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Dynamic modelling of the biomass gasification process in a fixed bed reactor by using the artificial neural network

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ABSTRACT

Biomass gasification enables the transformation of biomass feedstock into syngas suitable for further energy conversions. Mathematical models of gasification are not only valuable tool for the design and optimization of the processes, but could be also employed for online prediction and process control. In this work, the potential of using nonlinear autoregressive networks with exogenous inputs (NARX) for predicting the gasification process when a lower amount of experimental data is available was studied. The analysis of using an open-loop NARX network for an online prediction of the syngas composition in a downdraft gasifier at different data recording frequency was performed. The predicted results showed that by decreasing the data recording frequency, the prediction error increases. Furthermore, the possibility of improving the NARX network at lower data recording frequency was analysed by expanding the training dataset to reduce discrepancies between predicted and measured results. Inclusion of four data sets made neural network more robust and flexible for operating with fewer data points. Practical significance of results can be seen in the application of open-loop network for online prediction and control of the gasification process at lower data recording frequency as a part of a model predictive control module.

1. Introduction

Ever since the industrial era, CO_2 has been released into the atmosphere at an alarming rate causing disastrous global climate changes and release of permafrost carbon stored in Arctic and sub-Arctic regions (Schuur et al., 2015). In order to decrease the global average temperature rise and maintain it below 2 °C compared to pre-industrial levels, actions have been taken through technological advancement and sustainable development as part of the Paris Agreement (Rogelj et al., 2016). Ever-increasing energy demand has encouraged the energy sector towards a cleaner and more efficient renewable energy sources (Sen and Ganguly, 2017). Biomass has shown itself as an environmentally abundant energy source, and in combination with other renewables, namely solar, water, wind and geothermal energy, represents one of possible replacements for fossil fuels. Biomass can also be used as a feedstock in various synthesis processes of chemicals such as hydrogen and its derivatives (Guo et al., 2015).

Biomass gasification is a highly efficient and clean conversion technology used to convert biomass feedstock of various origins and compositions into products of known chemical compositions suitable for further energy conversions (Fózer et al., 2020). Biomass gasification systems produce by-products which are readily marketable and not toxic to the environment. The gasification process is a thermochemical conversion by which feedstock in combination with gasifying agents at an elevated high-temperature undergoes partial oxidation, and is thus converted into a gaseous mixture named syngas composed out of hydrogen, carbon monoxide, carbon dioxide, methane and other light hydrocarbons (Mikulandrić et al., 2014). Biomass characteristics such as moisture content, ash and char content, thermal conductivity, organic and inorganic constituents cause slight differences in the performance of

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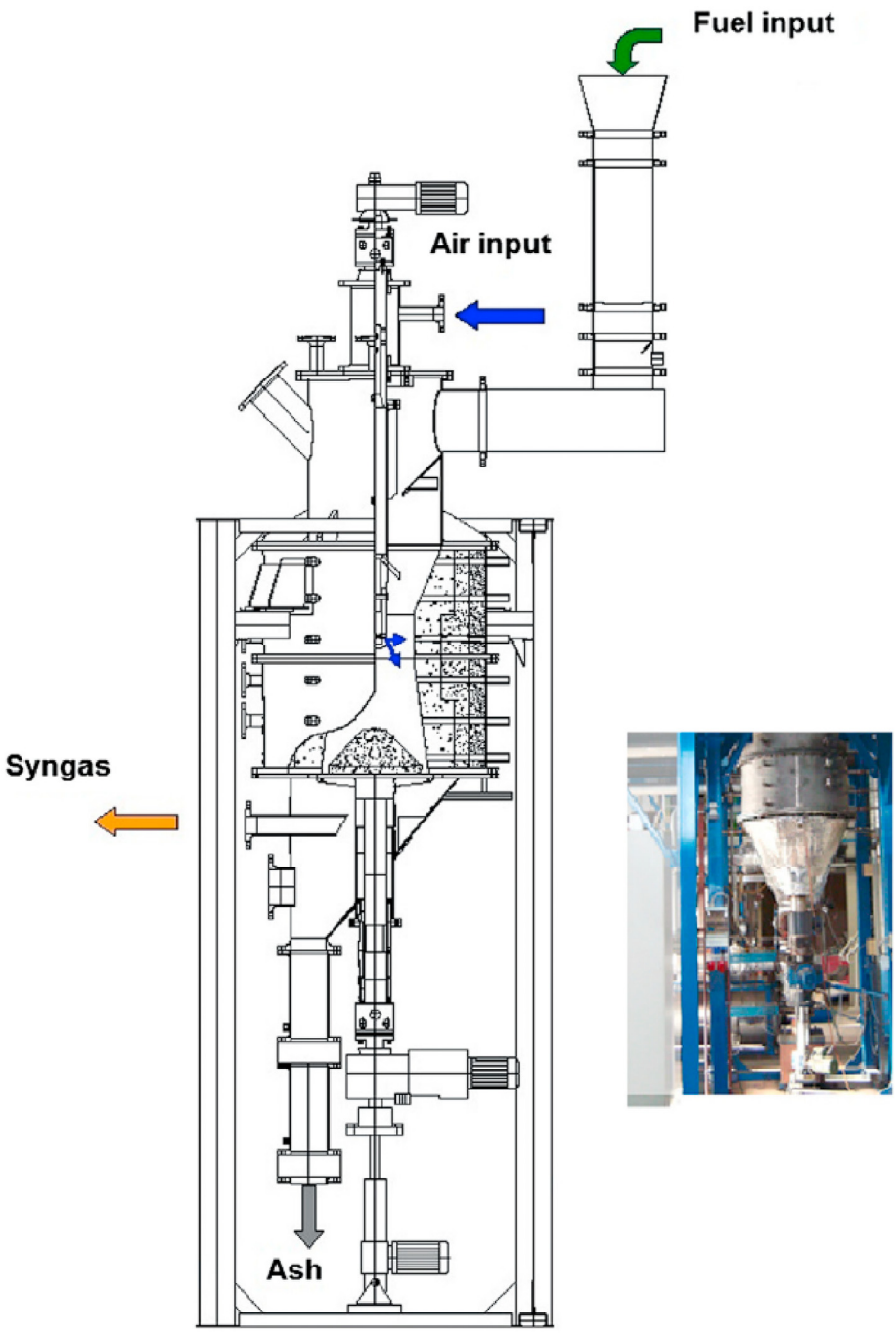

Fig. 1. Downdraft gasification reactor scheme (Mikulandrić et al., 2016).

Table 1
Biomass ultimate analysis.

Ultimate analysis, wt%	
Carbon	47.4
Hydrogen	5.63
Moisture	7.87
Ash	0.55
Chlorine	0.01
Oxygen (by difference)	38.54

individual biomass feeds. The design of the reactor, as well as operating parameters, strongly influence performance, produced syngas composition and system efficiency during the gasification process (Baruah et al., 2017). Albeit, gasification being a well-known technology, there still exist hurdles to pass for its complete utilization, as well as integration into modern energy production. Issues such as high investment costs and the necessity for pre-treatment and cleaning of syngas, show the need for further research and should be resolved to increase gasification share in the global energy consumption (Ruiz et al., 2013). Biomass gasification technology can economically meet energy demands in undeveloped regions, while consequently lowering their waste products (Ejiofor et al., 2020).

Gasification reactors can be classified into several groups, most notably auto-thermal and allo-thermal reactors which can be further divided into fixed bed, fluidized bed and entrained flow gasifier (Farzad et al., 2016). Selection of a particular type of gasifier has serious repercussions on particle residence time, as well as on heat exchange inside

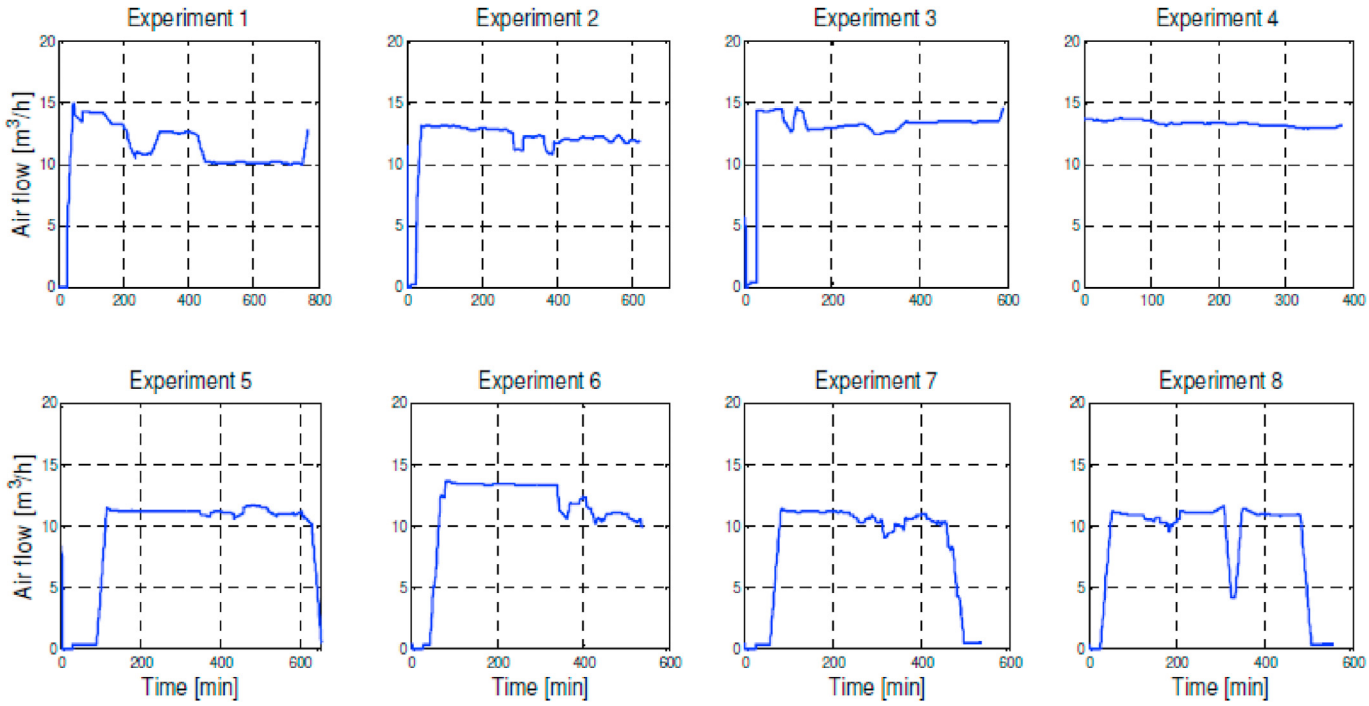

Fig. 2. Air volume flow for all experiments (Mikulandrić et al., 2016).

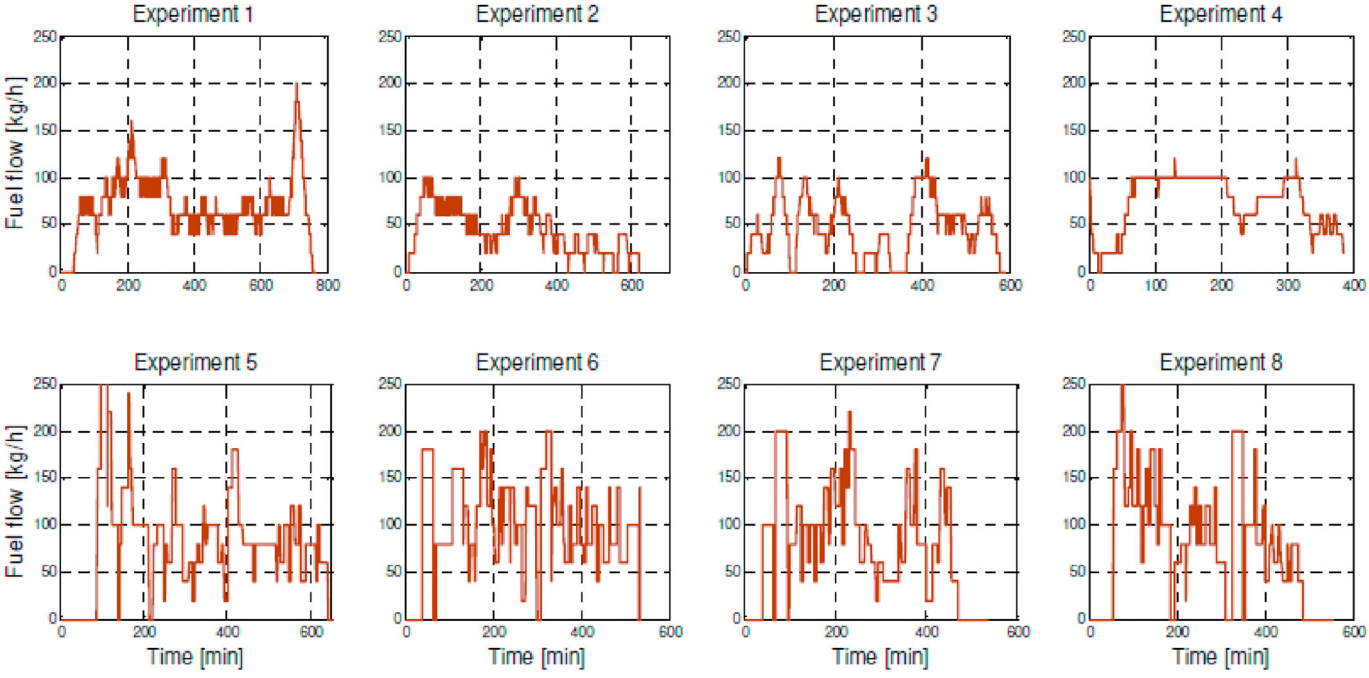

Fig. 3. Fuel mass flow for all experiments (Mikulandrić et al., 2016).

the reactor. Fluidized bed gasification may show better results than fixed bed gasification due to the bed temperature being held under the ash slagging temperature, thus reducing the volatilization of elements such as sodium and potassium (Gabra et al., 2001). Fixed bed reactors are more favourable for economics at the small-scale, showing longer particle residence time than their fluent bed counterparts, as well as slower heat exchange due to slower particles velocity through the reactor (Wang et al., 2008).

Numerical models are developed to virtually simulate the gasification process in order to improve its overall efficiency, as well as to ensure the quality throughout a various range of operating conditions. Moreover, numerical models are recognized as a valuable tool for the optimization process, which is emphasized as an important step in the development of manufacturing process, and also separate processes, like biomass gasification (Perković et al., 2017). Predictions of a variable's influence on the overall system can be achieved by simulating different scenarios and thus valuable information may be gained quickly and safely. Artificial neural networks (ANN) represent a non-physical modelling approach with the ability of machine learning to correlate experimental input and output data to approximate any continuous function to an arbitrary precision

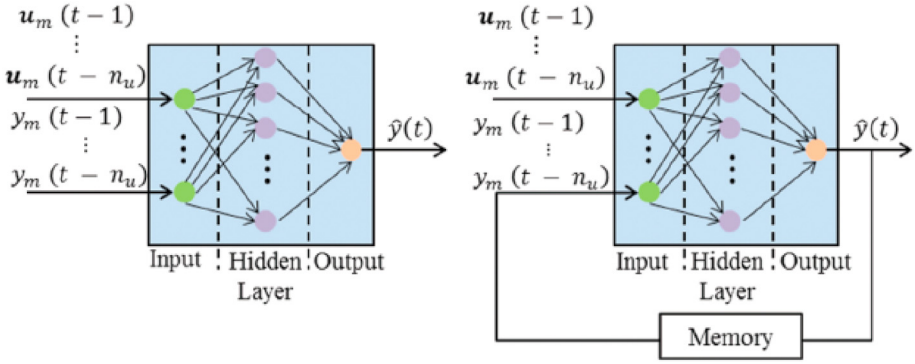

Fig. 4. Open-loop (left) and closed-loop (right) NARX network (Salah et al., 2016).

Table 2
Experimental data preparation.

Data recording frequency, min	Time delay, min	Number of time steps in all experiments
0.5 (original)	1	3,033
1	2	1,514
1.5	3	1,009
2	4	754
2.5	5	604
3	6	502

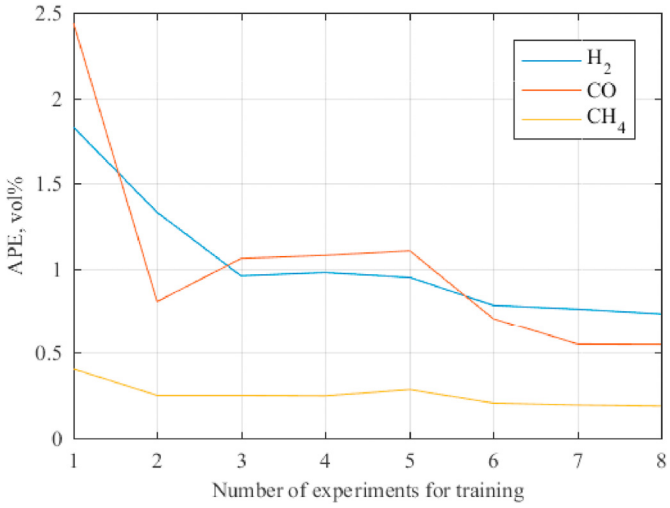

Fig. 5. Determination of experimental dataset for training procedure.

Table 3
APE for the different data recording frequency.

Case	Data recording frequency, min	H_2 APE, vol %	CO APE, vol %	CH_4 APE, vol %
1	0.5	0.9575	0.9796	0.2731
2	1	0.963	2.0434	0.4637
3	1.5	1.1864	1.9182	0.6606
4	2	1.6587	1.9426	0.6698
5	2.5	1.3995	2.0990	0.9190
6	3	1.4145	2.4050	0.8008

even without prior knowledge on the structure of the function for the process in question (Ponton and Klemeš, 1993). ANN models are widely known and accepted as a technology able to work with non-linear problems, and after a training period, may predict model outputs at high speeds. More efficient plant design, emission reduction and biomass power efficiency may be achieved as more research is conducted for biomass gasification modelling (Dang et al., 2021). These models have recently proven their worth in energy-related processes such as biodiesel production (Piloto-Rodríguez et al., 2013), distillation processes (Klemeš and Ponton, 1992) and predicting net output power from a system using various biomass feedstocks, and also at various operating conditions (Safarian et al., 2020). In a study by Pandey et al. (2016) syngas yield was predicted, in addition to which the lower heating value of gas and other gasification products such as tars and entrained char were predicted.

Dynamic neural networks are effective at predicting time-variable relationships for short-term prediction (Mohebbi et al., 2019). These networks are different as the output does not only depend on current inputs, but previous values as well. By using feedback loops and/or recurrent connections a degree of the memory capacity of the network may be shown (Salah et al., 2016). Nonlinear autoregressive networks with exogenous inputs (NARX) represent dynamic types of neural networks which can be used to describe process dynamics of non-linear chaotic systems. NARX relates current values of a time series to both past values of the same series and current and past values of the externally determined series that influences the series of interest, thus offering greater versatility and adaptability (Billings, 2013). These models have limited feedback architectures in comparison to other recurrent neural models, while research of Siegelmann et al. (1997) has shown promise for comparable results to Turing machines. NARX models have seen success in various engineering areas. Methane generation rates for a landfill in Regina, SK, Canada were predicted using a two-stage time series model (Fallah et al., 2020). The research focused on the influence of missing data imputation coupling with time series NARX models. Potential benefits of missing data estimation were evaluated using multilayer perceptrons coupled with the NARX model. Shahbaz et al. (2020) used a NARX model to determine syngas composition from a fixed bed downdraft gasifier using waste bottom ash as a catalyst. Impact of various process parameters on gas yield was investigated, namely temperature, airflow rate and catalyst loading. Study found that usage of NARX model can assist in optimizing process parameters before undertaking commercial-scale development and thus reducing development time and potential costs. Syngas production rates for a reactor using bagasse wash water were predicted using a NARX network to model unsteady state behaviour of the reactor (Jain et al., 2015). Developed model represented dynamic behaviour of the reactor and was able to recursively predict and forecast syngas production rate. In the research by Mikulandrić et al. (2020) a NARX model was developed to predict syngas temperature and composition in a fixed bed gasifier. The NARX model required only a limited amount of data for training and was able to accurately predict syngas temperature in changing operating conditions. The study suggests that for further improvement of the NARX prediction capability sub-models for separate reactor regions must be developed. NARX models appear to be a promising approach to describe non-linear systems with significant delays in which mass and energy accumulation

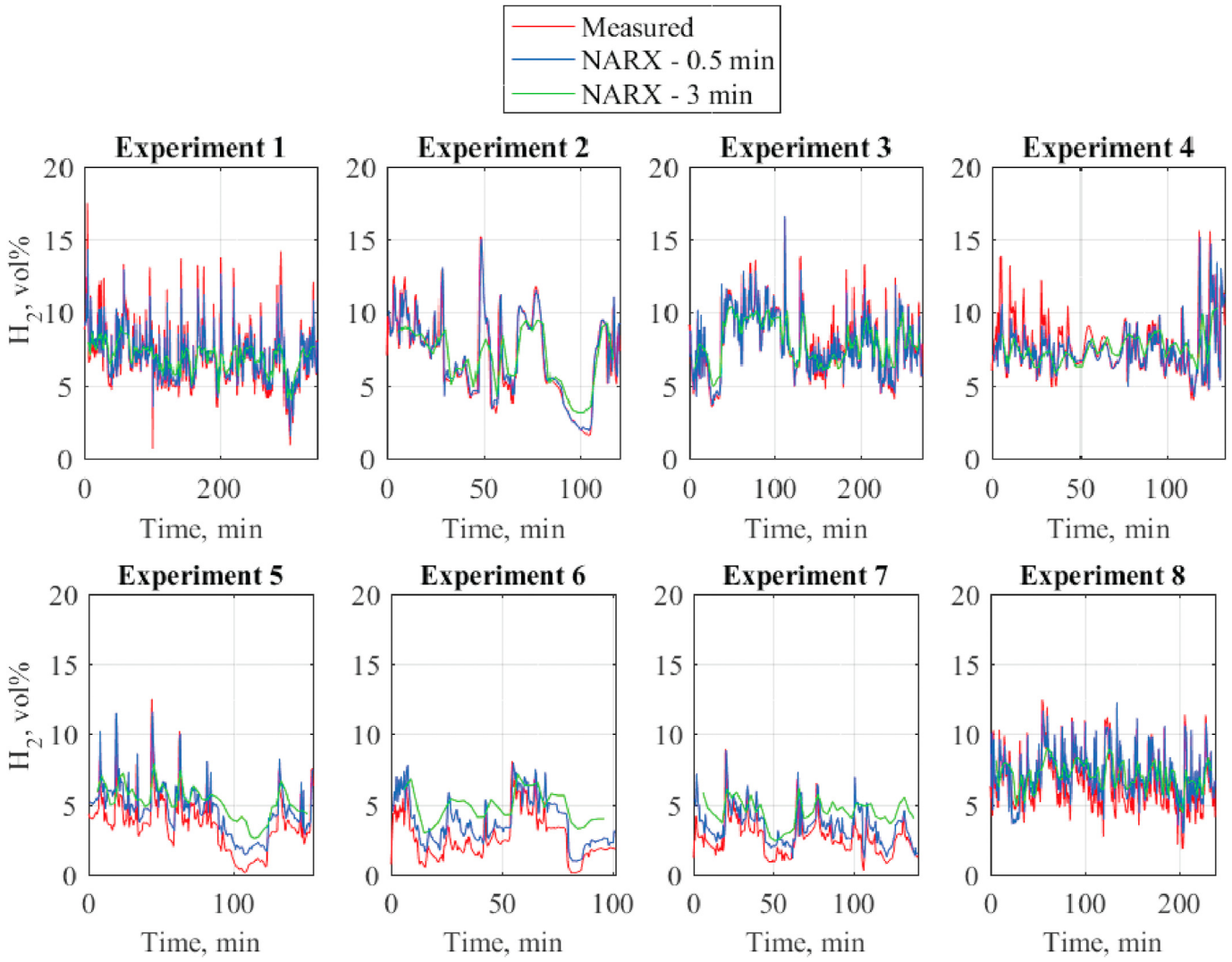

Fig. 6. NARX H_2 predictions for different data recording frequency.

needs to be considered. In the study by (Yucel et al., 2019) NARX neural network model was used to predict the gasification process in a fixed bed downdraft gasifier. Using experimental gasification data, the networks were trained and validated. Authors concluded that using temperature distribution in NARX and ANN-based models led to an increase in prediction accuracy for gasification products.

Considering overview of the recent literature given above, biomass gasification represents a promising technology suitable to enhance the penetration of renewable energy sources into the energy sector. Also, the provided literature review indicates increase in utilizing the ANN modelling approach in the past few years to simulate the biomass gasification process. Mentioned researches mostly showed a good capability of using ANN models for improvement of the gasification process, especially NARX networks were used to simulate the dynamic behaviour in the reactor. The analysis of using NARX neural network when a lower amount of experimental data is available is not available in literature. Consequently, the potential of using NARX neural network for an online prediction of syngas composition in a downdraft gasifier at different data recording frequencies was studied in this work. The results showed that by decreasing the data recording frequency, the prediction error increases. It was necessary to expand the experimental dataset used for training accordingly to take into account various operating conditions.

2. Materials and methods

A proper method for building ANN cannot be generalized, as it highly depends on the process itself and on the preparation of the experimental data. The ANN simulation method can be divided into few steps. Firstly, a previously structured ANN is trained on the training set of experimental data, and after this, trained neural network is applied on a completely new set of experiments (Hudson Beale et al., 2017). ANNs can be classified into static and dynamic networks. Static neural networks calculate the output directly from the input data through the feedforward connection. Including some delays or taking into account the influence of past values through the feedback loop is not possible. On the other hand, the calculated output of dynamic networks depends also on previous inputs and outputs of the network. In this work, a dynamic neural network will be used, since the observed biomass gasification process should be mathematically described over operating time.

Following subsections are structured as follows. Firstly, the gasification reactor with its operating conditions is described, then the simulation setup of a dynamic NARX neural network used in this work is given. Finally, the preparation method of measurement data required for the ANN modelling procedure will be provided.

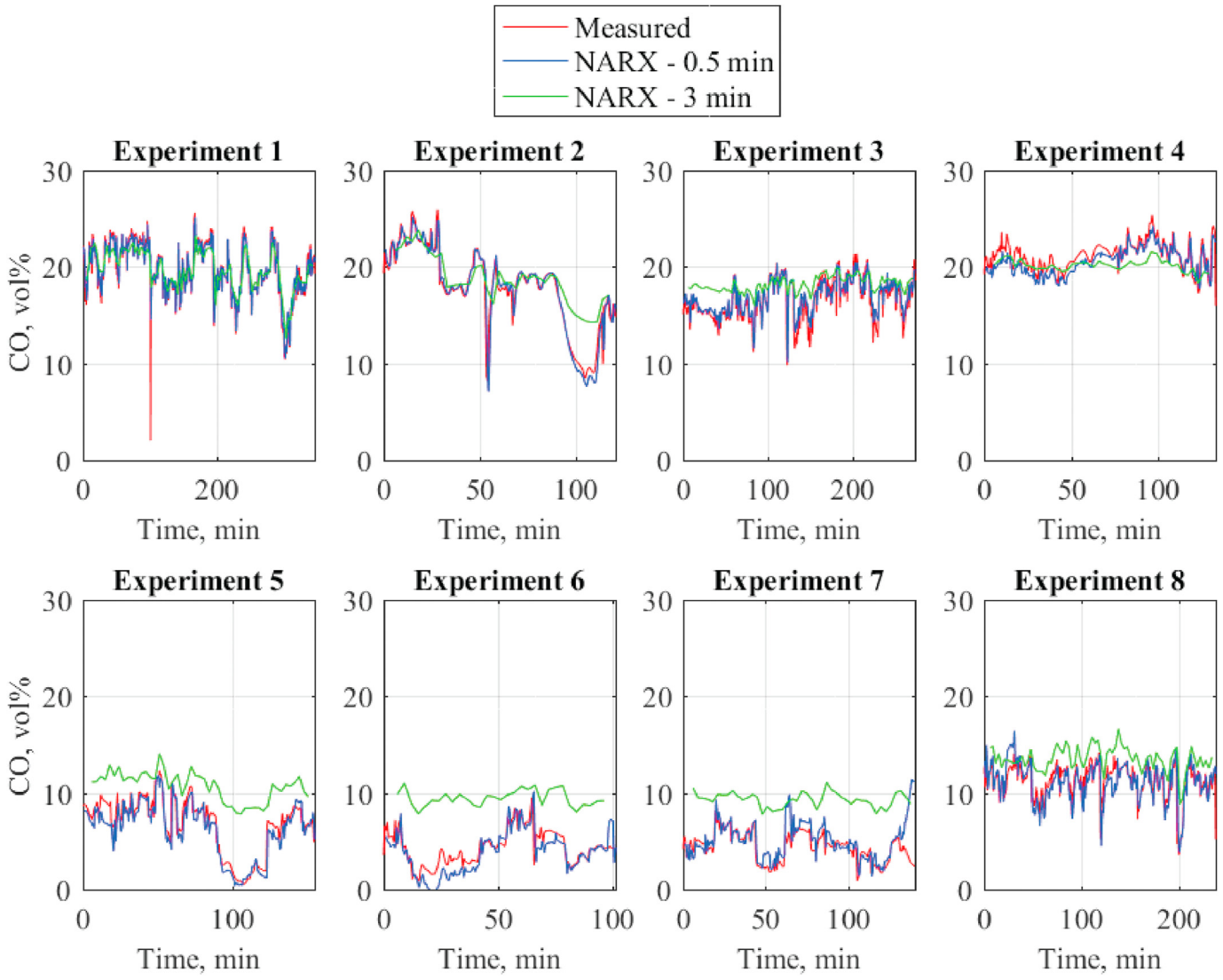

Fig. 7. NARX CO predictions for different data recording frequency.

2.1. Gasification plant and operating conditions

Measurement data for modelling purposes were taken from the literature (Mikulandrić et al., 2016). The observed gasification plant is a fixed bed downdraft gasifier located in Pirna, Germany operated by TU Dresden with a thermal input of 75 kW_{th}. The biomass feedstock is fed into the storage container, located in the front of the biomass feeding control system. When the amount of biomass in the reactor drops below a certain level, a manually controlled valves in the feeding control system are opened and biomass enters the shredder. After the shredding process, biomass is continuously fed into the gasifier. In the gasification process, air is used as a gasifying agent, while the distribution and the flow rate are controlled by air pumps. At the bottom of the reactor, ash is collected manually through the ash valve. The whole gasifier scheme is shown in Fig. 1. For modelling purposes in this work, two sets of experiments were taken into consideration. Both sets have 4 experiments, where the first set was measured in 2006 (Mikulandrić et al., 2014), and the second one was measured in 2013 (Mikulandrić et al., 2016). A more detailed description of the plant, along with experiment sets used in this work can be found a research by Mikulandrić et al. (2016).

Wood chips were used as a biomass fuel in all experiments. Biomass analysis is available only for the first set of experiments (1–4) from 2006. Biomass lower heating value is 17.473 MJ/kg while the ultimate analysis on wet basis performed at TU Dresden laboratory is shown in Table 1. In experiments from 2013, the same type of biomass was used as in experiments from 2006, although the precise composition is unknown.

The gasification plant is equipped with measuring devices to track various process parameters over time, such as air volume flow rate, fuel mass flow rate, pressure drop in the reactor, syngas temperature, composition at the gasifier outlet and the air inlet temperature. The data measurement frequency is 30 s, while the experiment duration depends on the initial state of the gasifier. Input values used for the model development were air volume flow and fuel mass flow, while the syngas composition (H_2, CO and CH_4) was the modelling output. Air flows for all experiments are shown in Fig. 2, while fuel flows are shown in Fig. 3. While comparing two sets of experiments, higher fuel flow rates and lower airflow rates were noticed in the second experiment set from 2013. Mikulandrić et al. (2020) concluded that this behaviour was indicated due to the shift of complete combustion process in the experiment set from 2006 to the incomplete combustion process in the experiment set from 2013. They prescribed this shift to the possible change of biomass quality, different amount of ash sintering or some unknown reason.

2.2. Dynamic NARX model

In dynamic neural networks calculated output values are a function of

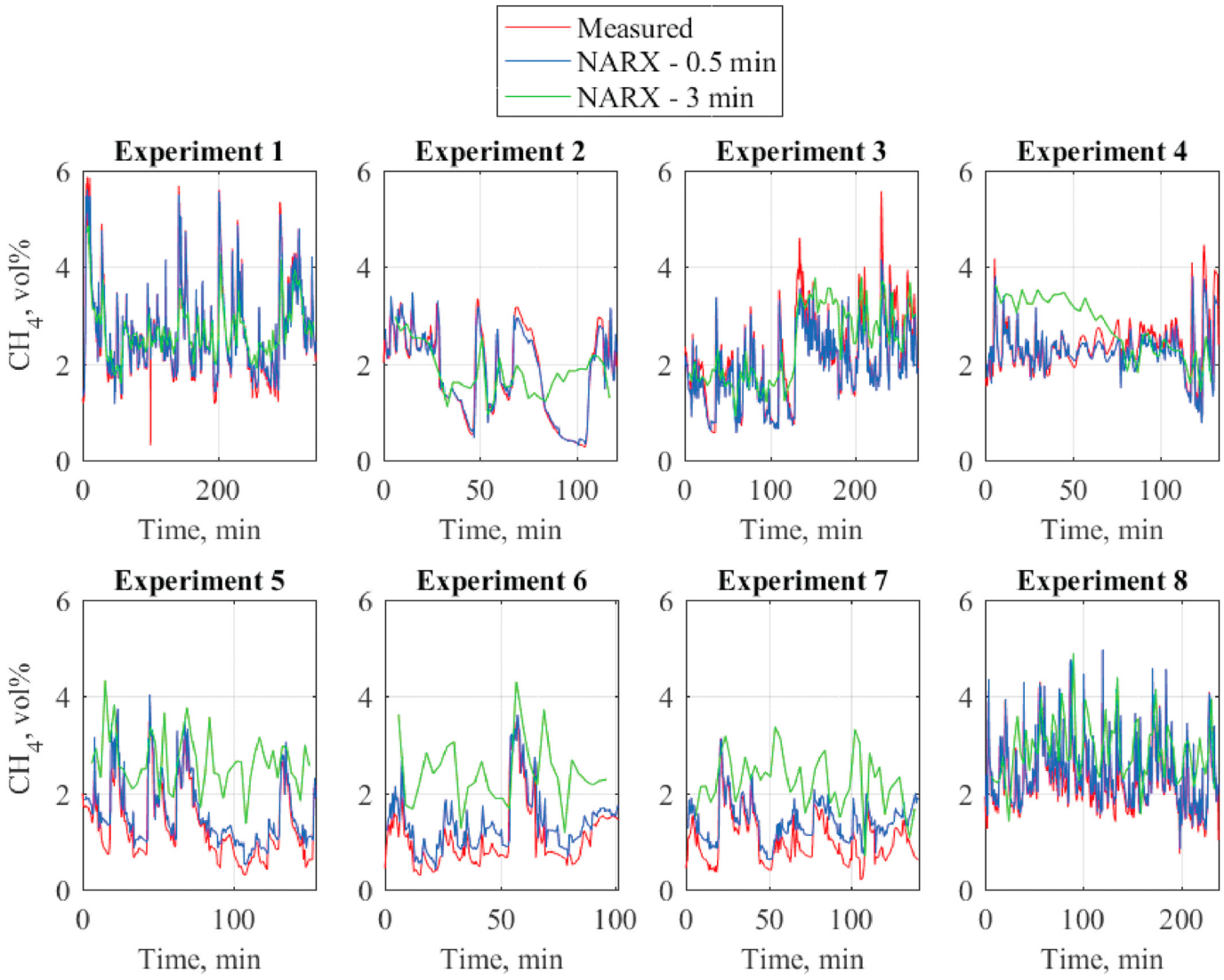

Fig. 8. NARX CH_4 predictions for different data recording frequency.

Table 4
APE for different number of experiments as training dataset.

Case	Experiments for training	H_2 APE, vol%		CO APE, vol%		CH_4 APE, vol%	
		1.5 min	3 min	1.5 min	3 min	1.5 min	3 min
2	**1–2**	–	–	1.9182	2.4050	0.6606	0.8008
3	**1–3**	1.1864	1.4145	1.5193	2.0875	0.5732	0.9286
4	**1–4**	**1.5630**	**1.3953**	**1.7538**	**2.1410**	**0.5645**	**0.6586**
5	**1–5**	1.5344	1.3545	1.8830	1.7602	0.5416	0.6812
6	**1–6**	1.0820	1.2208	1.9242	1.1559	0.3648	0.4518
7	**1–7**	0.9926	1.0684	0.8812	1.0744	0.3425	0.4256
8	**1–8**	0.9739	1.0563	0.8654	1.0612	0.3262	0.4057
9	**1–2, 5–6**	**1.2025**	**1.1449**	**1.1373**	**1.3896**	**0.3806**	**0.4973**

the current input data along with previous values of input and output data through the feedback loop and/or recurrent connections, so-called delays. In this work, a dynamic NARX network was used. NARX is a recurrent dynamic neural network suitable for modelling nonlinear dynamic processes (Hudson Beale et al., 2017), like biomass gasification. The output value for a time t is determined by the following expression:

$$\hat{y}(t) = f\left(y(t-1), y(t-2), \ldots, y\left(t-n_y\right), u(t-1), u(t-2), \ldots, u(t-n_u)\right), \quad (1)$$

where terms n_y and n_u are the number of output or input delays. Usually, the number of input delays is equal to the number of output delays, $n_y = n_u$. Those implemented delays represent the memory ability of the network. Training procedure of the NARX network can be performed in two steps as shown in Fig. 4.

The first step is an open-loop training process for creating the series-parallel network architecture. The feedforward multilayer network is trained on experimental input and output data using the backpropagation algorithm. Inputs of the model are input vector $\boldsymbol{u}_m$ (fuel flow and airflow) with a certain amount of delays (n_u) and measured output value y_m, again with its delays. After, trained open-loop network can be applied for on-

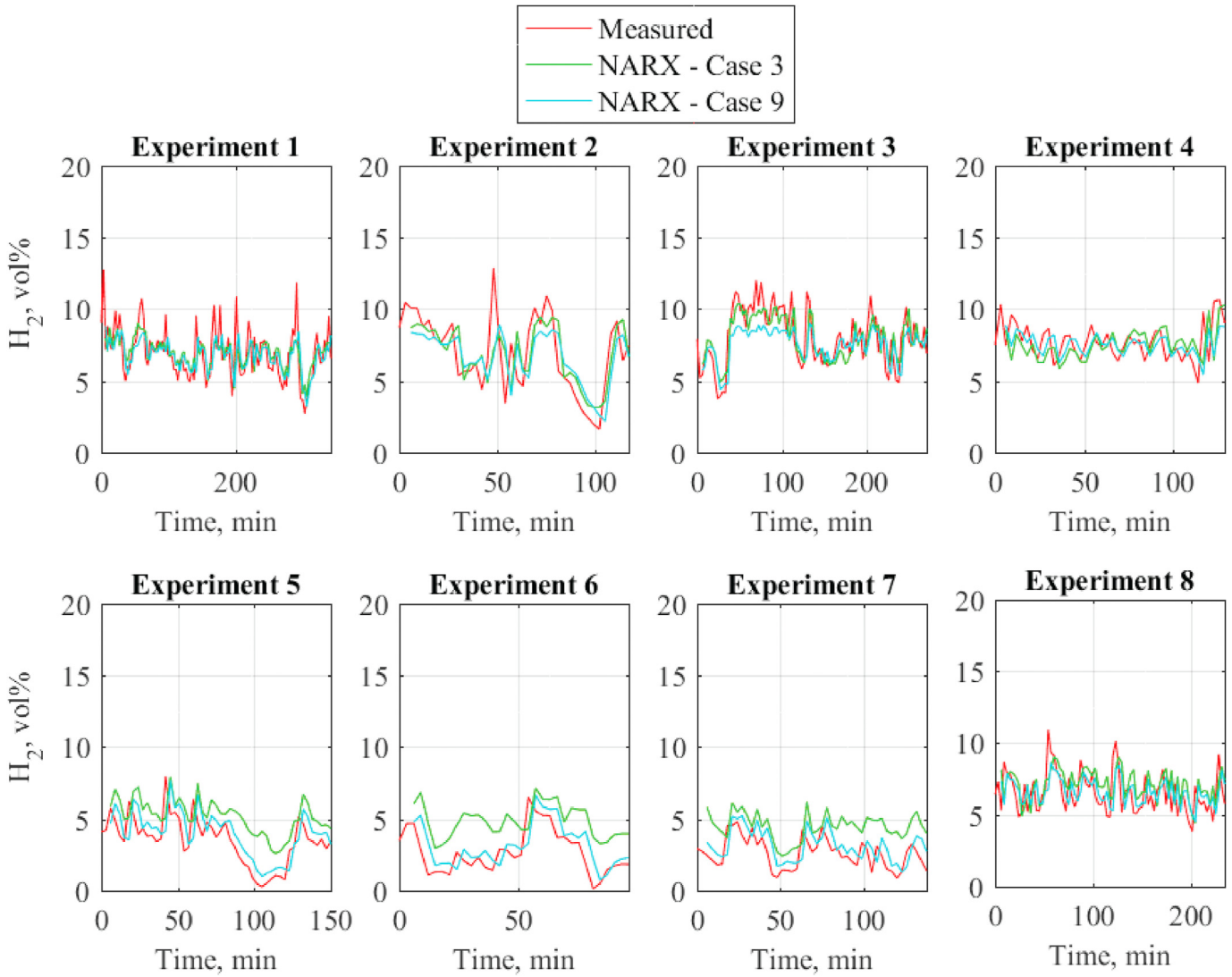

Fig. 9. NARX H_2 predictions with the improved training procedure.

line prediction of the process on a completely new set of input data if measuring the output data is available in a real-time. Previously trained network can be closed by implementing the feedback loop, as shown on the right-hand side in Fig. 4 and generating the fully parallel network architecture. When using a closed-loop network there is no need for measuring the output data in the real-time, thus it can be applied to offline prediction of the output value.

In this work, an open-loop network was used to realise the potential of using NARX neural network for online prediction of the biomass gasification process. The NARX network was structured as follows; input and output layers were connected with one hidden layer of 5 neurons and two delays were taken for the calculation. For a connection between hidden and output layer, a tan-sigmoid transfer function was used, while the linear transfer function was used in the output layer. Bayesian regularization method was used as a training algorithm, and a maximum number of training epochs was set to 600 to avoid the model overfitting. The training data was divided using the function 'divideblock' into three contiguous dataset blocks, namely training set, validation set and test set. The training set was used for the calculation of gradient and updating the network weights and biases. The validation set was monitored through the training and its error normally decreased during the training process, but when the network started to overfit the data, the validation set error started to increase. At the end of the process, the weights and biases at the minimum of the validation error were taken. On the other hand, a test set was monitored during the training process to see if its error reaches a minimum at a significantly different iteration number than the validation set error, which might indicate a poor division of the data set (Hudson Beale et al., 2017). The training process was running in several training sessions. Each session started with different initial weights and biases, and a different division of training dataset. These different conditions can lead to a different solution of the same problem and the session with the lowest prediction error was picked. The final trained network was then applied again to the same training dataset and to a completely new experiments set. The preparation of the data for training and using the network in online prediction procedure is described in the next section.

2.3. Preparation of the experimental data

In all experiments measurement of the syngas composition started when the syngas temperature at the outlet was around 250 °C or above. The aim of the experiment was to ensure a stable syngas production for approximate 3 h, although it was not completely achieved in all experiments (Mikulandrić et al., 2020). For that reason, the amount of experimental data used for training the neural network is reduced compared to the data shown in Figs. 2 and 3. The duration of experiments varied from 107 min for experiment 6 up to 345 min for experiment 1. The purpose of this study was to analyse the possibility of predicting the syngas composition for lower recording data frequency. Originally, the

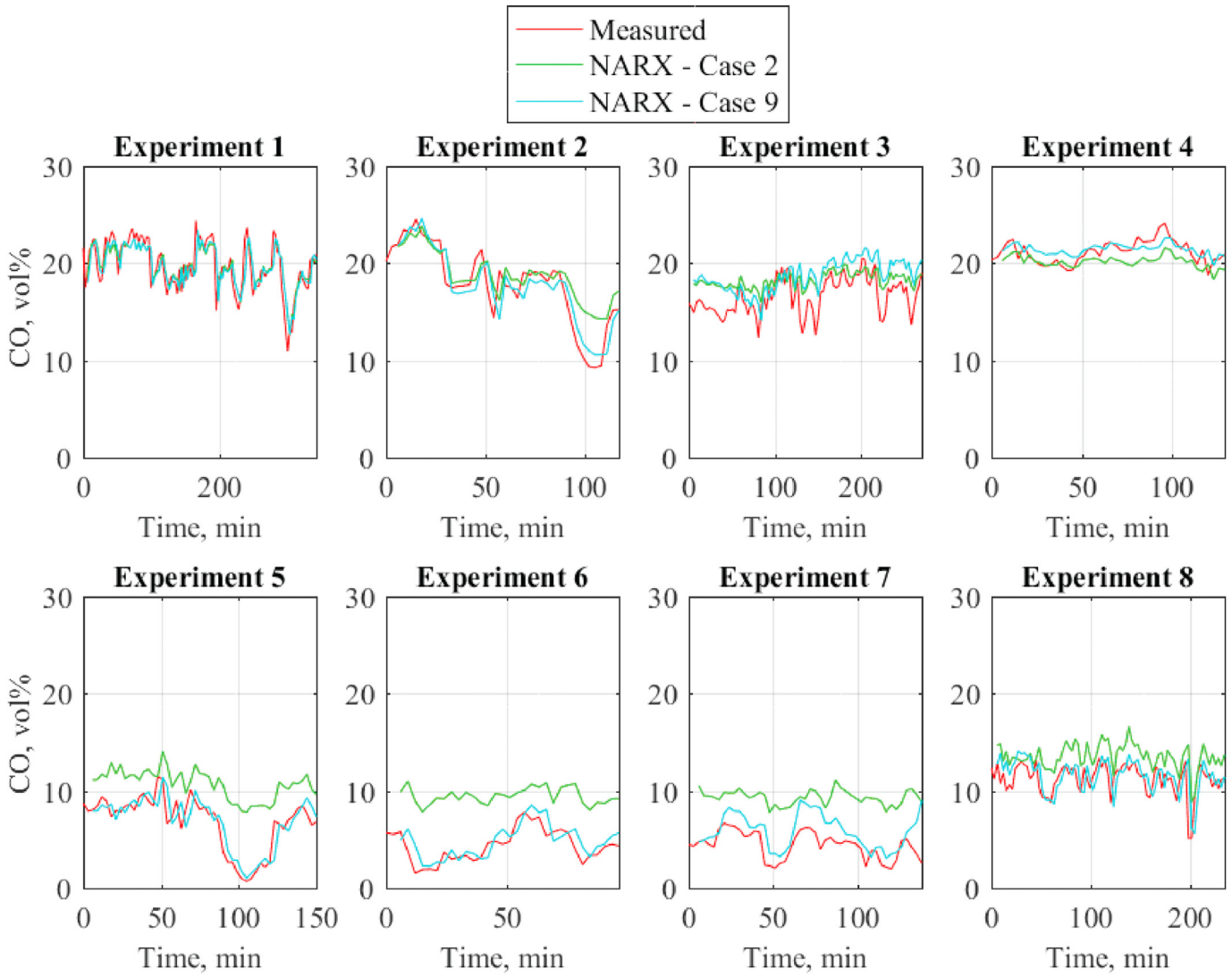

Fig. 10. NARX CO predictions with the improved training procedure.

experimental data was recorded every 30 s, while in this study, the recording frequency varied from 30 s up to 3 min. Accordingly, the experimental data was prepared as an average value during the selected time period. All information about the prepared data is shown in Table 2.

3. Results and discussion

Previously explained experimental data was used for creating and using NARX ANN model for the syngas composition. The output of the model is a syngas composition, expressed as the volumetric fraction (vol %) of H_2, CO and CH_4. The main parameter to evaluate the developed neural network model was Average Prediction Error (APE), which represents averaged absolute error for all experiments, expressed in vol% of gas content. This section is divided into three parts. Firstly, the experimental dataset for training procedure was determined. In the second part, the influence of different data recording frequency was analysed. In the last section, the possibility of improving NARX predictions with lower recording data frequency was studied.

3.1. Determination of experimental dataset for the training procedure

Firstly, the number of experiments for a training procedure, to provide satisfactory prediction accuracy, needs to be determined. The dataset with an original data recording frequency of 30 s is used for analysis. The number of experiments for training procedure is varied from using only experiment 1 to using experiments 1–8. Separate NARX networks are created for H_2, CO and CH_4. In Fig. 5, the change of APE by increasing the training dataset is shown. It can be noticed that in either case, the first experiment is not sufficient to provide the desired accuracy. According to the presented figure, for H_2 predications first 3 experiments are taken as the training dataset, while for CO and CH_4 predictions experiments 1 and 2 are sufficient as the training dataset.

3.2. Data recording frequency analysis

As it was shown before in Table 2, the amount of data is significantly reduced while decreasing the data recording frequency. To analyse the influence of data recording frequency on NARX predictions of H_2, CO and CH_4, six different cases are simulated as stated in Table 3. Data recording frequency is varied from 30 s (original data) to 3 min. APEs for all cases are shown in Table 3. While observing H_2 predictions, it can be noticed that a lower data recording frequency increases the APE, with the exception of Case 4 which resulted in the highest average error. Also, it is interesting to notice that Case 2 achieved similar APE as the original Case 1, despite reducing the dataset in half. CO prediction errors are higher for all cases compared to Case 1, which indicates the necessity for further

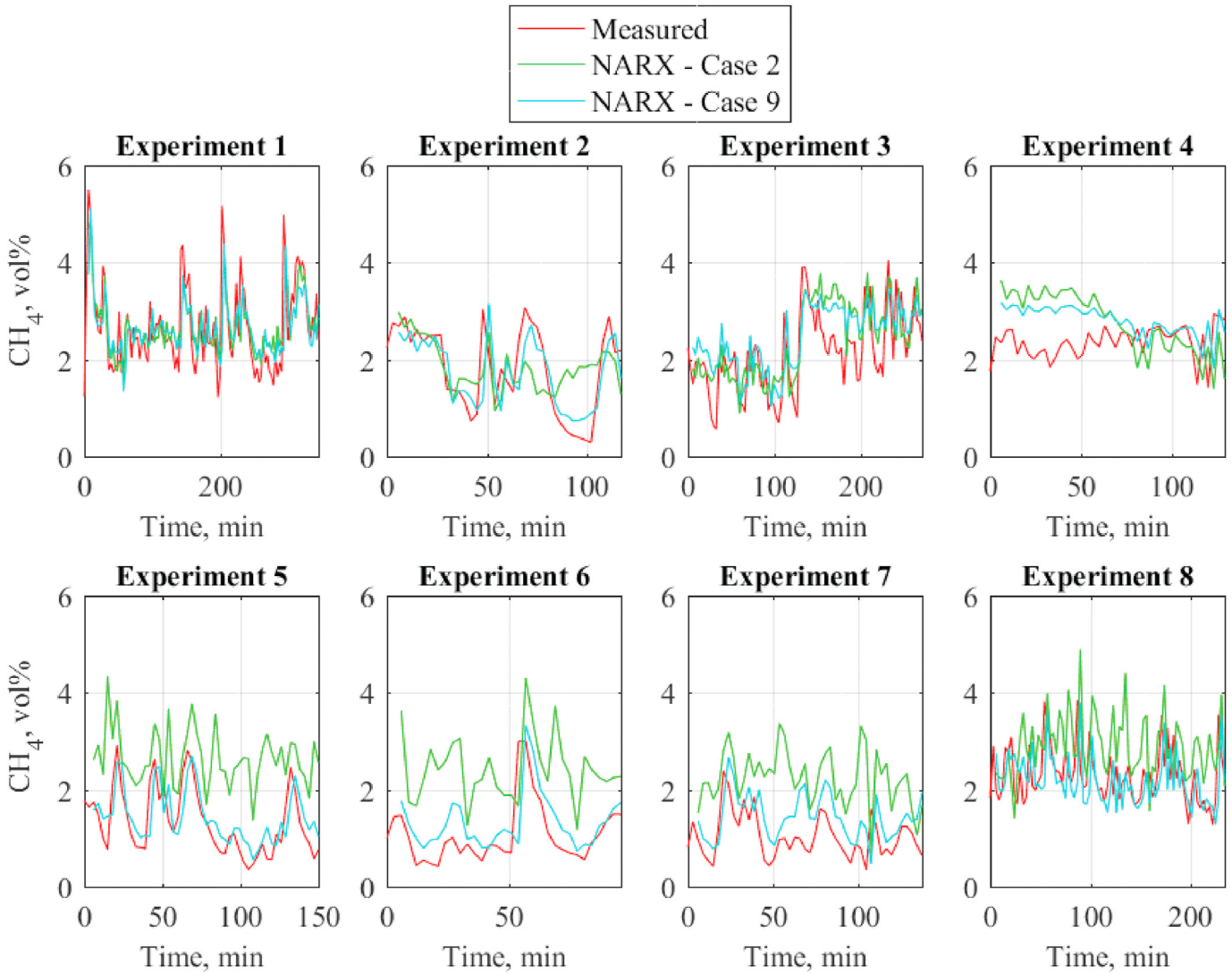

Fig. 11. NARX CH_4 predictions with improved training procedure.

improvement of the model. APEs of CH_4 predictions increase in a similar trend as for H_2 predictions, while the highest prediction error is recorded in Case 5.

In the following figures, dynamic NARX predictions of H_2, CO and CH_4 volume fractions from Case 1 (original data recording frequency) and Case 6 (the lowest data recording frequency) are compared to the measurement data. Generally, the highest prediction error of H_2 is recorded within experiments 5, 6 and 7 for both cases, as it is shown in Fig. 6. Also, deviations of Case 6 are much higher compared to Case 1 for all experiments, which is in a correlation with results given in Table 3. It can be noticed that in experiments 5–8, Case 6 deviates more compared to experiments 1–4. This is can be prescribed to a lack of experiments from 2013 (5–8) in the training dataset.

When CO predictions in Fig. 7 are observed, it can be noticed that Case 1 matched the measurement data for all experiments with satisfying accuracy. On the other hand, CO predictions with Case 6 deviate mostly for all experiments, except for the first two experiments which are used as the training dataset. CO predictions highly deviate for experiments 5–8 due to the same reason of lacking the experiment from 2013 in the training dataset, as mentioned in H_2 predictions. Since the predictions with original data recording frequency provide satisfactory matches with the experimental data in all experiments, it can be concluded that decreasing the data recording frequency implies the necessity for NARX model improvements in a way of expanding the training dataset.

Similar to CO predictions, CH_4 predictions with Case 1 matched the measurement data for all experiments as it is shown in Fig. 8. Again, by reducing the data recording frequency to 3 min, modelling results significantly deviate from the measurement data, especially for experiments 5–8 due to the same reason stated before. To decrease deviations of NARX predictions at lower data recording frequency, a training dataset needs to be expanded which is studied in the next section.

3.3. *Improvement of NARX predictions*

Possibility of improving NARX predictions at lower data recording frequency is analysed by expanding the training dataset. As it is shown in Table 4, the training dataset was varied from the referenced dataset used in the previous section to a dataset with experiments 1–8. Additionally, Case 9 is proposed where 4 experiments are used as the training dataset, first two experiments from 2006 (experiments 1–2) and first two experiments from 2013 (experiments 5–6). APEs are analysed for two data recording frequency cases 1.5 min and 3 min. While observing APEs, it can be noticed that expanding the training dataset, significantly reduces the error. Logically, the lowest APE is achieved with Case 8 where all experiments are used as the training dataset. This neural network doesn't provide a promising solution, since there is no additional dataset where

the network could be tested. Case 9 is chosen as an optimum solution since only 4 experiments are used as the training dataset, while the APE is lower compared to Case 4, where the same number of experiments is used. This could be addressed to including experiments from 2006 to 2013 in the training dataset, which makes the trained neural network more robust and flexible to predict syngas composition at different operating conditions.

Comparison of referenced case predictions (Case 3 for H_2 predictions and Case 2 for CO and CH_4 predictions) with Case 9 predictions and the measurement data is given in Fig. 9 (H_2), Fig. 10 (CO) and Fig. 11 (CH_4). The data recording frequency is 3 min, while the measured data represent time average values of 3 min for easier comparison of the predictions. It can be noticed that in Case 9 deviations are reduced for all observed gasses and experiments. It is important to notice that in Case 9 H_2 prediction deviations are significantly reduced in experiments 5–8, compared to Case 3.

Before mentioned high deviations of CO predictions in experiments 5–8 are reduced also. It is visible that including the experiments from 2013 into the training dataset in Case 9, highly reduced CO prediction errors compared to Case 2.

CH_4 prediction deviations are reduced in Case 9 for all experiments. Including the experiments from 2013 (5–6), highly improved the prediction capability for all experiments, similar as stated before for H_2 and CO predictions.

Considering the overall results, it can be concluded that the NARX neural network is suitable for online prediction of syngas composition in biomass gasification process at lower data recording frequencies. While lowering the data recording frequency, the training dataset needs to be expanded to train the network for various operating conditions.

4. Conclusion

Biomass gasification process enables conversion of bulky raw material into more suitable energy source of syngas. Mathematical models of gasification are not only valuable tool for the design and optimization of the processes, but could be also employed for online prediction and process control. With that aim, present contribution investigated the possibility of using NARX ANN in the fixed bed downdraft gasifier to predict the syngas composition for lower recording data frequency. An open-loop network consisting of input and output layers connected with one hidden layer of 5 neurons was taken for the calculation. Sensitivity analysis concerning data recording frequency in the range from 30 s to 3 min revealed severe disagreement between measurement data and predictions, especially for CO and CH_4 concentrations, which motivated second sensitivity analysis of training dataset expansion. Expansion of the training dataset by including four sets of data made the neural network more robust and flexible to predict syngas composition at different operating conditions. Practical significance of results can be seen in application of open-loop network for online prediction and control of the gasification process. Future work should investigate implementation of NARX network in the model predictive control module and analysis of possible benefits reached by such an approach.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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