Modeling of Nitrogen Oxide Emissions in Fluidized Bed Combustion Using Artificial Neural Networks

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Abstract

The reduction of harmful emissions is affecting increasingly the modern-day production of energy, while higher objectives are set also for the efficiency of combustion processes. Therefore it is necessary to develop such data analysis and modeling methods that can respond to these demands. This paper presents an overview of how the formation of nitrogen oxides (NO_x) in a circulating fluidized bed (CFB) boiler was modeled by using a sub-model -based artificial neural network (ANN) approach. In this approach, the process data is processed first by using a self-organizing map (SOM) and k-means clustering to generate subsets representing the separate process states in the boiler. These primary process states represent the higher level process conditions in the combustion, and can include for example start-ups, shutdowns, and idle times in addition to the normal process flow. However, the primary states of process may contain secondary states that represent more subtle phenomena in the process, which are more difficult to observe. The data from secondary combustion conditions can involve information on e.g. instabilities in the process. In this study, the aims were to identify these secondary process states and to show that in some cases the simulation accuracy can be improved by creating secondary sub-models. The results show that the approach presented can be a fruitful way to get new information from combustion processes.

Keywords: Fluidized bed, Artificial neural network, Self-organizing map, Multilayer perceptron, Clustering

1. INTRODUCTION

Nowadays the efficiency of energy plants is considered an important topic due to environmental issues and increasing production costs. Efficient combustion of fuels with lower emissions is a challenging task in the modern-day production of energy, especially when inhomogeneous fuels such as coal, bark, or biomass are used. Fortunately, process data can involve important information on the behavior of the process and on different phenomena that affect the emissions and the energy efficiency of a combustion process. This information is valuable when optimizing the process. For this reason, new methods are needed for data processing, analysis and modeling.

Artificial neural networks (ANN) have shown their usability and power in the modeling of industrial processes [1]–[4]. ANNs have provided serviceable applications in diverse fields of industry, for example in energy production, chemical and electronics industry, and even in waste water treatment [5]–[11]. The variety of neural network applications is wide due to their strong advantages including flexibility, nonlinearity, adaptivity, applicability, a high computing power and a high tolerance of faults [2], [12], [13]. These benefits make ANNs a valuable choice for modeling method in industrial processes.

The use of a self-organizing map (SOM) [12] in the analysis of process states has produced a variety of applications in the past years. In 1992, Kasslin et al. [14] have first introduced the concept of process states by using a SOM to monitor the state of a power transformer. Later on, Alhoniemi et al. [15] have broadened the field of SOM-based applications by using the method in the monitoring and modeling of several industrial processes.

Furthermore, our earlier findings [8], [16] support the fact that different states of the fluidized bed combustion process can be discovered in process data. In reality these states can be for instance start-ups, shut-downs, idle times and different states of normal process flow. The behavior of the process, e.g. the quantities of different emission components, can be diverse between these conditions. However, these upper level process states also include secondary process states, where for example the bed temperature is unstable or the steam flow is lower than usual. It is momentous to learn to identify these states as well, because the performance of the process can fluctuate also in a smaller scale but regardless in a way that has an effect on the model accuracy.

Studying sub-models in parallel to more generic models opens an interesting view to modern-day process analysis. This is because process states and their corresponding sub-models can include valuable information on the performance of the process, as our earlier results concerning the activated sludge treatment and the wave soldering process indicate [6], [11]. The sub-model - based approach is a realistic option for instance in cases where it seems apparent that less detectable but still important phenomena are hidden under the generic behavior of the data. In spite of being more difficult to recognize, these phenomena can have a substantial effect on certain events in the combustion process. Fortunately, this kind of underlying information can be exposed by identifying different process states and creating sub-models, progressing from universal to more detailed models.

In this study, ANNs were used to identify the different states of a circulating fluidized bed (CFB) process and to create sub-models where the nitrogen oxide content of the flue gas was simulated. The obtained sub-models were then compared to the generic process model to see whether the accuracy of simulation could be improved by using this method. In the approach used, self-organizing maps [12], k-means clustering [17] and multilayer perceptrons [2] were combined sequentially to form an ANN method that benefits the good characteristics of all these methods.

2. PROCESS AND DATA

Fluidized bed combustion is a widely-used combustion technology used in power plants and designed primarily for solid fuels. A typical circulating fluidized bed (CFB) boiler consists of a combustion chamber, a separator and a return leg for the recirculation of the bed particles. The fluidized bed is characteristically composed of sand, fuel ash and a matter for capturing the sulfur. This mixture is fluidized by the primary combustion air brought in from the bottom of the chamber. Because of high fluidizing velocities, the bed particles are persistently moving with the flue gases. The particles are driven through the main combustion chamber into a separator, where the larger particles are extracted and returned to the combustion chamber. Meanwhile, the finer particles are separated from the circulation and removed from the flue gases by a bag-house filter or an electrostatic precipitator located downstream from the boiler's convection section.

One of the advantages of fluidized bed combustion is the large heat capacity of the bed, which ensures steady combustion. Only the start-ups involve the use of supporting fuels such as oil or gas. The purpose of the strong turbulence in the circulating fluidized bed is to support the mixing and combustion of fuel. The typical combustion temperature in CFB boilers is between 850 and 900 °C. The process data from the coal-burning CFB under study comprised 10 000 data rows with a 15 minute time interval, the number of variables being 36.

3. METHODS

3.1 Self-Organizing maps (SOM)

Kohonen's self-organizing map (SOM) [12] is a well-known unsupervised artificial neural network algorithm. The common purpose of SOM is to facilitate data analysis by mapping *n*-dimensional input vectors to structural units called *neurons* for example in a two-dimensional lattice (map). The map reflects variations in the statistics of the data set and selects common features which approximate to the distribution of the data samples. On the SOM, the input vectors with common features are associated with the same or neighboring neurons, which preserves the topological organization of the input data. The common properties of a map neuron can be presented with an n-dimensional, neuron-specific reference vector (prototype vector). The size of the map, or the number of neurons, can be altered depending on the purpose; the more neurons, the more details appear.

The SOM analysis is premised on unsupervised learning. At first, the preliminary reference vectors are initialized randomly by sampling their values from an even distribution whose limits are defined by the input data. During learning the input vectors are then grouped one by one into best matching units (BMU) on the map. The BMU is the neuron whose reference vector has the smallest *n*-dimensional Euclidean distance to the input vector. At the same time, the nearest neighbors of the activated neuron become likewise activated according to a predefined neighborhood function (e.g. Gaussian distribution) that is dependent on the network topology. At the final phase, the reference vectors of all activated neurons are updated.

In this study, the SOM was used as a pre-processor to compress information, to remove noise, and to visualize the data. The fluidized bed boiler data were coded into inputs for a self-organizing network, and a SOM having 384 neurons in a 24 x 16 hexagonal arrangement was constructed. The linear initialization and batch training algorithm were used in training, and the neighborhood function was Gaussian. The map was taught with 10 epochs, and the initial neighborhood had the value of 6. The SOM Toolbox (http://www.cis.hut.fi/projects/somtoolbox/) was used in the analysis under a Matlab version 7.6 software (Mathworks Inc., Natick, MA, USA, 2008) platform.

3.2 Identification of Process States

K-means clustering [17] was used to cluster the SOM reference vectors. The algorithm is initialized by randomly defining *k* cluster centers, and then directing each data point to the cluster

whose mean value is closest to it. The Euclidean distance is generally used as a distance measure in these comparisons. At the next stage, the mean vectors of the data points assimilated to each cluster are calculated and used as new centers in an iterative process. Clustering was performed twice, first to reveal the primary process states, and secondly to discover the secondary process states within the primary states.

There are several computational methods to determine the optimal number of clusters, one of the mostly used being the Davies-Bouldin -index [18]. Small values of the DB-index refer to compact clusters whose centers are far from each other. Hence the optimal number of clusters is the number where the index reaches its minimum. The computation of the optimal cluster structure is useful because thus it is not necessary to know the clusters beforehand.

The difference between two separate cluster center vectors represents the factors that separate the clusters. Therefore, this operation can be used to identify the reasons for the determination of different process states. In practice, this calculation is performed so that the comparable individual vector components of the center vectors are subtracted from each other. This produces a vector of differences, which can be used to identify the clusters as process states.

3.3 Multilayer perceptrons (MLP)

Multilayer perceptrons (MLP) are a widely-used [2], [3], [19], [20], supervised ANN methodology that can be used for example to create prediction models. MLPs consist of processing elements and connections. The processing elements are comprised of at least three layers: an input layer, one or more hidden layers, and an output layer. In training, the inputs are processed forward through consecutive layers of neurons. At first, the input layer distributes the input signals to the first hidden layer. Next, the neurons in the hidden layer process the inputs based on given weights, which can either weaken or strengthen the effect of each input. The weights are determined by a supervised learning process, which means learning from examples, or data samples. The inputs are next processed by a transfer function, which is usually nonlinear, providing the method with the ability to distinguish data that are not linearly separable. After that, the hidden neurons transfer the outcome as a linear combination to the next layer, which is generally the output layer. At the last stage, the performance of the model is evaluated with an independent validation data set. This is done by simulating the known data samples by using the model, and comparing the simulated output values with the real ones by using some model performance measure.

MLP neural networks must be trained to a given problem. One of the mostly used training techniques is the back-propagation [21] algorithm. In back-propagation, the network's output value is compared with the original sample to compute the value of a predefined error function. In the iterative training process the network weights are adjusted to a level that minimizes the error value between the actual and expected output for all input patterns.

A MLP network consisting of an input layer, an output layer and a hidden layer with 15 hidden neurons was used to simulate the flue gas nitrogen oxide (NO_x) content in the primary and secondary process states defined earlier by clustering. Variance scaling was used for pre-processing the data. The pre-processed data was divided into training, training test and validation sets. The training data set, being 60 % of the total 10 000 samples was used for training the network, while 20 % of the data set was put to the separate test set to be used in the back-propagation error calculations. The validation data set included the remaining 20 % of the samples, and was used as an independent test set for testing the model.

The parameters for the neural network were determined experimentally. The hyperbolic tangent sigmoid (*tansig*) transfer function was used in the hidden layer, and the linear (*purelin*) transfer function in the output layer. The resilient back-propagation (*trainrp*) algorithm was operated in the training procedure, and the mean squared error (*mse*) as the error function in training. Matlab version 7.6 (Mathworks Inc., Natick, MA, USA) software with the Neural Network Toolbox (version 6.0) was used in data processing. At the final stage, the prediction performances of the primary

and secondary models were compared to prove the usefulness of the presented method. Index of agreement [22] was used as the model performance measure.

4. RESULTS

The identification of the primary and two examples on the identification of the secondary process states in the CFB process are illustrated in Figure 1. Figure 2 and Table 1 present the NO_x prediction performance of the main model and the sub-models of the levels 1 and 2 in clusters III and 7.

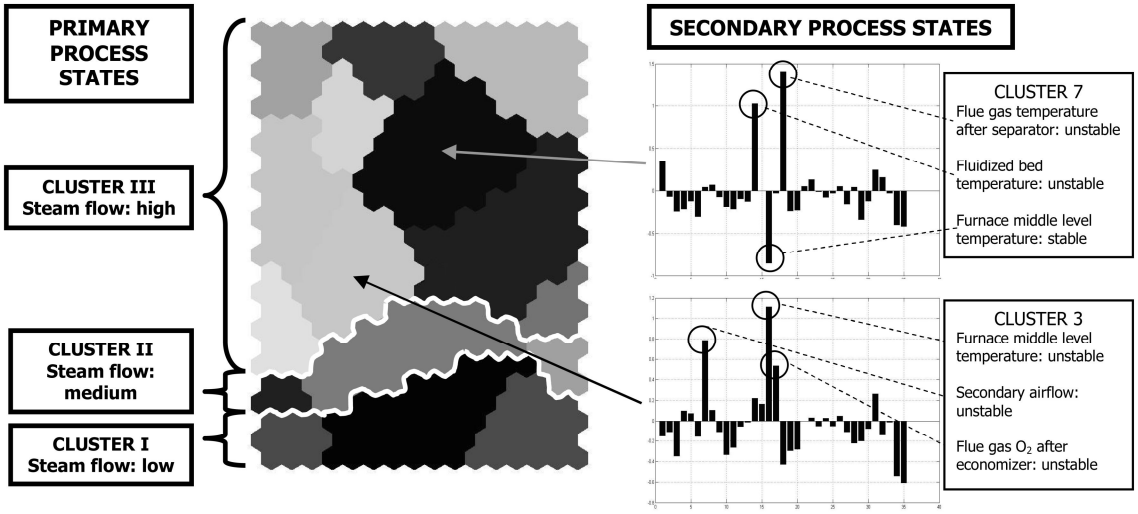

FIGURE 1: Example on the identification of primary and secondary process states on the SOM. The bar graphs represent the difference between the cluster center vector of the secondary process state and the cluster center vector of the primary process state (high steam flow). A considerable positive difference of standard deviations indicates instability in the corresponding variable.

Main model	Level 1 sub-model (Cluster III)	Level 2 sub-model (Cluster 7)
0.950	0.956	0.979

TABLE 1: The goodness (index of agreement) of models a, b and c presented in Figure 2.

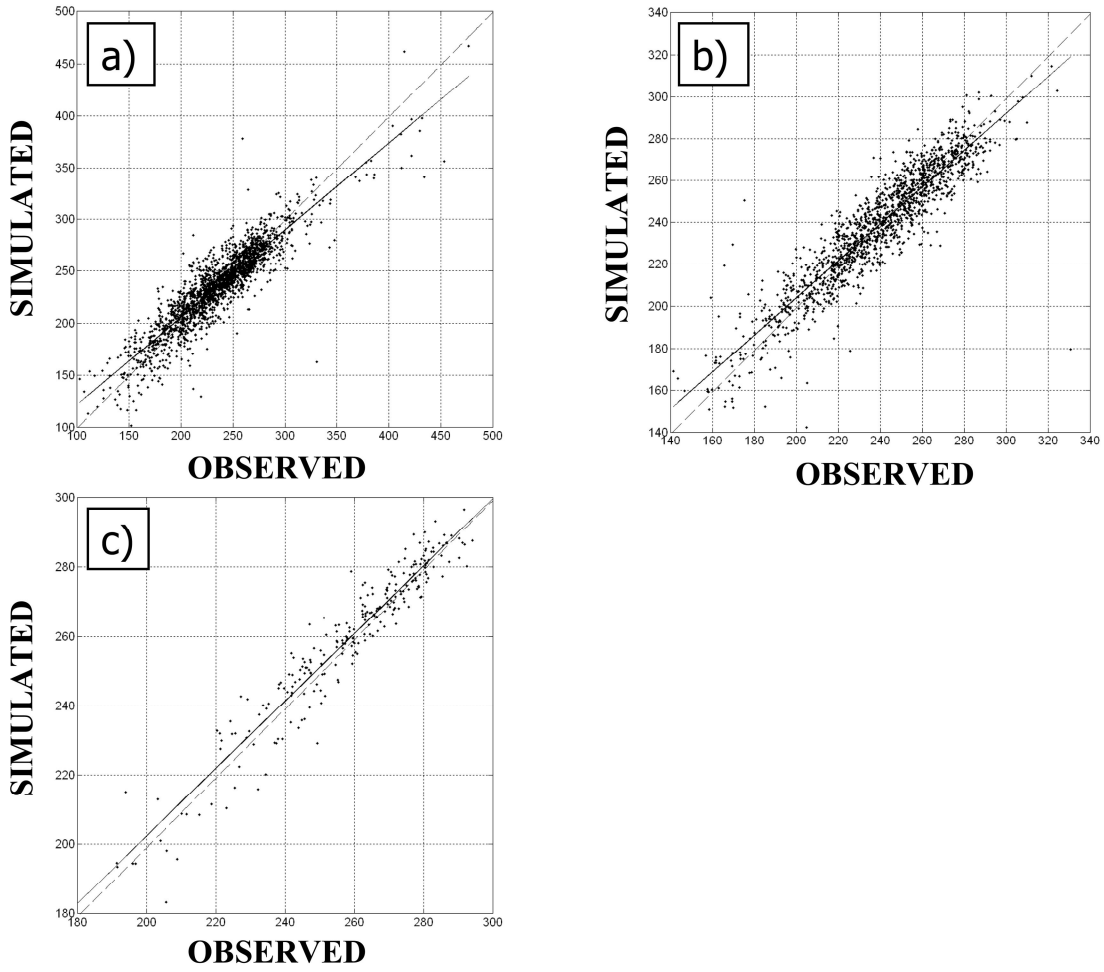

FIGURE 2: Simulated vs. observed flue gas NO_x content in different models. a) indicates the generic main model where the whole data is involved, b) is the level 1 sub-model (Cluster III, high steam flow), and c) is the level 2 sub-model (Cluster 7). Solid line describes least squares and dotted line perfect fitting.

5. DISCUSSION

Present-day energy industry is confronting many challenges, including the tightening legislation on reducing environmental pollution, pressure to increase the energy efficiency of energy plants, and new fuels that are demanding in terms of efficient combustion. The situation is complicated because changes in the combustion process may cause phenomena that have surprising side-effects. For instance, the process may fluctuate to an unstable state where the combustion is inefficient. Unfortunately, an inefficient conversion of fuel to energy often leads to an increased level of emissions. On the other hand, there are also situations where the process works optimally regarding to the efficiency and stability of combustion. It is useful for energy plants if the archived process data can be exploited for advanced process monitoring and diagnostics.

The SOM has been considered a functional, visual and efficient method when it comes to process monitoring, diagnostics, and optimization of circulating fluidized beds [5], [8]–[9], [16]. The findings presented in this study support our earlier results. As a whole, the SOM and k-means provide a simple and functional means to visualize and study the combustion process. Moreover, the results show that the method can be used to define process states and illustrate them in a visual way. All together, it is practical to observe the alteration of process states, because they

provide supplementary information on the operational use of the energy plant and its side-effects, e.g. changes in the levels of nitrogen oxide emission.

The behavior of the CFB process data showed strong distribution of the process events into three principal process states. These states are defined best by high, low and medium steam flow, as can be seen in Figure 1. This kind of principal clustering behavior can be referred to as separation into primary process states. However, the strong grouping of data samples caused by the characteristics of the data means that some interesting phenomena can remain undetected under those strongly defined states. Despite their inconspicuousness, these phenomena can be important in respect to the performance of the combustion process and certain combustion-related events like the formation of emissions. In Figure 1, we have presented one way of revealing this sort of underlying information by identifying the secondary process states. The identification is possible by comparing the cluster center vectors as shown in the figure.

In the literature, experimental models have been successfully developed to model the formation of NO_x in fluidized beds [23]–[26]. In this study we managed to gain good generic models (IA = 0.95) by exploiting real operational data from a coal-fired CFB boiler. However, the accuracy of the NO_x simulations can be improved even as much as 3 % by creating secondary states of process and their sub-models, as can be seen in Figure 2 and Table 1. This means that the model can be improved gradually by getting deeper into the process states and their corresponding sub-models. In this respect, the results support our results concerning the wave soldering and the activated sludge treatment processes [6], [11].

The results suggest that it is reasonable to perform clustering in several successive steps to reveal the unnoticeable phenomena that otherwise may not be recognized. These hidden phenomena are not automatically perceivable without creating sub-models, but may still have a significant effect on certain factors in the process. In other words, the model of a more general level can be sufficient in certain situations, but a more detailed model can be more suitable for describing other phenomena.

In summary, the data analysis scheme used is illustrated in Figure 3. Firstly, the raw process data are pre-processed. Preprocessing includes all the necessary actions, such as data filtering and normalization of variables, to prepare the data for modeling. Next, the SOM and k-means clustering are used and combined with expert process knowledge to obtain the primary process states and their MLP sub-models. After this, the secondary states of process and their corresponding sub-models are formed using the same approach.

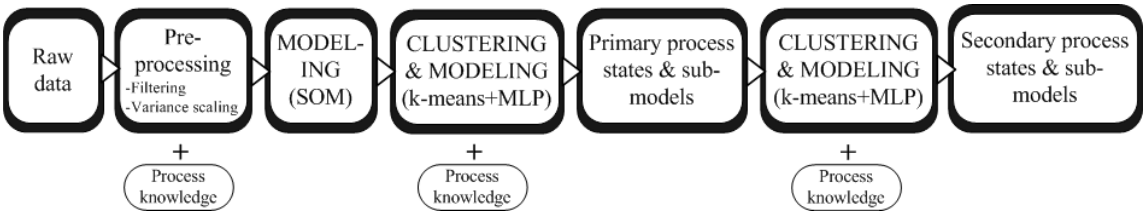

FIGURE 3: The data processing chain in a nutshell

The results show that the universal-to-detailed data analysis method presented can be excellent in cases where high simulation accuracies are required. In addition, the gradual penetrating analysis ensures that the best model is always found for each case in spite of its specific level. The classification of data samples into different subcategories, or process states, provides extra accuracy to the emission model. Furthermore, the ability of the method to reveal nonlinear and multivariate interactions entails additional value to the model. For these reasons, the data analysis method presented offers a powerful option to model industrial processes.

6. CONCLUSIONS

It is apparent that in the future also the energy plants have to be capable of producing energy with a lesser amount of harmful process emissions. Developing new data-based modeling methods for the energy industry is important because there is a growing need for improving the energy conversion processes. In this sense, the utilization possibilities of the approach presented include a wide spectrum of applications. One of them is process diagnostics, which exploits measurement data and has become an essential part of process improvement. Alternatively, the method provides an option for precise modeling of emissions in circulating fluidized bed boilers. The results presented in this study show that the modeling approach used is a fruitful way to model the coal-burning circulating fluidized bed process and to simulate its emissions.

The CFB boiler used as the case process is a coal-fired facility. In the future, it would be appropriate to test the methodology in other CFB processes incinerating different types of fuels, such as bark, biomass and even waste. This is because these inhomogeneous fuels are extremely challenging when it comes to efficient and stable combustion, while their use is also bound to increase in the future. Applying the method more widely would offer the opportunity to validate the method and make it a general approach for data-driven diagnostics and modeling of CFB boilers.

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