Towards Data-Driven NARX ANN Simulation for Optimal Control of the Flue Gas Desulphurization for Coal Power Plants

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KEYWORDS

SO_X absorption, data-driven modeling, and simulation, semi-dry gas desulfurization, optimal control, artificial neural network

ABSTRACT

This paper presents the ANN-based algorithm for data-driven optimal control of desulfurization of the flue gases from Coal Power Plants. We have proposed the NARX recurrent neural network with experimentally selected feedback connection length as the black box model for the first stage of the control process. Then simple brute force algorithm was used to find the optimal level of the reagent added into the system to keep the SO_X concentration outlet below the assumed level. This procedure was designed for a known level of SO_X concentration inlet. The proposed approach was tested on real data collected from the selected Coal Power Plant in Poland. The simulation that was made confirms that such an approach is effective for coal power plants to increase their energy efficiency and meet the appropriate environmental standards.

I. INTRODUCTION

Sulfur oxides pollute the air and have a negative impact on human health [1] and ecosystems [2]. Desulfurization of flue gases with SO_X (SO_2 and SO_3) emissions is one of the main challenges for the energy industry. The main source of sulfur dioxide emissions is the combustion of coal for energy production. In Poland, half of the SO_X emissions are attributed to the energy industry (according to the national report [3]). The reduction in the amount of SO_X emissions is linked to Poland's accession to the European Union and compliance with the Industrial Emissions Directive on emission limits. Current standards allow emissions from flue gas desulfurization plants at 200 mg/Nm^3.

This study aimed to develop a nonlinear autoregressive exogenous Neural Network model (NARX ANN) learned from industrial field data of the process of semi-dry flue gas desulphurization with soft-burned quicklime. The required quantity of reagent (CaO) for the purification of sulfur discharges produced by a Coal Power Plant was forecasted. Our objective pertains to the enhancement of technological processes with the aim of optimizing reagent consumption, which leads to a reduction in own costs but also affects the protection of the environment.

II. PROBLEM FOMULATION

The control problem for the flue gas desulfurization is based on the fact that SO_X emissions depend on two factors: the level of SO_X concentration inlet and the amount of the reagent added to the working system, see tab. 1, and fig. 1. The more reagents added the less SO_X concentration outlet is produced. However, adding more reagents results in an increase in the cost of the process. Moreover, the SO_X concentration outlet must be kept below a certain level, given by international norms and standards. Optimal Control of the Flue Gas Desulphurization for Coal Power Plants may be formulated as follows:

- SO_X concentration outlet(reagent amount) $<$ SO_X concentration outlet critical value;
- reagent amount $\rightarrow$ min.

For solving this problem data-driven approach was adopted. It does not require modeling the system using closed mathematical formulas. Instead, ANN (artificial neural network) was used as the black-box model for the dependence between SO_X concentration outlet, SO_X concentration inlet, and reagent amount. ANN was trained to predict the level of SO_X concentration outlet (ANN targets) based on reagent amount SO_X (first element of ANN input) and SO_X concentration inlet (first element of ANN input).

Data	variable name
reagent	$input_{ca}$
SO_X concentration inlet	$input_s$
SO_X concentration outlet	$output_{so2}$

TABLE 1: Considered data description and variables used in Matlab simulation

The next stage is to use the trained ANN as the black box model for the simulation of the working system and

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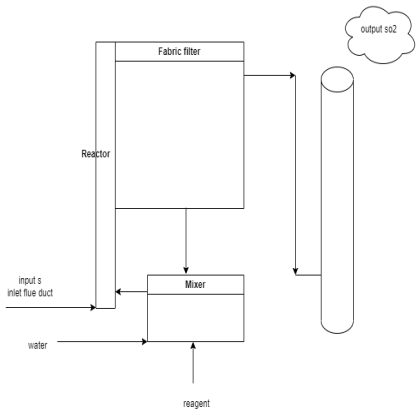

Fig. 1: Flue Gas Desulphurization for Coal Power Plants schema

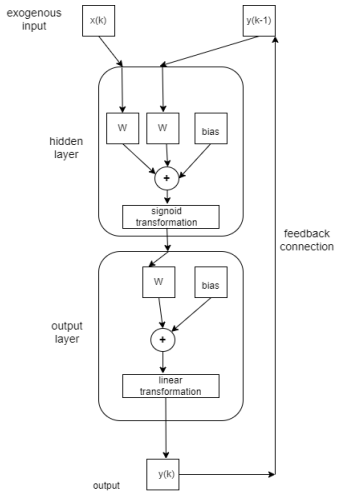

Fig. 2: The nonlinear autoregressive network with exogenous inputs (NARX), a recurrent dynamic network, with feedback connections enclosing several layers of the network

the prediction of the amount of the reagent for the given level of SO_X concentration inlet. The aim is to determine the impact of different reagent amounts on the level of a SO_X concentration outlet. Based on those simulations, the system may be controlled for the next stage of operation. For this aim, the nonlinear autoregressive network with exogenous inputs (NARX), see fig. 2, a recurrent dynamic network with feedback connections enclosing output and input layers, was used, [4]. Such ANN is reported to obtain very good results in time-series modeling. To verify the quality of modeling, the mean squared error (MSE) and R coefficient of variation were used for the learning and testing process separately, [5]:

$$MSE = \sum_{k=1,...,K} (ANN_{target}(k) - ANN_{output}(k))^2/K \quad (1)$$

and the $meanErr$, the mean absolute of the testing errors obtained from the testing process:

$$meanErr = \quad (2)$$

$$mean_{k=1,...,K}|ANN_{target}(k) - ANN_{output}(k)| \quad (3)$$

where $k = 1, ..., K$ denotes the kth sample from the training/validation/testing set.

III. RELATED WORK

There are several methods using different absorbents to flue gas desulfurization, of which the most popular is limestone for economic reasons [6]. Taking into account the sorbent dosing method, as well as the reception of the product formed during flue gas desulfurization, calcium-based methods are classified as dry, semi-dry, and wet. These methods use the reaction between calcium oxide and sulfur dioxide to reduce SO_X emissions [7]. The industrial process that combines CaO to reduce pollutant emissions from the Coal Power Plant is described below. Acidic pollutants from flue gases are removed by introducing hydrated or burnt lime $Ca(OH)_2$. This lime reacts with sulfur dioxide (SO_2) and hydrogen chloride (HCl) to form hydrated calcium sulfate ($CaSO_3$) and calcium chloride ($CaCl_2$), which are then transported by the gas flow:

$$SO_2 + Ca(OH)_2 \rightarrow CaSO_3 \cdot 0,5H_2O + 0,5H_2O \quad (4)$$

$$2HCl + Ca(OH)_2 \rightarrow CaCl_2 \cdot 2H_2O \quad (5)$$

Dry and semi-dry methods produce desulfurization product in a dry state, called End Product. In semi-dry methods, the temperature has a significant impact on the product state. Wet methods result in a suspension or slurry. Due to its higher efficiency and lower costs, the semi-dry method is the most commonly used in the energy industry [8]. At the same time, the effectiveness of SO_X removal is complex and depends on many factors. The reactivity of the calcium-based sorbent is variable. The process, as an exothermic reaction, depends on changes in temperature, humidity, and the contact time of the sorbent with SO_X [9]. Modeling the desulfurization process can be useful in predicting and assessing the impact of parameter changes on its efficiency, diagnosing problems, and, of course, predicting emissions under changing conditions. Modeling these elements optimizes the sulfur removal process and, in practice, serves to minimize SO_X emissions into the atmosphere. Modeling the desulfurization process can be useful in predicting and assessing the impact of parameter changes on its efficiency, diagnosing problems, and, of course, predicting emissions under changing conditions. Modeling these elements optimizes the sulfur removal process and, in practice, serves to minimize SO_X emissions into the atmosphere. The choice of the appropriate modeling method depends on the adopted goal, process scale, data availability, computing power, and time. In the literature, one can find models based on kinetic equations directly related to the calcium sorbent - SO_X reaction [10], [11] flue gas flow simulations [8], [12] and machine-learning based models [13], [14].

It is worth noting that models based on kinetic equations do not take into account the many variables affecting the desulfurization process and are difficult to implement for changing process conditions. Flow simulation requires consideration of equipment geometry, adequate knowledge, and significant computational resources. Simple regression models are easy to implement but less accurate as they do not consider the process dynamics. An alternative solution that takes all these elements into account is machine learning models. Regarding the availability of process data, the results obtained by these methods are also more realistic.

IV. ALGORITHM FOR CALCULATING THE IMPACT OF REAGENT INTO SO_2 CONCENTRATION OUTPUT

The algorithm for finding the optimal level of reagent for the Kth consecutive step of the plant operation was formulated as follows:

- Set $output_{so2}^{critical}$ critical value for SO_X concentration outlet, set the number N of possible values of $input_{ca}$ (reagent) to be examined, set the optimal $input_{ca}^{opt}$ as $max\{input_{ca}(k), k = 1, 2, .., K-1\}$ the maximum amount of reagent added to the system for $k = 1, 2, .., K-1$. Denote the NARX last memory state of the depth d $[output_{so2}(K-1), ..., output_{so2}(K-5)]$ by $MEM^d(K-1)$

- Train/Validate/test Narx with all samples $k < K$

- Retrieve NARX weights and the $meanErr$

- Set Kth value of the $input_s(K)$ of the new amount of SO_2 concentration inlet

- For i=1,2,..N calculate the
$ANN_{output}(K) =$
$ANN(input_{ca}(i), input_s(K), MEM^d(K-1))$
if $ANN_{output}(K) + meanErr < output_{so2}^{critical}$ set
$input_{ca}^{opt}$=$min(input_{ca}(i), input_{ca}^{opt})$

V. NUMERICAL SIMULATION

A. NARX training and testing

The analyzed data were collected from 29.12.2019 (00:00:00) until 10.01.2020 (23:43:00) every minute. That resulted in 18706 observations; see tab.2 and fig.3.

Variable name	min	max	units
$input_{ca}$	0	1945	kg
$input_s$	0	2401	mg/Nm^3
$output_{so2}$	0	1388	mg/Nm^3

TABLE 2: Considered data range and units used in simulation

All the data were consecutive in time measurements. We denoted $input_{ca}(k)$ as the kth consecutive measurement of the variable $input_{ca}$.

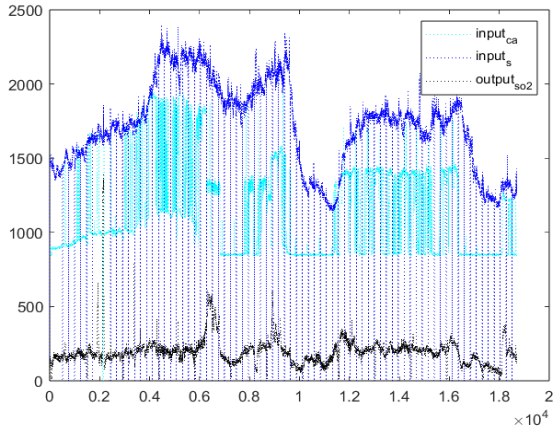

Fig. 3: Data collected from the system: SO_X concentration outlet, SO_X concentration inlet, reagent level

After the introductory test nonlinear 2-15-1 autoregressive exogenous Neural Network model (NARX ANN) with sigmoidal activation functions in the hidden layer and linear activation function for the output. Five (d=5) autoregressive units were selected as the NARX memory depth.

Inputs and targets for NARX ANN were introduced as:

$$ANN_{input}(k) = \tag{6}$$

$$[input_{ca}(k), input_s, output_{so2}(k-1), ..., output_{so2}(k-5)] \tag{7}$$

$$ANN_{target}(k) = [output_{so2}(k)] \tag{8}$$

for k=1,2,....K-1 (K=18706). 70% of data was randomly taken for NARX training, 15% for validation, and the remaining 15% for testing. The NARX model was trained by three concurrent methods: Levenberg–Marquardt algorithm, Bayesian Regularization, and a scaled conjugate gradient algorithm in Matlab environment, [16], see tab. 4, 3. The obtained results for best selected NARN ANN are shown for selected data samples from the testing set, see fig. 4-7.

MSE	LM	Bayes	SCG
Training	104.59	96.67	206.29
Testing	102.03	126.86	211.34

TABLE 3: The results of NARX ANN, Mean Squared Error for training and testing sets

R	LM	Bayes	SCG
Training	0.9942	0.9949	0.9905
Testing	0.9950	0.9929	0.9867

TABLE 4: The results of NARX ANN, the correlation coefficient for training and testing sets

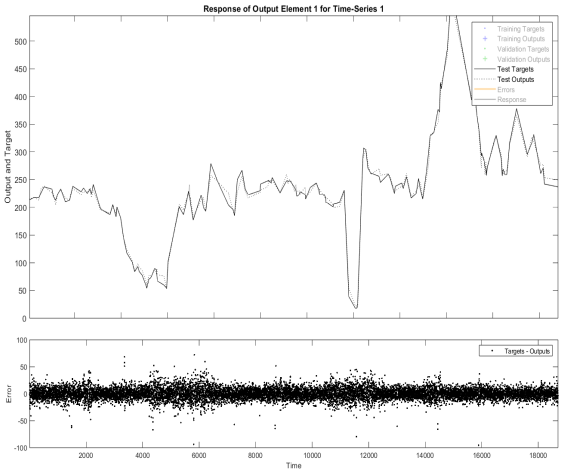

Fig. 4: Chosen results of NARX testing, predicted and measured SO_X concentration outlet level

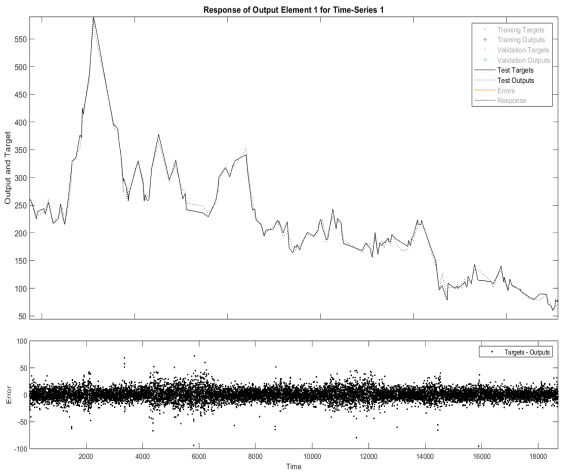

Fig. 5: Chosen results of NARX testing, predicted and measured SO_X concentration outlet level

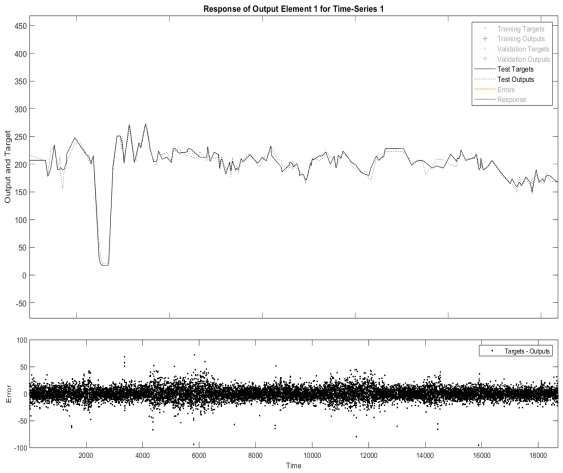

Fig. 6: Chosen results of NARX testing, predicted and measured SO_X concentration outlet level

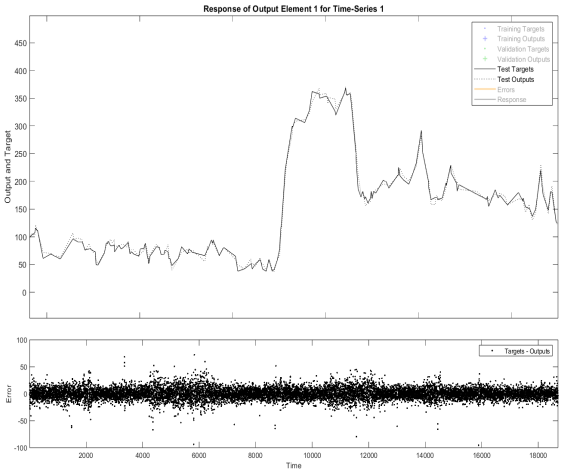

Fig. 7: Chosen results of NARX testing, predicted and measured SO_X concentration outlet level

B. Finding the value of reagent consumption

The simulation was made as follows:

- $output_{so2}^{critical}$=130 critical value for SO_X concentration outlet, N=201 of possible values of $input_{ca}$ (reagent) to be examined, that is $input_{ca} \in [0, 1350]$ set the optimal $input_{ca}^{opt}$ as $max\{input_{ca}(k), k = 1, 2, .., K-1\} = 1945$ the maximum amount of reagent added to the system for $k = 1, 2, .., K-1$.

- Train/Validate/test Narx with all samples $k < 18706$

- Retrieve NARX weights and the $meanErr = 7.53$

- $input_s(18706) = 1406$ of the new amount of SO_X concentration inlet

- For i=1,2,..201 calculate the

$ANN_{output}(18706) =$
$ANN(input_{ca}(i), input_s(18706), MEM^d(18706-1))$
if $ANN_{output}(18706) + 7.5 < 130$ set
$input_{ca}^{opt}$=$min(input_{ca}(i), input_{ca}^{opt})$

The best-selected reagent level obtained from the above simulation was 550 kg. The predicted SO_X concentration outlet for SO_X =1406 for different levels of regent in the range [200, 1200] is depicted in fig. 8. As we can see, adding more reagents results in decreasing the SO_X concentration outlet level. However, the simulation detected nonlinear behavior in the interval [800, 900] kg. The possible origins of this anomaly should be investigated in the next stage of the research. Potential causes of this in the context of the desulfurization process could be the chemical and physical properties of the reagent, process conditions (such as changes in

temperature, humidity, or flue gas flow rate), or contamination of the reagent, for example, by ash. All of these factors can affect the effectiveness of SO_X removal [17]. We have set the critical threshold at 130 mg/Nm^3 because Poland is required to lower its emissions to that level by 2030. Considering the critical level 130 and taking into account the mean NARX error equals 7.5, the lowest save level of the reagent should result in SO_X concentration outlet equal 122 mg/Nm^3. For this level, the reagent level simulated by NARX ANN shows strongly decreasing behavior. Therefore the solution to the minimalization problem is singular.

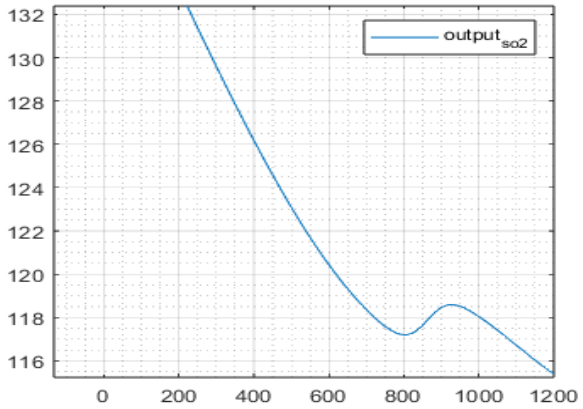

Fig. 8: Predicted SO_X concentration outlet for selected SO_X concentration inlet equal 1406 mg/Nm^3 for different levels of reagent in the range [200, 1200] kg

VI. CONCLUSIONS

In this paper, we presented data-driven modeling techniques using a nonlinear autoregressive exogenous Neural Network model. The data pertaining to the process originated from the flue gas desulfurization coal power plant.

Results indicate that:

1. NARX ANNs can therefore be used to build models of the semi-dry desulfurization process, used in practice for optimizing reagent consumption reaching in our case a coefficient of determination of up to 99% for the efficiency. In our opinion, further research should focus on optimizing the performance of NARX ANN models.
2. The obtained forecasts indicate the possibility of more efficient use of sorbent in the semi-dry desulfurization process.
3. By reducing the amount of reagent used in a process, Power Plants can save money on reagent purchases and reduce their overall water and electricity usage. This, in turn, can help to reduce the environmental impact of the process, as well as the costs associated with end product utilization. Indirectly, lower media usage decreases CO_2 emissions.
4. Thanks to process optimization, coal power plants can increase their energy efficiency and reduce the costs associated with maintaining appropriate environmental standards. Further investigations may involve the use of other process control variables - for example, optimization of process temperature and water consumption.

Symbol	Description
ANN	artificial neural network
NARX	autoregressive exogenous ANN
MSE	mean squared error
R	coefficient of variation
$meanErr$	mean absolute of testing errors
$input_{ca}$	reagent
$input_s$	SO_X concentration inlet
$output_{so2}$	SO_X concentration outlet
$output_{so2}^{critical}$	critical val. SO_X concentration outlet
k	measurement number
$ANN_{output}(k)$	output of ANN for the k input
$ANN_{target}(k)$	true value of $output_{so2}(k)$
$ANN(x)$	output of ANN for the x vector input
$K-1$	the last data used for NARX training
d	the depth of NARX network memory
$MEM^d(K-1)$	$[output_{so2}(K-1), ..., output_{so2}(K-d)]$
K	the data for the control
SO_X	SO_2 and SO_3

TABLE 5: Numenclature

References

[1] Jain R K, Cui Z., Domen J. Environmental Impact of Mining and Mineral Processing Butterworth-Heinemann; 2016. p. 53-157

[2] Wookey P.A., Ineson P., Mansfield T.A. Effects of atmospheric sulphur dioxide on microbial activity in decomposing forest litter Ecosystems & Environment; 1991. p. 263-280 vol.33

[3] https://www.kobize.pl IOŚ-PIB; 2021 [in Polish]

[4] Cooper S. Neural Networks: A Practical Guide For Understanding And Programming. Data Science; 2019.

[5] Haykin S.O. Neural Networks and Learning Machines. Pearson; 2008.

[6] Kallinikos L.E., Farsari E.I., Spartinos D.N., Papayannakos N.G. Simulation of the operation of an industrial wet flue gas desulfurization system Fuel Process. Technol.;2010. p. 1794–1802, 91 (12).

[7] Li X., Han J., Liu Y., Dou Z., Zhang T. Summary of research progress on industrial flue gas desulfurization technology Separation and Purification Technology; 2022. 119849, vol 281.

[8] Li C., Xu Z., Wang X., Bai H., Han L., Zhou Y. Numerical simulation and optimization of semi-dry flue gas desulfurization in a CFB based on the two-film theory using esponse surface methodology Powder Technology; 2022. 117268 vol. 401.

[9] Wichliński M., Włodarczyk R. Assessment of the Impact of Modification of Calcium Sorbents and the Possibility of Their Use in Desulfurization for Oxy-Fuel Combustion Process Minerals; 2021. 1284:11.

[10] Zhao Z., Zhang Y., Gao W., Baleta J., Liu Ch., Li W., Weng W., Dai H., Zheng Ch., Gao X Simulation of SO2 absorption and performance enhancement of wet flue gas desulfurization system Process Safety and Environmental Protection; 2021. p 453-463 vol.150.

[11] Du J., Yue K., Wu F., Ma X., Hui Z., Li M. Numerical Analysis of Semi-dry Flue Gas Desulfurization Process in the 3D Spouted Bed Chemical Engineering Transactions; 2020. p 1-6 :81

[12] Wu F., Yue K., Gao W., Gong M., Ma X., Zhou W. Numerical simulation of semi-dry flue gas desulfurization process in the powder-particle spouted bed Advanced Powder Technology; 2020. p 323-331 vol. 31.

[13] Ribeiro V.M. Sulfur dioxide emissions in Portugal: Prediction, estimation and air quality regulation using machine learning Journal of Cleaner Production; 2021. 128358 vol. 317.
[14] Gassner M., Nilsson J. , Nilsson E. , Palmé T. , Züfle H. , Bernero S. A Data-Driven Approach for Analysing the Operational Behaviour and Performance of an Industrial Flue Gas Desulphurisation Proceedings of the 24th European Symposium on Computer Aided Process Engineering – ESCAPE 24 June 15-18, 2014.
[15] Nguyen D., Widrow B. Improving the learning speed of 2-layer neural networks by choosing initial values of the adaptive weights. In: 1990 IJCNN International Joint Conference on Neural Networks; 1990. p. 21–26 vol.3.
[16] Demuth H., Beale M. Neural Network Toolbox for use with MATLAB. MathWorks. 2000;9.
[17] Rodríguez-Albelo L.M., López-Maya E.,Hamad S.,Ruiz-Salvador A.R.,Calero S., Navarro J.A.R. Selective sulfur dioxide adsorption on crystal defect sites on an isoreticular metal organic framework series Nature Communications; 2017. 14457 vol. 8.

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