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Hybrid Models for Efficient Control, Optimization, and Monitoring of Thermo-Chemical Processes and Plants

Thomas Freudenmann [1,*], Hans-Joachim Gehrmann [2], Krasimir Aleksandrov [2], Mohanad El-Haji [1] and Dieter Stapf [2]

[1] EDI GmbH—Engineering Data Intelligence, Wöschbacher Str. 73, 76327 Pfinztal-Berghausen, Germany; el-haji@edi.gmbh
[2] Institute for Technical Chemistry, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany; hans-joachim.gehrmann@kit.edu (H.-J.G.); krasimir.aleksandrov@kit.edu (K.A.); dieter.stapf@kit.edu (D.S.)
* Correspondence: freudenmann@edi.gmbh

Abstract: This paper describes a procedure and an IT product that combine numerical models, expert knowledge, and data-based models through artificial intelligence (AI)-based hybrid models to enable the integrated control, optimization, and monitoring of processes and plants. The working principle of the hybrid model is demonstrated by NO_x reduction through guided oscillating combustion at the pulverized fuel boiler pilot incineration plant at the Institute for Technical Chemistry, Karlsruhe Institute of Technology. The presented example refers to coal firing, but the approach can be easily applied to any other type of nitrogen-containing solid fuel. The need for a reduction in operation and maintenance costs for biomass-fired plants is huge, especially in the frame of emission reductions and, in the case of Germany, the potential loss of funding as a result of the Renewable Energy Law (Erneuerbare-Energien-Gesetz) for plants older than 20 years. Other social aspects, such as the departure of experienced personnel may be another reason for the increasing demand for data mining and the use of artificial intelligence (AI).

Keywords: numerical model; oscillating combustion; NO_x reduction; artificial intelligence (AI)

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1. Introduction

To master the constantly growing amount of information from sensors and measurement systems, intelligent evaluation and optimization tools are playing an increasingly important role in the field of thermo-chemical processes to reduce costs and improve efficiency. One common tool involves modeling processes numerically based on their theoretical principles and validating these models with experimental data. However, it has been shown that the adjustment of systems and components requires longstanding expert experience combined with relevant parameters that are measured online. There is a lack of numerical simulations for specific plant behavior. In particular, the behavior of air and material flow in big plants cannot be adequately depicted, and a long calculation time for each operating point is required.

The combination of a data-driven (i.e., empirical) approach with expert knowledge of the plant and of thermo-chemical and physical principles could be a solution to better understand the behavior of the plant and thermo-chemical processes. This approach is referred to as the artificial intelligence (AI)-based hybrid model.

The combination of white and black box models and the resulting challenges have been presented in other works [1–4]. In most cases, the focus was increasing the transparency and accuracy of neural networks to obtain a better understanding of model behavior.

In this paper, the focus is on the formalization of expert knowledge and its use for test design and integration into different machine learning (ML) algorithms. The formalization of expert knowledge from different domains (e.g., expertise regarding plant mechanical processes and knowledge about thermo-chemical and other physical mechanisms of chemical processes) is particularly challenging and reveals the uniqueness of the presented approach. Due to the lack of data, deep neuronal networks cannot always be trained, and other ML algorithms must be combined to quantify and expand expert knowledge from different domains.

Figure 1 shows the continuous learning procedure and the interaction between the different parts of an AI-based hybrid model, i.e., data measurement, expert knowledge, and ML algorithms with special metrics for automated evaluation (autoML) [5]. With this procedure, expert knowledge can be continuously quantified, and the understanding of the plant and chemical processes can be expanded.

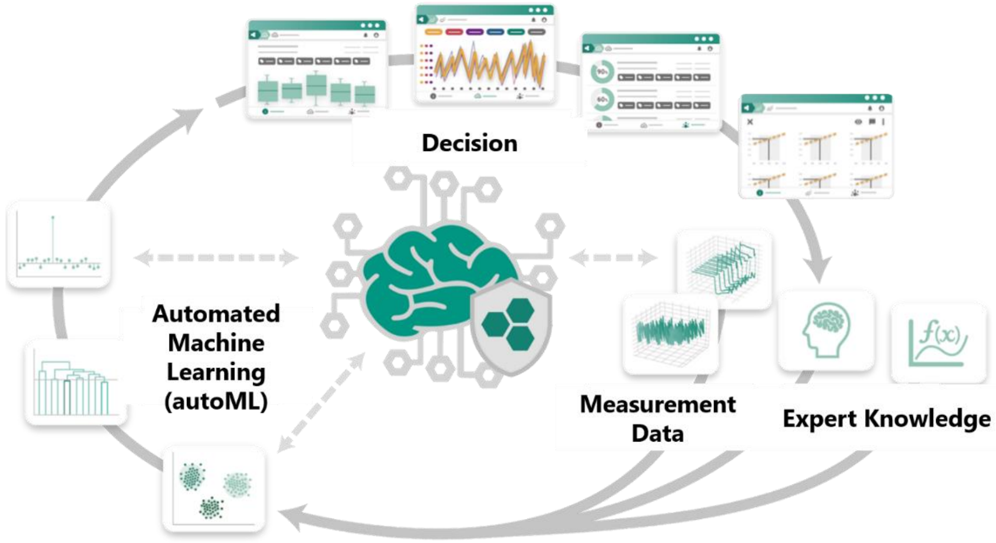

Figure 1. Procedure of continuous learning in the artificial intelligence (AI)-based hybrid model.

Along with a cloud-based IT solution from Engineering Data Intelligence (EDI Ltd., Pfinztal-Berghausen, Germany) called the "EDI hive Internet of things (IoT) Framework" (short EDI hive), the process of capturing expert knowledge and the integration of process engineering fundamentals, AI-based modeling, and the subsequent application of the AI-based hybrid model in power plant operation can be achieved. In this paper, the advantages of AI-based hybrid models in industrial applications are discussed, the experimental results are presented together with the modeling results, and the continuous software-based support of this process through EDI hive is demonstrated.

2. Materials and Methods

2.1. Procedure and Methodology

First, the modeling background, the structure of the logic, and the application to the combustion process are described. In this context, the pilot plant is briefly introduced, and the test program is presented.

2.2. AI-Based Hybrid Model

AI-based algorithms are calibrated in a hybrid model through formalized expert knowledge, which enables robust and technically meaningful predictions for the optimal control of a process, even with a small database. The structure and possibilities of a hybrid model are illustrated in Figure 2.

In a thermo-chemical process, it is often not possible to directly measure and record all of the parameters relevant for control and monitoring. These parameters include local high temperatures and pressures, or concentrations of unstable intermediate products. Frequently, data that can be measured in principle cannot be captured for design reasons.

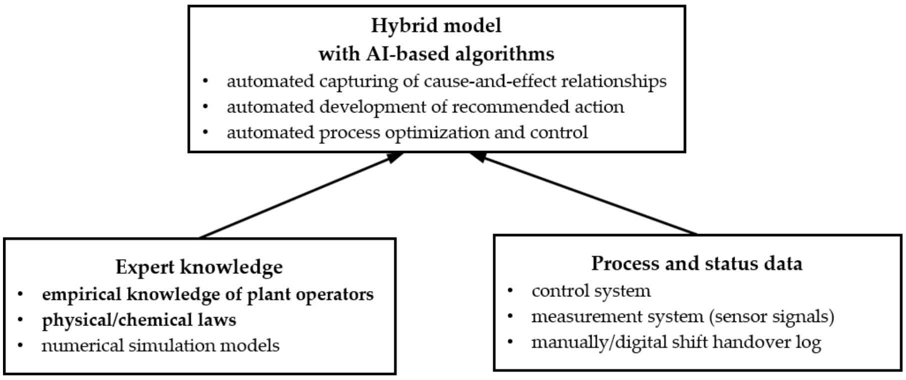

Figure 2. AI-based hybrid model.

In contrast, relevant status data can be calculated or predicted from simple measurable parameters using valid simulation models or based on expert knowledge. The acquisition of such parameters can be referred to as a soft sensor supporting the AI algorithms, which can then be trained with a larger and technically more meaningful database and be calibrated for prediction [6,7].

The relevant process and status data from a plant are often available in heterogeneous form, e.g., in different dimensions, formats, and partly in databases that are not time-synchronous. In some cases, important process and status data are only available in manually kept shift handover logs. However, the continuous collection and use of data is considered key for future competitiveness, especially in the process industry [8].

2.3. EDI hive Internet of Things (IoT) Framework

The EDI hive IoT framework is a cloud system based on the latest microservices architecture, which allows for a flexible orchestration of resources. This means that many user groups with large amounts of data can access the platform for different applications without performance restrictions. For data safety purposes, the platform can be operated as a private cloud on- or off-premises [9]. In addition to general use, role/rights, measurement data from management functions (e.g., aggregated measurement data), etc., the EDI hive offers other generic applications that can be used to optimize and control processes (Figure 3). In particular, the "EDI hive Cause-and-Effect Chain Editor" can be employed to formalize existing expert knowledge and use it for the calibration of AI-based models [10]. With the EDI hive standard names application, the system and system parameter names in the EDI hive can be semantically networked with regard to different languages. Furthermore, specific and frequently abbreviated control and measurement system channel names can be translated into different languages.

The EDI hive can be directly connected to the control systems of machines or plants and can thus be used as an IoT platform [11].

In the following section, the "EDI hive Cause-and-Effect Chain Editor" and the "EDI hive Model Generator" are described in more detail.

2.4. EDI hive Cause-and-Effect Chain Editor

As large databases are not always accessible, relevant correlations can partly be derived via known physical/chemical laws; thus, existing databases can be extended by further parameters, similar to the derivation of dimensionless characteristics. In particular, the knowledge of experienced plant operators or researchers with specific process knowledge should be formally recorded in cause-and-effect chains and used for the calibration of AI-based algorithms (Figure 4).

Figure 3. Generic applications of the Engineering Data Intelligence (EDI) hive Internet of Things (IoT) framework.

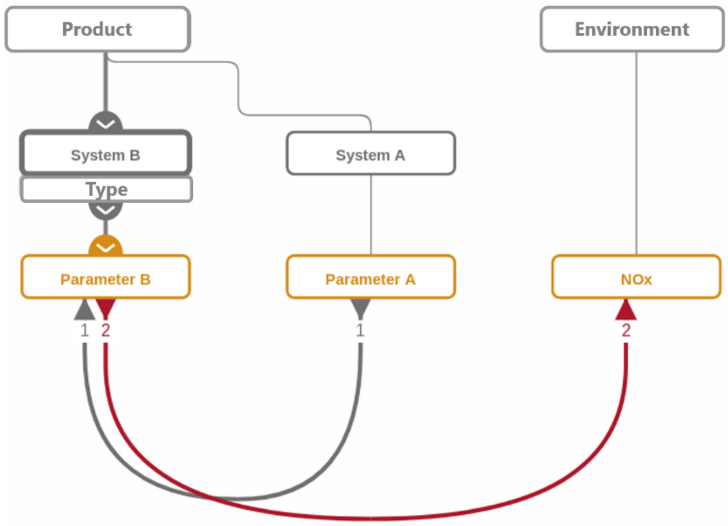

Figure 4. Example of a simplified cause-and-effect chain.

In the context of this project, a patented solution developed through EDI was used to formalize expert knowledge using the "EDI hive Cause-and-Effect Chain Editor". The specific knowledge of the experts from the BRENDA pilot plant regarding nitrogen oxide (NO_x) reduction in combustion processes was clustered in workshops and formally linked via cause-and-effect chains. This allows expert knowledge to be captured in semantically networked categories in a way that is understood by the computer, which is an essential prerequisite for the meaningful clustering and calibration of AI algorithms.

The determined cause-and-effect chains support a guided statistical design for experiments that allow for the quantification of the presumed correlations between the parameters at a lower test expenditure. Figure 4 shows a simplified cause-and-effect chain, which can represent a cause–effect relationship between the parameters relevant to NO_x reduction through oscillating combustion.

In a cause-and-effect chain, systems and their characteristics are represented by gray boxes, and system parameters (e.g., parameter A) by yellow boxes. The relationships between the systems and the system parameters are marked by simple lines. Relations show how the system parameters interact; gray relations denote relevant context and red relations are the focus of the cause-and-effect chain, which are referred to as test relations. The direction of the arrow indicates whether a system variable is an input variable (e.g., parameter A for the context relation) or an output variable (e.g., NO_x for the test relation).

In the subsequent application case, parameter B represents the oscillation frequency, while the system parameter NO_x is the target parameter to be minimized (NO_x concentration depends on the oscillation frequency). Further system parameters are the hard coal mass flow, flue gas temperature, and the conveying air for generation of the swirl. In addition, further physical/chemical laws or relevant legal requirements can be stored with their respective relations, e.g., the correct conversion of the volume content of oxygen according to the 17th Federal Emission Control Act (17th BImSchV). In this way, knowledge can be captured sustainably and reused for experiments at a later stage.

The capture, evaluation, and quantification of expert knowledge with the generated data, and visualization of the data model for the decision-making process are used in the AI-based hybrid model procedure in the following steps:

1. Formalization and capture of thermo-chemical expert knowledge, as well as expert knowledge about the technical boundaries of the plant (Figure 5).

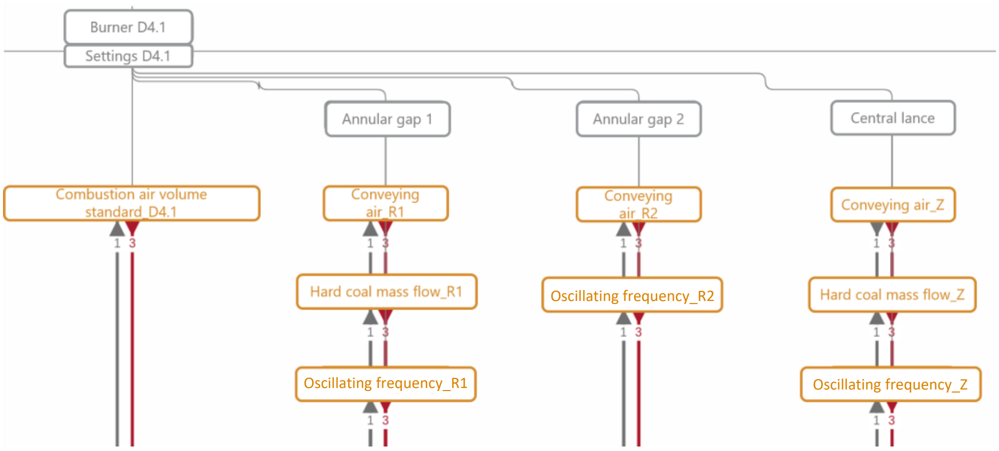

Figure 5. A selection of the cause-and-effect chains.

Experts know that the parameter oscillating frequency x_Z has a significant influence on NO_x reduction, so this expert knowledge is formalized with a variable and is included in the cause-and-effect chain.

2. Definition of the test design considering the expert knowledge and the time and cost restrictions of the dedicated technical system (BRENDA facility).

A D-optimal test plan was selected [12], where the combination of other relevant parameters (coal mass flow, combustion, air distribution) and the oscillating frequency parameter x_Z were varied on three discrete levels to describe the quadratic influence and the interactions between the other parameters. From the point of view of the test plan, a frequency of 6 Hz is desirable, but for the BRENDA facility, this frequency is not feasible. Here, the expert knowledge of the team was required to make the decision to operate at maximum frequency of 3 Hz. The pinch valve, applied here, is too inert to operate at frequencies higher than 3 Hz.

3. Generation of a defined test design.

In this step, the defined test design has to be filled with data to train the hybrid model. These data can be collected either from a database or from new experiments.

To evaluate the completeness of the expert's assumption with regard to the relevant parameters, a hierarchical cluster algorithm and a principal component analysis were carried out on all (measured) data, and no parameters were identified that were superior to the expert's assumption.

4. Quantification of expert knowledge regarding the influence of the parameters using a multiple regression model with limited numbers of operational points.

In this step, mathematical models correlate the main influencing parameters on NO_x concentration and weigh their impact.

5. Visualization of the quantified parameter for decisions in interaction diagrams.

Interaction diagrams show the results of the hybrid model in a simplified and clear way to obtain the crucial information of the best operational parameters for the technical system.

A hierarchical cluster algorithm was used, and component analysis was carried out [13] to evaluate significant parameters.

With the systematic test design using the "EDI hive Cause-and-Effect Chain Editor" coupled with the experimental setup, a regression model with nonlinear functions is used according to Equation (1):

$$y = \beta_0 + \sum_{i}^{n} \beta_i \cdot x_i + \sum_{i}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} \cdot x_i x_j + \sum_{i}^{n} \beta_{ii} \cdot x_{ii}^2 + \ldots + \varepsilon \tag{1}$$

The factor β considers the effects of the influence of the parameters x_i, x_{ii}, and x_j, and can be described as follows:

$$Effect = 2 \cdot \beta \tag{2}$$

Effect represents the value of an influencing parameter on the target parameter (NO_x), e.g., if the *Effect* is equal to zero, the parameter has no influence.

The coefficient β is determined using the least squares method, where:

x_i i = 1, e.g., oscillation frequency; i = 2, e.g., coal mass flow;
x_j j = 1, e.g., the interaction between oscillation frequency and coal mass flow;
n sum of all parameters;
${x^2}_{ii}$ considers possible quadratic correlations of the oscillation frequency;
ε deviation, which has to be minimized by the algorithm;
y target parameter (NO_x).

The "EDI hive Cause-and-Effect Chain Editor" thus enables simple formal modeling of relevant systems with specific characteristics and system parameters with their value ranges and their relationships via relations, which can be defined as context or test relations. Through stored rules, the user is systematically guided to a meaningful context, which can be quantified, e.g., within the framework of an experiment. In addition, the implemented similarity algorithms continuously display similar cause-and-effect chains to the user, i.e., similar experiments that have already been carried out. This ensures that the existing knowledge can be built upon and relevant contexts and relationships are not forgotten. This method of formalizing knowledge has already been demonstrated in other projects, and its benefit has been highlighted [14,15].

2.5. EDI hive Model Generator

Based on the collected measurement data and the formalized expert knowledge, the implemented AI-based algorithm can be used to quantify and intuitively visualize the relationships in the measurement data.

The overview of the model shown in Figure 6 illustrates the data set used, the target, and influencing parameters, as well as the quality of the model.

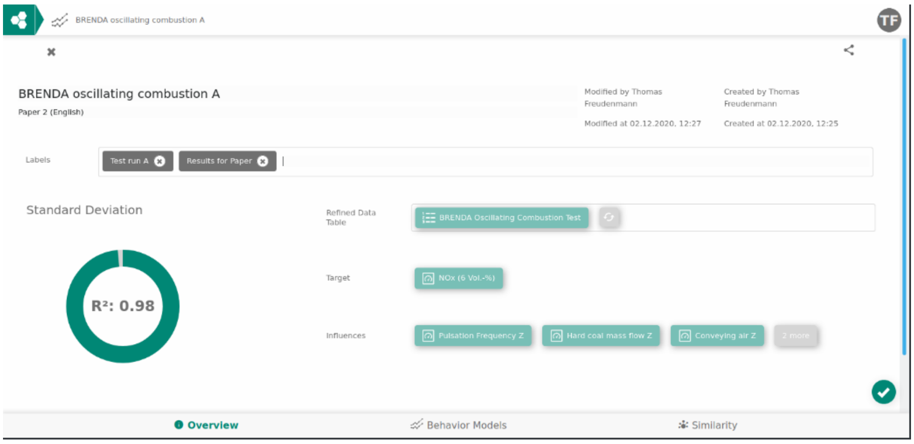

Figure 6. Exemplary overview page of the EDI hive model generator.

2.6. BRENDA Pilot Plant and Balancing

The BRENnkammer mit DAmpfkessel (BRENDA) pilot plant (a combustion chamber with a steam boiler) consists of a rotary kiln furnace with a thermal output of 1.5 MW, to which a vertical combustion chamber with two antiparallel burners with a total output of 1 MW is connected. One of the two burners is designed as a multi-fuel dust burner (Figure 7) through which different fuels can be conveyed simultaneously [16]. In the flow charts, this burner is named burner D4.1 (Figures 5 and 7).

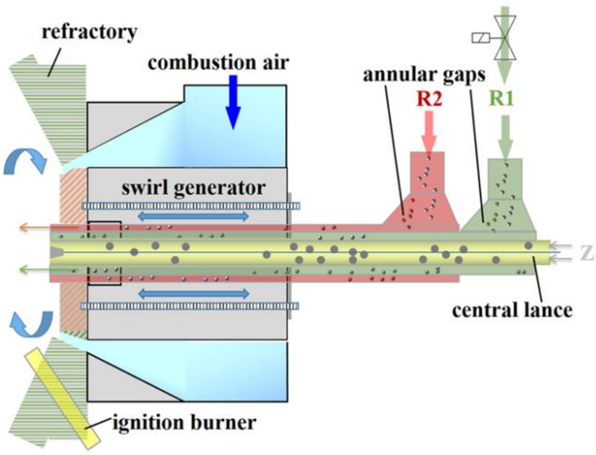

Figure 7. Schematic of the swirl-type burner.

In this investigation on nitrogen oxide reduction through oscillation, a pinch valve was inserted in the annular gap R1, which periodically interrupted the coal flow. Airflow was supplied centrally in the annular gap R2 and outside, and in addition, the combustion air can be swirled. Nitrogen oxide and oxygen concentrations were measured immediately downstream of the boiler in the raw gas; carbon monoxide was determined after about 5 seconds residence time in the flue gas upstream of the dust burner. Both parameters are mainly used to describe the oscillating combustion process.

2.7. Experimental Program

For the experimental program, the presumed relevant systems, system parameters, and relationships were formalized for systematic planning using the "EDI hive Cause-and-Effect Chain Editor". The section of the cause-and-effect chain displayed in Figure 8 shows the most important influencing variables that were systematically changed in the course of the study. The burner, which has a central lance, is equipped with an annular gap 1 (R1) and an annular gap 2 (R2) and was the focus of this investigation. In addition to the large air volume flow and combustion air volume flow, feeding air can also be introduced into the combustion chamber via the annular gaps and the central lance. The feeding air from annular gap 1, annular gap 2, and the central lance can be oscillated with a defined frequency. In this way, oscillating combustion can be realized.

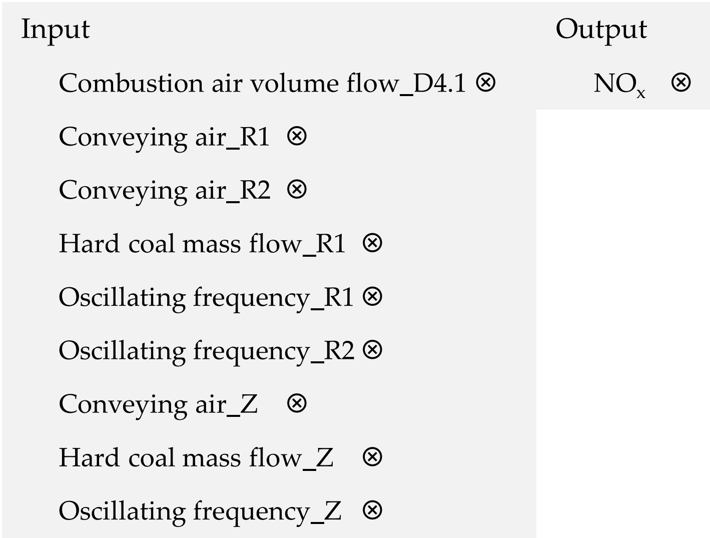

Figure 8. Relevant influencing and target variables of the campaign.

Figure 8 shows all relevant influencing variables (input) and the target variable (output), which were formalized within the study and varied in a targeted, constant, or systematic manner in the corresponding design area during the experiments (Table 1) according to step 1 of the EDI hive cause-and-effect chain.

Table 1. Experimental program.

Test Series	Coal Mass Flow	Hard Coal Supply	Feeding Air	Feeding Air	Feeding Air	Combustion Air	Oscillation	Oscillation Frequency R1	Oscillation Frequency R2
			Z	R1	R2		Frequency Z		
	(kg/h)			(Nm^3/h)				(Hz)	
					Variation Range				
A	70 80 90	Central Z	70 80 90	70 80 90	0	500	0 1 2 3	0 1 2 3	-
B	70 90	Annular gap R1	0 70 90	70 90	0 70 90	420	0 3	0 3	0 3

Although flue gas temperature, O_2 concentration in flue gas, and swirl are relevant parameters influencing NO_x formation, they were considered invariant since they did not change much during the experiment. The experimental program was developed according to and in coordination with EDI, considering temporal, technical, and economic constraints. The experimental program comprised two test series, A and B, which differed in the number of varied parameters according to Table 1.

From previous experiments with oscillating combustion, experts know the main parameters influencing NO_x reduction. Besides the oscillation frequency, the impact of these parameters on the oscillation of fuel or the combustion air (feeding air) is recognized. However, the best frequency to minimize NO_x for this plant was not known. To obtain specific information about this target, the parameters were varied according to Table 1 within the range of the technical possibilities of the plant. This procedure refers to step 2 of the EDI hive cause-and-effect chain. To reduce the number of tests, a combination of parameters was implemented in the hybrid model.

The coal used in these experiments was a hard coal with a net calorific value of 32 MJ/kg. The nitrogen content was analyzed and found to be 1.6 wt % dry base, and the medium particle diameter (d_{p50}) was about 50 µm.

For test series A, the influencing variables shown in Table 1 were partly varied at three or four factor levels. A quadratic influence on the target variables was observed. Test series A focused on the influence of the oscillating frequency on NO_x. Twenty-six factor combinations were set, and the corresponding measured values were recorded via the control system and additional measurement systems. Considering the technical and thermo-chemical boundary conditions, the number of necessary tests could be achieved using a modified D-optimal test plan. This test plan describes the necessary system behavior with sufficient accuracy.

In test series B, the focus was the influence of the local air supply via the different feeding possibilities (Z, R1, and R2). Due to the limited test time, all factors were varied on two levels only, and the test was therefore composed of 36 individual tests.

3. Results

A snapshot from the test series showing the change from non-oscillating operation to oscillating operation is shown in Figure 9. The partial model tree of the hybrid model is shown in Figure 5, and the calculated function for determining the optimum operating point for the burner using the example of frequency is shown in Figure 9. The experimental data were collected according to step 3 of the EDI hive cause-and-effect chain.

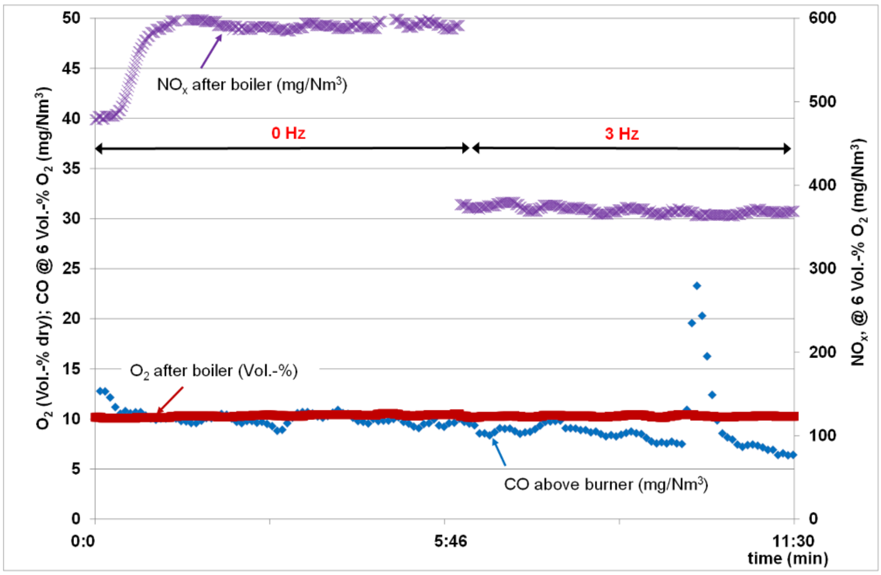

Figure 9. Concentrations of CO, NO_x, and O_2 for non-oscillating and oscillating operation.

From test series B, an exemplary period was selected, which shows the influence of oscillation on nitrogen oxide concentration (Figure 9). The left y-axis shows the oxygen content downstream of the boiler in percent by volume (dry basis), and the CO content upstream of the burner standardized to 6% by volume oxygen. The NO_x downstream of the boiler is plotted on the right y-axis opposite the test time. The reduction in NO_x through oscillation at 3 Hz from around 600 mg/Nm^3 to 370 mg/Nm^3 based on 6% volume O_2 is clearly visible. In this case, the hard coal mass flow dosed via the annular gap R1 was oscillated. However, the different combinations of fuel mass flow and air volume flow according to Table 1 changed the total air ratio at the burner. The local air ratio, which is crucial for the NO_x reduction potential, could unfortunately not be measured.

Based on the EDI hive cause-and-effect chain (step 4 and Equations (1) and (2)), the values (*Effects*) for the most significant parameters are shown for test series A in Table 2.

Table 2. Calculated effects of the parameters on the multiple regression model.

Parameter	Effect
Conveying air R1	+5.74
Conveying air R1 × conveying air R1	−5.54
Oscillating frequency R1	−0.10
Oscillating frequency R1 × oscillating frequency R1	+0.07
Conveying air Z	+5.04
Conveying air Z × conveying air Z	−4.52
Coal mass flow Z	+1.02
Coal mass flow Z × coal mass flow Z	−1.12
Coal mass flow Z × conveying air Z	−0.42
Oscillating frequency Z	−8.34
Oscillating frequency Z × oscillating frequency Z	+7.12

The target parameter NO_x is reduced if the sign is negative and increased if the sign is positive.

For an efficient decision-making process, the multiple regression model was rearranged for the individual parameters, resulting in an interaction diagram that allowed for the intuitive visualization of the influences and interactions between parameters. From test series A, the interaction diagram (based on step 5 of the EDI hive cause-and-effect chain) shown in Figure 10 provides an example of the oscillating frequency Z and the hard coal mass flow Z. It clearly shows the sensitive effect of the oscillation frequency of the conveying air from the central lance on the NO_x target value corrected by the O_2 reference, since the curve has a large gradient within the design range. With a defined setting for the other parameters, an O_2-corrected NO_x emission of about 483.79 mg/Nm^3 was achieved at 0.54 Hz and a 70 kg/h hard coal mass flow. The optimum oscillating frequency for oscillation of the air and coal mass flow in the central lance was 1.8 Hz, with a significant NO_x reduction being achieved and only approximately 380 mg/Nm^3 being produced when the settings for the other parameters remained unchanged.

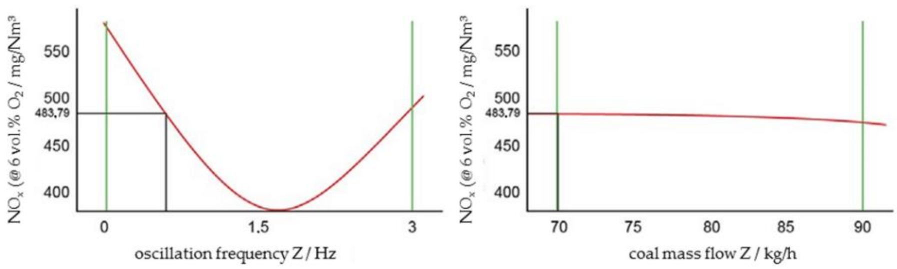

Figure 10. Determination of the optimum frequency of the oscillation with respect to NO_x.

Figure 11 shows that the additional air supply from annular gap 1 has a sensitive effect on NO_x, and that NO_x reduction can be achieved by means of an appropriate supply.

Due to the effect of oscillating the coal flow in the central lance, the influence of the oscillation of the air supply in annular gap 1 was rather small and, for the experimental set-up and parameter settings described, must be considered statistically insignificant.

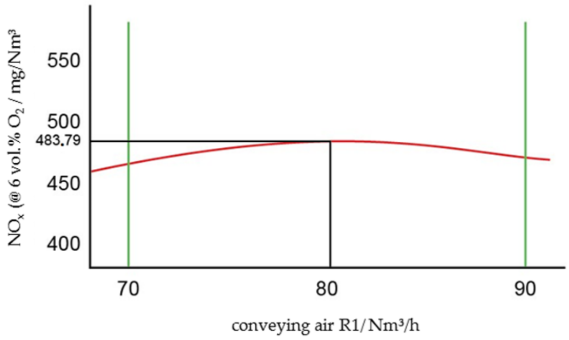

Figure 11. Sensitivity in the case of additional conveying air via annular gap 1 with respect to NO_x.

4. Conclusions

With the AI-based hybrid model, which embeds expert knowledge as well as the specific boundary conditions and characteristics of the technical system, an innovative approach was presented to quantify the interactions between the main influencing parameters of the technical system and a target parameter, which, in this case, was NO_x concentration.

The hybrid model enabled us to reduce the expensive operation time of the BRENDA facility to find the minimum NO_x concentration as a function of the main influencing parameters within the design area. Based on the quantified characteristics of the plant, this model can easily be used to derive measures for the efficient operation of the plant, or to evaluate further thermo-chemical optimization potential.

With the EDI hive IoT framework, an efficient test design and evaluation of the data guaranteed that all influencing parameters and the interactions between them were presented and evaluated. In this case, the AI-based hybrid model was used to examine the reduction potential of oscillating the coal mass flow to reduce NO_x emissions. The campaign consisted of a screening trial, where the data were used to identify relevant influencing parameters. Based on these results, a second trial was initiated to further investigate the optimal test settings and the reproducibility of the test setup. The formalized expert knowledge, measurement data, and the decisions for all iterations were captured sustainably through the AI-based hybrid model procedure, which is supported by the EDI hive. With the statistical planning of the trial and the use of statistical analysis algorithms, it was possible to identify significant influences, such as the best oscillation frequency. In this case, it was found to be 1.8 Hz for coal oscillation to reduce the NO_x concentration to 380 mg/Nm^3.

In the future, these quantified AI-based hybrid models could be used to optimize and control the plant, enabling the automated control of the optimum oscillating combustion. Through the automated application of autoML algorithms with defined metrics, the degree of automation can be increased and other influencing factors from the power plant that have not yet been recognized can be discovered.

More investigations are needed to identify whether, in addition to quantified influences (Figures 9 and 10), there are secondary minima where a minimum NO_x concentration could only be achieved by oscillating the annular gap air instead of the coal mass flow. Periodic interruption of the coal flow is not practical with the pinch valve used. Further experiments could add to the database for the model and thus enable more robust control of the plant in the future.

Investigations with an inert gas as the oscillating air could be a promising approach to reduce NO_x emissions using the same output of the power plant.

Expert knowledge was expanded, formalized, and quantified with EDI hive regarding the system behavior of innovative oscillating combustion. With the parameter settings discovered here, a reduction of up to 50% of NO_x emissions is possible.

In summary, applying statistical algorithms and expert knowledge lead to a quick and reliable prediction result to apply to process control systems, avoiding a costly Computational Fluid Dynamics (CFD) simulation. However, to fully understand different thermo-chemical phenomena, more valuable measuring instruments and a simulation based on these measurements are needed.

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