Proceedings of the 2024 Winter Simulation Conference
H. Lam, E. Azar, D. Batur, S. Gao, W. Xie, S. R. Hunter, and M. D. Rossetti, eds.

SIMULATION-BASED DIGITAL TWINS: AN ACCREDITATION METHOD

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ABSTRACT

The simulation-based Digital Twin (DT) has been gaining prominence in recent years and represents a revolution in decision-making processes. In this context, increasingly fast and efficient decisions are made by mirroring the behavior of physical systems and using advanced analysis techniques. On the other hand, this article draws attention to the challenges of ensuring the accreditation of simulation models over time, as traditional approaches do not consider the periodic updating of the model. Therefore, this work proposes an approach based on the periodic evaluation of these models using Machine Learning and control chart. More specifically, the authors adopted the K-Nearest Neighbors (K-NN) classifier, combined with a *p*-chart. The proposed approach has been tested in theoretical and real case studies, allowing us to monitor the DT results and ensuring its accreditation. The broad applicability of the proposed tool is highlighted, which can be used in simulation-based DTs with different characteristics.

1 INTRODUCTION

Digital Twins (DTs) to support decision-making have gained prominence in recent years due to technological advancements and the need for increasingly intelligent and efficient tools (Tao and Zhang 2017). The concept of a DT is based on the virtualization of physical systems through highly integrated digital models. In this case, DTs enable mirroring these systems through sensors, smart devices, and databases, allowing for more efficient and effective decision-making (Santos et al. 2021). In this scenario, we observe applications across several sectors such as manufacturing, services, logistics, and healthcare (Wright and Davidson 2020).

Notably, within the context of Industry 4.0, decision-making based on DTs has become one of the pillars of this new industrial era (Zhong et al. 2017). Furthermore, for the design of DTs, besides commercial packages, the use of computational simulation is highlighted, especially Discrete Event Simulation (DES) and Agent-Based Simulation (ABS) (Santos et al. 2022). In this case, the authors reveal that such an approach has stood out for the flexibility and cost-effectiveness of simulation software and packages.

However, when considering simulation-based DTs, some characteristics and functionalities must be ensured for the model. In addition to the virtual model being capable of capturing physical changes and adapting, it is also necessary to ensure the correct functioning of these models over time. In this sense, the model accreditation must be ensured over time (Tao and Zhang 2017). For Sargent (2020), the accreditation goes beyond validation methods since it considers that the model must be ready to be interpreted and provide reliable results. Finally, Santos et al. (2022), through a systematic literature review on the topic, pointed out the need for methods and systems to periodically evaluate simulation models used as DTs.

Therefore, this work proposes a new approach for monitoring-based accreditation of simulation models used as DTs. An alternative for evaluating complex systems with multiple variables is using classifiers, and in this case, this work adopts the K-Nearest Neighbors (K-NN) classifier due to the simplicity and efficiency of this Machine Learning technique. Furthermore, the use of the *p*-chart is also proposed to monitor the behavior of models over time.

Finally, to evaluate the proposed approach, it was applied in theoretical cases and also in a real case study where the DT supports decisions in an automated production cell. The remainder of this article is organized as follows: Section 2 provides a theoretical framework, while Section 3 presents the proposed approach. Section 4 is dedicated to presenting the application of the proposed tool in theoretical and practical cases. Finally, Section 5 contains the conclusions of the work.

2 THEORETICAL BACKGROUND

2.1 Simulation-based DTs

The use of simulation models as DTs is not a recent concept but has been gaining prominence in recent years due to technological advancements (Santos et al. 2022). According to Wright and Davidson (2020), what differentiates a traditional simulation model from a DT approach is the ability to extend its use across time scales as well as its integration with the physical environment allowing the model to adapt according to changes in these environments. In this case, by connecting the model to physical systems, we have a synchronized copy that adapts according to the current state of the physical systems (Ashrafian et al. 2019). Finally, Santos et al. (2021) add that the model responses can be autonomous or semi-autonomous (requiring human decisions), and real-time and near real-time approaches are valid.

According to Tao and Zhang (2017), although there are different DTs varying in the level of integration between physical and virtual environments, all of them are based on four main components: (i) Physical System (PS), consisting of humans, materials, and processes; (ii) Virtual System (VS), consisting of models representing physical behavior; (iii) Service System (SS), including the structure capable of enabling communication between physical and virtual environments; and (iv) Data System (DS), a set of data and information transmitted between the PS and the VS.

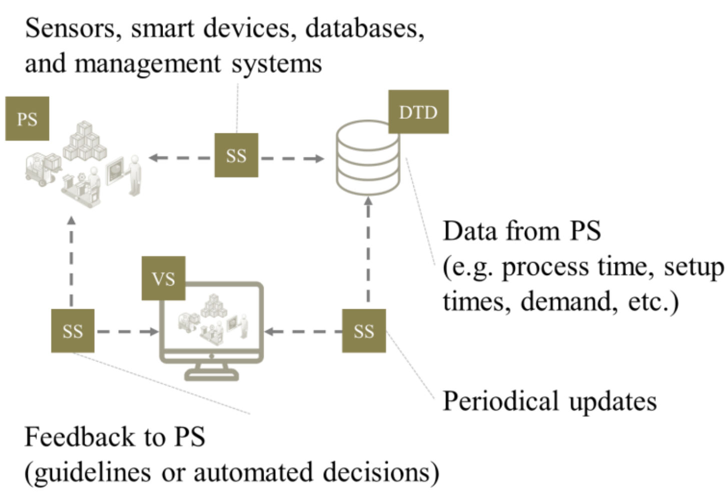

Figure 1: General structure of a DT (adapted from Tao and Zhang (2017)).

Simulation-based DTs have two distinct stages: model building and model operation (Montevechi et al., 2020). During the model building phase, the focus is on integrating it with physical systems and validating it to ensure that it adequately represents physical behaviors. On the other hand, in the operation phase of the DTs, it is assumed that the model is valid and will be used periodically to support decision-making. In this case, Tao and Zhang (2017) reveal that the model's periodic verification, validation, and accreditation (VV&A) routines are necessary.

While the verification and validation stages aim to ensure the correct functioning of the computational model and its satisfactory correspondence with physical systems, respectively, the accreditation phase is a more complete approach since it is related to the decision process and evaluates the model's reliability and usability to guide decisions (Sargent 2020). In this regard, Tao and Zhang (2017) emphasize that the results of physical and virtual systems should be frequently compared to ensure the accreditation of DTs during their operation.

Despite the importance of ensuring such accreditation routines during the operation of the DT models, Zhuang, Liu, and Xiong (2018), Onggo et al. (2018) and Santos et al. (2022) highlight that methods and techniques for this purpose are still lacking. Cho et al. (2019) adapted a traditional validation approach to monitor the validity of a simulation-based DT. In this case, at each decision-making interval, the authors conduct hypothesis tests to compare physical and virtual environments. However, this approach has limitations since its adoption might become unfeasible according to the complexity of the DT. Moreover, this approach proposes a punctual evaluation and comparing DT data with the physical system using only descriptive statistics (i.e., mean and standard deviation) can lead to erroneous conclusions (Chen et al. 2019).

Thus, the need for techniques and tools focused on monitoring and evaluating simulation models used as DTs over time becomes evident. Furthermore, the authors highlight the use of classifiers integrated with monitoring tools, such as control, charts as an innovative approach. Therefore, this work is based on a Machine Learning technique, the K-NN classifier and Control Chart p to develop a monitoring tool focused on ensuring the model's accreditation throughout its operation.

2.2 K-NN Classifier and *p*-chart

The K-NN is a Machine Learning technique that relies on the labels of the 'K' nearest neighboring data samples (training data) to classify test data (Kumar et al. 2020). Although K-NN is one of the simplest classification algorithms (Lee et al., 2020), it was chosen for the proposed approach due to its robustness and suitability for problems with multiple classes (Zhang et al., 2021). K-NN uses the Euclidean distance, calculated by Equation 1, to define the nearest neighboring data and then predict the classification of test data according to the labels of these nearest neighbors (Gong et al., 2020).

$$D = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2} \tag{1}$$

Where D represents the distance between two vectors of dimension n, $\mathbf{X} = (x_1, x_2, \ldots x_n)$ and $\mathbf{Y} = (y_1, y_2, \ldots y_n)$.

Additionally, the accuracy of the K-NN indicates how well the algorithm can classify the data (Boontasri and Temdee 2020). In this case, it is expected that the accuracy increases as the algorithm can correctly classify the data (target of 100%). On the other hand, if there is no clear majority of training data with a particular label, the algorithm assigns a random label to the test data, and the classifier accuracy tends to 50% (Kumar et al. 2020). Therefore, as the proposed approach suggests monitoring K-NN accuracy over time, it is necessary to adopt a monitoring technique, and in this case, Control Charts stand out.

According to Montgomery (2009), control charts are one of the main techniques of statistical process control, useful for monitoring the output variable(s) in systems subject to sources of variability. Basically, samples are regularly taken from the process, and the value of a monitoring statistic is calculated. Then, this statistic is plotted on a chart. If it is plotted beyond the control limits of the chart, the process is considered out of control, and corrective actions must be taken (Apsemidis et al. 2020; Zwetsloot and Woodall 2021).

Control charts have been used in various areas, such as manufacturing, healthcare, and services. Moreover, considering the peculiarities of these areas, different charts have been developed (Abbas et al. 2019; Chukhrova and Johannssen 2019). Several approaches explore monitoring quality characteristics expressed on a quantitative scale and are classified as "Variable Charts". On the other hand, some quality characteristics are expressed as qualitative variables, and in this case, we have the so-called "Attribute Charts" (Montgomery 2009).

Considering K-NN accuracy as a process parameter to be monitored, the authors adopted the "*p* control chart". According to Chukhrova and Johannssen (2019), the *p*-chart focuses on monitoring characteristics that fit the Binomial distribution, that is, evaluating a proportion of points that are or are not in accordance with a certain evaluated characteristic. This choice is justified since K-NN accuracy can be obtained by considering the proportion of errors and correct classifications of the classifier when trying to separate data from physical and virtual systems. The control chart's limits are called the Upper Control Limit (UCL) and Lower Control Limit (LCL), and the Center Line (CL) is given by the proportion of the evaluated characteristic given a set of data (Abbas et al. 2019). Figure 2 illustrates a typical p control chart and we can observe several points plotted over time, with a point outside the limits of the chart being considered an "out of control signal" and indicating that some special cause may have affected the monitored system.

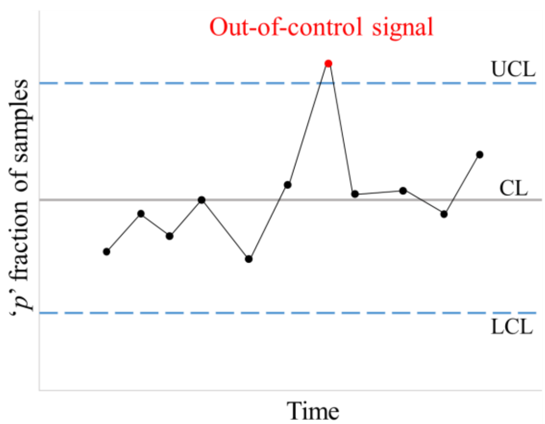

Figure 2: Control chart illustration (adapted from Montgomery (2009)).

3 PROPOSED METHOD

This work proposes an approach based on three main phases: Definition of the evaluation variables of the DT (where key system variables are selected and prepared); Monitoring interface setting (involving the creation/configuration of an interface that allows the classification of physical and virtual data using K-NN, as well as the plotting of classifier accuracy on a p control chart); and Periodic monitoring (where the interface is updated and used periodically).

3.1 Definition of Evaluation Variables for the Digital Twin

The evaluation variables are the parameters of the DT that can represent the similarity of the virtual model to the physical environment. Their selection represents a critical step, as the monitoring system will be built and configured based on this stage. According to Sargent (2013), the evaluation variables of a simulation model are related to the model's purpose, i.e., those associated with decision-making. Therefore, when considering the use of simulation as a DT for production processes, some of the most common evaluation variables include: process times, waiting times, resource utilization rate, among others.

Furthermore, the selection of variables should be done in pairs, meaning it is important to ensure that each variable is available both in the virtual and physical systems, in the same proportion. In other words, the same data collected from the model must be collected in the physical environment. Thus, it is possible to compare the two environments and infer the validity of the DT through the monitoring interface. In this case, we must provide the collection of these same variables in the physical system, either through sensors, smart devices, databases, among others. Finally, it is worth noting that an advantage of the proposed method is that it allows for different types of variables, i.e., numerical and categorical, integer and real.

3.2 Monitoring Interface Setting

The monitoring interface was designed to be a user-friendly tool and was coded in Python, using the Scikit-learn library (Pedregosa et al. 2011). The interface is expected to perform several activities, as illustrated in Figure 3.

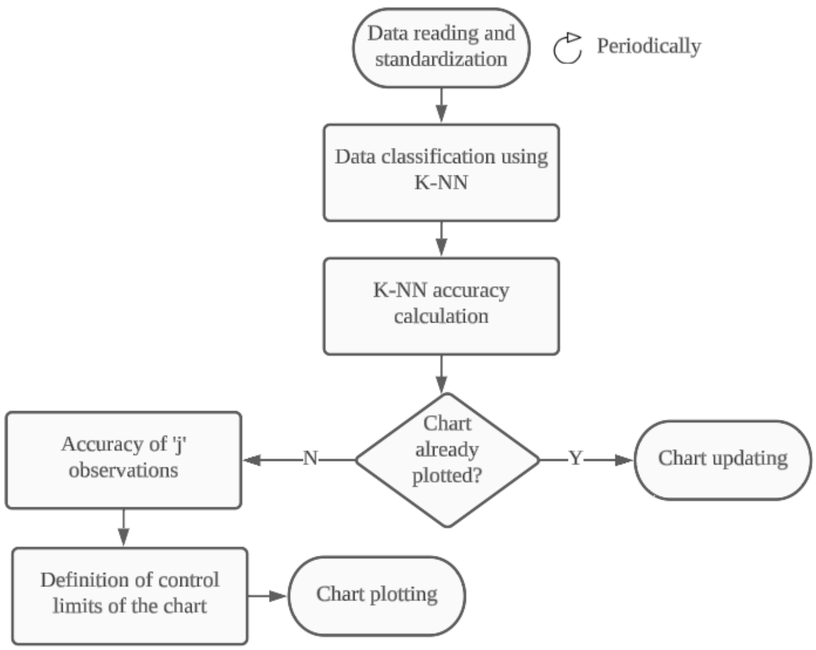

Figure 3: Activities performed by the monitoring interface.

Firstly, physical and virtual data are collected, and before being classified, they are standardized using the Robust Scaler method (Raju et al. 2020). The K-NN is then trained using the dataset, and for this purpose, the optimal value of 'K' is defined using the cross-validation method, as suggested by (Zhang et al. 2021). Once trained, the K-NN will attempt to separate the data from physical and virtual environments. In this case, if the model data is perfectly realistic, the K-NN will not be able to identify which data is from the model and which is from the physical system, and will then classify each observation randomly (accuracy of around 50%). However, if the DT data is not realistic, the classifier may easily separate them from the data of physical systems (accuracy of around 100%). In other words, the accuracy of the K-NN increases as the DT model becomes invalid.

It is worth noting that the classifier training and accuracy calculations are carried out using data samples of size n=100 (including data from both the physical and virtual environments). Considering a p-chart, the central line (CL) of the graph refers to the proportion 'p' of an evaluated characteristic. In this case, the value of 'p' was considered as 0.5 for the proposed approach, since it refers to the K-NN accuracy target. In other words, it is expected precision to vary around 0.5 (CL) on the control chart. We also set the distance (L) of the control limits from the center line of 3 standard deviations, and the magnitude of the process shift (δ) of 0.15 (to guarantee the accreditation of the DT). In this way, it was obtained n = 100. This value was defined through the equation 2, proposed by Montgomery (2009).

$$n = \left(\frac{L}{\delta}\right)^2 p(1-p) \tag{2}$$

Once the K-NN accuracy is obtained, the *p*-chart is built (with the first '*j*' observations, and in this work, '*j*' was adopted as 25, as suggested by Montgomery (2009). Finally, after the set phase, the *p*-chart will be updated with K-NN accuracy over time, as described in the next section. The entire process described is cyclical and periodic.

3.3 Periodic Monitoring

Periodic monitoring is the primary objective of the proposed approach. Different from traditional simulation validation, the goal is not to ensure model accuracy during the model building phase, but rather its accreditation over time as a DT. In this case, it is important to define some issues, such as the monitoring frequency and actions considering potential issues with the DT models.

On one hand, the definition of the monitoring frequency does not depend on the characteristics of the DT. Given the ease of data collection when considering the operation of simulation models as DT, monitoring should be conducted as the monitoring sample size (n=100) is reached. In other words, data is collected continuously, and each time the monitoring sample size is reached, the monitoring process described in Figure 3 is carried out again, forming a cyclical process. It is important to highlight that the frequency of this monitoring process depends on the characteristics of the DT, such as the synchronization level, update intervals, number of evaluation variables, etc.

On the other hand, when considering actions in the face of potential DT issues, it is important to note that the proposed tool aims to indicate when the model does not behave as expected but does not act to fix the system's errors. This is because, in cases where the model is not valid, problems beyond the model may occur, such as failures in physical systems or communication interruptions. In this case, it is up to decision-makers to assess and correct any issues that may arise. Figure 4 illustrates the proposed approach architecture and more details about the monitoring tool and its main characteristics can be found in the works Santos et al. (2023) and Santos et al. (2024). It is possible to observe in Figure 4 that data from both physical and virtual systems are periodically collected (evaluation variables) to input the K-NN, which tries to differentiate the data. Then, the K-NN accuracy (proportion) will input the *p*-chart.

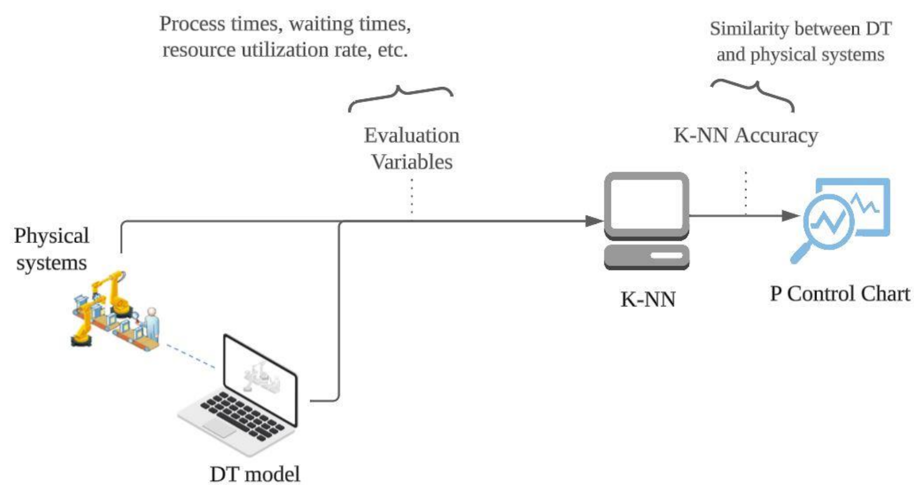

Figure 4: Proposed approach architecture.

4 APPLICATION

The proposed approach was initially implemented in theoretical cases to demonstrate its applicability. In this regard, the behavior of the monitoring tool was assessed when subjected to special causes that would impact the results of a DT model. Subsequently, the monitoring tool was adopted in a real-world case study.

In this sense, the aim was to complement the DT with an auxiliary supplement that allows for monitoring of its results over time, ensuring its accreditation and bringing robustness to decision-making processes.

4.1 Theoretical Cases

Data were emulated referring to both physical and virtual environments. In this scenario, two theoretical cases were emulated considering standard statistical distributions. In other words, samples were created in order to represent both physical and virtual systems data and, in this case, these samples were designed to fit standard statistical distributions. Moreover, the authors followed the proposed three stages for each case: selecting the evaluation variables, monitoring interface setting, and periodic monitoring. We opted for a simpler case (using a lognormal distribution) and a more complex case (multivariate normal distribution), justified by their common usage in simulation projects. Table 1 presents the adopted distribution parameters.

Table 1: Parameters of the distributions adopted in the theoretical cases.

Case	Standard distribution	Parameters
I	Lognormal	*Location* = 0 and *Scale* = 1
II	Multivariate Normal (3 variables)	*Means* = [60, 500, 40] and *Covariance matrix* = [[9, 60, 20], [60, 1600, 350], [20, 350, 100]]

About 100 observations with a sample size of 100 were emulated for each case, representing data collected over time from both the physical and virtual environments. In other words, each sample had 50 lines representing physical systems data and 50 lines representing virtual systems data. In this scenario, the data were stored in different databases for input into the monitoring interface. For Case I, the dataset has one data column representing a single evaluation parameter ("x"), while in Case II, we have three data columns representing three evaluation parameters ("x_1," "x_2," and "x_3").

For both theoretical cases, a special cause (10% variation) was induced in observation No. 50 (only in the dataset representing data from the physical system) to evaluate the performance of the monitoring tool in identifying such a cause. It is important to note that a 10% difference between the physical and virtual environments is generally considered common in simulation projects. However, considering that using simulation as a DT is associated with high-impact decisions, it is important to monitor its operation and identify signals that may be causing such variation. Figures 5 and 6 present the control charts for Cases I and II, respectively.

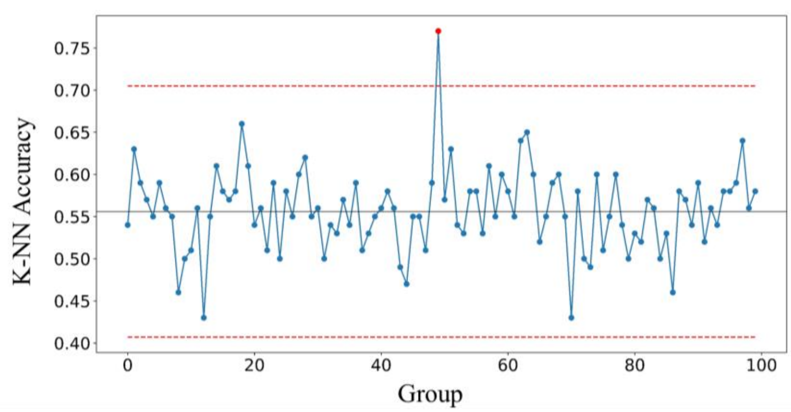

Figure 5: Case I control chart.

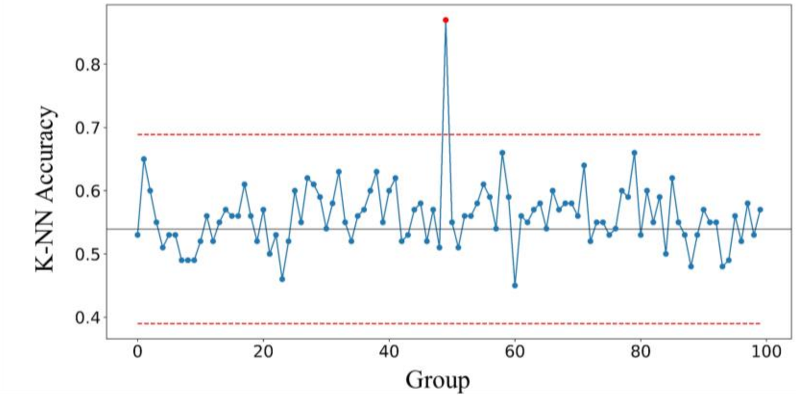

Figure 6: Case II control chart.

It is noted that, for both cases, the monitoring interface works as expected. Initially, the average K-NN accuracies for both cases represent a valid DT, demonstrating that the classifier can identify the similarity between what would be the virtual and physical data. Furthermore, considering a slight variation in the dataset representing the physical data (observation No. 50), the classifier identified this special cause, as shown by the out-of-control signal on both charts. The same analysis was carried out 1000 times maintaining the special cause and we noted a special cause in about 97% of the control charts.

4.2 Real Case Study

When considering an automated production line, ensuring the proper functioning of all equipment and systems is crucial. In this context, the selected DT is based on a DES model and focuses on monitoring a production cell. This cell has a simple structure, with two workstations manufacturing two types of products, across three shifts. Initially, raw materials arrive at the arrival area (A) and are dispatched to the supply areas (B and D), which provide raw materials to the workstations (C and E), respectively. An automated conveyor carries out transportation between areas, and movement between these areas and the workstations is facilitated by robotic arms (R1 and R2). The workstations are automated by computer numerical control (CNC). Figure 7 illustrates the production flow of the cell and its 3D simulation model, which was modeled in FlexSim®.

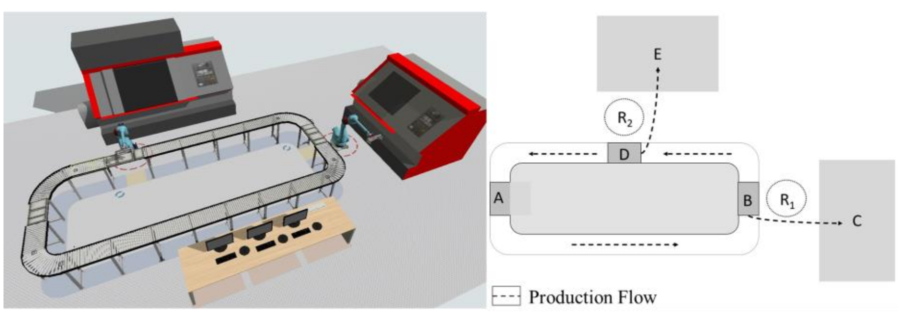

Figure 7: Production line and its 3D DES model (Real case study).

According to Santos et al. (2022), the use of virtual models to monitor production systems and evaluate metrics during their operation is one of the main applications of simulation models as DTs. In this case, the model was designed to support the production cell through key performance indicators (KPIs), such as total lead time, downtime, production rate, and overall equipment effectiveness. Process data is collected in real-time through sensors and intelligent systems and stored in the local database. Information regarding work-in-progress (WIP) products is used to update the DES model in near-real-time with a few minutes delay, mirroring the cell in a virtual environment and allowing comparison between expected and real behavior. According to the literature, near-real-time approaches can be considered a DT and the synchronization delay must be smaller than the decision-making intervals (Santos et al. 2021).

In this case, we have a non-autonomous approach since the DT is used to evaluate the process but not to infer about it. Additionally, a decision dashboard was also adopted to enable integration between the DES model and physical systems. Figure 8 illustrates the architecture of the analyzed DT.

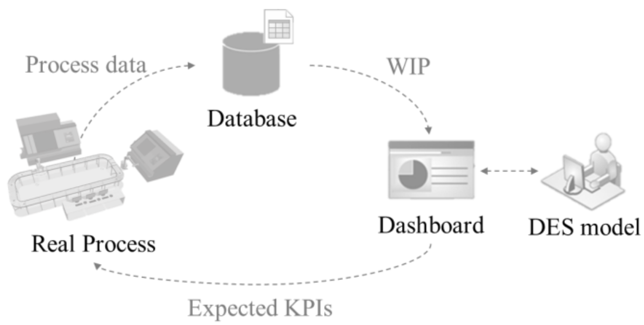

Figure 8: DT architecture (Real case study).

The three steps of the proposed approach were applied: the evaluation variables were selected, the monitoring tool was developed, and finally, periodic evaluation of the DT was possible. Regarding the selection of evaluation variables, Waiting Times and Processing Times for each product were chosen, considering both workstations C and E (totaling four variables). These variables were continuously collected by sensors and intelligent systems (physical system data), and the DES model periodically provided the same information (virtual system data).

The average demand of the production cell (per shift) is around 110 items (including the two types of products produced), and the monitoring tool was planned to collect data from both the physical and virtual environments in samples of 50 during the working day, totaling datasets of size n=100. The monitoring tool was updated with each sampling, and the entire process described in section 3 was carried out periodically. For this work, observations from about 50 shifts were recorded, and the first 25 observations were used to define the control chart limits, while the remaining observations were used in the monitoring process. It is important to highlight that 50 shifts were considered for this experiment, but the tool is prepared to continuously monitor the process over time. Figure 9 shows the control chart considering the described period.

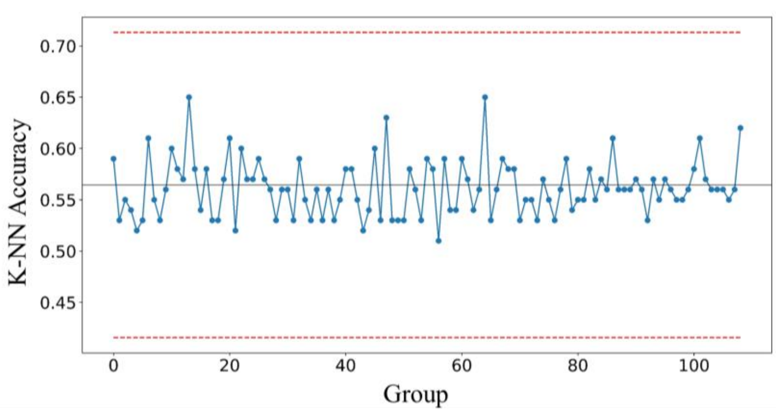

Figure 9: Real case study control chart.

Similarly to the theoretical cases, it was observed that the monitoring tool functioned as expected. The monitoring tool was able to compare the physical and virtual environments and identify their similarity, as indicated by the average K-NN accuracy. The tool indicated a valid model, aligning with expectations since no special cause was induced and the process was operating under control.

5 CONCLUSIONS

Despite the wide applicability of simulation-based DTs for decision support, the operation of the simulation model should be monitored over time to ensure its accreditation during its use as a DT. This is especially important because DT-based decisions often have a significant impact on the systems in which they are implemented. However, the authors identified a lack of work in the literature with this purpose. Thus, this work proposed an approach based on Machine Learning and control charts to enable the evaluation of simulation models during their operational phase as DTs.

More specifically, the K-NN classifier was used to compare the virtual model with the physical systems, and through the *p*-control chart, it was possible to monitor the accreditation of the model over time. The proposed approach is based on three main stages, starting with the selection of evaluation variables to be monitored. Then, there is the stage of monitoring interface set, which compares the data from physical systems with the model data, and based on the K-NN accuracy, it is possible to infer the validity of the simulation model. In this case, this accuracy is plotted on the *p*-control chart over time to allow monitoring of the model's accreditation.

Finally, the last stage of the approach corresponds to periodic monitoring. The proposed tool was tested in theoretical and real-world case studies. It is concluded from the results the versatility and flexibility of the proposed approach, being compatible with different DTs, encompassing models that operate in real-time/near real-time and with different characteristics of connection, integration, and complexity. In this case, with just one parameter (the K-NN accuracy), which is plotted on the *p*-chart, the decision-maker can quickly assess the DT accreditation through several evaluation variables (with different characteristics).

ACKNOWLEDGMENTS

The authors would like to express their gratitude to CNPq, CAPES, and FAPEMIG for their support throughout this research.

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