IEEE Access
Multidisciplinary : Rapid Review : Open Access Journal

Received 8 September 2023, accepted 1 October 2023, date of publication 9 October 2023, date of current version 16 October 2023.

Digital Object Identifier 10.1109/ACCESS.2023.3322926

RESEARCH ARTICLE

Model-Based Simulation Framework for Digital Twins in the Process Industry

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This work was supported by the European Union's Horizon 2020 Program through the Project Energy-aware Factory Analytics for Process Industries (FACTLOG) under Grant H2020-869951.

ABSTRACT A process modelling and simulation theoretical framework of general use for the study of continuous process industrial systems is introduced. The proposed process modelling methodology is based on Material Flow Networks and is implemented on a Process Simulation Modelling Tool developed for this purpose. The tool introduced can also serve the requirements arising for online use of the models as digital shadows of the physical systems, in the context of digital twinning the process industry. The implemented models in conjunction with tools from other scientific fields can be used for monitoring, root cause analysis, performance optimization, limitation and recovery of the behaviour of systems. An application example of the proposed methodology is provided and useful conclusions arise. Finally, extensions of the proposed method and potential challenges are discussed.

INDEX TERMS Analytics, continuous process systems, digital twins, industrial systems, Industry 4.0, Internet of Things, material flow network, optimization, process modelling, simulation.

I. INTRODUCTION

The main target of the current research is to introduce a formal methodology of general use for the development and operation of complex models of continuous process industrial units through an analytically defined procedure. Process modelling and simulation comprise a valuable tool for studying systems from a variety of areas. The latest advances on scientific domains such as Industry 4.0, Analytics, Big Data Management, Internet of Things and Sensors extend the modelling power and the possible fields of application of process modelling and simulation in the context of Digital Twins (DT). In this context the process models are not considered any more as a passive tool that is exclusively for what-if analysis but become a valuable part of any system, which through efficient infrastructures and algorithms can monitor, mirror the dynamic state of the system (or of certain components of it) and control its behaviour through the realization of certain actions.

The associate editor coordinating the review of this manuscript and approving it for publication was Chaitanya U. Kshirsagar.

The proposed method has been developed in tandem to the one introduced in [1] that refers to the construction and operation of dynamic process models of discrete industrial systems. However, because of the different characteristics and behaviour in general of continuous process industrial models, the methodology has been customized with respect to them and is introduced as a completely independent methodology in the current work. This broadens the applicability of the previously proposed method, providing a general, easily adaptable framework in the context of Digital twins, for modeling, monitoring, study and management of industrial systems.

A. CONTRIBUTION

In summary, the most important contribution of the current work are the following the following:

1. Introduces a generic step-by-step continuous process modeling and simulation methodology following a number of well-defined steps.
2. Defines the necessary data sets, their role and their utilization in the implementation of the above methodology.

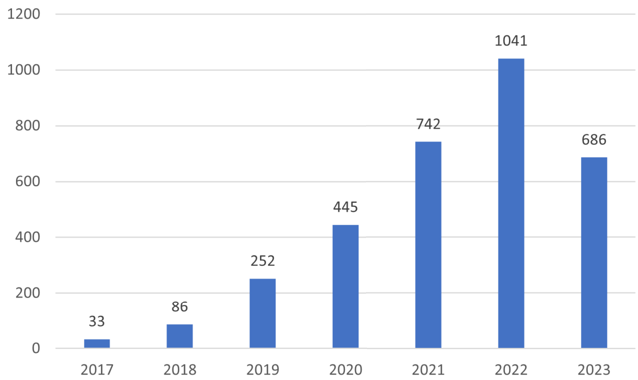

FIGURE 1. **Publication trend on process modelling and digital twins.**

3. Describes the interactions with tools and algorithms from other fields, such as Analytics and Optimization.
4. Enables the operation of the constructed models not only offline as most modelling and simulation tools and methods but also online with the respective physical system, through the provided Application Programming Interface (API).
5. Introduces a process modelling and simulation tool that enables the development of process models with different levels of detail, their execution and the calculation of KPIs and output parameter values.

B. STRUCTURE

The rest of the paper is organized as follows: Section II presents an overview of the main concepts behind process modelling and simulation, the fundamentals of Digital Twins, the advanced capabilities arising from the implementation and operation of process models within the context of DTs as well as the main principles of Material Flow Networks (MFNs) which have been adapted in the developed Process Modelling Simulator. Section III discusses the role of process modelling and introduces the scope, the assumptions and the steps composing the proposed process modelling procedure. Section IV describes the process modelling and simulation Tool and the corresponding API. Section V displays the application of the previously presented methodology in the development, operation and evaluation of models in a production scenario of a continuous chemical system. Finally, Section VI concludes the paper and discusses open issues, future steps and challenges.

II. RELATIVE LITERATURE

A. PROCESS MODELLING AND SIMULATION

Advances in fields like Internet of Things (IoT), Cyber-Physical Systems (CPS), Industry 4.0, Big-Data analytics, and hardware (especially sensors), have enabled the application of DT paradigm in a number of fields and for a variety of purposes. Among these fields, process modelling and simulation have received increased interest from the research community within the concept of Digital Twins.

In Figure 1 the number of publications per year (trend) for articles found under the query "Digital Twins" AND "Process Modelling OR Simulation" from the Scopus database, is presented. This bar-chart shows a high increase in the number of manuscripts, especially after 2019 (252 publications) until 2022 (1.041 publications) where the maximum number of relative to the query manuscripts is met. The same trend continues in 2023, where there are already 686 publications although there are 4 more months left. Between the years 2019 and 2022 the number of query results are almost doubled per year while in the year 2023 this increase is almost 40%. This illustrates the increased interest of several researchers for Digital Twins and Process modelling and Simulation.

Process models are popular tools for improving the understanding of a system and of facts, events, and behaviors taking place in it and also for testing the effects of changes and disturbances from applying alternative strategies and corrective actions in its operation and efficiency. For this reason, representation of system characteristics is attempted, tested and validated while the detection of not obvious mechanisms that govern its behavior and performance comprises one major challenge. Some of the most popular application fields that process modelling and simulation can play an active role, include smart industries, resource efficiency optimization, predictive maintenance, supply chain optimization as well as anomaly detection. Further applications, challenges, categorizations and details on the specific topic can be found in survey papers [2], [3], [4].

System modelling and efficiency optimization first of all has to do with the characteristics that will be studied as well as with the metrics that will be used for its performance evaluation. A model has to be realistic without having unnecessary complexity, and that's why only critical variables that govern its behavior are defined and studied. Three components enable the above particularly the model, the simulator and the experimental frame.

A model is a quantitative expression of system's static characteristics and dynamic parameters that is necessary in order to calculate results comparable to real world data. Typically, a model consists of a set of interacting entities involved in its operation whose behavior is limited to a (finite or not) set of states in which the physical system can be driven through the appearance of system's internal and/or external, scheduled and/or random, controllable and/or uncontrollable events.

Simulators are agents that imitate the system and entities response and operation from the continuous update of the defined critical variables.

The experimental frame describes the specification of the conditions and state under which the system is observed. During scenario simulation, system-wide as well as local (between process units) model flows are calculated. Simulation is performed for understanding the behaviour of the system, for testing the effects of parameter values changes or of changes in event sequences, for testing possible limitations in the operations of the system and finally for aiding decision making through alternative strategies evaluation.

This work is the first attempt, according to the author's knowledge, to introduce a generic step by step methodology for building and operating a process model of a realistic continuous system in the context of Digital Twins. An analytical methodology as well as the necessary input data are defined and the application of the produced process models online with the real system, far beyond the traditional process modelling and simulation scopes is enabled, in order to monitor and dynamically manage the behavior of a system and evaluate its performance.

In the literature there is a limited number of studies regarding process modelling and simulation of realistic continuous systems in the context of Digital Twins. The majority of these methods are application specific (e.g. [5] that refers to a digital twin of a continuous direct compression line for solid drug product and process design) or focus on subjects considerably different from the ones presented in the current work (such as application of machine learning methods, process planning, performance monitoring, failure detection etc). Some representative such works are presented in this section.

In [6] authors study the literature related to the implementation challenges of Digital Twins in apparel manufacturing industries. Then they introduce a discrete evet-based methodology for implementation of such DTs in a multi-stage sequential production procedure applied to the case of a shirt factory. The proposed method is rather non-detailed and the input, output types are not defined explicitly, while KPIs considered are limited. In [7] authors introduce a multidimensional modeling framework for machining processes (dimensions have to do with different models used in several stages of the machining products lifecycle), to improve processing performance. This method is considerably different from the approach proposed in the current work as it is mainly applied to machining processes with completely different characteristics from the ones of the processes considered here. In [8] authors propose a semi-automated methodology to generate digital twins for process plants using available P&ID engineering documents. They mainly focus on the construction of the model using a number of software tools and not on it's application online with the physical system.

B. DIGITAL TWINS

Probably the first operational Digital twin can be identified in NASA's Apollo program where mirrored systems were used to monitor the behaviour of unreachable objects and find solutions to problems they faced using tools from the field of simulation and analysis. The term Digital Twins (DT) was introduced in 1997 at [9] for the production of 3D digital models of civil engineering designs and the way these overcome drawbacks inherent to the conventional design process. However, real attention was given in digital twins on 2002 by Michael Grieves, during an industrial presentation at University of Michigan Executive Course on Product Lifecycle Management [10]. DTs are also closely related and share many common features with the rather early introduced Cyber Physical Systems (CPS), that have been described as multidisciplinary systems used to conduct feedback control on widely distributed embedded computing systems by the combination of computation, communication and control technologies [11].

DTs have become extremely popular the last 3-4 years with a large volume of publications on this field and rather less practical applications. According to one of the most explanatory definitions for DTs met in literature "a DT is a comprehensive software representation of an individual Physical Object". It includes the properties, conditions, and behaviour(s) of the real-life object through models and data. A DT is a set of realistic models that can simulate an object's behaviour in the deployed environment. The DT represents and reflects its physical twin and remains its virtual counterpart across the object's entire lifecycle [12]. Survey on definitions, characteristics, applications, design implications, open issues and challenges of digital twins can be found in [13]. In [14] authors conduct a bibliometric study on the 100 most cited articles in digital twin domain in smart manufacturing in order to detect the main research directions, limitations and challenges concerning digital twins in the examined field. DT applications can be met in a variety of fields including Manufacturing, Aviation, Energy, Smart Cities, Industry, Telecommunications, Buildings, Healthcare, Vessels, Asset management, Lifecycle management, Traffic management, Project management, Education and study of human behaviour and its interaction with the environment. A survey on the application of Digital Twins in 13 different industrial sectors is presented in [15] while in [16] the authors studied the scholarly literature of digital twin research using a scientometrix approach.

The main field of interest of the current research concerns applications of Digital Twins in process industries where the applications are still limited. In [17] the authors study relative literature in an attempt to detect the barriers and the enablers of the implementation of DTs in process industry as well as the relationships between them. In [18] and [19] a semi-automatic methodology for generating a steady state digital twin of a brownfield plant is proposed and validated through a water process plant case study while in [20] the authors demonstrate the development and application of a DT for process simulation and production scheduling of a food processing industry. Finally, [21] presents an overview of different aspects of the current status of DT application in stages of Pharmaceutical and Biopharmaceutical Manufacturing.

C. PROCESS MODELLING AND SIMULATION WITHIN THE CONCEPT OF DIGITAL TWINS

Process models comprise a popular tool for engineering system analysis, design, and control development, as they enable virtual experiments that provide realistic results for evaluation when physical experimentation is not applicable [22].

The advanced capabilities arising from Industry 4.0, Sensors and Internet of Things extend the usability of the process models that now can be used online with the modelled physical system as part of a digital twin. In this case the current state of the system can continually be updated with incoming data from the operating environment (through sensors or data feeds) to monitor and mirror the current status and evaluate its performance. Through the projection of the current state of the system, a process model can be efficient in predicting the upcoming behaviour of a physical system in conjunction with tools from other fields including big data management, analytics, artificial intelligence and optimization techniques in quasi real time. This operational extension combined with the advanced capabilities of sensors and actuators create an interactive bidirectional relationship between process models and the physical system, as they become a tool for modifying systems future behaviour [23]. According to [24] regarding DT process models, three categories are met in literature and in particular, (a) creation of DTs, (b) synchronization between physical and digital assets, and (c) operationalization of the DT. In [8] authors introduce a methodology and implement the necessary tools and software for extracting required process information, for generating a steady state simulation model and creating a digital twin for a paper process system. From the analysis provided, it becomes evident why process models in the context of DTs are a crucial factor and a key trend in realization of intelligent industrial system process management [25].

D. MATERIAL FLOW NETWORKS

Industrial processes can be distinguished in two general categories; discrete and continuous. Continuous industrial processes do not have stationary behaviour, are time-varying, display non-linear and dynamic properties and are functioning at diverse operating points. These characteristics are taken into account during system design, monitoring and control. Since such processes have a wide range of operating conditions, it is very important to consider data models and exploit specific features from all available measurements [26]. Thus, modelling of continuous systems, has been proven quite complicated and in the past sometimes process modelling was often regarded as ''more art than science'' or ''more art than engineering'' [27]. The accumulated experience and knowledge from the various system models developed and used has been insightful to provide a set of rules that helps engineers and researchers develop process models of continuous systems.In order to create a process model that will successfully serve its intended purpose, one has to fully understand the modelling goal(s) as well as the effects of those goals on the process model together with the required elements of the model, i.e. the model equations and any starting and terminating conditions.

In order to represent and interpret the material and energy flows in a particular process industry, it makes sense to base such analysis on business accounting methods. Material Flow Networks approach can be considered as an accounting system, in which instead of financial flows, material and energy flows are considered [28] and has been initially developed at the University of Hamburg [29]. Material flow models have been applied in industrial material flow management, for structured data assessment and visualization of optimization potentials [30]. This approach requires the inclusion of energy and material stocks in order to be possible to track the material and energy flows and stocks within a company or between different companies within a value chain [31], [32].

MFNs is a graphical modelling notation based on the Petri-Net (PN) formalism (which is summarized in [33]) that describes the material flow of a single or a selection of multiple products or components within plants [34]. A material flow network, for a given time period, can be implemented by adding all used process units and connecting all pairs of these, between which, raw or semi processed materials are transferred [Forecasting Changes in Material Flow Networks with Stochastic Block Models]. The main structural elements (building blocks) of a PN are places, transitions and connecting arcs. Analogy of these elements to MFNs is implemented by considering that:

- The locations where material and energy transformations are taking place are equivalent to the transitions on a PN.
- Storage locations and connections without material transformation are equivalent to the PN places.
- The material and energy flows are equivalent to the arcs connecting places to transitions and transitions to places in the PN.

III. PROPOSED METHODOLOGY

In this part of the manuscript the framework of process modeling and simulation is described and then the respective general use methodology is introduced. Initially the application of the methodology for model building and operation is presented and its interactions (through data exchange) with tools from other scientific fields are defined. In addition, the types and the exact categories of the necessary input data as well as the outcomes from the scenario simulations using the implemented process models are defined. The main target of this part is to explain the prerequisites, the steps that should be followed for the construction of the process model and the outputs arising from its simulation online with the real system and in relation with tools from other fields that also operate in real time and in parallel to the system.

A. DESCRIPTION OF PROCESS MODELLING AND SIMULATION ROLE

Process Simulation and Modelling (PSM) denotes a generic field with all related methods, algorithms, mechanisms, services and tools, integrated into an overall approach. According to the proposed approach, PSM interconnects and interacts with external Analytics, Optimisation, Machine Learning and other tools in order to manage the current states and the desired behaviour of the cyber and the physical system under a certain scenario. Figure 2 outlines the data and information exchange between the physical system and its digital shadow as well as the data transformations and actions performed in a DT enabling actions from the cyber to the physical system. In particular, the specified data are transferred from the physical system to the data management module of the digital shadow. In this, data are cleansed, stored, classified according to specifications and then appropriately selected, combined and formatted. The cognition procedure that follows, utilizes techniques and algorithms from the fields of Analytics, Process Modelling & Simulation and Optimization in order among others to define the strategy that should be followed, produce schedules, calculate Key Performance Indicators (KPIs), make predictions, define the values of specific parameters and for reasoning purposes. The calculated outcomes are utilized directly from the Digital Shadow and indirectly from the physical system in the form of corrective actions and supporting information streams.

The interactions between PSM and Analytics refer to the estimation of KPIs for assessing (*a*) the performance of the current system (or process-by-process), either at regular intervals or upon request, and/or (*b*) the performance of a simulated scenario. In addition analytics provide forecasted data streams to be simulated and approach the characteristics (durations and appearances) especially of uncontrollable and unpredictable events using statistical and AI tools. Upon an anomaly is detected, PSM can either verify or refine (or both) this inference running a scenario regarding the current state of the system in isolation from the digital shadow, in order to evaluate what-if scenarios. Such scenarios may refer to (i) partially modified data streams starting from system's current state, (ii) in the past to retrace the system's behavioural history, or (iii) in the future to calculate results, predict outcomes and evaluate alternative actions and strategies. In the case of optimization service, there is a repeated interchange of data, where PSM produces alternative scenarios, provides them to optimization for evaluation and according to the results may receive feedback for further scenario creation. The most important cognition related roles of process models are to operate as Dynamic Digital Shadows in parallel with the physical system, to support AI inference, to help efficiency evaluation, to represent interacting entities and to manage the systemic knowledge taking into consideration the data, the states of the interacting entities and their behaviour [35].

B. CONTINUOUS PROCESS MODELLING AND SCENARIO DEFINITION METHODOLOGY

Physical and/or chemical processes are mainly taking place in a continuous industrial system. Modelling of such a system

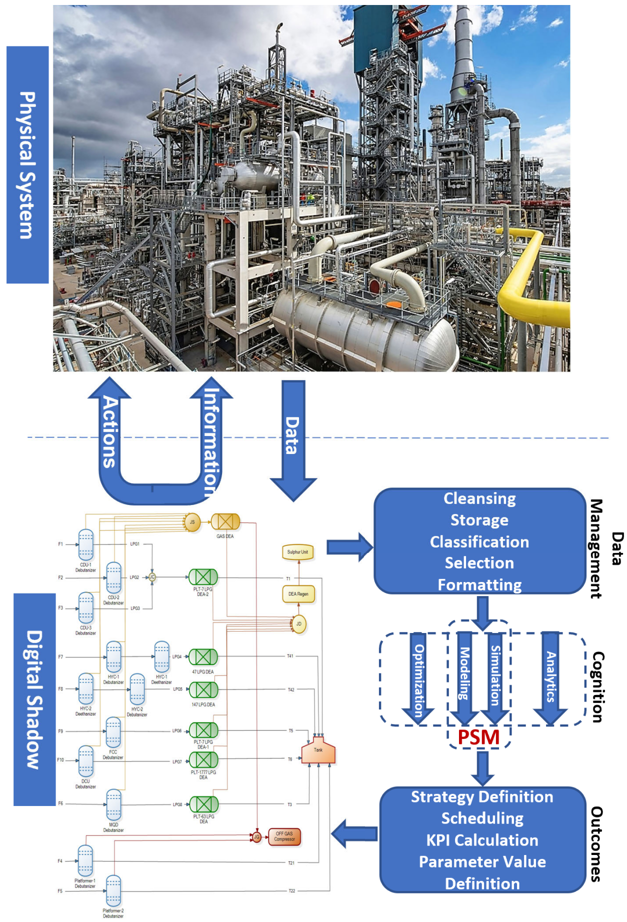

FIGURE 2. Physical system - digital shadow communication and services interoperation.

can be considered in different scales, from a whole process plant and its environment, or limited to a specific part of the plant, or even a specific operating unit or equipment. Hence, the inputs, outputs, the physio-chemical processes taking place in it and the boundaries of the system have to be clear and concise. The most popular way to model continuous process systems is by the use of a flowsheet, since information regarding the operating units and their internal connections and interactions are usually available beforehand.

In order to create efficient and useful models a step-by-step modelling and simulation approach is introduced. The development of generic modelling frameworks is common in literature and is applicable to a variety of systems with partially common characteristics that share a common number of features and operations. Development of generic frameworks enables the reuse of the developed models (especially when modular models of system entities have been developed), composition of the developed models following a well-defined procedure in order to model and study complex systems, easiness of simulation of the developed models and definition and calculation of a number of local or global KPIs through simulation [36].

An example of generally developed simulation frameworks includes [36], where a framework using Component-based Model Driven Approach is used to promote rapid development and effective reuse of developed models. In [37], authors introduce agent-based modeling framework for developing agent-based simulation models of energy business ecosystems and apply the proposed framework to demonstrate how an ecosystem with several actors and objects can be translated into an agent-based simulation model. Finally, in [6] authors introduce a methodology for applying Digital Twin (DT) technology in apparel manufacturing plants following certain steps, with primary goal the conduction of dynamic simulations to reduce bottleneck operations. Generally, in apparel industries, line balancing is crucial for maximizing efficiency and reducing labor costs.

Modelling is inherently an iterative process, and some or all of those steps may be repeated in order to resolve problems or incorporate potential changes and alternatives. Assuming that the problems features and parameters have been defined in detail (physical process, modelling goal(s) and validation criteria) the guidelines are elaborated in a structured way depicted in the flowchart introduced in Figure 3. These instructions when followed can guide the interested stakeholder to create a flexible, measurable and efficient process model of a continuous industrial system, that can be used online with a physical system or offline for what-if analysis, root cause analysis and comparative evaluation of alternative designs or decision making strategies. In the second case, step 8 of the introduced methodology is not mandatory. The main steps of this methodology and the procedures performed in each step are the following:

1. **Define the System**: During system definition, a refinement of the described system as well as the modelling goal(s) takes place. Additionally, inputs and outputs of the model, hierarchy, spatial distribution, range and accuracy and time characteristics are solidified.
2. **Identify controlling factors and mechanisms**: The physical/chemical process being modelled is identified and studied in relation to the modelling goal(s). Some indicative controlling factors in process modelling are chemical reactions, mass diffusion, heat conduction, heat transfer and material flow.
3. **Evaluate data**: Usually models of industrial process systems are a combination of first-principles and data-driven models, so process data or estimated values are required. These data need to be cleansed, organized and evaluated in order to be meaningful.
4. **Develop the model**: The models are based either on first-principles, corresponding to conservation balances (e.g. heat and mass balances), chemical reactions, etc. corresponding to the physical process being modelled or on historical data. Ideally the combination of historical data and some principal equations create the most accurate models, which are called hybrid models.
5. **Select solution methodology**: The procedure to solve the mathematical models need to be established and implemented carefully in order to avoid high complexity problems and to lead towards the simplest and fastest solution possible.

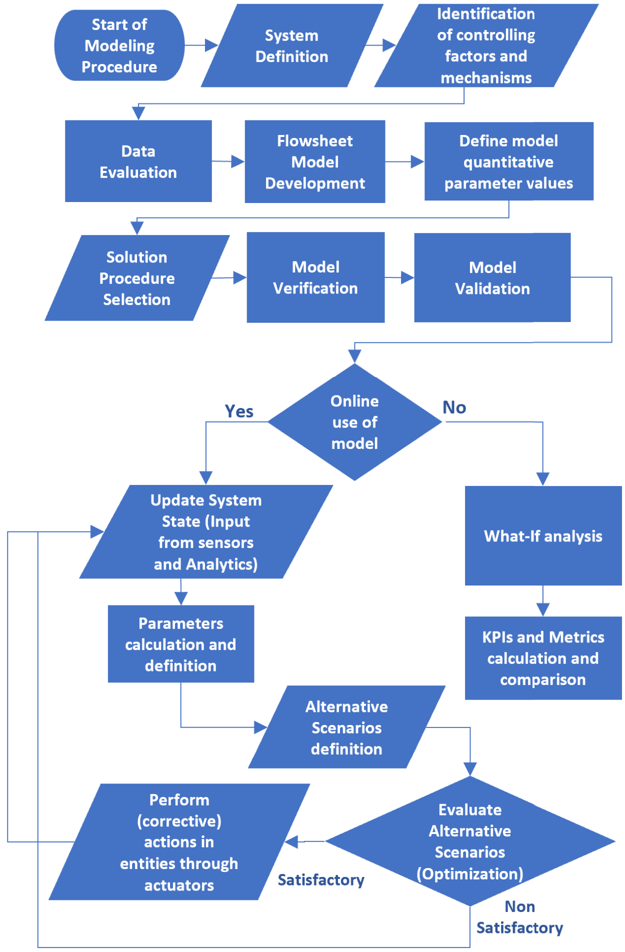

FIGURE 3. Model building and operation procedure.

6. **Verify model**: At this point the model needs to be verified that it is behaving as intended and has been implemented correctly.
7. **Validate model**: When the model is ready it's time to validate it against reality. The most common ways to validate a model are experimental validation, comparison between model and physical process, comparison between models solving a common problem or even direct comparison with process data.
8. **Utilize associate tools and algorithms output data**: At this stage addition of extra information and definition of additional parameters' values in order tof define more realistic scenarios takes place. Such input data, mainly comprise of output results from associate tools and algorithms (processed data from real-time Analytics, Optimization, Machine Learning).

In order to implement the above described process modelling methodology, 3 main data sets are required:

(a) System static data (structural)

Initially, the structure of the model has to be defined. The main target is to represent the entities from which the physical system is composed as well as their physical connections and interactions and to define the channels for the exchange of resources and information between them. These data are static and not updated frequently (this can happen when machines are added or removed from the system). The most common categories of such data, with respect to their role, include (but are not limited to) the following: i) Industrial system structure data. These include the available resources of the physical system, possible categories (families) and their capacities. Physical connections (permanent or product specific) between resources are also necessary in order to construct the structure and to define the type of the system under study (e.g., production line, job shop, continuous flow process production system, and continuous flow assembly production system) as the simulation algorithm makes use of this characteristic. To obtain these types of information, flow charts and non-structured data can be used as well as knowledge graphs that provide a collection of interlinked descriptions of the entities of the industrial system. ii) Product-related static data. Products belong to families with similar or partially common characteristics (setup durations, tools and resources used, specifications and physical or chemical characteristics, etc.). Also, setup times and types (e.g. sequence dependent, family dependent etc.) and ideal production times of all possible products in each processing unit must be defined. Finally, if ancillary equipment is considered, data concerning its use should be provided (for example, speeds and transfer capacities of cranes for moving parts between resources and buffers). iii) Constraints regarding the use of specific subsets of resources for the performance of a subset of jobs. In this category also, priorities between products must be recorded and constraints related to flexibility between production stages, maximum batch sizes, unit operational limits, resource sharing, resource management and control policies followed, etc.

(b) System dynamic data (quantitative parameters)

Quantitative parameters are necessary to represent a specific dynamic situation in the system and define the initial state of the scenario(s) that will be evaluated through simulation. Such dynamic data types comprise the following: i) Industrial system dynamic data that refer to the current states of the resources (if machines are operational or under maintenance), current values of system parameters (temperatures, pressures, etc.), current types of processes performed in each machine (as setup times can be sequence-dependent) and machine availability because of scheduled maintenance activities in the considered time horizon. In addition, if certain resources operate with efficiencies lower than the ideal ones (e.g., for safety or energy consumption reasons), this has to be taken into account in order to define the realistic values of working speeds and process durations. ii) Set of orders under process. This is the most important type of dynamic data as this would be used as input from the optimisation service to define the schedule that will be then simulated (in fact, this is the definition of the specific problem under study every time as the first stage is static and is not repeated generally). Production order set represents the customers' requirements (external or internal according to market needs forecasting) and refers to the types and quantities of products that have to be produced as well as to their due dates. iii) Initial raw materials, in-process products, products, tools and other material inventories. This refers to the initial levels of internal buffers of the system as well as in process products in the processing units and is used to define some additional operational constraints that have to be taken into account to improve the system's efficiency, as resource idleness may increase in other cases. In addition, raw materials quality is taken into account as specific parameters of the industrial system's operation have to be specified according to this (for example, in a chemical plant the quality of the raw materials affects operational parameters such as temperatures and pressures).

(c) Associate tools and algorithms output data

The third stage refers to adding extra information and defining the values of additional parameters to the model whose initial state has been defined through associate tools and algorithms. They are necessary to describe the scenario(s) under study and make them even more realistic. The main types of such data are: i) Optimisation output. In the case of Continuous process industries based on historical data from units, models are created, and their behaviour is described. Process modelling and Simulation service produces a set of alternative operational scenarios with a given step for each operating condition. These scenarios are then transferred to the optimisation module that utilises them to solve the corresponding on-specs recovery problem. Then the alternative scenarios are evaluated, and the dominant one is selected for simulation in order to define the production strategy. Matter of optimal planning also may be the scheduled preventive maintenance activities in the equipment used in the industrial system. ii)Non-scheduled maintenance activities (machine breakdowns) from analytics. Analytics can provide data concerning the appearance of non-scheduled machine breakdowns as well as the duration of their repair in the time horizon of the scenario. Analytics and machine learning models typically use historical data to detect patterns and predict future outcomes when they receive a company's data.

IV. PROCESS SIMULATION MODELLING TOOL

The Process Simulation and Modelling Tool (PSM) has been developed to address modelling and simulation requirements in the process industry, as an extension of the tool initially introduced in [38] and [39]. It has been designed according to the needs and the features of the introduced methodology in order to facilitate its application in realistic continuous industrial systems. PSM Tool enables the parametric definition of models of any complexity, the graphical representation with different detail levels, the bidirectional exchange of data between Process Modelling and Simulation and tools from other fields and the calculation and real time graphical

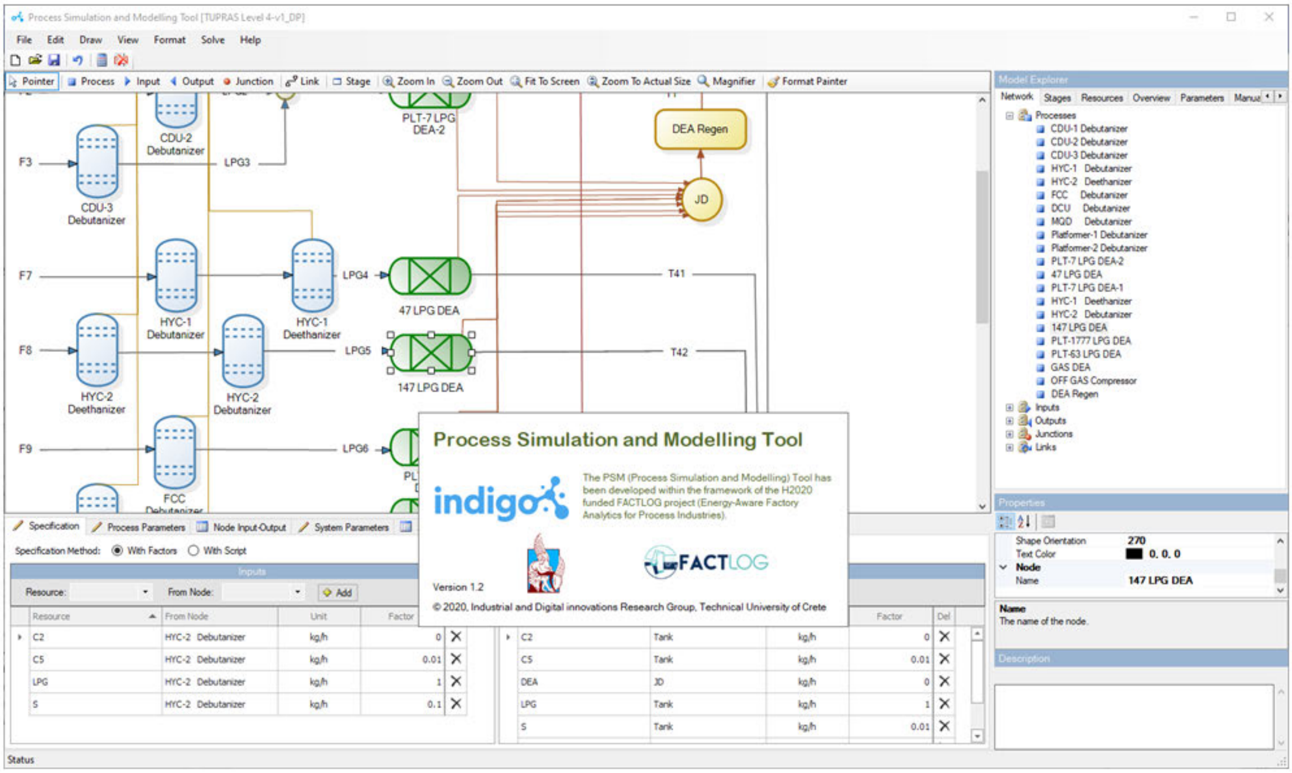

FIGURE 4. PSM tool interface and splash screen.

visualization of the variable values. In addition, the developed tool has already been used by our research team to analyze networks dependencies and assess the system's risk with dependency risk graphs in order to build a security-aware framework for industrial processes [40].

PSM Tool operation is based on the principles of MFN, a domain used to model material and energy flows in production chains, that enables the calculation of estimations regarding associated economical or environmental factors for example, based on the resources consumed or the corresponding emissions. Model entities are organised into a Hierarchical Inheritance Registry that provides prototype reconfigurable building blocks for building any industrial system model. A PSM model describes the procedure of transforming resources, such as raw materials, energy or other inputs into outputs with given specifications. This flow of the aforementioned material characterizes such a system. PSM mainly utilizes two different types of vertices; processes and places:

- Processes correspond to PN transitions. Various materials (input) are converted into new or modified materials (output). Through this processes manage to link material consumption to production.
- Places can be interpreted as storage for resources within the network and can be interpreted as input nodes (sources towards processes), output nodes (targets of processes) and junctions (connecting processes).

Processes and places are connected with links, which represent material flows from a place to a process or vice-versa and can be grouped into stages, in order to consider a bounded part of the model as an individual unit. This is equivalent to modeling capabilities of Hierarchical Petri nets.

The PSM tool (splash screen shown at Figure 4) is developed as a distributed application, including a desktop and a web application. The desktop application is implemented in the *.NET* framework using *C#*. Its core functionalities are (*a*) the design of the model, following a graphical approach, by drawing the elements on a canvas; (*b*) specification of material and energy flows to and from processes as well as interrelations between input and output; (*c*) calculation of the flows system-wide as well as between process units; (*d*) processing units and overall system KPIs calculation; and (*e*) result presentation and reporting not only in tabular format but also in other common formats for further processing.

The desktop application communicates and interacts with the web application back-end through an Application Programming Interface (API) for uploading and processing industry models and scenarios with alternative parameters to the web application. The web application exposes functionality through the API that allows users and/or systems to simulate, monitor in real-time, and modify the operation of a process model on demand. More importantly, it transforms the process model into an active component that can bidirectionally interact with the physical systems. It achieves that by allowing various parameters to be configurable on the process level based on the initial modelling.

The actual value of the PSM API is illustrated by presenting the life-cycle of a model in Figure 5. Initially,

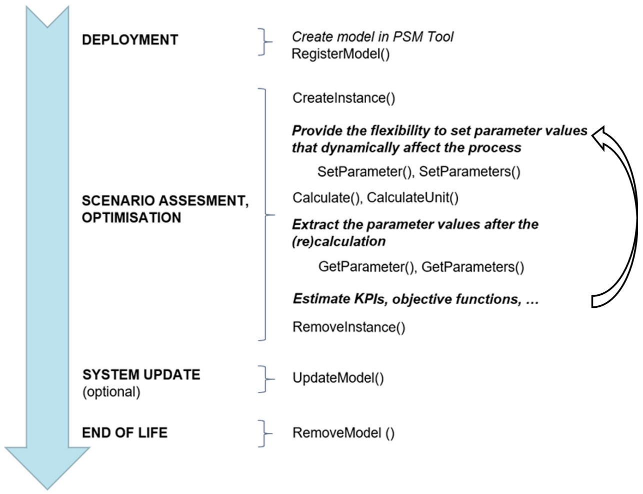

FIGURE 5. Lifecycle of a model.

the model has to be developed with the PSM desktop application. It is then registered within the platform providing the representation of the model as produced by the PSM desktop app. The next step is to grab an instance at the specific time frame important for the specification assessment or optimisation effort using the *CreateInstance*() function. The API provides the flexibility to set parameter values that dynamically affect the process by using *SetParameter*()/*SetParameters*(). When the values are set we can call *Calculate*()/*CalculateUnit*() (depending if we are looking for a specific unit or the whole model values) to run the simulation and then call *GetParameter*()/*GetParameters*() to read those calculated values. With these results we are able to calculate KPIs or objective functions and of course depending if the results are satisfactory or not we can repeat the calculations altering the parameter values. When we are done with our calculations regarding the specific instance we can call *RemoveInstace*() to discard it. In case the registered model needs to be updated we can call the *UpdateModel*() function however that is not going to update any instances already created before the update but only the model itself. Finally, when we have completed every simulation and experimentation and we don't require the model any more we can call *RemoveModel*() and completely remove the model from the system marking the end of the life-cycle in discussion.

V. CASE STUDY

A. LPG PURIFICATION PLANT OVERVIEW

The case study presented studies an oil refinery, a representative example of a continuous process industry. Modeling and Simulation of oil refineries receives increased interest in literature, mainly targeting in the increase of refinery productivity and reduction of resources usage such as energy. Typical such works are [41] where authors use Matlab and Aspen to develop a simulation and optimization model and [42] where the hydrogen unit in a domestic refinery

TABLE 1. LPG product specifications.

LPG Specifications				
Total Impurities $(^{vol}/_{vol})$	Vapour Pressure (kPa)	C_2 $(^{vol}/_{vol})$	C_5 $(^{vol}/_{vol})$	Sulphur $(^{mg}/_{kg})$
5.0%	1430	3.0%	2.0%	50

based on the mass and energy balance equations at steady state condition is used to calculate the optimal operational conditions of the unit. The majority of published works refer to specific installations (and do not propose a general framework) and make use of well-established commercial software tools or first principle models, of limited flexibility for integration with digital technologies and data exchange.

The refinery under study produces various petroleum products such as gasoline, diesel, naphtha and Liquefied Petroleum Gas (LPG). Generally, a refinery is composed of multiple units, each one serving a specific role in the production process (e.g., production of LPG, purification, storage). This use case focuses on the LPG purification, i.e., on the various processes that have to be applied to turn *crude* LPG to *refined* LPG in order that meets specific market quality criteria. LPG is a mixture of hydrocarbon gases, mostly propane (C_3H_8) and butane (C_4H_{10}) with various other hydrocarbons usually also present in small concentrations. By the end of the production process, various impurities remain in the *crude* product. Such impurities render the product unsuitable for the market and have to be removed in order to adhere to the standards and regulations of the petroleum market. These specs are summarized in Table 1. During the purification process, LPG passes through various steps of refining and uses additional organic compounds such as diethylamine (DEA) to withhold unwanted substances.

B. MODEL DEVELOPMENT

For the development of this LPG purification system process model, the units and the processes taking place have to be identified. Initially we have to identify the sources of the LPG streams being studied:

1. Atmospheric or Crude Distillation Unit (CDU)
2. Hydrocracker (HYC)
3. Fluid Catalytic Cracking (FCC)
4. Delayed Coker Unit (DCU)
5. Maximum Quality Diesel (MQD)
6. Platformer

The basic components used in the model development are presented in Figure 6. Entities used in the tool have been adapted to resemble well established chemical engineering symbols in order to facilitate the easier use of the tool from the process engineers and other stakeholders. In particular, debutanizer/deethanizer columns remove C_2 and C_5 impurities from the LPG streams. Tanks are used in different parts of the refinery to represent storage of products that have received a

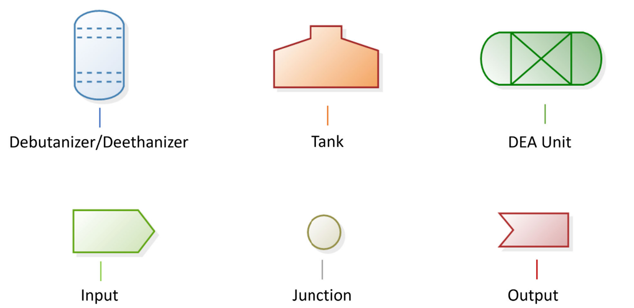

FIGURE 6. **Basic components of the model.**

number of processes. DEA units remove Sulphur from LPG using diethylamine organic compounds to retain H_2S from the LPG. This amine is deteriorating and loses its absorption capabilities over time, while it can be regenerated and reused for the refinery processes with the help of steam. Input and Ouptut entities are used to introduce and remove resources to/from the process model, while junction block enables the sum of multiple flows in a single one. The entities are interconnected through links, represented as arrows, which refer to material and energy flows between them.

PSM Tool provides the opportunity to set parameters for specific processes or for the whole model. Typical such parameters include flowrates, control parameters of the process units (e.g. temperature, pressure), time horizon of the simulation, quantities of the used resources, energy consumption and primary (products) or secondary outputs (emissions, byproducts).

The modelling of the processes taking place in the refinery has been implemented in four levels of detail, each one with additional details compared to the previous. Those four levels have been developed not only for easier comprehension of the processes taking place but also because different services (optimisation, analytics, simulation) using these process models require different levels of abstraction, as certain subsets of parameters provide adequately accurate results. In Figure 7 those four levels are presented through the dashboard of the PSM Tool. In each model level the number of entities considered as well as their interactions are presented in greater detail. Figure 8 summarizes the characteristics of the different model levels, describing in detail the main entities added separately in each one of the extension models (not grouped as an universal entity).

C. SIMULATION AND RESULTS

In order to demonstrate the functionality of the PSM Tool and the applicability of the proposed methodology, we consider a representative example focusing on the LPG stream *FlowA* and the processes taking place in Debutanizer A (removal of C_5) and Deethanizer A (removal of C_2), as shown in Figure 9, part of Level 2 model introduced earlier. The specific example does not refer to the whole process of the LPG purification, since the scope here is to present the applicability of the developed methodology and the outcomes but to a certain part of the process. The application example summarizes the overall functionality of the PSM Tool and can be extended for process modelling of complex systems without restrictions.

Stream *FlowA* is carrying LPG fed to Debutanizer A of the refinery. According to the assumptions adopted and the information provided by the process engineers, the quality of *FlowA* is uncontrollable, can not be affected from any actions and is considered static, although the quantity is known. Debutanizer A and Deethanizer A units are installed sequentially and the output of the first unit is the input of the second. The process taking place in these units is controlled by three variables: temperature, pressure and reboiler flow. The parameter values are continuously monitored using appropriate sensors (in all process units), and the received output quality characteristics are compared to the set specifications in order to evaluate system state and if corrective actions should be taken. Sulphur Absorption 1a unit is responsible for removal of S from the LPG and its control variables are temperature and pressure. In Figure 10 a snip of Debutanizer A and Deethanizer A control variables values is visualized, covering a 6 hour period. The variables do not follow any specific patterns and are continuously adjusted either automatically, through MPC controllers or by the process engineering team. The implemented process models can be an additional tool to support process engineers to the decision making procedure.

FlowA stream is set to have a flowrate of LPG at 11.42 m^3/h, C_2 a concentration of 2.07 % m^3/m^3, C_5 a concentration of 5.65 % m^3/m^3 and S 83.12 mg/kg. These values are mean values resulting from the real time measurement on the input of Debutanizer A, and are crucial since C_2, C_5 and S are the contaminants that have to be reduced in order to have the LPG on-specs. The process parameters have been set at 10.82 kg/cm^2 for pressure, 60.51 $°C$ for temperature and 5.54 m^3/hr for the reboiler flow. Similarly, these values represent mean values from the recorded data provided. The impurities on the input stream of *FlowA* and the process parameters of Debutanizer A are presented in Figure 11.a and 11.b.

Having set the inputs and the process control values, the simulation can now take place. It must be noted here that PSM Tool offers three different ways to define how the calculations will take place. The first one is to define ratios that will calculate the output based on an input; the second is to create a script in C# and the third is to use API endpoints to integrate machine learning models. In this example, the third one has been used integrating the models created by the project partner responsible for their implementation. These are hybrid models created with the historical data provided by the refinery with the purpose to predicted the concentration of C_2, C_5 and S in the output of a process unit according to the control parameters, i.e. temperature, pressure and reboiler flow. More details on the used machine learning models can be found in [43] and [44].

By performing a simulation, in order to evaluate a current scenario with specific process parameters, the aforemen-

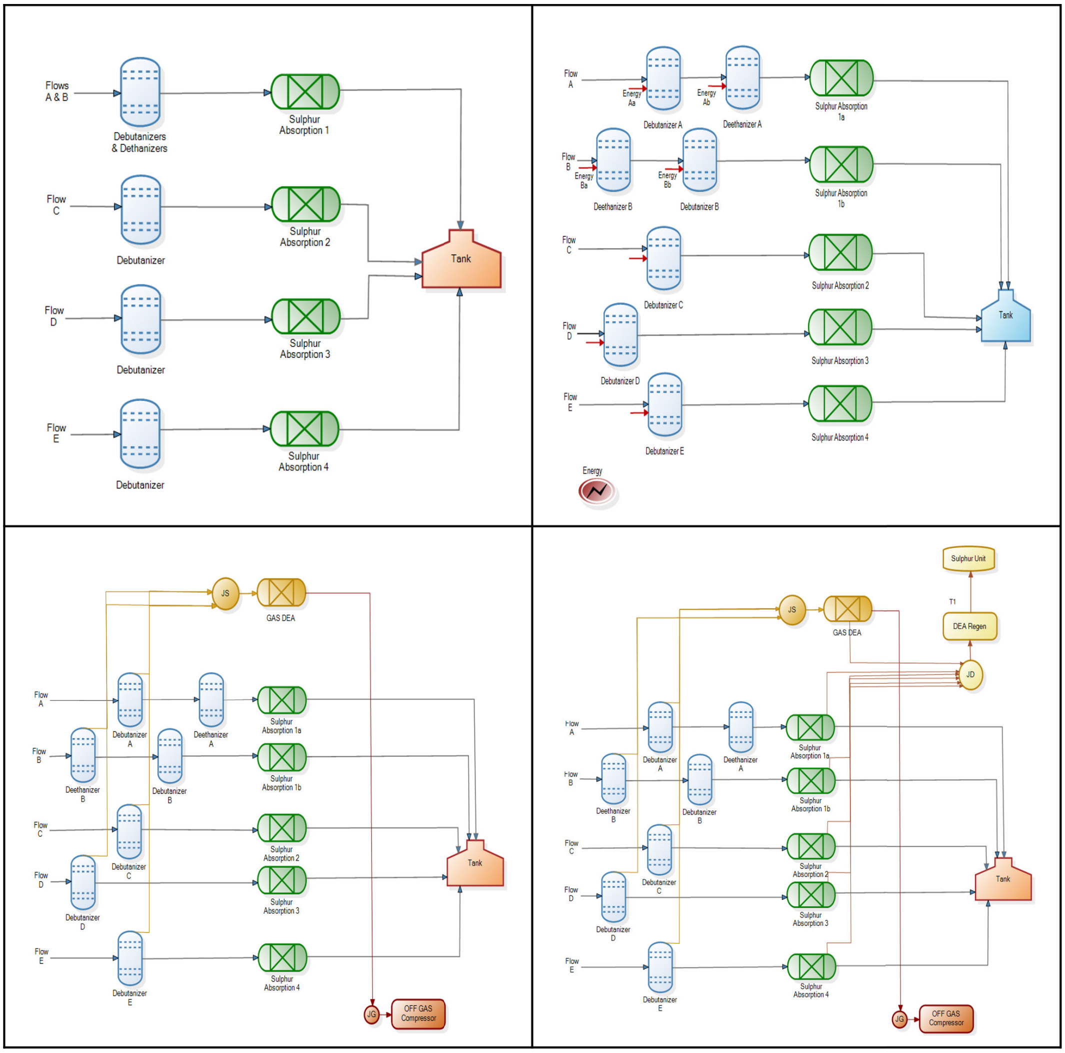

FIGURE 7. Visualization of the different modelling levels.

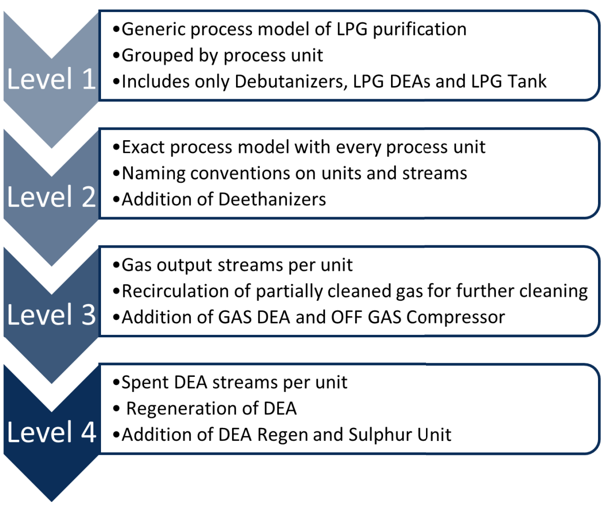

FIGURE 8. Modelling levels characteristics.

tioned models are called through the API and the results of each unit are calculated and presented through the tool with Debutanizer A output visualized in Figure 12.a, Deethanizer

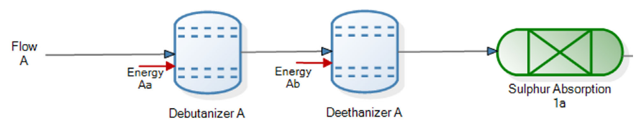

FIGURE 9. Focus area of the example.

A in Figure 12.b and Sulphur Absorption 1a in 12.c. Studying these results we can identify the processes taking place in the aforementioned LPG refinement process, where Debuatnizer A reduces C_5, Deethanizer A reduces C_2 and Sulphhur Absorption 1a reduces S.

PSM tool produces a variety of tables that capture the evolution of the values of parameters referring to features of systems' entities. These data can be exported for use from associated tools and algorithms but can be also accessed through an API endpoint in order to allow the seamless integration with associated services, such as optimization and analytics.

Another use of the proposed methodology concerns the definition of multiple alternative scenarios required for the

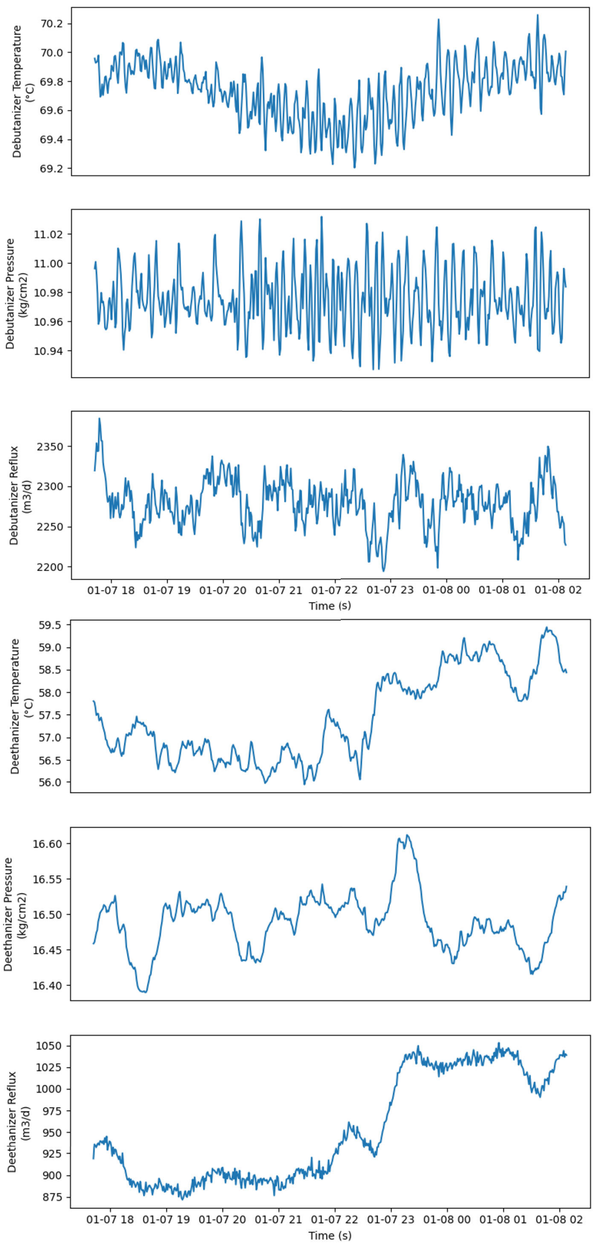

FIGURE 10. Recording of Debutanizer A and Deethanizer A control variable values for a six hour period.

optimization services. A set of alternative scenarios with different values of pressure, temperature and reboiler flow are produced and fed to the optimization service. Then, optimization evaluates them and selects the optimal (or near-optimal) based on predefined evaluation criteria (e.g. least amount of energy consumed). The optimal (or near-optimal) scenario is then validated through simulation, KPIs are calculated and results are provide to decision makers. The scenario creation process has been integrated in the PSM Tool described earlier and runs continuous simulations based on the alternative parameters provided. Two output files in *.json* format are created, one that contains the parameters for each scenario and one with the simulation results. In Figure 13 the scenario creation tab can be seen where the user selects

Resource	Flow	Unit
C2	2.07	% m^3/m^3
C5	5.67	% m^3/m^3
LPG	11.42	m^3/h
S	83.12	mg/kg

a.

Symbol	Is Read Only?	Value	Unit	Description
PRESSURE	☑	10.82	kg/cm^2	Top Pressure (47PIC1504.PV)
REFLOW	☑	5.54	m^3/hr	Reboiler Flow (47FIC1524.PV)
TEMPERATURE	☑	60.51	C	Top Temperature (47TI1532.PV)

b.

FIGURE 11. PSM tool input parameters values and initial assumptions.

Resource	From Node	Flow	Unit
C2	Flow A	2.07	% m^3/m^3
C5	Flow A	5.67	% m^3/m^3
LPG	Flow A	11.42	m^3/h
S	Flow A	83.12	mg/kg

a.

Resource	From Node	Flow	Unit
C2	Debutanizer A	2.07	% m^3/m^3
C5	Debutanizer A	0.76	% m^3/m^3
LPG	Debutanizer A	11.42	m^3/h
S	Debutanizer A	83.12	mg/kg

b.

Resource	From Node	Flow	Unit
C2	Deethanizer A	1.24	% m^3/m^3
C5	Deethanizer A	0.76	% m^3/m^3
LPG	Deethanizer A	11.42	m^3/h
S	Deethanizer A	83.12	mg/kg

c.

FIGURE 12. PSM tool calculated results through simulation.

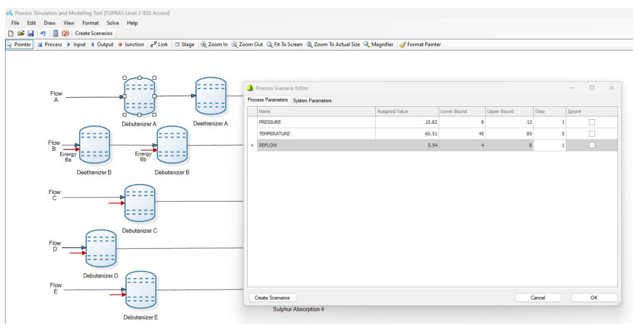

FIGURE 13. PSM tool scenario creation screen.

the parameters that wants to be included in the alternative scenarios, the range between the minimum and the maximum parameter value as well as the number of produced scenarios.

VI. CONCLUSION

In the current research, a process modelling and simulation theoretical framework for continuous industrial systems has been proposed. The proposed framework is generic, well defined and allows a graphical representation, with different levels of detail of systems, or system entities, simulation, product specification and state monitoring. In the context of the proposed methodology, a Process Simulation and Modelling Tool based on Material Flow Networks has been developed and verified for monitoring, evaluation and interaction among entities purposes. The proposed method is considerably distinguishable compared to previous research since the constructed models not only have the typical offline use but can also be used in the context of Digital Twins online with the physical system. The implemented models in conjunction with tools from other fields can be used for monitoring, root cause analysis, limitation, performance optimization and recovery of the behaviour of the system.

In the upcoming steps of our research more complicated cases of real systems will be studied analytically and under different operating conditions. Such a study would evaluate and quantify, using crucial KPIs, the behaviour of a system as determined from the interaction with its digital twin in comparison to its current state. There still exist challenges for extending specific features of the proposed method, such as data management and decision making in interaction with tools from the areas of Analytics, Machine Learning, Multicriteria Decision Making and Optimization. Possible extensions and variations regarding ways results are calculated, manipulated and visualized in the PSM Tool will be further developed.

ACKNOWLEDGMENT

The authors would like to thank the members of Industrial and Digital Innovations Research Group (INDIGO) of the School of Production Engineering and Management, Technical University of Crete and the partners in FACTLOG Project. The publication of the article in OA mode was financially supported by HEAL-Link.

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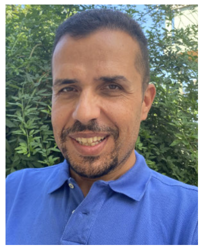

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