IEEE Access
Multidisciplinary : Rapid Review : Open Access Journal

Received July 21, 2021, accepted August 5, 2021, date of publication August 11, 2021, date of current version August 18, 2021.

Digital Object Identifier 10.1109/ACCESS.2021.3104058

Framework for Automated Data-Driven Model Adaption for the Application in Industrial Energy Systems

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This work was supported in part by the Cooperative Doctoral School through the Smart Industrial Concept (SIC!) (https://sic.tuwien.ac.at/), and also in part by the TU Wien Bibliothek through the Open Access Funding Program.

ABSTRACT Increasing flexibility and efficiency of energy-intensive industrial processes is generally seen as a big lever towards a decarbonized energy system of the future. However, to leverage these potentials, the accurate prediction of unit behavior is essential to be able to close the gap between supply and demand. Not only pose nonlinear relations a serious challenge in thermal systems engineering and optimization but real-world unit behavior furthermore changes during operation due to wear, fouling and other effects. In the present work, a novel framework for automated data-driven model adaption is presented which is capable of automating fast and accurate predictions of current system behavior. The framework is based on open protocol bidirectional live communication and mechanistic grey box modeling. While especially thermal energy storage is considered a solution to increase flexibility, it is very challenging for operation optimization. A packed bed thermal energy storage operated under severe conditions leading to continuous fouling acts as proof of concept of the proposed framework. The obtained results indicate major improvement for storage output prediction with the novel framework compared to a conventional approach without readjustment. Furthermore, the presented framework is perfectly suitable and an essential foundation for live condition monitoring, fault prediction, predictive maintenance, and operation optimization.

INDEX TERMS Automated model adaption, data-driven modeling, industrial energy systems, OPC UA.

ABBREVIATIONS AND SYMBOLS

$\dot{m}$	Mass Flow of the Heat Transfer Fluid.
l_i	Vertical Distances between the Measurement Layers.
T_{1-4}	Inner Temperatures of the Test rig.
T_b	Temperature on the bottom of the Test rig.
T_{in}	Input Temperature of the Test rig.
T_{out}	Output Temperature of the Test rig.
T_t	Temperature on the top of the Test rig.
V_i	Partial Volumes of the Test rig.
PBR	Packed Bed Regenerator.
PI AF	PI Automation Framework.
PI DA	PI Data Archive.
PLC	Programmable Logic Controller.
RMSE	Root Mean Square Error.
SCADA	Supervisory Control and Data Acquisition.
SM	Storage Medium.
TES	Thermal Energy Storage.

The associate editor coordinating the review of this manuscript and approving it for publication was Jamshid Aghaei.

I. INTRODUCTION

This Introduction presents a short motivation for the present work and a brief history and summary of related work that can be found in current literature, followed by highlighting the main contributions and the remaining structure of this paper.

A. MOTIVATION

Decarbonization efforts are a driving force for the energy-intensive industries to drastically increase energy efficiency. At the same time, we are in the middle of what is often referred to as the fourth industrial revolution or Industry4.0, driven by evolving Information and Communication Technologies [1]. Industry4.0 and the sustainable energy transition share important characteristics and can mutually benefit from each other [2], both being highly influenced

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by technological innovations [3]. Most researchers agree on the huge potential of digitalization for reducing energy consumption and for increasing economic sustainability [4]–[7]. As another paradigm of Industry4.0, Predictive Maintenance, achieved by real-time monitoring, can also positively affect the environment [3]. Preventive and predictive maintenance promoted by data analytics extends the lifespan of machinery, thus minimizing end of life waste [8].

The key foundation for Predictive Maintenance, as well as energy optimization is automated real-time data analytics, therefore achieving collaborative and real-time interaction between computational and physical processes [9]. Especially in thermal process engineering, so called *soft sensors* provide essential insights into the state of process operations especially in cases where the direct measurement of key process variables is very difficult, impossible or unreliable [10]–[12]. Such soft sensors have thus been developed to estimate key quality variables that are difficult to measure by constructing mathematical prediction models using the easy-to-measure process variables [13]–[15]. Predictive data, i.e. probable future values or states forecasted based on accurate models representing a given process, are therefore essential for numerous applications [16].

B. STATE OF THE ART

In the last decades, process analytics and condition monitoring have gained significant importance due to the increasing complexity of plants and machinery and vigorous economic competition. Condition monitoring can be described as ''the assessment of the current condition of a physical entity by employing measurement data'' [17], [18]. By preprocessing the raw data (normalization, PCA, Feature Extraction, sensor fusion, soft sensors, ...), valuable information about the current state of the physical entity is gathered and further utilized in several condition monitoring related services like fault detection, predictive maintenance, and operation optimization. Condition monitoring approaches have relied on specific measurements during plant and machinery operation (e.g. vibration analysis, strain measurement, and thermography) [18], [19]. Current developments in sensors and signal processing systems, big data management machine learning, and improvements in computational capabilities have opened up opportunities for integrated and in-depth condition monitoring analytics [19]. Latest concepts like cyber-physical systems [20] and digital twins [21] aim to take automation to the next level and achieve collaborative and real-time interaction between the real world and the digital world [22]. The foundation for this is the bidirectional connection between the real and the digital world [21] and, therefore, virtual model synchronization.

Automated model adaption in the context of condition monitoring is primarily applied to classify and detect system faults. Prominent examples are bearing fault detection for electric motors [23], fault detection for wind turbines [24], or general rotary machines [25]–[27]. Also, condition monitoring for electrical equipment like transformers [28], or the wear of cutting tools [29] has been the topic of machine learning studies where models have been trained for classification purposes.

In general, the goal of condition monitoring applications is to detect states of damage early or to initiate maintenance before actual damage occurs, based on learned characteristics [30]. So basically, the output of the beforehand trained analysis tools is a decision if the process is in a normal or abnormal state by determining if parameters (e.g. vibration signatures, forces or temperatures) exceed defined or learned borders. This is possible because the damage mechanisms behind the phenomena to classify are often well known and distinguishable.

Contrary to this, the automated data-driven model adaption approach presented in this work allows up-to-date prediction of the future behavior of the thermodynamic component, which extends the range of possible enhancements. Common mechanisms like fouling or abrasion within industrial thermodynamic machinery bear the challenge that they are often hard to monitor during operation and are likely to impact performance and change important physical properties like heat transfer. If these changes are not critical for the lifespan of a machine, the successive task is to adapt it's operation for maximum efficiency. Accurate predictions of the asset's performance gain importance for operational optimization, since the margins of energy and resource savings are shrinking. In case of inaccurate optimization results based on non up-to-date asset models, the forecasted savings are consumed by process control, needed to keep the real process in a physically feasible state [31]. To be able to meet the need for accurate predictions mentioned above, the aim of this study was to create an innovative framework for automated data-driven model adaption for industrial thermal energy systems.

Industrial thermal energy systems are often designed for long-time service life, which traditionally comes with communication problems between systems that become deployed decades apart from each other. Either the software of the suppliers is not compatible or even the communication standard has changed. To tackle this problem, the use of unified open protocol standards continuously gains shares in the industrial communications market [32]. The OPC UA standard is widely recognized in various industries to enable interoperability and communication in all operational layers. Because the hardware and software available during the research were compatible, and the free availability of the communication standard that enables barrier-free research, OPC UA was chosen as the base of the proposed framework.

C. MAIN CONTRIBUTIONS

Peres *et al.* [16] state that there is still a clear need to further combine real-time and historical data at both the resource and system levels, as well as closing the loop to autonomously act on the results of the predictive analytics. Furthermore, solutions should be highly adaptable, being capable of changing even after deployment by learning from newly generated knowledge [33].

To the best of the authors' knowledge, no automated data-driven model adaption framework for industrial thermal energy systems has been presented so far. We therefore consider our main contribution in presenting an automated continuous model adaption framework for the application on industrial energy systems that

- relies on open protocol live communication for maximum flexibility,
- features real-time analyzes and feedback considering the current physical properties of the system and,
- is fast and easily modified on models and systems for similar applications.

Compared to systems that rely on manufacturer-specific communication standards, the presented framework can be used with a wide range of devices or programs from different sources, as long as they support the open source OPC UA standard. Because the framework allows a continuous and automated adaption of prediction models to match the properties of the real physical system, less human intervention is needed compared to traditional condition monitoring systems.

D. PAPER STRUCTURE

The remainder of this paper is structured as follows: In Section II, the proposed automation framework is described. In the following Section III, the use case subject to the proof of concept is given. The results of the exemplary framework application are then discussed in Section IV, followed by Section V, where the conclusion and an outlook on future research is given.

II. AUTOMATION FRAMEWORK

The way measurement data is recorded has undergone a long series of changes and improvements. Starting from written recordings, the emerging of new information processing technologies led to new paradigms. As data storage became cheap and practicable enough, the storage of considerable amounts of raw measurement data started. Nowadays, it is clear that the simple storage of measured data without proper procession is not sufficient for detailed analyzes that are needed for improvements of efficiency or resource demand. The raw measurement data has to be enriched with semantic data like the accuracy of the used sensors, measurement position, calibration data, or control values. A framework for automatic data acquisition and model training for industrial energy systems based on OPC UA and other modern communication protocols has been implemented exemplary on an existing test rig to meet the requirements above.

A programmable logic controller (PLC) from hardware manufacturer B&R Industrial Automation GmbH provides the operational data of the test rig via an OPC UA server hosted on the PLC itself. The test rig is controlled via the XAMControl SCADA system from evon GmbH, whereas the data handling and storage are performed by the OSIsoft® PI System.

A complete illustration of the digital infrastructure of this framework is given in Fig. 1. The test rig is located in a laboratory of TU Wien. It is connected via the university network to the control and data processing server, located in a central server room in a different physical location.

The digital and analog sensor data of the test rig (on the left-hand side of Fig. 1) gets processed in the PLC and passed on to the OPC UA server, which supplies the data to possible clients in the same network. Along with every measured value of a data point, the timestamp of the measurement and the quality of the data are transmitted.

The so-called "PI Connector for OPC UA" of the PI system acts as an OPC UA client that requests the time-series data with all its associated information from the PLC in defined intervals. This information is then copied into a specific subsystem of the PI server, the PI Data Archive (PI DA), where it is stored as a PI point. The PI DA retrieves data and serves it in real-time to all components of the PI system. The PI Asset Framework (PI AF), which is the second part of the PI server, allows an object-orientated, consistent grouping of the measurements of assets. Within the PI AF, the first analyses with low complexity are performed. For example, suppose redundant temperature measurements on the same measurement position are compared, and the difference is higher than expected by known uncertainties. In that case, a warning will be generated that initializes external intervention or even emergency procedures if necessary. So-called event frames allow the classification of states like charging or discharging, making it easier to compare the behavior of an asset for recurring operation conditions. Another connector of the PI System, the PI SQL Data Access Server, is used as a gateway to pass time series data via SQL queries to MATLAB® (on the right-hand side of Fig. 1), where the actual model training and simulation takes place.

In the given use case, the query requests a defined amount of recently completed charging and discharging events to train the model with the current state of the test rig. The trained model is then used to predict the response of the PBR and thus its temperature curves for planned future operation. The resulting prediction is then transferred back into the PI system with the help of a universal file loading interface that reads the data points from a defined output file of the MATLAB® model and copies them into the PI DA (bottom right in Fig. 1).

The predicted values of the temperature measurements are stored as future control values, which can be seen as additional attributes of the measurements, allowing for a real-time comparison of the measured values and their prediction, taking the test rig's real condition into account. Decisions resulting from the analyses or comparisons are then sent back to the PLC and thus to the SCADA system via a custom programmed Python™ Wrapper that acts as connector between OPC and OPC UA, allowing the system to react to them directly.

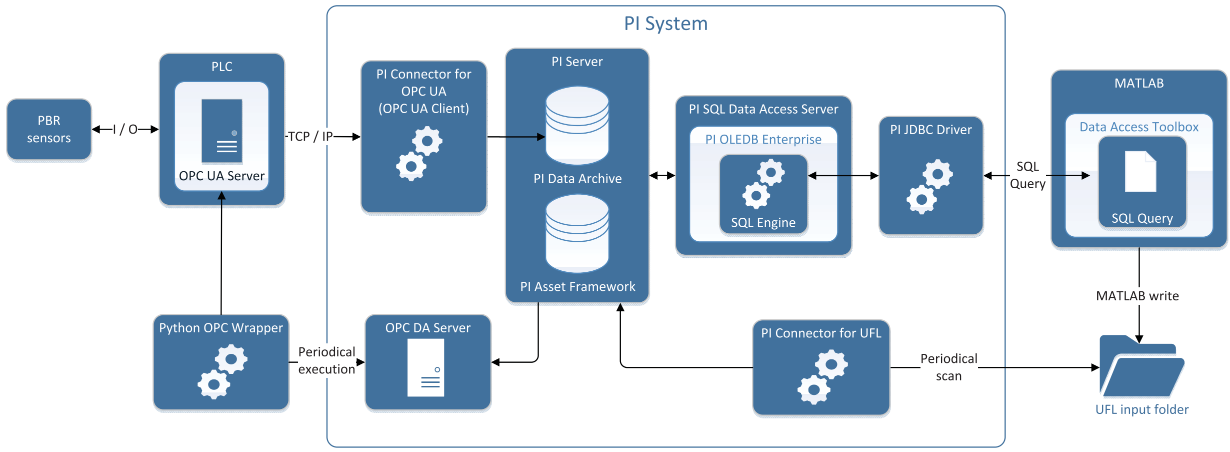

FIGURE 1. Digital infrastructure of the presented framework.

III. SELECTED USE CASE

Industrial energy systems typically consist of energy supplying components, energy storages, energy conversion components like heat pumps, and energy demanding components as exemplary depicted in Fig. 2. Therein, two processes, a fractionating column and a particle dryer, are fed with thermal energy by an energy supply component. Without the possibility of storage or conversion of energy, the energy supply has to satisfy the demands regardless of efficiency concerns to keep the processes running. As addressed in earlier work of Prendl *et al.* [34], energy demand and excess energy in industrial processes are often offset in time. Hence, heat recovery in combination with energy storage allows to reduce the external energy demand and, thus, the use of resources and the emission of CO_2. Furthermore, since different temperature levels often occur in energy-intensive processes and not only one temperature level like in Fig. 2, the integration and operational optimization of several different storage units is a common problem. Economic operation of such industrial energy systems is even more complicated by the increasing share of renewable energy sources and the resulting highly volatile energy prices. Therefore, increasing focus is laid on process control with optimized storage management, which is dependent on accurate predictions of component behaviour. In the following, this paper deals with the storage as central component.

A. PBR TEST RIG

As exemplary use case, an existing packed bed regenerator (PBR) thermal energy storage (TES) test rig situated in a TU Wien laboratory is used. It consists of an insulated conical metal container filled with gravel as a storage medium (SM) that is equipped with temperature measurement sensors in several layers as shown in Fig. 3. The PBR is charged by electrically heated air acting as heat transfer fluid (HTF) from top to bottom and discharged with ambient air from bottom to top. A detailed description of the PBR can be found in several scientific publications that dealt with different aspects of the storage and already provided insights on it's properties and behavior [35]–[39]. Also, different models for simulation [36], [37], [40] and optimization [31], [38] for the test rig have been created and validated in the past.

However, in real operation, deviations from ideal laboratory conditions can influence the behavior of machinery. Processes such as fouling or wear that occur over time are often hard to measure or quantify, especially in the running operation. In case of the PBR for example, deposition can occur if the HTF is polluted with particles smaller than the bed material. The passable cross section can change, flow channels can form, or the heat transfer to the bed material can be influenced. Further, the particle size of the bed material can change because of thermal degradation or abrasion. These or similar effects can occur during real plant operation and change the heat transfer inside the PBR. Thus, to maintain optimum operational capability, models used to predict the future behavior of assets must be kept up to date.

B. GREY BOX MODEL

Amongst the simulation models mentioned above, especially the mechanistic grey box model developed by Halmschlager *et al.* [40] is capable of fast and easy adaption to changed properties and is robust at the same time. This modelling approach is therefore used and adapted for the proof of concept of our framework and described in the following paragraph. For a detailed mathematical description of the applied modelling approach, we refer to the chapter "Extended Grey Box Model 2" in the original publication [40].

The mechanistic grey box model consists of physical relations/equations and uses measurement data to optimize specific parameters of these equations. While only a small number of equations needs to be solved for model training, the model shows excellent prediction performance and stands out compared to data-driven and physical models by its high accuracy, low computational effort and high robustness [40]. An illustration of the test rig and the vertical position of the measurement layers is given on the left hand side of Fig. 3. The model uses the inlet temperature T_{in} and the mass

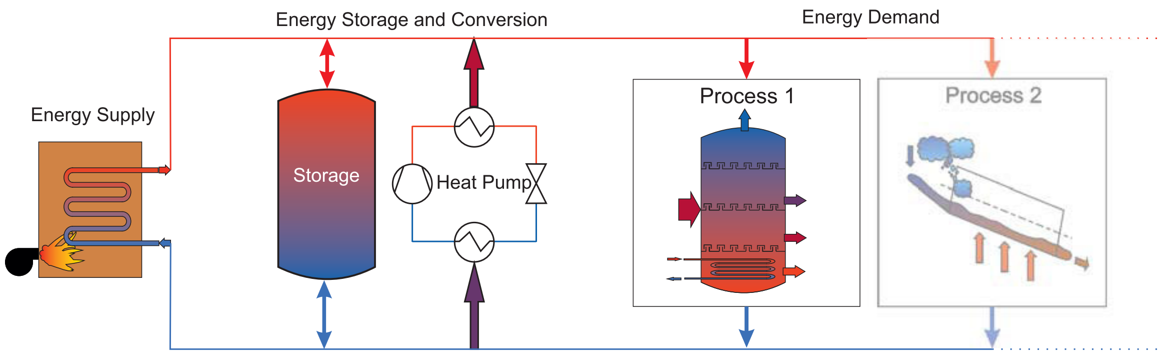

FIGURE 2. Exemplary industrial energy system, consisting of energy supplying components, energy storage components, energy conversion components, and energy demanding components.

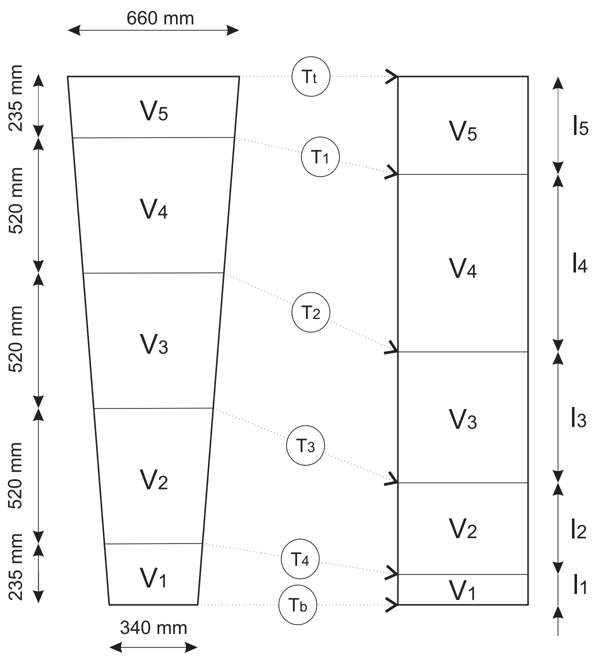

FIGURE 3. Actual conical shape of the PBR with the vertical position of the measurement layers in comparison to the cylindrical simplification of the grey box model.

flow $\dot{m}$ of the HTF to calculate the corresponding output temperature T_{out} of the PBR. During charging, T_{in} equals the temperature at the top of the PBR T_t and the T_{out} equals the temperature at the bottom of the PBR T_b. During discharging, T_{in} equals T_b and T_{out} equals T_t, since the direction of flow is reversed, as explained above.

If the model's target is to predict the output temperature, the cost function to be minimized consists of the root mean squared error (RMSE) of the model output temperature compared to the training data output temperature. In [40], existing measurement data of the PBR is used for the training and validation of the model. While predictions of T_{out} showed high accuracy, predictions of internal temperature values T_1 to T_4, which were not part of the optimization target, showed significant deviations. This is due to the fact that the conical vessel shape of the PBR was approximated to a cylindrical shape.

In case not only the output temperature of the PBR, but also its internal condition is of interest, the prediction of the internal behavior gains importance. In order to improve the prediction, the vector of the measurement positions is corrected in this work, in a way that the ratios of the volumes and thus the ratio of the masses between the measurement layers match the ratio of the volumes of the real conical shape. This transformation is depicted in Fig. 3. Because the heat capacity of the SM, the HTF, and the wall are included in the factors that are fitted during training, only the ratio of the volumes (V_i) and not the absolute values of them is of importance for the accurate prediction of the internal temperatures T_1 to T_4. The assumption of a cylindrical vessel causes the ratios of the distances (l_i) between the measurement positions to equal the volume ratio as expressed in (1). The correction introduced here has no significant impact on the prediction of T_{out} but results in a vast improvement of the prediction of the internal temperatures, which can be seen in Fig. 4. In the upper part of Fig. 4, a time series of simulated temperature measurements of the PBR compared with the predictions of the uncorrected model (dotted lines) and the new corrected model (dashed line) is shown. In combination with the prediction error plot below, it is visible that drastic improvement could be achieved. This shows the importance of choosing the right assumptions and simplifications for the development of models or correlations to meet specific demands.

$$\begin{aligned} V1 : V2 : V3 : V4 : V5 \\ = l1 : l2 : l3 : l4 : l5 \\ = 0.117 : 0.352 : 0.503 : 0.682 : 0.375 \end{aligned} \tag{1}$$

IV. EVALUATION AND RESULTS

For a comprehensive testing of the framework, a validated one-dimensional finite difference model of the PBR based on the modelling approach introduced by [39] is used to generate training and test data sets. The assumed load cycle as given in Fig. 5 is used as an exemplary measurement data. The charging temperatures vary between 170 °C and 260 °C whereas the discharging temperature is constant at a 22 °C ambient temperature. The HTF mass flow $\dot{m}$ is assumed constant at a value of 150 kg/h.

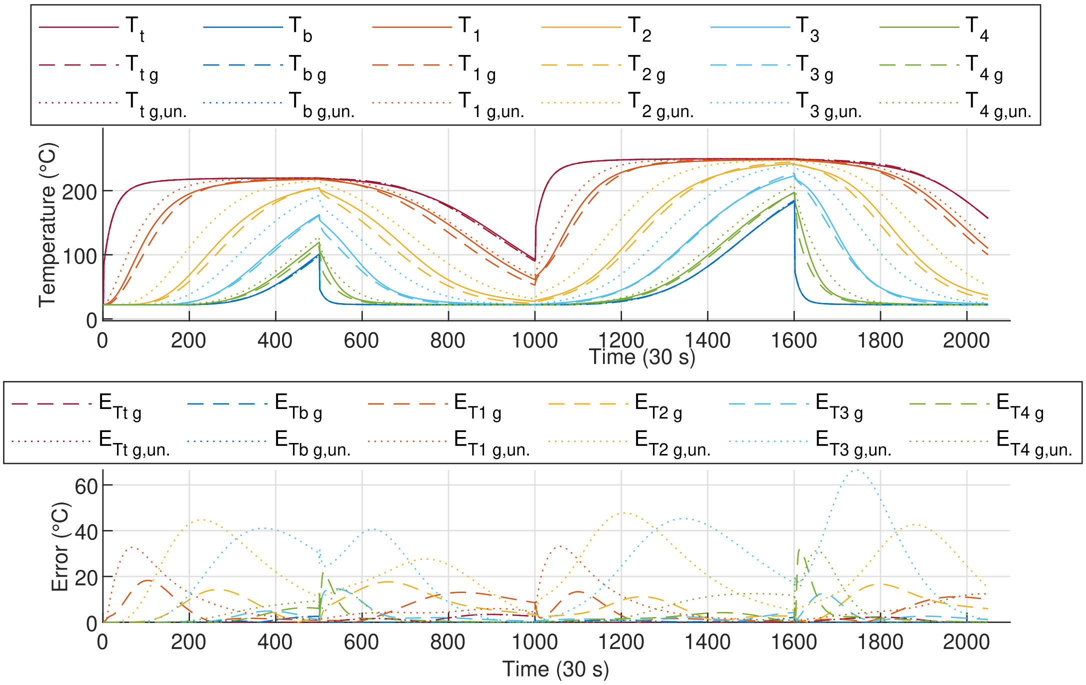

FIGURE 4. **Comparison of simulated inner temperatures with the uncorrected model ($T_{i\ g.un}$) and the corrected grey box model ($T_{i\ g}$) and their respective error compared to the measurement values (T_i).**

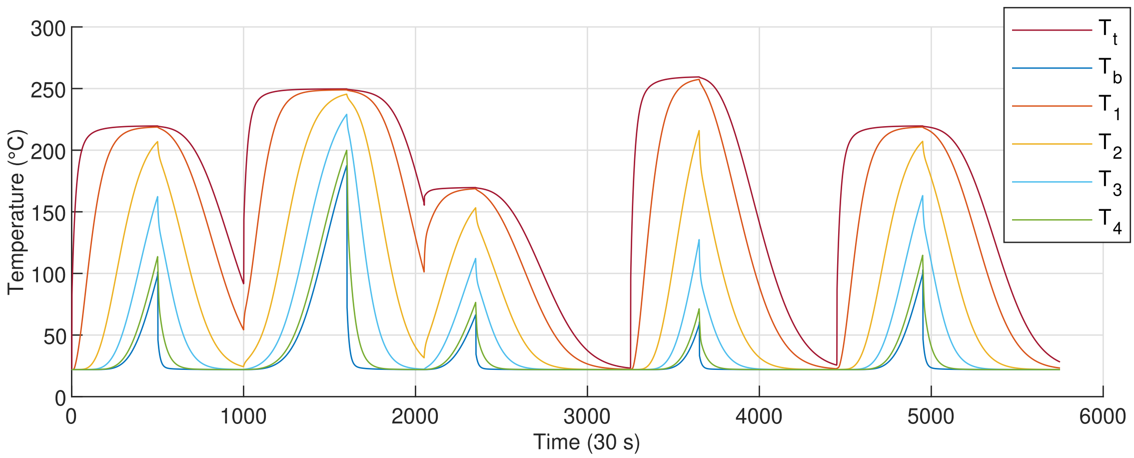

FIGURE 5. **Time series of temperature values of the assumed test data set.**

For the simulation of pollution or fouling, it is assumed that the given load cycle is repeated in a cyclical manner while the heat transfer coefficient between HTF and SM is gradually decreasing over time. Naturally, real pollution processes not only cause a reduction of the heat transfer coefficient. A variety of mechanisms lead to changes in the behavior of the PBR or the flow conditions of the HTF. However, in this work, the change of the heat transfer coefficient was chosen as pollution indicator, because of the clear impact and traceability of the simulated behavior change.

The temperature response of the PBR is simulated for 8 example cycles while the heat transfer coefficient between the HTF and the SM is reduced by 10 % in every cycle. The resulting temperature curves are then stored on the PLC and supplied to the framework as would be the case when using real sensor data.

Two different model training scenarios are assumed for evaluation of the proposed framework on real operation conditions. Firstly, a traditional model training approach is applied, where the model is trained only once with the initial data without reduced heat transfer coefficient. Secondly, a model is initially trained with the same data but is retrained after every full cycle with the measurements from the previous cycle in order to adapt to changes in the physical behavior caused by pollution. The predictions of the temperatures for the subsequent cycles of the only once trained model (in the following denoted as $T_{i\ g}$) and the continuously trained model (in the following denoted as $T_{i\ gtrain}$) are then compared to the simulated measurement data.

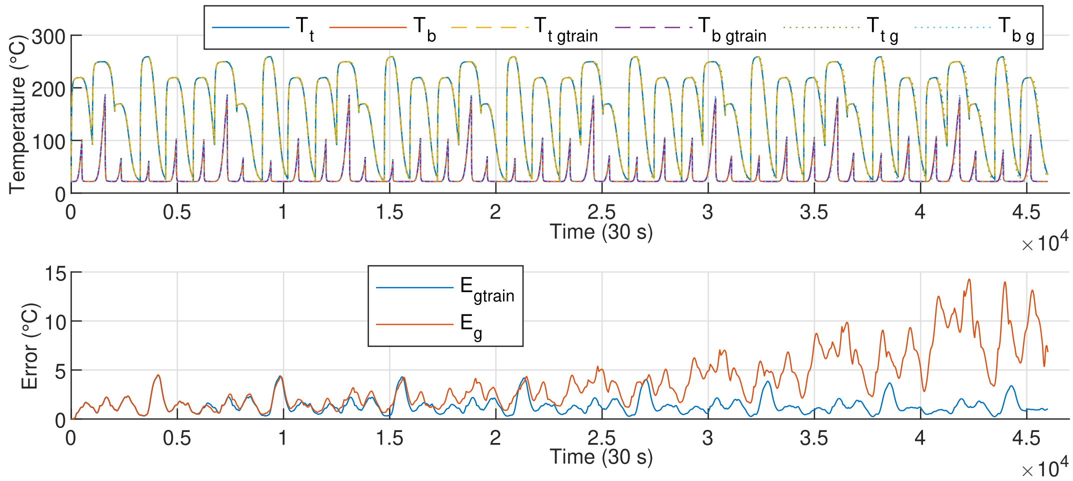

FIGURE 6. Comparison of simulation results for the input and output temperatures of the cyclical trained model ($T_{i\ gtrain}$) and the only initial trained model ($T_{i\ g}$) over the continuous sinking heat transfer between HTF and SM and their errors (E_i) compared to the generated measurements (T_i).

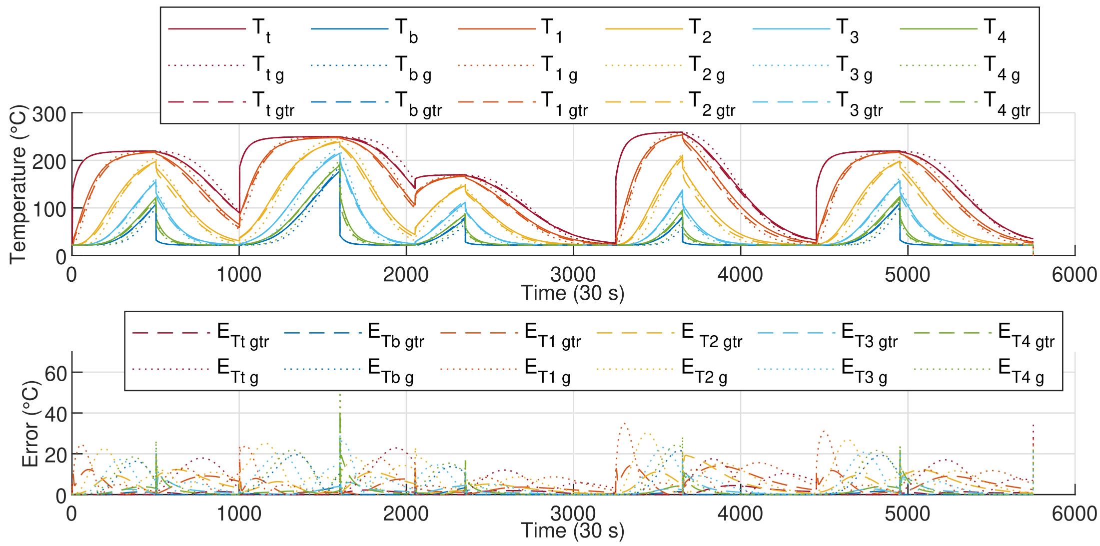

FIGURE 7. Simulation results of the cyclical trained model ($T_{i\ gtrain}$) and the only initial trained model ($T_{i\ g}$) for the cycle with the maximum pollution and their respective errors (E_i) compared to the generated measurement values (T_i).

In Fig. 6 the input and output temperature curves are given with their respective prediction results and the absolute errors between them. The values for the static model $T_{i\ g}$ are dotted, and the values of the adapted model $T_{i\ gtrain}$ are dashed. It is clearly visible here, that the absolute error of the once trained model is steadily increasing over time while the error of the continuously trained model stays in the same range. The error for $T_{i\ gtrain}$ even slightly decreases over time, which might be a consequence of more data that is available for model training.

For the sake of better visibility, the inner temperatures predictions are not shown in Fig. 6. However, to visualize the vast improvement the last test cycle with maximum pollution is given in detail with all inner temperatures in Fig. 7. One can see that the predictions of the static model (dotted lines) clearly differ from the measurements, while the predictions of the continuously trained model are hardly visible because of the small error. This also shows in the lower part of Fig. 7, where the errors of the predictions are displayed.

For quantitative analysis, the total RMSE (Root Mean Square Error) for all temperature predictions of the cycle with the highest pollution, given in Fig. 7, is calculated. For the untrained model, a RMSE of 9.10 °C was obtained whereas the retrained model featured a RMSE of 4.05 °C. This improvement in accuracy requires additional computational time of only a few seconds for retraining of the model, whereas measurement intervals for the PBR sensors of one minute are considered sufficient. Even this seemingly small difference of a few degrees in the model output can significantly change the optimum solution of optimization procedures like the heat exchange network synthesis (HENS) [34] or scheduling [31], resulting in deviating planning and control strategies.

V. CONCLUSION

A novel framework for the automated data-driven model adaption for industrial energy systems is presented. The framework's capability to autonomously collect measurement data, train a model, predict an asset's future behavior, and analyze the current system behavior is shown with the help of a PBR TES as a use case.

The automated model adaption is applied on an assumed cyclical operation of the storage where continuous pollution reduces the heat transfer between HTF and SM over time. The predictions of the model that was able to learn the changed behavior of the PBR due to the developed framework provide an accurate forecast and show considerable improvements in accuracy compared to a static model. The maximum absolute error of the static model was up to 14.2 °C whereas the maximum error of the learning model was only 4.3 °C. This means the prediction error could be reduced up to 70 % within the given boundaries. Considering that even small potential efficiency improvements add up to large monetary savings for the energy-intensive industry, improvements like this are gaining importance as the crucial factor in economic operation.

However, it is important to consider that automated model adaption comes with all its advantages and disadvantages. As long as a robust and suitable model is used, the automation reduces the operator's workload. However, if incorrect measurement data is not detected and then used for the model training, the resulting model and it's predictions are also incorrect. Thus, accurate and up-to-date predictions are needed to monitor the measurements and initialize immediate system response or external intervention if necessary.

The implemented framework can be seen as a foundation for real-time condition monitoring, fault prediction, predictive maintenance, and operation optimization, all of which rely on advanced communication.

The presented automation framework yields the potential to characterize similar TES with small adaptions and only little training data from initial measurements.

Furthermore, our framework is applicable for variable industrial energy systems, provided appropriate system models are used. For further evaluation of this topic, a research project concerning the enhancement of the test rig that allows for the contamination of the HTF with pollutants is already in the development state within the author's research unit. The real measurement data obtained by this enhancement of the test rig will allow for comprehensive comparisons of different prediction approaches for this problem and further evaluation of the framework presented in this work.

ACKNOWLEDGMENT

The idea of this publication was initiated during the work on the topics of the cooperative doctoral school Smart Industrial Concept (SIC!). The authors would like to thank OSIsoft® and evon GmbH for the supply of the software as well as comprehensive support within the course of SIC!.

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