Adaptation framework for an industrial digital twin

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Abstract

Digital twins for performance-oriented applications in industrial environments require systematic model maintenance. Model adaptation requires efficient optimization tools and continuous evaluation of measurement quality. The adaptation and model performance evaluation are based on the modeling error, making the adaptation prone also to the measurement errors. In this paper, a framework for combining model adaptation and measurement quality assurance are discussed. Two examples with simulated industrial-scale biopharmaceutical penicillin fermentation are presented to illustrate the usability of the framework.

Keywords: *digital twin, adaptation, framework, differential evolution*

1 Introduction

Simulation tools have efficiently been applied in various engineering problems such as in process design and production planning. Currently, the simulation tools are also developed to real-time utilization. In process industries, the simulation models are, for example, used as an open-loop decision support tool (scenario simulation, prediction). These models can be considered as digital twins as essentially, "the digital twin is a virtual and computerized counterpart of a physical system that can be used to simulate it for various purposes, exploiting a real-time synchronization of the sensed data coming from the physical system". (Negri et al., 2017)

The digital twins can be classified in terms of their utilization in different tasks and areas, for example, design twins, performance twins and product or production twins. An important classification can be made in terms of real-time integration between the twin and its physical counterpart. Digital twin needs to have a closed-loop, automatic integration to the real process. Otherwise the correct term is a digital model (without integration) or a digital shadow (an open-loop integration). (Kritzinger et al., 2018)

Foreseen possibilities applying digital twins in continuous processes have been discussed for example in (Sun et al., 2017). In case of digital twins and shadows in these kinds of performance-oriented applications, it is crucial that the simulation model represents the real system continuously. Therefore, the performance of the digital model needs to be evaluated and the model needs to be updated automatically to cope with unseen or unmodeled changes.

The continuous updating, namely model adaptation requires efficient data-analysis and optimization tools. In general, the adaptation can be based on several techniques (Kadlec et al., 2011). However, both the real-time requirements and the model complexity (interconnected measurements and parameters) can make the adaptation problem challenging. Several methods have been presented to match the physical process with the digital model (Ohenoja et al., 2018; Friman and Airikka, 2012; Pietilä et al., 2013; Schirrmacher et al., 2009), but with limited insight on the whole problem.

This paper elaborates the overall picture on development and maintenance of a performance digital twin in industrial processes. In real systems, the actual parameters are not known. Hence, the whole adaptation (model performance evaluation) can only be dependent on the modeling error, making the adaptation prone also to the measurement errors. It is assumed that the adaptation involves a multivariable optimization problem. The computational issues, such as the real-time requirements are out of the scope of this presentation. Figure 1 presents the discussed framework. In Sections 2—4, the different elements of the framework are treated more detailed. In Section 5, simulated examples are presented.

2 Measurements as a foundation for adaptation framework

Modern industrial automation system includes measurements with varying characteristics; There can be sparse or even discontinuous data from the online analyzers and laboratory measurements providing product quality measurements, continuous automation system data with even sampling interval, and data with very high sampling frequency that needs to be preprocessed before used for decision making and process control. In addition, soft sensors are often used to infer measurements from harsh environments or otherwise difficult locations, or they can be used parallel to physical measurement device for validation and backup purposes.

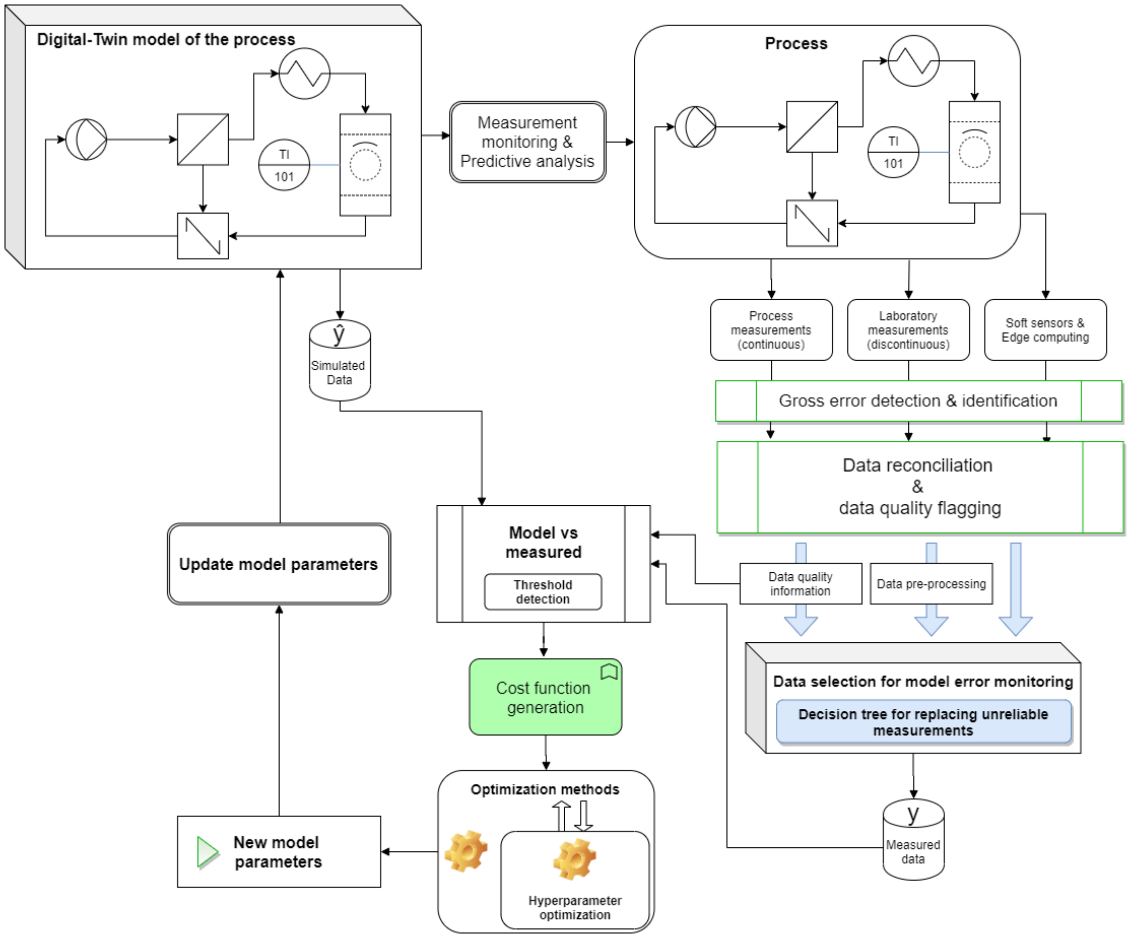

Figure 1. The concept for adaptation of industrial digital twin.

The concept for adaptation of industrial digital twin is presented in Figure 1. Different measurements from the real process on the right upper corner are used to monitor the modeling error of the digital twin on the upper left corner. Measurement quality is ensured by real-time monitoring and data reconciliation. Low quality or missing data is accounted in cost function generation.

Using a digital twin for decision making, robust self-diagnostics is required. Sensor malfunctions, measurement drifting, and other possible systematic error sources such as fouling may cause misinformation that leads to unreliable decisions. Measurement drift can be caused by ageing of components or environmental changes. Re-calibration is therefore important to maintain reliable information for a control system.

Soft sensors have always some error in their estimates or predictions. This error consists of modeling error and the quality of process measurements their model is based on. Similarly, physical sensors may perform acceptable at some defined measurement range, however their error can grow drastically when moving outside this working range.

Laboratory measurements are rarely used in automated control but can work as a basis for evaluating reliable process operation and for validating process measurements, as well building soft sensors. They are used as a basis for reliable decision making in many industrial processes. Sampling can induce large errors or variation in results if done improperly and inconsistently. Sample preparation and analysis should be done according to previously validated standard procedure to ensure the quality of data.

Intelligent measurement devices can detect if their data is reliable and possibly self-calibrate or alternatively alert the process operator or maintenance personnel. Modern automation system can include functionalities for detecting unreliable measurements and this is important aspect to consider when implementing digital twin. It is preferable to associate the information of the measurement quality with the measurement value for any kind of modeling and decision support.

3 Quality of measurements

Reliable measurement information is a prerequisite for the successful model adaptation. This requires online measurement quality monitoring. Unfit measurements can be removed or replaced. There are several methods for detecting differing measurement errors presented in chapter 3.1. If gross errors (Human mistakes, measurement errors, etc.) are also present in the process data, they must be identified and removed before data reconciliation (Sánchez et al., 2002).

Intelligent measurement devices with vast amount of data and real-time data processing demands require automated quality assurance (QA) and quality control (QC) methods. (Campbell et al., 2013; Morello et al., 2014) A high performance control system includes automatic quality control algorithms and a comprehensive flagging system to indicate data quality level, to identify errors, to highlight corrected values, and to make it easier for data users to identify suspicious and erroneous data, namely to make quality control more efficient and closer to real-time. (Vejen et al., 2002)

3.1 Gross error detection & identification

Measurement drift is a typical for phenomenon related to industrial measurements where bias between true and measured values is evolving during long period of time. Baena-García et al. (2005) presented two methods for drift detection; Drift detection method uses binomial distribution to calculate the number of errors. On the other hand, early drift detection method considers the distance between two errors classification instead of considering only the number of errors.

Nishida and Yamauchi (2007) considers previous methods and presents new more noise resilient option which works for sudden concept shifts and gradual changes. They continued their work in (Nishida and Yamauchi, 2009) and presented learning system that uses multiple online classifiers that can predict changes. In Dries and Rückert (2009), six methods for online concept drift detection were evaluated and three approaches that can detect data drift reliably were presented. Finally, different gross error detection & identification (GEDI) methods, based e.g. in Mean squared error (MSE), root mean squared errors (RMSE), correlation coefficient based methods etc. are presented in (Kadlec et al., 2011).

3.2 Quality flagging

QA and QC procedures are closely related, but each has a distinct meaning. QA is a process of data profiling to discover inconsistencies and other anomalies in the data and performing data processing to improve the data quality. On the other hand, the QC process decides whether data meet the requirements for quality outlined by the end users. Hereby, QA can be considered a proactive or preventive process to avoid problems and QC as a process to identify and flag suspect data after they have been generated. (Campbell et al., 2013; Scully-Allison et al., 2018)

The QC procedures can be applied at various stages of data flow from sensors to the end user and can be carried out by numerous methods. Observations can be flagged by several methods and various symbols and names can be used to indicate the quality control level. It is difficult to develop common guidelines for QC and flagging procedures that are applicable in all circumstances and so there are no universal standards, but they are specific to the type of the data, application and the location at which data is collected. (Campbell et al., 2013; Vejen et al., 2002). Hence, several QC methods for automatic tests have been reported (Vejen et al. 2002; Scully-Allison et al. 2018; Geuder et al., 2015; Lewis et al., 2018)

In addition to the simple and traditional QC procedures, methods utilizing machine-learning have also been developed. These methods represent a data-driven approach to QC, wherein statistical models or classifiers are trained using empirical data collected from sensors. Hence, little knowledge is required about the device hardware or the phenomena being measured. On the other hand, adequate amount of data that contains the examples of faulty and correct data for model training and validation is required. Artificial neural networks, support vector machines, decision trees, and probabilistic models among others are commonly utilized as machine-learning approaches (Kadlec et al., 2011; Campbell et al., 2013; McNutt et al., 2019) but also hybrid systems, for example combining QC flags and a fuzzy logic, are developed (Morello et al., 2014).

Defective or missing data are unavoidable and require decisions how to process the faulty data: should the erroneous values to be removed, adjusted, replaced with an estimated value (e.g. soft sensor) or ignored. Great care must be taken to ensure that all processing steps are well documented so that they can be evaluated. The raw unmanipulated data should also always be saved. The uncertainties may arise from missing data and for instance using the wrong methods to fill the gaps. In a quality control procedure, all invalid data should be marked, but it is essential to ensure that valid data are not marked or removed, for example when a real but rare and extreme value outside the expected range occurs. In device self-diagnostics one difficulty that often arises is in differentiating between normal deviations and component faults.

Uncertainty techniques can be applied to measure the impact of faults on measurement quality, which makes it possible in certain circumstances to continue to use a sensor after it has developed a fault. Setting QA/QC tolerances to minimize false detections is difficult, especially under changing conditions. Moreover, the values of many parameters are site-dependent. In many cases, too many or too few events may be detected and therefore, the results of automatic screening demand a manual check of an expert to ensure the validity. Expert knowledge and analyzing the circumstances under which false errors occur provides information that can be used to adjust the QC procedure and achieve more optimal performance. (Campbell et al., 2013; Geuder et al., 2015)

3.3 Data reconciliation

One possibility to monitor the quality of measurements is based on data reconciliation. Data reconciliation also offers means to correct or replace the erroneous and missing measurements. (Vasebi et al., 2014)

The main idea of data reconciliation is to adjust the measurements data to satisfy the mass, energy, or momentum balance equations. Steady-state data reconciliation is solved as an optimization problem, where the objective is to minimize the difference between the measured variables and the adjusted ones, weighted by the reciprocal of the variance. Objective function can be e.g. weighted least squares function (WLS). (Vasebi et al., 2014)

4 Adaptation

In real systems, the actual model parameters are not known. Hence, the whole adaptation (model performance evaluation) can only be dependent on the modeling error, making the adaptation prone also to the measurement errors mentioned in the previous Section. Therefore, the adaptation should preferably utilize the uncertainty estimates and quality flags of the measurements. In addition, the adaptation framework needs to consider when the adaptation is needed, how to cope with varying data quality and how to make the trade-off between the adaptation accuracy, stability, and computational load.

4.1 Triggering

The adaptation algorithm can be run consistently or there can be predetermined threshold based on the estimation error. The regular adaptation interval can be determined based, for example, on the minimum process delay or maximum sampling interval of the relevant measurements.

The thresholds for infrequent adaptation can be calculated between the actual process measurements and the model output values representing the measurements. Methods for triggering should be chosen according to case. For example, (Palomo et al., 1991) mentions residual analysis, variance distribution and coherency-based methods among others. Also, in this case, the quality information of the measurements can be utilized to guide the triggering.

4.2 Optimization methods

There is a vast amount of optimization methods. On the other hand, it has been stated that there is a lack of a single solver that can overperformance the others in variety of optimization problems (Rios and Sahinidis, 2013). The performance of solvers is strongly dependent on the problem dimensionality and non-smoothness of the function and bounds on the variables.

In typical engineering problems, the global optimum is a solution that outperforms its alternatives after a fixed number of cost function evaluations. It has been shown that the metaheuristic methods can overperform the deterministic methods especially with small budgets (Sergeyev et al., 2018). On the other hand, the deterministic methods have provable convergence abilities to any optimization problems with an unlimited budget, but metaheuristic method may not be able to find the global optimum despite increased budget. (Sergeyev et al., 2018)

One well-known metaheuristic (stochastic) optimization method is the Differential Evolution (DE) (Storn and Price, 1997). Its implementation is sufficiently straightforward, and DE has only several hyperparameters to tune the algorithm. DE is utilized in the adaptation examples in this paper, also since calculations proceed with real numbers. The optimization method selection was done in the previous study (Ohenoja et al., 2018).

4.3 Selection of model parameters and outputs

In large-scale processes and simulation models, the number of adjustable model parameters, together with number of possible measurements (model outputs) gets high and the optimization problem becomes too complex. It is important to be able to focus to the most relevant parameters and measurements to decrease the problem dimensions. Naturally, expert knowledge is needed to perform the selection of parameters and measurements to the model adaptation.

Systematic approach to reach a smaller subset of possible parameters and measurements could involve sensitivity analysis tools. In local sensitivity analysis (LSA), one individual model parameter is changed at the time and the effect to model outputs observed. However, this approach cannot account for parameter interactions. Global sensitivity analysis (GSA) for estimating input parameter effects on different process outputs can use, for example, Sobol method (Sobol′, 2001). It is based on variability observed from Monte Carlo simulation and therefore large-scale system may require extensive computational cost.

4.4 Cost function selection

In model adaptation the objective is to match the model outputs with real measurements. Hence, an intuitive selection of the cost function is the sum of output measurement errors. However, the cost function typically contains measurement values with totally different ranges and the measurements that have largest error, will define the model parameters that are preferred/overweighed in the adaptation. Therefore, the first requirement is to normalize the values from the data sources to compensate the different absolute values.

Secondly, the adaptation performance can be improved by weighting certain measurements according to their importance to selected model input parameters. The weighting can be based, for example, on expert knowledge or systematic testing of model parameter sensitivities.

Finally, the adaptation framework for an industrial digital twin discussed in this paper indicates that the quality information connected to measurements should also be utilized in the cost function formulation. The cost function measurement weighting can be changed accordingly if quality flagging describes measurement as unreliable. Alternatively, this unreliable measurement can be replaced with soft sensor if available.

4.5 Hyperparameters

The selection of hyperparameters of the optimization method is crucial for its convergence and computational performance. Some rule of thumbs exists for different optimization methods, but typically the selection is based on experience and intensive off-line testing. In some scenarios, it would be beneficial to automatically change these algorithm tuning parameters to compensate decreased data quality or when the optimization performance drops noticeably. In the case of DE, it can be done using the method itself for this task. First loop optimizes the model parameters and the second loop finds the best model parameters for the task. (Chachuat et al., 2009)

5 Illustrative simulation examples

5.1 Simulation model

Industrial Penicillin Simulator (IndPenSim) is a MATLAB® based model for industrial-scale biopharmaceutical penicillin fermentation simulation. IndPenSim constitutes of several m-files providing their own function for the simulator. This program is intended to be a benchmark simulator for researchers to compare and validate new controllers in the batch fermentation process. It also includes Raman spectroscopy simulation that can be used for advanced process control design. It has fault generation capability built-in so it can be used for testing fault detection algorithms and for process fault identification. (Goldrick et al., 2019; 2015)

This paper uses a modified version of the simulator. Measurement noise and random variations were removed to move towards deterministic model. This serves our purpose of testing adaptation algorithm with adaptive cost function. The effect of random noise and measurement faults will be studied in the future after we understand how this algorithm performs in optimal conditions.

The IndPenSim includes 105 model parameters in total and 67 model outputs. The number of model outputs were decreased to 17 based on expert knowledge. The use of expert knowledge here refers to consideration of which of those model outputs could be measured directly or indirectly in real-time without discontinuous laboratory sampling. The model parameters were narrowed down to six by using LSA. The system of six inputs and 17 outputs was then utilized in model adaptation and it was also executable for GSA.

5.2 Example with weighted objective function

This example aims to illustrate the effect of measurement weighting in the objective function (OF) of model adaptation. GSA was used to generate weighting factors for model outputs which represent different process measurements. Fractional sensitivity indices between the different model parameters and outputs were added up to form the weighting coefficient for each output. In the other scenario, all measurements were equally weighted.

The real process in this text refers to modeling results gained by a reference simulation with altered model parameters. Nominal model input parameters are used to represent the state of the digital twin to be adapted. The model input parameters are changed by 5% upwards to represent changed operating conditions of the real process. Adaptation algorithm is then used to find these new values using the error between process output measurements and model outputs.

Adaptation algorithm, realized with DE, compares the model output values from the simulated process to values received from different DE trials and starts to adapt the designated model parameters in an iterative way. Adaptation stops when maximum number of iterations is reached or if the cost function value reaches the predetermined threshold value (0.001), which relates to the total relative modelling error of 0.1%.

The cost function combines total relative difference between 17 model outputs and process measurements. The total error is a sum from a simulation period of 1150 samples. Adaptation performance is inspected using cumulative and dynamic output errors. In addition to model outputs, the adapted model parameter errors to known values are inspected (although not relevant in industrial implementations).

Preliminary work for this study includes selecting optimal adaptation window for minimizing the delay between adaptation cycles, while still maintaining a good performance. It was determined that 200 datapoints was enough to maintain good performance.

The results are presented in Figure 2 and Figure 3. Weighted OF lowers the total error in almost every measurement compared to nominal OF in Figure 2. Measurements with larger error compared to nominal OF have only small rise in total error while ‘NH3’, ‘PAA’, ‘a3’, ‘a4’, and ‘S’ have significant drops in total error. The total error with weighted OF is only 39% from the total error with nominal OF. The total error is still mainly influenced by single model output errors peaking at certain points of a batch process. Overall, all the measurements stay below the generally acceptable 5% error limit for the soft sensors, which indicates that the adaptation was successful.

According to results in Figure 3, the model parameters 'ratio_mu_e_mu_b' and 'K_diff' are the only ones to have larger error with weighted OF than with nominal OF. 'Y_PAA_P' has very large drop in error after measurement weighting.

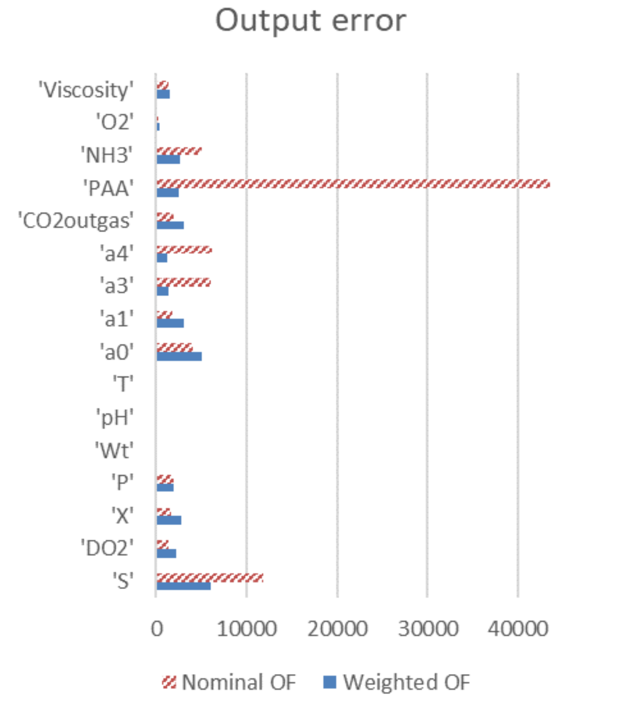

Figure 2. Total measurement errors between the model outputs and simulated process measurements using nominal and weighted output functions. The total error is a sum from a simulation period of 1150 samples.

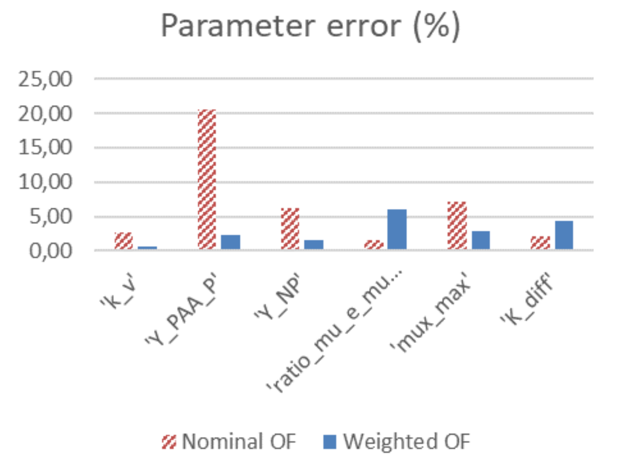

Figure 3. Model input parameter errors with nominal and weighted output functions.

5.3 Example with missing measurement

Adaptation performance is strongly dependent on the quality of measurement information. Loss of vital measurement information increases the adaptation error to a level where model is unreliable. This highlights the need for measurement quality monitoring and flagging. Adaptation robustness can be increased by implementing soft sensors that can be used to replace missing or faulty measurements.

Such a scenario is simulated here, where a vital measurement ‘a0’ is missing and replaced with a soft sensor. The soft sensor performs somewhat worse than the original measurement, as depicted in Figure 4.

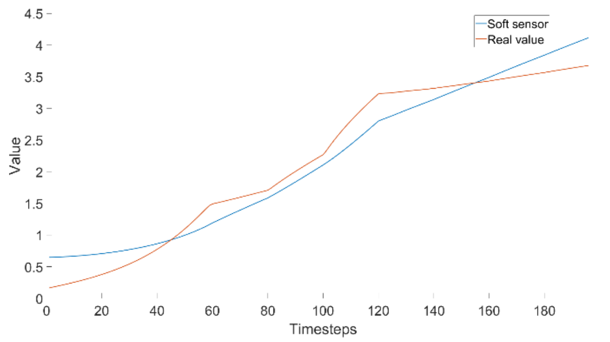

Figure 4. The comparison for soft sensor and real measurement in a0 value. The x-axis presents 200 samples with 12-minute sampling interval.

The adaptation result is presented in Figure 5. The missing measurement increases the output error tremendously. By replacing the missing measurement with a soft sensor, the adaptation performance can be maintained and the total errors in the model outputs can be noticeably decreases. Large errors in ‘a3’ and ‘a4’ are caused by the differences in measurement dynamics between the soft sensor and the real measurement.

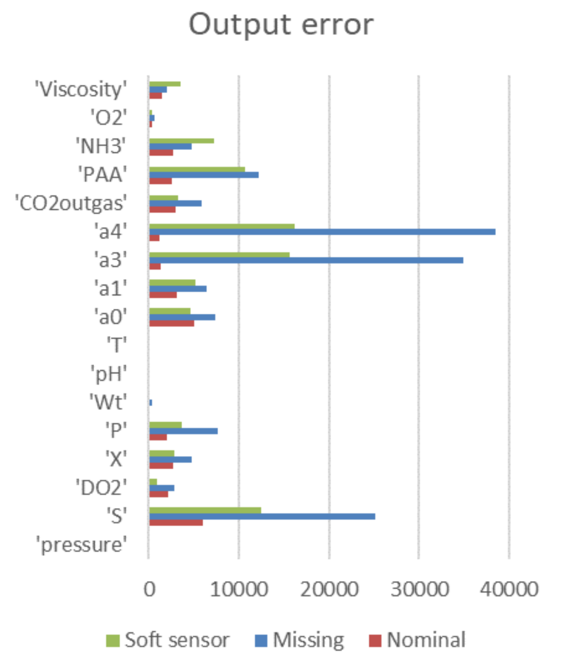

Figure 5. The effect of missing measurement information to adaptation performance.

6 Discussion and conclusions

The simulated results with modified IndPenSim are deterministic to some extent to be suitable for controlled testing of our adaptation framework. These results revealed the applicability of our LSA/GSA based approach for selecting the set of adapted model parameters and using GSA results for measurement weighting.

It was also depicted that the adaptation can be very dependent on a single measurement. This emphasize the importance of the reliable measurement information and real-time quality monitoring. Robustness can be improved by implementing data reconciliation and soft sensors to replace unreliable or missing measurements.

Work will continue with testing the adaptation with different measurement errors and by efficiently combining the measurement QA/QC information to model adaptation. The adaptation framework will also be stressed in mineral processing simulation models that represent real life process in Oulu Mining School enrichment pilot plant.

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