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Echo-state neural networks forecasting steelworks off-gases for their dispatching in CH_4 and CH_3OH syntheses reactors

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Abstract. In the era of European Green Deal, steelworks are committed to reduce their CO_2 emissions by preserving their competitiveness. One of the options to achieve such aim is the valorization of process off-gases. Methane and Methanol production can be obtained by coupling novel reactors with an advanced control system that dispatches these gases after enrichment with green hydrogen. Knowing in advance the gases availability and composition is fundamental. The paper present Echo State Networks based-models that are applied to this aim and achieve adequate forecasting accuracy also in case of highly dynamic processes.

1 Introduction

Steel is a fundamental material for modern society and progress. However, steelmaking industries currently accounts for 4-5% of the total world CO_2 emissions [1]. Therefore, steelworks are spending efforts for improving their sustainability. Research activities focus on valorization of by-products or energy efficiency optimizations to obtain environmental and economic advantages; integrated steelworks (IS) Process Off-Gases (POGs) can lead to achieve both the objectives. Indeed, considerable amount of Coke Oven Gas (COG), Blast Furnace Gas (BFG) and Basic Oxygen Gas (BOFG) are produced in IS. These are carbonaceous POGs, whose main components are CO_x, H_2 (similar to syngas) and N_2. Due to their characteristics, POGs are generally internally exploited for heating purposes or power production. Sometimes the POGs distribution among consumers is not optimized and surplus or lack of POGs are addressed, respectively, by flaring or buying natural gas. This is why, in the last years, investigations focused on optimization of POGs management or on new reuse paths. Some works dealt with development of offline [2], online or combined Decision Support Systems for improving off-gas management in a holistic way [3-4]. Interesting studies can be found also on a material basis recovery of steelworks POGs (e.g. for chemicals production). Considering the most recent works, many investigations concern use of POGs for CH_3OH production, such as treated in [5-7]. While, Rosenfeld et al. analyse POGs use for CH_4 production [8].

In the listed works, valuable technical and economic analyses were carried out, but a real application requires the coupling of breakthrough syntheses technologies [9] with an advanced Supervision and Control System (SCS). A SCS optimizes POGs distribution towards the internal power plant and the CH_4 and CH_3OH reactors, taking

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into account the constraints related to POGs internal uses. The SCS also governs the enrichment of POGs with H_2, which is often needed to satisfy the reactors requirements [10]. The overall objective is maximization of economic yield and minimization of environmental impact. Within the i^{3}upgrade European project a control system is developed, which is named Dispatch Controller (DC) and is based on an economic hybrid model predictive control approach. The DC, among other information, has to know in advance the POGs availability and their compositions (also of minor compounds that could poison the catalyst), which are strongly affected by the dynamics of the industrial processes. This information can be obtained through ad-hoc developed models that are able to reproduce the high dynamics of involved processes with the available continuous data. The paper shows how Machine Learning can be fundamental to reach this scope. It presents models based on Echo-State Neural Networks (ESN) that are integrated in the DC and allow forecasting POGs amount and compounds. Paper is organized as follows: Sec. 2 briefly provides a background on ESN-based models; Sec. 3 focuses on data preprocessing; in Sec. 4 numerical results are presented and discussed, while Sec. 5 gives concluding remarks.

2 Background on Echo-State Neural Network-based models

ESNs were selected for models development considering different aspects. Firstly, fast learning was necessary: re-training could be often required for the considered application. ESN's memory feature was suitable for the highly dynamic industrial processes to be modelled, whose states are strongly dependent from previous ones. In addition, good results were obtained by the authors in the forecasting of similar outputs [11-13] and ESNs gave better predictions compared to other methods (e.g. Long Short-Term memory) for the modelling of same nature processes [13]. Among Reservoir Computing methodologies, ESN architecture stands out as one of the most effective, both from the point of view of computational cost, and for the accuracy of the predictive models that can be developed. Compared to classic recurrent networks, ESNs differ in their structure essentially consisting of an input layer, one or more reservoir layers and the readout. Reservoir consists of a large number of sparsely and randomly connected neurons, which are excited by input layer and emit dynamics richer in frequency than the input signals. The large and rich set of dynamics is finally combined through the readout to calculate the network outputs. Starting from the shallow architecture (SESN) [14], several studies proposed an evolution exploiting concepts related to Deep Learning to improve models generalization and accuracy [15]. The resulting Deep ESNs (DESNs) have a structure similar to SESNs, but their reservoir consists of a set of reservoirs usually connected in series. The interesting aspect of ESN architecture lies in the fact that the training of the weights concerns only the readout layer, whose weights can also be calculated through non-iterative algorithms. In this work, Tikhonov regularization least square algorithm was exploited for networks training; it calculates the readout weights while minimizing the mean square error between the target and simulated output, through a standard well know linear regression method. To find the optimal model architecture in terms of number of layers, neurons, spectral radius and input factors, a random search methodology was exploited aiming at minimizing the following type of Normalised

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Root Mean Square Error (NRMSE) on the validation dataset that allows evaluating the error on the whole target range:

$$\mathrm{NRMSE} = \frac{100}{\max(T) - \min(T)} \sqrt{\frac{1}{N_s} \sum_{k=1}^{N_s} \left(T(k) - y(k)\right)^2} \quad (1)$$

where T is the output target, y is the output of the model, N_s is the number of samples. More in details, within the random search routine the hyperparameters are varied in the ranges: number of layers = [1 10], total reservoir neurons = [50 3000], spectral radius = [0.1 1], input factors = [0.01 10].

3 Data pre-processing and datasets preparation

Time ordered industrial data were collected according to staff experience concerning process variables affecting POGs amount and composition, by also taking into account the issues related to the online availability of data flows in the data storage. A preliminary data pre-processing stage aimed at removing and correcting outliers (data quality was improved), as well as organizing and splitting into two datasets groups devoted the first one to variable selection (VS), and the second one to models development, by balancing the information content of all possible processes operating points (state dynamics diversity was guaranteed). VS was performed on the first datasets group. For processes characterized by a large set of descriptive variables, the approach of Cateni et al [16] was applied, which is articulated in two steps. Firstly, the feature space is reduced through a redundancy analysis in order to include only non-redundant variables. Then a genetic-based wrapper VS is applied, which selects relevant variables in a reasonable time reducing drastically the feature space. This process of reducing the space of the variables is necessary to avoid the overfitting phenomenon, to increase models accuracy and to improve process knowledge. For processes characterized by a limited set of variables, the VS was performed through an exhaustive search: optimal wrapper method that takes into account all variables combinations; it can only be performed for reasonable non-redundant variables number and by taking into account available data amount, to avoid training of models which are sensitive to overfitting. After VS, second datasets groups, describing the operating point of each gas producing process for 6 months of operation, was divided into 3 different time ordered subsets holding 40%, 30% and 30% of the available data, respectively, for the models training, validating and test stages.

4 Results and Discussion

Developed models provide a prediction on a forecasting horizon of 120 min and their accuracy is assessed through the NRMSE defined in equation (1). In the considered IS, 3 Blast Furnaces (BF) are in operation (one large - BF_A and two smaller - BF_B, BF_C) and more monitored data are available for the larger BF. Therefore, two models were developed for forecasting BFG: the first one forecasts BFG produced by BF_A (BF_AG), while the second one, cascaded to the first one, forecasts the total BFG (BFG_{Tot}) produced by the 3 BFs. BF_AG forecasting model allows predicting outputs reported in Table 1 by using 7 parallel and independent SESNs. Each ESN forecasts

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one target, to improve the accuracy and reduce the computational burden, and is fed by the scheduling plan of BF operation 120 min ahead in the form of a binary variable (1 means that BF is in operation), and by current values of the following variables: blast pressure, moisture and temperature, cold blast volume flowrate, injected O_2 volume flowrate, fed coal mass flowrate, injected plastic mass flowrate, BF_AG temperature, volume flowrate, CO, CO_2, H_2, O_2, H_2S and dust content. Results of this model in terms of prediction of 120 min ahead of volume flowrate, CO, CO_2 and H_2 content are fed to 4 further SESNs with the 3 BFs scheduling to predict the behavior of BFG_{Tot}. Predicted BF_AG minor compounds is considered suitable also for BFG_{Tot}, as lack of data prevented development of ad-hoc model. Results are good as evident from the validation and test NRMSE (*vNRMSE* and *tNRMSE*) listed in Table 1. Lower amount of data is the reason for higher errors in forecasting H_2S content. An example of prediction is given in Figure 1a, which depicts the CO_2 content in the BFG_{Tot}.

Model	Type	Outputs (t=1…120 min)	vNRMSE [%]	tNRMSE [%]
BF_AG	SESN	Volume flowrate	0.28-2.48	0.33-2.87
		CO	0.57-5.86	0.61-6.75
		CO_2	0.31-3.08	0.35-3.80
		H_2	0.57-5.23	0.68-6.17
		O_2	0.33-3.97	0.41-5.02
		H_2S	0.79-7.35	1.75-10.07
		Dust	0.68-5.80	0.92-7.03
BFG_{Tot}	SESN	Volume flowrate	0.13-1.55	0.10-1.61
		CO	0.64-3.22	0.73-3.55
		CO_2	0.75-5.19	0.94-6.82
		H_2	0.44-3.56	0.87-4.99
$BOFG_{Tot}$	SESN	Volume flowrate	7.52-10.52	8.23-11.47
		CO	1.10-5.68	1.87-6.94
		CO_2	0.81-10.78	0.81-13.24
		O_2	0.86-19.22	0.82-20.35
COG	DESN	Volume flowrate	1.68-4.83	1.74-4.91
		CO	3.31-4.70	3.34-4.80
		CO_2	2.37-2.65	2.28-2.66
		H_2	1.73-4.62	1.85-4.59
		O_2	3.44-3.97	3.65-4.13
		CH_4	3.60-5.25	3.88-5.47

Table 1: Models performances in terms of NRMSE on validation and test sets.

Model forecasting BOFG global amount ($BOFG_{Tot}$) is based on 4 independent SESN (one for each target) and provides $BOFG_{Tot}$ volume flowrate, CO_x and O_2 content, by using as inputs the binary representation of O_2 injection in the 3 converters for 120 min ahead (1 means that O_2 is injected) and current values of following variables for each converter: movable skirt position, O_2 injection, cumulative mass of fed pig iron, lime, FeSi and raw magnesite, $BOFG_{Tot}$ volume flowrate, CO_2, CO and O_2 contents. Figure 1b shows an exemplar comparison between 120 min real and predicted $BOFG_{Tot}$ amount. BOF process high dynamic is the main reason why the NRMSE values of the $BOFG_{Tot}$ model (Table 1) are higher, as well as of the fact that some

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predictions in Figure 1.b are under/over-estimated. However, the predictions are still suitable for DC purposes considering the amount of available monitored variables and data (for higher accuracy, more data are required). Only for O_2 content, NRMSE is significantly high but it is not an issue due to the very low amount of O_2. In the COG case, different models were developed to forecast COG production in terms of volume flow and composition of the gas in terms of H_2, CO_2, CO, CH_4 and O_2 contents. For each variable of interest, a single DESN based model was developed. Each model forecasts its specific variable for 120 min ahead by exploiting the past 120 min of the specific variable timeseries, through an autoregressive approach. Test results show the validity of DESN approach for forecasting each specific variable. In particular, COG volume flow and composition is forecasted with an accuracy described by NRMSEs in Table 1. For all the models, highest NRMSEs refer to 2 h ahead predicted values.

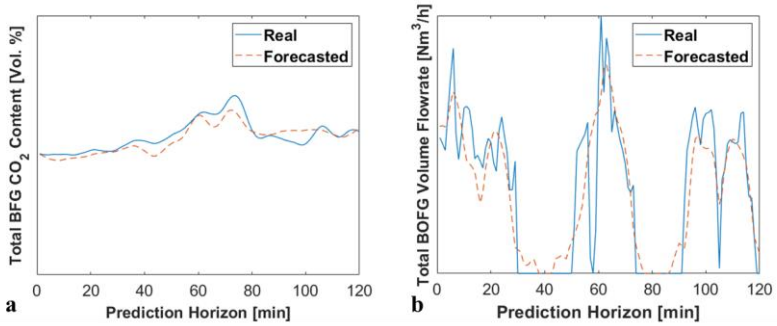

Fig. 1: Prediction example of BFG_{Tot} and $BOFG_{Tot}$ models (y-axes values are not shown for confidentiality constraints)

5 Conclusions and Future Works

In this work a set of ESN-based models are presented, which forecast volume flow and composition of main POG available in IS. Each model was trained, validated and tested by exploiting real industrial data. These models are included in a SCS that aims at optimizing the distribution of POGs, enriched with H_2, for maximizing the economic yield of their exploitation in CH_4 and CH_3OH reactors, while minimizing the environmental impact in terms of CO_2 emissions. Although some models show an accuracy with a *tNRMSE* in the order of 11-20% (i.e. for the high dynamic processes), all the obtained results show that they can be effectively used within the developed SCS, demonstrating the validity of the presented approach. This work also shows that Machine Learning can be a powerful enabler within systems aimed at improving environmental sustainability of industrial processes.

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