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Short Communication

Prediction of trace compounds in biogas from anaerobic digestion using the MATLAB Neural Network Toolbox

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Abstract

The outlook to apply the highly energetic biogas from anaerobic digestion into fuel cells will result in a significantly higher electrical efficiency and can contribute to an increase of renewable energy production. The practical bottleneck is the fuel cell poisoning caused by several gaseous trace compounds like hydrogen sulfide and ammonia. Hence artificial neural networks were developed to predict these trace compounds. The experiments concluded that ammonia in biogas can indeed be present up to 93 ppm. Hydrogen sulfide and ammonia concentrations in biogas were modelled successfully using the MATLAB Neural Network Toolbox. A script was developed which made it easy to search for the best neural network models' input/output-parameters, settings and architectures. The models were predicting the trace compounds, even under dynamical conditions. The resulted determination coefficients (R^2) were for hydrogen sulfide 0.91 and ammonia 0.83. Several model predictive control tool strategies were introduced which showed the potential to foresee, control, reduce or even avoid the presence of the trace compounds.
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Keywords: Biogas; Prediction; Hydrogen sulfide; Ammonia; Modelling; Neural networks; MATLAB Neural Network Toolbox; Anaerobic digestion

1. Introduction

1.1. Anaerobic digestion

Anaerobic digestion is a world-wide applied principle to stabilise municipal sewage sludge, treat organic wastes, products and waste-waters from industries, households and farms. Thereby a highly energetic biogas is produced which is used in combined heat and power generators. The advanced application of biogas into fuel cells will result in a significantly higher electrical efficiency (NETL, 2000) and can contribute to an increase in renewable energy production. However, besides methane and carbon dioxide, biogas can contain by-products like hydrogen sulfide, ammonia, halogens and non-methane organics, which will reduce the fuel cells life time dramatically (NREL, 2001). Therefore, the prediction of these trace compounds is necessary so the right precautions can be taken. Applying suitable models in a predictive control tool can result in a biogas were compounds are controlled, reduced or even avoided. Holubar et al. (2002) demonstrated this kind of application for methane composition and biogas production optimisation.

1.2. Hydrogen sulfide

Hydrogen sulfide (H_2S) is the end product of the reduction of sulfate and other sulphur containing

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compounds in anaerobic digestion. Concentrations in biogas up to 5.7 vol.% H_2S were reported (Braun, 1982). Hydrogen sulfide is one of the main toxicants because of the frequent presence in biogas and toxicity for all common fuel cells (NETL, 2000). At this moment no effective tool exists to prevent hydrogen sulfide production during the anaerobic treatment of sulfate-rich wastewater (Hulshoff Pol et al., 2001). Even the in practice applied measures of sulfide precipitation with iron salts (Stachowske, 1991) or air injection (Chambers and Potter, 2002) are not effective enough to reach the fuel cells tolerances of a few ppm H_2S (NETL, 2000). From this point of view a pre-treatment technology, like a bio-scrubber combined with a chemical cleaning, is a good possibility to upgrade the biogas quality to fuel cells tolerances. Therefore, predictive model based control will be necessary so H_2S in biogas production is regulated and pre-treatment functioning is assured.

1.3. Ammonia

Ammonia (NH_3) is the end product of ammonification processes in anaerobic digestion. As a component in biogas it has not been researched until now. Still there is no literature available which constitutively demonstrates the presence of ammonia in biogas. Only Schomaker (2000) noted that 450 ppm ammonia was measured at a biogas plant. Nevertheless, from the Henry constant of ammonia (Stumm and Morgan, 1996) and possible reactor conditions it was easily calculated that, when gas transfer limitation is excluded, ammonia should be present in the biogas phase. Some fuel cells tolerate ammonia as a fuel, but other fuel cells like the Proton Exchange Membrane Fuel Cell (PEMFC) (Austrian Energy Agency, 2004; FAL, 2004) or the Phosphoric Acid Fuel Cell (PAFC) (Fuel Cells, 2000, 2004), are certainly not resistant to ammonia (NETL, 2000). For these type of fuel cells research of the ammonia production and prediction in biogas is required.

1.4. Modelling

Basically, there are two ways in which a model can be established: it can be derived in a deductive manner using laws of nature, called mechanistic modelling, or it can be inferred from a set of data collected during a practical experiment with the system, called black-box modelling. There is considerable valuable development and application in mechanistic modelling of anaerobic digestion processes (Batstone and Keller, 2003; Fedorovich et al., 2003) based on the standard Anaerobic Digestion Model No. 1 (Batstone et al., 2002) as well as in black-box modelling with, for example, artificial neural networks (Holubar et al., 2003). Both methods are based on a different philosophy and have their specific characteristics. When circumstances or processes occur which are not understood well enough or parameter determination is unpractical and required, there will be a distinctive advantage for black-box modelling (Strik et al., 2004). This is especially the case in the complex processes of anaerobic digestion where the number of parameters is high and variable. So far there is very little information available about gas–liquid mass transfer coefficients which are required for describing the processes of biogas formation (Merkel and Krauth, 1999). Also there is inadequate information available about H_2S and NH_3 toxicity and adaptation to toxicity of these compounds (Speece, 1996). These considerations justify the use of black-box modelling methods. Black-box models like the artificial neural networks are very attractive. They do not require prior knowledge about the structure and relationships that exist between important variables. Moreover, their learning abilities make them adaptive to system changes (Zupan and Gasteiger, 1999). Up to now, there is an interesting amount of applications of neural network models in the field of environmental engineering (Steyer et al., 2000; Holubar et al., 2002, 2003) and much potential for application in the whole environmental sector.

In this research the two compounds, H_2S and NH_3, have been produced in biogas and the processes modelled with artificial neural networks. Therefore, the MATLAB Neural Network Toolbox was used, because it is flexible and easy to apply. The prediction of the models under dynamical circumstances will be presented and discussed. Finally an outlook will be given of the models' application in predictive control tools.

2. Materials and methods

2.1. Artificial neural network background and modelling

A neural network is by definition: a system of simple processing elements, called neurons, which are connected to a network by a set of weights (Fig. 1). The network is determined by the architecture of the network, the magnitude of the weights and the processing element's mode of operation. The neuron is

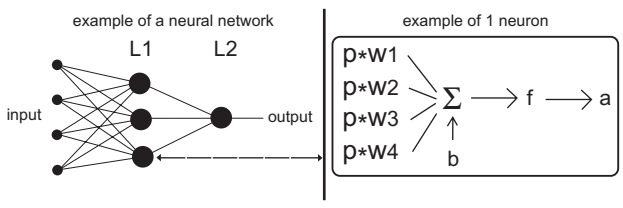

Fig. 1. Scheme of a full connected neural network with an input of 4 elements, 2 layers (L1 with 3 neurons and L2 with 1 neuron), 1 output element and the example of a single neuron (Hagan et al., 1996).

a processing element that takes a number of inputs (p), weights them (w), sums them up, adds a bias (b) and uses the result as the argument for a singular valued function, the transfer function (f), which results in the neurons output (a). The most common networks are constructed by ordering the neurons in layers, letting each neuron in a layer take as input only the outputs of neurons in the previous layer or external inputs. To determine the weight values, a set of examples is needed of the output relation to the inputs. Therefore, a set of data was produced describing the whole operating range of the system. All important parameters which were measured and used as input in the neural network modelling of the trace compounds are shown in Table 1.

The knowledge of the neural network is encoded in the values of its weights. The task of determining the weights from these examples is called training and is basically a conventional estimation problem. For this purpose, the back-propagation strategy has become the most frequently, and here, used method which tends to give reasonable answers when presented with inputs that they have never seen. Standard back-propagation is a gradient descent in which the network weights are moved along the negative of the gradient of the performance function. The term back-propagation refers to the manner in which the gradient is computed for non-linear multiple-layer networks. The typical performance function that is used for training feed-forward neural networks is the mean sum of squares of the network errors between the network outputs and the target outputs (Zupan and Gasteiger, 1999). In this work the batch gradient decent with momentum algorithm (Demuth and Beale, 2000) was used as the training function. This and other training functions gave good results in earlier neural network modelling of anaerobic processes (Domnanovich et al., 2004).

After the networks training the model needs to be validated with a representative set of data which was not used during the training of the model. Since the weight initialisation at the start of the modelling was a random process and was influencing greatly the results (data not shown), 50 repeats of each different model were done. The performance of the neural network model was evaluated with the root mean square error (RMSE) and determination coefficient (R^2) between the modelled output and measures of the training and validation data set. When the RMSE is at the minimum and R^2 is high, ≥ 0.8, a model can be judged as very good (Kasabov, 1998). Secondly, was the comparison between the modelled output and the measured output heuristically reviewed. These methods were occasionally used in neural network model validation (Norgaard et al., 1999; Hagan et al., 1996). Before the best model was found, a trial and error process was followed where different inputs and inputs-combinations were tested. By graphical representation of all results, the best input combination was selected. Hereby all reasonable combinations of input parameters were validated. Finally the architecture of the neural network model was optimised by applying different amounts (1–10) of hidden neurons. When the increase of hidden neurons did not improve the model anymore, the model with the smallest amount and maximum performance was chosen as the best model.

Table 1
Parameters which were measured for use as input in the neural network modelling of the outputs H_2S and NH_3 for the next day ($t + 1$)

Input for predicting H_2S $t + 1$	Input for predicting NH_3 $t + 1$
Sulfate loading rate [g SO_4-S m^{-3} d^{-1}]	Nitrogen loading rate [g N m^{-3} d^{-1}]
H_2S in biogas [ppm]	NH_3 in biogas [ppm]
Total sulfides in reactor [mg S^{2-} l^{-1}]	Ammonia in reactor [mg N-NH_3 l^{-1}]
Biogas-productivity [m^3 Biogas m^{-3} d^{-1}]	Ammonium in reactor [mg N-NH_4^+ l^{-1}]
pH	Total inorganic nitrogen in reactor [mg N-NH_4^+ + NH_3 l^{-1}]
Organic loading rate [kg COD m^{-3} d^{-1}]	Biogas-productivity [m^3 Biogas m^{-3} d^{-1}]
	pH
	Organic loading rate [kg COD m^{-3} d^{-1}]

2.2. Software

For development of the neural network models the Neural Network Toolbox 5 and MATLAB 6.5 (The Mathworks Inc. USA) were used. A MATLAB script was written which loaded the data file, trained and validated the networks and saved the models architecture and performance in a file ready for use in Microsoft Excel. The input and output data were normalised and de-normalised before and after the actual application in the network. The MATLAB script is available free of cost from the corresponding author. The PC with a 800 MHz processor and 512 Mb intern memory took about 1 min for the processing of one neural network model. The Neural Network Toolbox offers a broad variety of parameters for neural network development which can be chosen flexibly. The toolbox is provided with a practical user guide by Demuth and Beale (2000).

2.3. Reactors set-up and feed composition

To gain data for model training and validation, two 20 l lab-scale anaerobic Completely Stirred Tank Reactors (CSTRs) were operated at 60 °C (Fig. 2) with a hydraulic retention time of 40 days. One reactor (R-H_2S) for the hydrogen sulfide production and one reactor (R-NH_3) for the ammonia production. The process control software Labview 6.5 (National Instruments, Austria) was used for monitoring and controlling

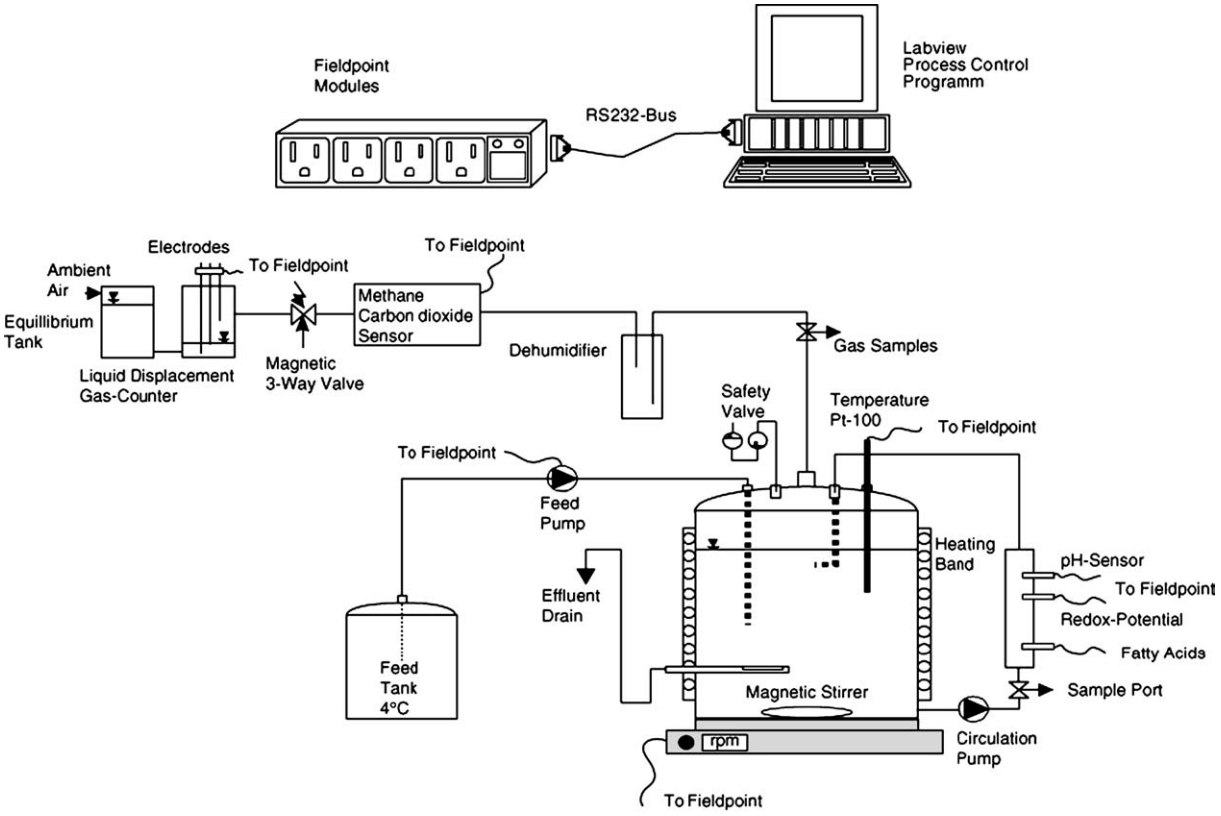

Fig. 2. Scheme of the anaerobic continuous stirred tank reactor.

the laboratory reactors. All devices used were connected to Field-point modules (National Instruments, Austria), and via an RS232 interface to the controlling PC. The reactor was mixed with the magnetic stirrer MR1 (IKA labortechnik, Austria). Reactor temperature was maintained at the set-point temperature by a heating band of type WB 185 (Winkler, Germany) and a Pt-100. Two peristaltic pumps (Verder, Germany) were used as feed- and circulation pumps. The reactors were fed with a pH adjusted (pH = 7.5) medium containing ($mg\,l^{-1}$): $MgSO_4{\cdot}7H_2O$ (100), $CaCl_2$ (10), H_3BO_4 (0.2), $FeCl_2{\cdot}4H_20$ (8), $ZnCl_2$ (0.2), $MnCl_2{\cdot}4H_2O$ (2), $CuCl_2{\cdot}2H_2O$ (0.152), $(NH_4)_6Mo_7O_{24}{\cdot}7H_2O$ (0.2), $CoCl_2{\cdot}6H_2O$ (8), $NiCl_2{\cdot}6H_2O$ (0.568), $Na_2SeO_3{\cdot}5H_2O$ (0.656), EDTA (4), $AlCl_3{\cdot}6H_2O$ (0.36), Resazurine (2) and HCl 37% ($0.008\,ml\,l^{-1}$). In the medium of R-NH_3 also $FeCl_3{\cdot}6H_2O$ (600–3000) was present. In the feed of R-H_2S were added KH_2PO_4, flour Type W480 and peptone from casein in different amounts in a ratio of 1:25:1 (g). In the feed of R-NH_3 were added NH_4Cl, KH_2PO_4, flour Type W480, peptone from casein and starch in different amounts in a ratio of 5.15:1.5:40:10:10 (g). Feeding was done automatically and split over the day into 5 or 10 smaller charges. The amount of feed was weighted with a Satorius Industry weight device. The feed was continuously mixed (IKAMAG REO, Austria) and cooled in a refrigerator at about 4 °C. The thermophilic digesting sludge was achieved from the waste water treatment plant of Altenmarkt (Germany).

2.4. Analytic

The chemical oxygen demand (COD) and total nitrogen (Tot-N) of the feed were analysed using, respectively LCK114 and LCK338 test-kit (Dr. Lange, Austria). Measurement of the amount of produced biogas was done by a liquid-displacement counter according to Veiga et al. (1990). Ammonium and ammonia in the reactor were determined with a gas-sensitive electrode NH500/2 (WTW, Germany) and pH measurement with a Sensolyt-SE electrode (WTW, Germany). Total sulphides in the reactor were determined colorimetrically after reaction with *N*,*N*-dimethyl-*p*-phenylenediamine oxalate according to the method described by Trüper and Schlegel (1964). The hydrogen sulfide and ammonia in biogas were measured daily with Dräger tubes (Dräger, Germany). An extra online biogas ammonia sensor (Iras, Germany) was temporarily installed to gain insight into the ammonia dynamics. Acetic acid, propion acid and total volatile fatty acids in the reactor were measured with a Fourier Transform Infrared spectrometer using a ZnSe Crystal (Perkin Elmer, Austria).

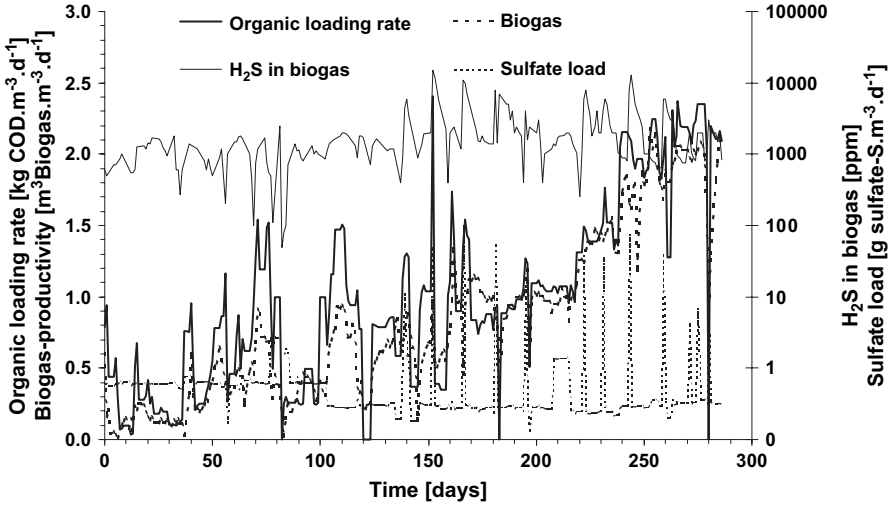

Fig. 3. Experimental course of R-H_2S.

3. Results and discussion

3.1. Experimental course and H_2S and NH_3 production

Both reactors were fed with a varying feed to gain the necessary dynamics in the data. To produce data which were distributed over the whole operating range, the COD/SO_4-S ratio, organic- and sulfate-loading rates varied for R-H_2S over time. Fig. 3 shows the experimental course and some of the data production of R-H_2S. The high sulfate-loading rates were reached by adding Na_2SO_4 to the reactor. As a result, the H_2S increased during the next days and gradually decreased afterwards.

For R-NH_3 the feed composition was constant but the amount varied during the experiment. Fig. 4 shows the experimental course and data production of R-NH_3. In the period from day 46 to 61, a lye pump controlled and increased the pH in the reactor by dosing 20 ± 10 ml of 6 M NaOH per day. This resulted in the increase of free ammonia and consequentially the increase of ammonia in the biogas. On day 88 the maximum concentration of 93 ppm of NH_3 was measured. The volatile fatty acids concentrations in the reactor (data not shown), which are indicators for reactor unbalance caused by overload or toxicity, were quite fluctuating. However, the biogas production (data not shown) was not severely affected.

3.2. Modelling

Several thousands of models were trained and validated until the best input parameters and best fitting input structure, architecture and MATLAB Neural Network Toolbox settings for the models were developed (Table 2). With the inclusion of the sulfate and organic loading rate $t + 1$ (value of the next day) in the H_2S model, it will be possible to embed the model in an optimisation algorithm whereby the parameters can be adjusted until a specific H_2S for the next day is

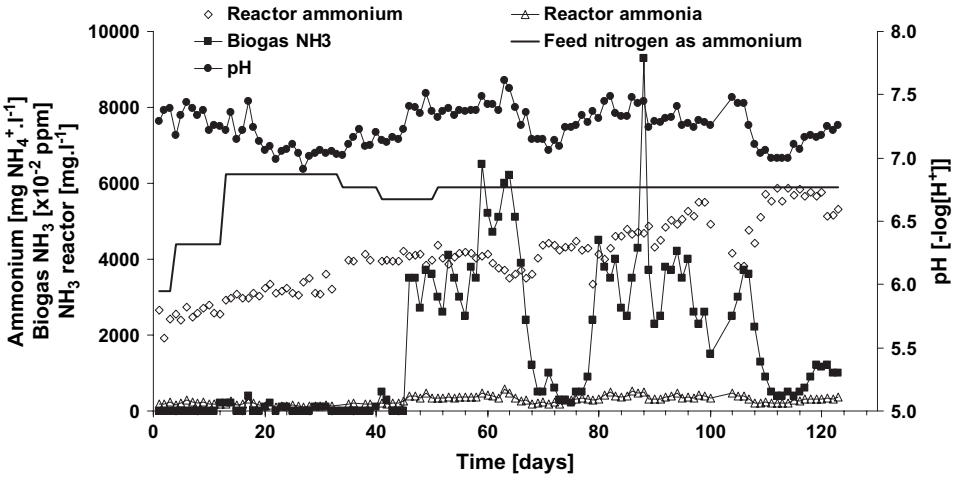

Fig. 4. Experimental course of R-NH_3.

Table 2
Structure, architecture and settings of the best found models predicting, respectively, H_2S and NH_3

	H_2S model	NH_3 model
Inputs[a]	Sulfate loading rate [g SO_4-S m^{-3} d^{-1}] $t-1$, t, $t+1$ Organic loading rate [kg COD m^{-3} d^{-1}] t, $t+1$ H_2S in biogas [ppm] $t-1$, t	Total nitrogen loading rate [g N m^{-3} d^{-1}] $t+1$ Organic loading rate [kg COD m^{-3} d^{-1}] $t+1$ NH_3 in biogas [ppm] t Biogas-productivity [m^3 Biogas m^{-3} d^{-1}] t pH $t-2$, $t-1$, t Ammonia in reactor [mg N-NH_3 l^{-1}] t
Output	Hydrogen sulfide in biogas [ppm] $t+1$	Ammonia in biogas [ppm] $t+1$
Layers	2	2
Hidden neurons	5	7
Transfer functions	*Tansig*/*purelin*	*Tansig*/*purelin*
Train function	*Traingdm* (batch gradient descent with momentum algorithm)	*Traingdm* (batch gradient descent with momentum algorithm)
Learning rate	0.001	0.001
Train epochs	5000	5000
Performance goal	0.02	0.02
Minimum performance gradient	1×10^{-8}	1×10^{-8}
Momentum constant	0.9	0.9
Maximum performance inc	1.04	1.04
Number of train data	100	131
Number of validated data	35	27

[a] $t-2$: value of two days before; $t-1$: value of one day before; t: value of present day; $t+1$: value of the next day.

calculated. The same principle will be possible with the NH_3 model, where the total nitrogen and organic loading rate can be adjusted for predicting the NH_3 in the biogas for the next day. In these ways a biogas plant operator can use the models in a predictive control tool. The results of the models' prediction were shown in Figs. 5 and 6. The one step ahead prediction of H_2S was even good when the H_2S increased fast (see e.g. days: 73, 82 and 94). The applied sampling time distance of one day was enough to describe all process dynamics. The increase of H_2S (after a sulfate pulse) took mostly several days. From data of the online ammonia sensor (data not shown) it was seen that the ammonia dynamics were captured with the one daily measurement.

The training determination coefficients (R^2) of both the models show that the neural networks learned the relation between input and output good. The validate R^2 of both models was even better which means that the generalisation capacity of the models was very good. That the training R^2 was worse than the validate R^2 was most probable due to noise in the training data. The RMSEs of the models were minimal and smaller than 6% of the maximum measured value. Both models were, from a heuristic point of view, following the dynamics in the system well and therefore suitable for doing predictions even under dynamical circumstances.

4. Conclusions

This paper confirmed the expectation that ammonia can be present in biogas in a range up to at least 93 ppm. Both researched trace compounds in biogas from anaerobic digestion were modelled successfully using

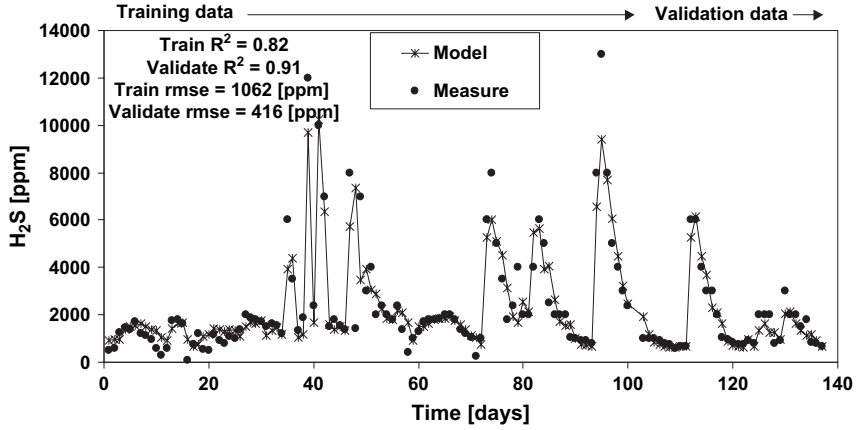

Fig. 5. Prediction of the H_2S in biogas with the best found neural network model.

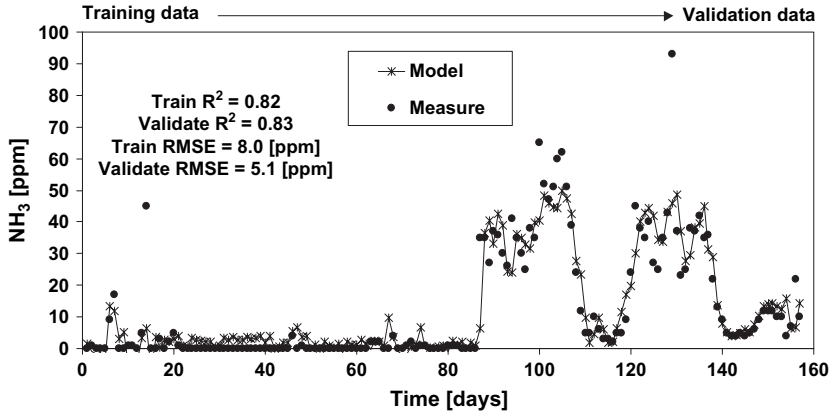

Fig. 6. Prediction of the NH_3 in biogas with the best found neural network model.

the MATLAB Neural Network Toolbox. By applying the developed MATLAB script it was possible to search for the best model in an easy manner. H_2S and NH_3 were predicted very well and the developed neural network models are therefore suitable in predictive control tools as was previously proposed by Steyer et al. (2000). With these kinds of tools an operator is able to take every day, in a few minutes time, the right precautions. For example, when a specific high nitrogen containing feed is offered the operator can calculate how much of this can be co-digested without producing ammonia in the biogas. The same counts for a high sulfate containing feed, where the operator can decide how the feed profile should be changed or otherwise it can be decided to add more iron salts so produced sulfide is precipitated. Another application way is possible when a pre-treatment technology for the H_2S cleaning is installed. The model can then be applied to predict and optimise the H_2S concentration so the pre-treatment will function optimally. Thus, with the proposed model based applications it will be possible to foresee, control, reduce or even avoid the production of the toxic trace compounds for fuel cells, H_2S and NH_3.

Acknowledgements

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