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Towards a Systematic Path for Dynamic Simulation to Plant Operation: OPC UA-enabled Model Adaptation Method for Tracking Simulation

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Abstract— A tracking simulator is an online simulation system that utilizes dynamic parameter estimation for calibrating model parameters to achieve state synchronization with the process. It can be utilized as a plant-wide virtual sensors or as a predictive tool to provide production forecasts based on the current state of the plant. The appearance of industrial applications based on tracking simulators has been hindered by high development cost and time-consuming sustainability of simulation models. In order to overcome this, dynamic simulation models developed during the process design and engineering stages could be used for implementing industrial tracking simulators. However, before these models can be utilized online, they require going through a model adaptation procedure where their structure and parameters are updated. This paper presents a model adaptation method for the implementation of tracking simulators which utilizes OPC Unified Architecture to adapt simulation models developed during the engineering phases of the process plant and apply them at the operation and maintenance stages. In this work, the method is described, implemented and tested using a representative process.

Keywords—*process simulation; model adaptation; online simulation; OPC Unified Architecture; tracking simulation;*

I. INTRODUCTION

In process and power generation industries, dynamic first principle simulation models are mainly developed during the engineering phases of the plant lifecycle where they are used for various applications, including process design, procurement planning and model-based testing of control applications. In recent years, online simulation configurations, shown in Fig. 1 (a), have been applied during the process operation and maintenance phases for model-based testing or data reconciliation [1]. Yet another promising industrial application based on online simulators is tracking simulation. A tracking simulator, shown in Fig. 1 (b), is an online simulation system that uses dynamic parameter estimation for calibrating model parameters in order to achieve a permanent state synchronization with the process. They can be utilized as plant-wide virtual sensors where non-measured process information can be derived or as a predictive tool to provide production forecasts based on the current state of the plant. Tracking simulators are a powerful industrial application for precise operation, monitoring and diagnosis of modern production plants [2, 3].

The appearance of industrial applications based on tracking simulators has been hindered by the high

Fig. 1. (a) Online and (b) Tracking simulation systems.

development cost and time-consuming maintenance of first principle models (FPMs) [1]. In order to overcome this, simulation models developed during the process engineering could be used for implementing tracking simulators [4]. However, because these simulation models are created when the plant is not yet functioning, their results cannot be tuned using measurements from the targeted physical system and only data series of similar process plants are used as a reference. Consequently, the original model results do not closely match the measurements of the operational process. Moreover, in the operation and maintenance stages, processes often undergo structural modifications causing the previously created model to not correspond to the process current layout. Additional model adaptation procedures are required before the previously generated simulation models can be used for tracking simulation.

This paper presents a model adaptation method for the implementation of tracking simulators that leverages on the information accessibility that the OPC Unified Architecture (OPC UA) [5] industrial interoperability standard offers in order to enable a systematic path for dynamic simulation models to process operation. The model adaptation method proposed utilizes OPC UA to seamlessly connect the simulation system to the physical plant without disrupting the process operation and to retrieve historical data of the plant in a systematic manner.

This paper is structured as follows. Section II provides an overview of related work. Section III presents the proposed model adaptation methodology including the description of the model structure update and the model tuning steps. The description of the experiments and its results are shown in Section IV. The conclusions are presented in Section V.

Fig. 2. Comparison of the plant lifecycle and the tracking simulation models implementation stages. The proposed model adaptation method is comprised of the model structure update and the model tuning steps.

II. RELATED WORK

Model adaptation is the procedure in which dynamic models update their underlying structure and re-estimate their parameters in order to represent a newly observed behavior of the physical system [6]. Therefore, model adaptation can be understood as a two-steps method targeted to mend outdated models for their results to closely match the behavior of the studied process. First, in the structure update, the model configuration is changed to correspond to the current physical process structure. Next, during the parameter re-estimation, new observations are used to tune model parameters in order to reduce model residuals.

Tracking simulators can be based purely on FPMs or use a combination of first principle and data-driven models [2]. FPMs are those based on fundamental physical principles. Data-driven models (DDMs) focus on determining the relationship between the output and input data of the system. In the data-driven modelling field, various methods have been developed for model adaptation in different application domains [6-8]. Recent developments in computational intelligence have reduced the development time of DDMs. As a result, it has become easier to create DDMs from recent information than to apply adaptation methods to re-use previously developed models. Moreover, since DDMs are highly dependent on the quality of the data, they can be adapted only when the process undergoes few changes during the period covered and these changes are limited to process operation regions where reliable data has been collected.

Model adaptation of FPMs has been mainly studied as a model validation problem that concerns the level of agreement between mathematical descriptions and the real system. Model validation is a procedure in which the model is iteratively refined until the behavior that best represents the physical system is found. In [9-11], various model validation methods for FPMs are reviewed. However, in those studies, validation is mainly focused in the comparison of model results and physical process outputs and they assume that new simulation models of the process are created on demand for the specific application. Therefore, the structure update step of the model adaptation is neglected. Moreover, the methods reviewed in these surveys do not consider the online or tracking simulation applications in which the direct communication between the simulation system and the actual process can be used to reduce the time and effort needed for model adaptation. In contrast, this paper presents a model

adaptation method for the implementation of tracking simulators that is applicable to simulation models developed during early stages of the plant lifecycle and in which the availability of process data is exploited to perform an update of the model structure and a re-tuning of model parameters. The adaptation methodology presented in this work is tested using a tracking simulator based on FPMs. However, the method is extensible for tracking simulators that combine FPMs and DDMs.

III. MODEL ADAPTATION METHODOLOGY

The development stages of industrial tracking simulation systems and its comparison with the process plant lifecycle is presented in Fig. 2. As previously explained, simulation models are created in the process design. During this stage, models are developed and tuned following data from similar plants and then used for engineering applications. Tracking simulators are further developed during the operation and maintenance stages of the targeted plant lifecycle when historical time data series and real-time measurements of the operational process are available. At the model adaptation, the simulation models are updated to represent the current process behavior. Next, in the model initialization, the current process state is mapped into the simulation model. Finally, at the tracking and predictive simulation stages, the tracking simulation is run together with the process, calibrated online and used to obtain predictions.

This work focuses on the adaptation of previously developed simulation models. Fig. 3 presents the model adaptation methodology proposed. The adaptation method presented is comprised of two steps: model structure update and model tuning. During the model structure update, the current process layout is mapped into the simulation model. This is a complex procedure that must be carried out manually by a process expert following the information available from various data sources. On the other hand, in the proposed method, the model tuning is done automatically by first accessing and selecting relevant process historical data and then applying a grey-box model optimization.

A. Model structure update

Process plants often go through configuration changes during their operation due to modifications made for maintenance purposes, for achieving efficiency improvement

Fig. 3. Model adaptation methodology.

Fig. 4. OPC UA client-server communication of the tracking simulation system during the model tuning. The connection between the client of the simulation system and the process server is needed only during the tracking simulation stage.

Fig. 5. OPC UA-enabled model tuning method.

or for coping with fluctuations in production demand. These changes do not only involve adjustments in controlled variables set points but may also include modifications of the actual process physical layout or replacement of process components. For this reason, simulation models developed during the early development stages of production plants do not correspond exactly to the functioning process. In the model structure update phase of tracking simulators development, the structures of previously developed simulation models are brought up to date for their layout to coincide with the current configuration of the process plant.

Accessing information of the current configuration of the plant is a challenging task due to the different tools and data formats in which this information is available. However, standardized machine-to-machine (M2M) communication protocols, such as OPC UA, can be used to provide a unified interface for accessing these data. OPC UA is an M2M industrial communication protocol standardized in IEC 62541. It enables secure and reliable transport of information between heterogeneous data sources. It is a platform independent standard widely adopted for vertical and horizontal communication in many industrial domains [8]. OPC UA has been selected as the only standard for the communication layer in the reference architecture model for Industry 4.0, which will furthermore consolidate its relevance in the future [12]. Authors in [13] present a platform that utilizes OPC UA to provide an homogeneous access to various plant information sources such as P&ID, control application and simulation systems. The platforms user interface is built with the existing 3D model of the plant. The tool presented in [13] could be utilized in order to reduce the time needed to access the current plant information. However, because up to date information of the configuration changes are available in different plant data sources, updating the simulation model structure must be carried out manually by a process expert after comparing and combining information derived from various data sources.

B. Model tuning

Model tuning refers to adjusting the model for reducing residuals. In tracking simulation, model tuning is an offline multi-parameter model calibration procedure directed to decrease the difference between simulation model results and the physical process outputs. This differs from the online calibration performed by the dynamic parameter estimators as online calibration is usually limited to adjusting only a few model parameters in order to achieve a permanent state synchronization with the process [2]. The model tuning method presented in this work utilizes OPC UA to connect the simulation system with the historian and to access historical process data in a systematic manner. OPC UA is a service oriented and client-server-based communication standard in which a server provides access to an information model with which multiple clients can subscribe and interact to access data and functions through a set of standardized services [14]. Fig. 4 shows the interactions between the OPC UA servers and clients of the tracking simulation system during the model tuning. The client of the historian subscribes to the simulation system and process servers to collect their data. The client of the simulation system connects to the server of the historian to retrieve historical process information. The process historian stores information of the process and the simulation system into an SQL database.

The model tuning method proposed is presented in Fig. 5. It begins by connecting the simulation environment to the process historian. Next, the process historical data is retrieved using OPC UA historical access (OPC UA HA) functions. OPC UA HA is based on the original OPC historical data access specification [5]. It is designed mainly for processing and analyzing data collected from a PLC/controller and OPC UA servers but it is also possible to obtain and operate historical events information. The OPC UA HA specification

Fig. 6. Algorithm of the data selection method followed during the model tuning.

Fig. 7. Model optimization method used for model tuning.

defines three functions: read, update and subscribe. The model tuning method retrieves process historical data using the read function of the specification. This function is designed to retrieve historical time data series of the specified nodes in a single request. The read function call should specify the start and end timestamps of the requested data as well as any other aggregate function invoke. The aggregate functions are operations that can be applied to process the retrieved data. Example of these functions are Average, Min, Max.

The model tuning thereof is performed by a model optimization method based on two algorithm variants which combine features from QNSTOP [15] and the Levenberg-Marquardt [16] algorithms. QNSTOP is a gradient-free scalar optimization method which is aimed at derivative-free stochastic optimization. The Levenberg-Marquardt (LM) algorithm is used for non-linear least-squares optimization. The employed algorithms combine the idea of an anisotropic trust-region from QNSTOP and a step direction selection from the LM algorithm. This method is in charge of estimating a set of model parameters that represent the closest the behavior of the process for a given operating region defined by process transients. Therefore, data series of various process transients are searched and selected from the retrieved historical process information before they are provided to the optimization method. The data selection algorithm is presented in Fig. 6. The data series needed for the model optimization are obtained by first, identifying in the historical process information the timestamps of events that cause transients such as set points modifications, production load changes or measured disturbances. Second, process data series delimited by the obtained timestamps are retrieved. Finally, the retrieved data series are provided to the optimization method along with an instance of the updated simulation model for performing the model tuning as shown in Fig. 7. Most commercial process historians store information only when there is a change in the monitored value, causing the historical process data to have irregular time steps. Thus, in cases where the time steps of the

TABLE I
PARAMETER VALUES BEFORE AND AFTER THE MODEL TUNING PERFORMED BY THE OPTIMIZATION METHOD

MODEL COMPONENT	PARAMETER	PARAMETER VALUE BEFORE	PARAMETER VALUE AFTER
		TUNING	TUNING
Y102	Nom. Mass Flow	0.04	0.050755
Y501	Nom. Mass Flow	0.02	0.0134688
P100	Form Loss Coeff.	100	161.468
P200	Form Loss Coeff.	0.0	93.80901
P300	Form Loss Coeff.	0.0	45.68852

data is not constant, the data series must be processed before they are provided to the optimization method. After the model optimization execution, an optimal set of parameters are written into the simulation model. The model optimization reduces the difference between simulation results and measured time data series of the process after recursively adjusting multiple model parameters and then evaluating model outputs.

IV. EXPERIMENTS AND RESULTS

The model adaptation methodology proposed was tested using a laboratory-scale heat production plant (HPP). The P&ID of the process is shown in Fig. 8. The HPP is a small process where water is heated and then pressurized before it is ready for its consumption. Changes in the load of hot water consumption are mimicked by regulating the position of a proportional valve (Y501). The water is heated in an open tank (B100) and then sent to a feedwater tank (B200) where the water level (L200) is controlled using two PID controllers connected in cascade by adjusting the flow (F100) between the B100 and B200 tanks. The water is pressurized in the tank B300. The model of the process was implemented in the simulation environment Apros [17]. The OPC UA process historian used was the Prosys Historian [18]. The model structure update step of the model adaptation was carried out manually following an up to date version of the PI&D which was available as a physical document. Thus, no OPC UA interface was required for this step.

The model tuning experiments started by connecting the simulation model to the process historian through their OPC UA interfaces. Next, historical process information was retrieved using OPC UA HA. Fig. 9 shows the retrieved historical time data series of the L200 process variable that corresponds to the water level of the open tank B200. Fig. 10 shows a close-up view of the data included inside the ellipse drawn in Fig. 9. After the data selection algorithm retrieves historical process information, the data selection algorithm finds changes in the controlled variables set points and identifies and selects data of various process transients as shown in Fig. 10. This is done by obtaining the timestamps of the set point changes and then retrieving all other process variables information delimited by such timestamps. Fig. 11 shows the data selected of one of the identified transients caused by a change of the water level L200 setpoint. This is the initial transient used for the model tuning.

The process historian used for these experiments has an event based data log mechanism. This means that the historian will only store information after there is a change in the monitored process variable. Moreover, the historian does not support any aggregate functions to operate the retrieved historical data. Thus, the retrieved data cannot be operated

Fig. 8. P&ID diagram of the HPP process.

Fig. 9. Process historical time data series.

Fig. 10. Close-up view of the process historical data included inside the ellipse drawn in Fig. 9. The data enclosed by the circles are the transients identified by the data selection algorithm.

Fig. 11. One of the identified transients in the water level L200 process variable.

Fig. 12. Interpolated data of the transient depicted in Fig. 11.

Fig. 13. Interpolated data of flow F100 during transient of Fig. 12

using one of the aggregate operations defined in the *Read* function of the OPC UA HA specification. For these reasons, the data series obtained from the historian do not have a

TRANS.	DESCRIPTION	PROCESS VARIABLE	SSE BEFORE MODEL TUNING	SSE AFTER MODEL TUNING
1	L200 = 0.14m-0.15m	L200	3.11	1.9
		F100	16.39	4.63
2	L200 = 0.15m-0.16m	L200	10.64	2.49
		F100	32.42	3.67

constant time step, as shown in Fig. 11. To overcome this, the data selection algorithm is also in charge of operating the retrieved data series of the transient before providing it to the optimization method. Fig. 12 shows the processed data of the transient depicted in Fig. 11 along with the data of the setpoint causing the transient. Fig. 13 shows the processed data of the process variable F100 during the transient shown in Fig. 12.

After the processed historical data along with the simulation model of the process are selected, they are provided to the optimization method for model tuning. The model optimization runs automatically and finds a set of model parameters that minimizes the difference between the simulation results and the actual process measurements. Table I shows the optimal parameter values calculated by the optimization method. Fig. 14 and Fig. 15 compare process measurements and simulation model results during the process transient caused by a change in the set point of the controlled water level L200 (Transient 1 of Table II). Fig. 14 corresponds to the water level L200 and its set point. Fig. 15 depicts the flow F100 during the same transient. Similarly, Fig. 16 and Fig. 17 compare process measurements and simulation models results for the second transient selected for model tuning (Transient 2 of Table II). Table II compares the sum of squared errors between the process measurements and the simulation model results before and after the model tuning for both transients. The results show that the model tuning procedure followed is able to substantially reduce the difference between the process and simulation outputs. After the model adaptation is completed, the simulation model can be connected to the process to be used as a tracking simulator.

V. CONCLUSIONS

This paper presented an OPC UA-enabled model adaptation method that eases the utilization of previously developed dynamic simulation models as tracking simulators for process operation and maintenance support. The proposed adaptation methodology is a two-steps procedure that starts with a model structure update and it is followed by a model tuning. The structure update is targeted to modify the model for its configuration to correspond to the current process structure. Although the proposed model structure update must be carried out manually by a process expert, OPC UA-based platforms, where data from various process information sources is available, can be used to support this adaptation step. The model tuning method proposed takes advantage of the information availability that OPC UA offers to seamlessly connect the simulation environment with the operational process and its historian as well as to retrieve process historical data through the OPC UA historical access (OPC UA HA) functions. The model tuning thereof is carried out by a model optimization method that iteratively evaluates a previously created simulation model and compares its results

Fig. 14. L200 comparison of process measurement and simulation model results before and after model tuning for Transient 1.

Fig. 15. F100 comparison of process measurement and simulation model results before and after model tuning for Transient 1.

Fig. 16. L200 comparison of process measurement and simulation model results before and after model tuning for Transient 2.

Fig. 17. F100 comparison of process measurement and simulation model results before and after model tuning for Transient 2.

with the selected historical process data in order to find a set of model parameters that reduces model residuals. The model tuning results show that the model optimization method is able to find a set of parameters that bring the simulation results very close to the current process outputs. Consequently, the adapted model can be connected to the operating process to be used as a tracking simulator. The model adaptation method described in this work aims to address the need for systematic procedures required to bring the FPMs developed during the engineering phases of the process plant to the operation and maintenance stages for tracking simulation applications. Future work will focus on the parallelization of the execution of the tuning method to reduce the time needed for this task.

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