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Digital twins for process industries

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Introduction

The term process industry is used to refer to a broad range of applications involving the storage, transportation of processing of liquids or gasses. Common components found across such industries include vessels for storage and processing, pipes connecting the vessels and valves and pumps for moving materials between vessels. It is notable that the material that is being processed, e.g. oil, is of a continuous nature, so it is not possible to identify discrete items that are distinct from other items. This is the major difference between process industry and manufacturing industry. In manufacturing, a resource such as a robot may perform an operation such as pick-and-place on a workpiece. However, such operations do not occur in an industrial process, as there are no workpieces. Instead, the process acts on the substances being processed through *control loops*. Key elements of a loop are a *measurement*, *controller*, *setpoint* and *actuator*. Before discussing digital twins of industrial processes, it is necessary to discuss fundamental concepts such as process *equipment*, models of the physical process, *instrumentation* and *control systems*. Process industry domain terms that are important for the eventual discussion on digital twins are *italicized* when first used.

Fundamental concepts of industrial processes

An example case: a laboratory water process

The simplest kind of process only manages water in its liquid state. Such a laboratory process for heating, pressurizing and circulating water is shown in Figure 1. It has been developed at Aalto University for research and educational purposes by Mr. Jukka Peltola (Peltola et al., 2011; Vepsäläinen et al., 2010), and it will be used to introduce key concepts and techniques that are encountered in all kinds of industrial processes. This will be essential background for understanding the subsequent discussion on digital twins for industrial processes.

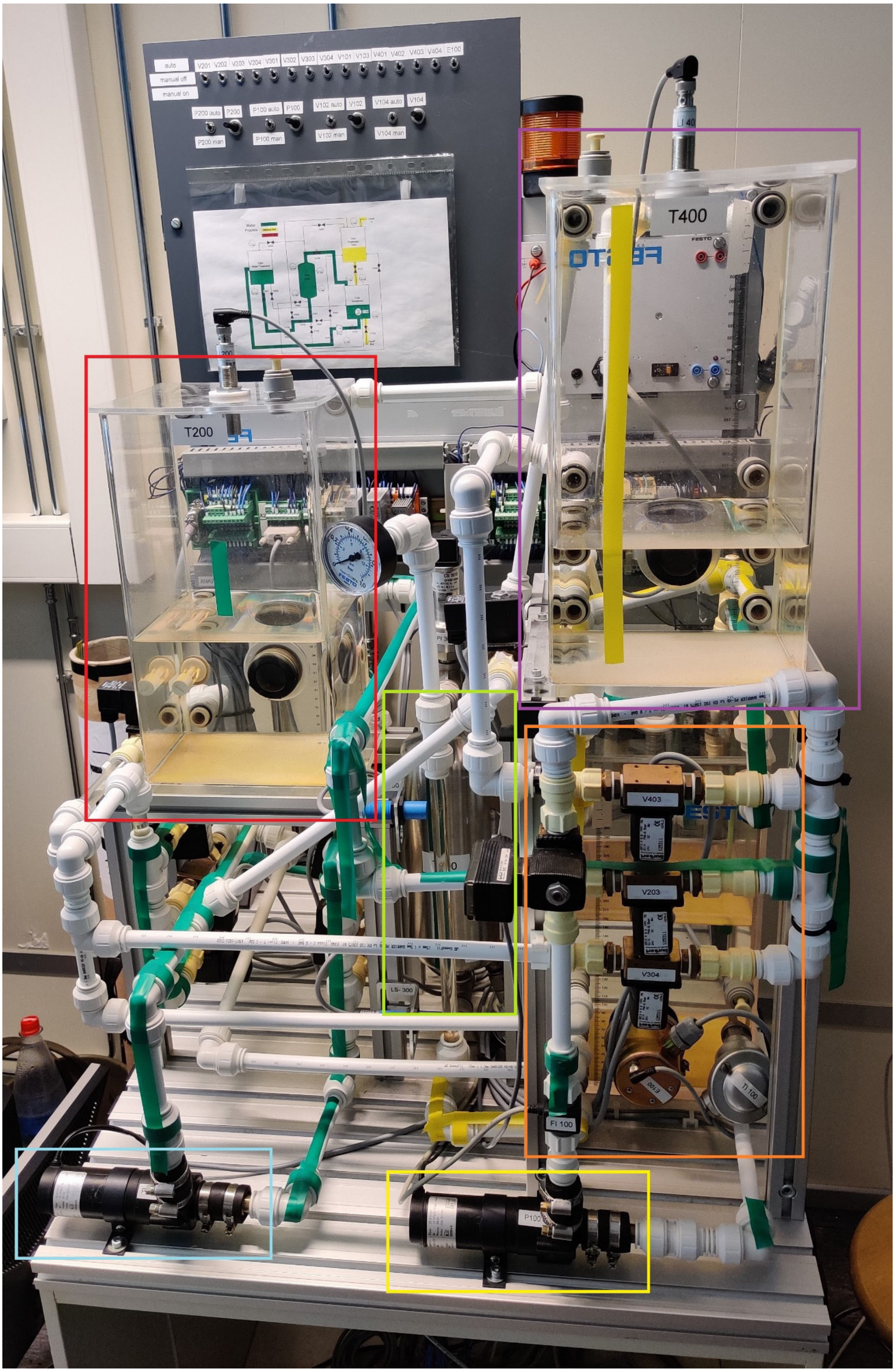

Figure 1 Laboratory process at Aalto University for heating, pressurizing and circulating water. Process equipment is marked with colored rectangles for further reference in Figure 2.

ALT TEXT: a water process consisting of 3 open tanks, one of which has a heating element, a pressure vessel, 2 pumps and piping and valves for circulating the water between the tanks.

The piping & instrumentation diagram

Figure 2 shows a *P&ID (Piping & Instrumentation Diagram)* of the process in Figure 1. By comparing the figures, it can be seen that the P&ID only includes some of the pipelines, namely the lines that comprise the primary circulation. There are additional pipelines which are needed when executing *sequences* for startup, shutdown, cleaning and maintenance purposes, which have not been modelled in Figure 2. As P&IDs are essential source information for building digital twins, this raises an important question: which pipelines of the process should be modelled? The answer depends on the intended usage of the digital twin. However, this illustrates the importance of scoping the source information before proceeding with a digital twin project.

The elements in the P&ID in Figure 2 are as follows:

- Vessels
    - Atmospheric tanks TK100, TK200 and TK200. The tanks have a lid, but they are not watertight, so overflow must be avoided. It is thus not possible to pressurize the tank above 1bar.
        - TK100 contains an electrically powered heating element E100
    - Pressure vessel TK300. In Figure 2, there is an outlet nozzle at the top of the tank. The layout of the P&ID does not in general provide information about pipe routing or nozzle placement, but in this case the nozzle actually is at the top of the tank. In normal operation the tank is full of water and pressurized by pump P200 in the inlet pipeline. The control valve V104 in the outlet pipeline provides resistance.
- Valves. 3 types of valve symbols are present in the diagram:
    - Manually controlled valve V-105 used to drain the process.
    - Automatic control valve, e.g. V102, which can be adjusted to any partially opened state by an analog signal from the control system.
    - Automatic binary valve, e.g. V203, which can only be fully opened or closed by a binary (on/off) signal from the control system.
- Pumps P100 in the pipeline from TK100 to TK200 and P200 from TK200 to TK300. The pumps are capable of continuous control based on an analog signal from the control system.
- Sensors in the circles. The significance of the code is as follows:
    - Temperature, Pressure, Level and Flow sensors are indicated in P&IDs with initial letters T, P, L and F, respectively.
    - The second letter is I or S standing for indication or switch respectively. Indications are analog measurement. For example, LI determines the surface level of the tank and is implemented with an analog ultrasound sensor at the top of the tank measuring the distance to the surface. The switches in these case are binary sensors, all of which are related to level. They activate when the surface level is below or above a predefined threshold. The suffix _H signifies a high level threshold and _L a low level threshold.
    - The number code relates the sensor to a process equipment or control loop.

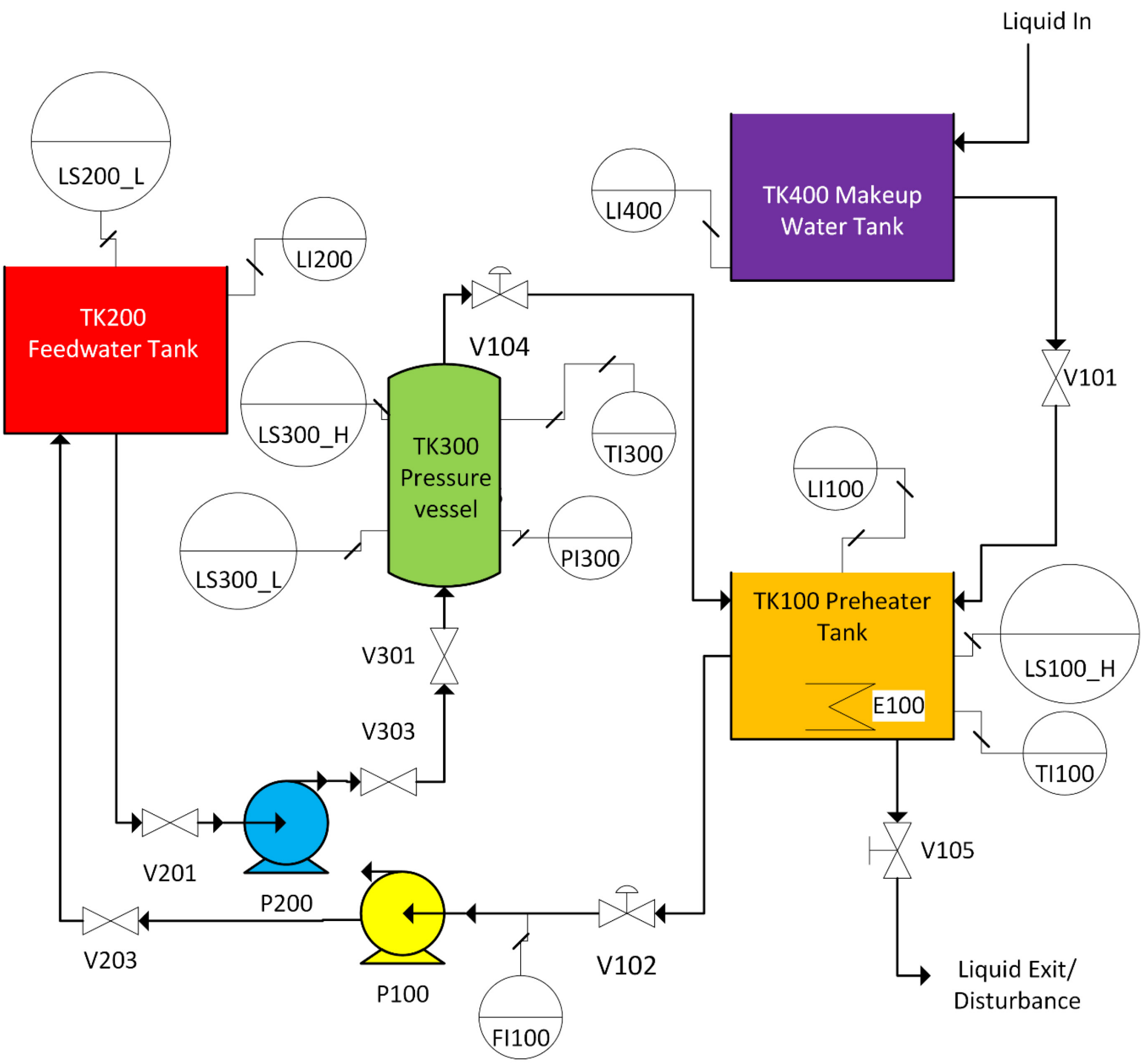

Figure 2 Process & Instrumentation diagram of the process in Figure 1

ALT TEXT: Process & Instrumentation diagram of the process in Figure 1 showing process equipment (tanks, vessel, pumps, heating element), valves and sensors for temperature, pressure, flow and level.

Modelling the physical process

Now that the control loops have been discussed, the main functionality of the process is understood, and it is possible to discuss the modelling of the physical process. There are two fundamentally different approaches: *steady state* and *dynamic*. The former does not consider time dependent phenomena and thus does not model control loops. The latter does consider such phenomena and is useful for investigating how the process reacts to *transients* such as changes to the setpoint of a control loop, operation of binary actuators, or various kinds of failures of the process components.

Steady state modelling can be beneficial especially for designing new plants and retrofits to reduce operating costs (Pinto-Varela, 2017), energy consumption (Wang et al., 2020), CO2 emissions (Min et al., 2015) freshwater consumption (Faria & Bagajewicz, 2009) and environmental pollution (Men et al. 2020). It is an open question that what could be considered a steady state digital twin. Sierla et al. (2020C) present a roadmap towards generating such a twin, using the process in Figure 1 as a case study. In this case, the digital twin would involve an online capability of synchronizing the steady state model parameters based on recent measurement data from the control system history database.

As digital twins involve a real-time connection to the physical process, the dominant modelling approach in this context is dynamic. The task is simplified in the context of our example process, in the sense that the only substance in the pipes and vessels is water in its liquid phase. The pressure and temperature of the water is of interest in all of the tanks and pipelines. Flow is of interest in the pipelines and surface level is of interest in the vessels. To capture how these quantities vary in time and how they are affected by the actuators requires building a simulation model with a thermo-hydraulic solver (e.g. Hänninen & Ahtinen, 2009). The dimensions of the vessels, interior diameter of the pipelines and the routing of the pipelines are essential information for building a thermo-hydraulically accurate model, but this information is not available from a P&ID. In particular, the pressure losses within the pipelines are crucial parameters to the model. Calculating them requires detailed information on the elevations of the nozzles at the beginning and end of the pipeline, interior diameter of the pipeline, number and angle of bends in the pipeline (known as *elbows*) and junctions where the pipeline branches in two ways (known as *tees*). Martínez et al. (2018A) present a detailed explanation of the pressure loss calculation and apply it to the process in Figure 1.

It is notable that steady state and dynamic simulation are not mutually exclusive. Some authors use steady state simulation as a precursor of dynamic simulation analyses (Cui et al., 2019; Yoon et al., 2020; Chisalita & Cormos, 2018; Kender et al., 2021).

In addition to physics-based approaches for modelling the process, it is possible to apply black-box approaches and machine learning models to determine input-output relationship of industrial processes or subprocesses. As the term digital twin has some marketing value, some such industrial products have been branded as digital twins. However, the twins are only valid when the process is operating in the same conditions as it was when the data was collected for the black box model. This is counterproductive to the objectives of using digital twins to ensure the desired operation of processes, especially in abnormal situations. Thus, in this section we adhere to the original NASA definition of digital twins that requires the use of the best possible physical models (Shafto et al., 2010).

Engineering design source information for modelling the physical process

Building an accurate simulation model or digital twin of an industrial process requires relevant engineering design source information beyond a P&ID. At this point, the nature of this source information and its availability for real industrial processes is discussed. It is important to distinguish between *greenfield* plants that are being designed from scratch and *brownfield* plants that are already operational. As process plants frequently have a lifecycle of several decades, the brownfield plant will be an important context for applying digital twins, so the availability of engineering design information in both greenfield and brownfield situation needs to be discussed. There are several ways of obtaining the required engineering design source information, depending on what is available at a specific plant:

- A recent version of a 3D process CAD (computer aided design) tool is able to export the pipe routing information in an open, standard and machine-readable format. In particular, the PCF (Piping Component File) format for 3D isometrics is supported my major 3D process CAD tool vendors, and Sierla et al. (2020A) developed a software application for parsing such a file for the process in Figure 1. The tool was able to extract the elbows, tees and elevations of the nozzles and thus obtained the information required to compute the pressure losses for these pipelines. Unfortunately, at the time of writing, PCF file can only be exported by recent versions of CAD tools and are thus available only for greenfield plants and very recently commissioned brownfield plants.

- Process plants have a lifecycle of decades, so a plant which has been operational for many years may not have any 3D CAD model, or it may be in an older format, from which it is not possible to export a machine-readable file such as a PCF file (Chen et al., 2018; Arroyo et al., 2016). Constructing a high-fidelity digital twin for such a plant will be laborious. For example, Martínez et al. (2018A) measured the dimensions of the components for the process in Figure 1 and manually reverse engineered the 3D CAD model.
- Laser scanning of industrial facilities is a viable approach for brownfield plants. The challenge is to automatically extract the process components from the raw point cloud data from the scan. Xiong et al. (2013) accomplish this for the building, identifying floors, walls, doorways and ceilings. Kawashima et al. (2011) accomplish the same for pipelines, identifying components of interest for our purposes, such as tees and elbows. Even if 3D CAD data is available, one advantage of using point clouds instead of 3D CAD models is that the latter describes the *as-designed* state of the plant whereas the former captures the *as-is* state of the plant. There can be a significant difference between these two configurations at a brownfield plant in which several retrofits have been made over the years. For the purposes of developing a digital twin, the as-is configuration is relevant, as the twin should be synchronized in real time to the physical process rather than to any historical previous embodiment of the process.

Putting it together: integrating the control system to the physical process or a simulation model thereof

The control system needs to be integrated to the physical sensors and actuators at the process. For simulation purposes, the integration needs to be done to the sensors and actuators of the simulation software. Understanding these integrations is a starting point for understanding how digital twins can be deployed. The information technologies and architectures for this purpose are beyond the scope of this book; Martínez et al. (2018B) discuss these aspects in the context of the process in Figure 1. The capability to interface a process control system to a simulation model of the physical process as well as to the physical process is prerequisite to building and deploying digital twins. This task is complicated due to the fact that source information for building the control systems comes mainly from the P&ID whereas the source information for the simulation model comes from a 3D CAD or a laser scan. The same components need to be matched in these different sources before the information can be integrated and the correct interfaces can be built. In general, it cannot be assumed that industrial practitioners use consistent naming conventions across different tools such as P&IDs and CADs (Rantala et al., 2019), so automatic matching of tags (e.g. 'V102' or 'E100' in Figure 2) is not a viable methods for integrating these two sources of information. Tags are also not present in the output of a laser scan. Doing this work manually is very laborious, so the engineering cost of building a digital twin can be very high if even the basic task of correctly integrating the different sources of information poses significant challenges. Recent research towards this end involves the generation of graphs from P&IDs and 3D CAD models, reducing both sources of information to the same abstraction level (Sierla et al., 2020B). Graph matching methods (Wen et al., 2017) can be applied as the next step to identify the same process components from the P&ID and CAD. It is notable that the techniques discussed in this subsection are a field of ongoing research rather than commercially mature technology.

Types of industrial process

The process in Figure 1 served the purpose of introducing elements that are generally found in industrial processes across industrial sectors. In this section, some main industrial sectors are discussed. Aspects of these processes that were not present in our example process are discussed.

A *combustion power plant* is in many ways a straightforward extension of the process in Figure 1 (Starkloff et al., 2015). Fuel such as coal is burned to generate heat in a vessel containing water at a high temperature and pressure. The water at the top of the steam evaporates despite the high pressure. The steam is led by a pipeline to a turbine for generating electricity. The low-pressure steam after the turbine needs to be condensed before it can be pumped back to the vessel. A *heat exchanger* is used for this purpose. The exchanger involves a winding pipe going through a tank of cool water. The heat is exchanged through the walls of the pipe, resulting in the steam cooling down and condensing. The high pressures and temperatures justify the investment to a SIS. The modelling of high-pressure steam is more difficult than the modelling of pressurized and heated liquid water in the example process in Figure 1. Thus, a higher fidelity thermo-hydraulic simulator would be required. The accurate modelling of the high-pressure steam is a challenging task, especially for recent efforts to increase the flexibility of coal fired plants to adapt rapidly to changes in renewable generation to the grid (Zhao et al., 2018; Wei et al., 2021). Dynamic simulation is identified as an appropriate technology for this task (Alobaid et al., 2017). Building on this trend, a recent research direction on dynamic simulation of coal-fired power plants is the solar-aided plant, in which solar generation complements the combustion (Yan et al., 2021).

Another development on the conventional combustion power plant with a steam turbine is a gas turbine driven by high pressure gas obtained by burning methane or natural gas, so that the remaining heat from the gas exiting the turbine is used to generate steam that is fed to another turbine (Henry et al., 2021).

The various types of *chemical processes* involve other substances in addition to water and steam, as well as chemical reactions that occur between the substances. Dynamic simulations have been used for a variety of purposes. Ge et al. (2021) develop and validate environmentally friendly flaring methods reducing the amount of unburned hydrocarbons, NOx, CO2 and CO released to the environment. Olivier-Maget et al. (2021) investigate boiler overpressure and flooding scenarios in propylene glycol production process. Khaled et al. (2021) investigate various fault and disturbance scenarios for an offshore gas processing plant. Wanotayaroj et al. (2020) simulates transients in temperature, pressure and tank level to validate and tune controllers for a Chemical looping combustion (CLC) process separating carbon dioxide from flue gas. Yoon et al. (2020) reduce waste and energy consumption in a Natural Gas Liquid (NGL) recovery process, while investigating potentially hazardous transients. Fluid catalytic cracking (FCC) is a main process in petroleum refineries converting crude oil into end products such as gasoline. Cui et al. (2019) simulate external disturbances to this highly safety critical process to validate that SIL requirements are met. Zhu et al. (2020) simulate potentially hazardous control actions by the human operators of the process. Chisalita & Cormos (2018) use simulation to predict the behaviour of a novel combustion process with carbon capture. Raimondi (2019) model the stratification of liquid and gas fractions in an underwater natural gas pipeline.

Digital twins in the process industry

Based on the introductory material in previous sections and italicized terms, it is possible to analyze recent works on digital twins for process industries. This analysis considers the objectives for the digital twin, the design approach and new capabilities that the digital twin provides above and beyond state-of-the-art industrial process simulations, such as the ones reviewed in the previous section. In the following, recent state-of-the-art works are analyzed. At the time of writing, the research on digital twins in process industry is in its early stages. Thus, the goal of this chapter is to demonstrate to the reader how previously introduced concepts of industrial process simulation can be applied to understand and critically assess this literature. A later edition of this book may discuss well-established approaches for developing digital twins for process industries, but at the time of writing, such approaches do not yet exist.

A digital twin for the case process in Figure 1 is described in (Martínez et al., 2018A; Martínez et al., 2018B; Martínez et al., 2018C). Sensor measurements are compared to state values of the dynamic simulation of the process that is running in parallel. A PI (proportional-integral) controller computes the error between the state and the measurement and adjusts some parameters of the dynamic simulation model such as the pressure losses in the pipelines. This is the same kind of controller that has been used in the continuous control loops in Table 1. The authors reported a very accurate performance at these points in the process. The digital twin can be disconnected from the physical system and run faster than real time under specified operating conditions, in order to determine the future state of the process if such operator actions would be applied to the physical process. It is unclear how well the dynamic simulation has been synchronized outside of the points at which there was a physical sensor to make an adjustment, so it is not possible to make strong claims about being able to use this digital twin as a soft sensor (i.e. to measure the process state in locations in which there is no physical sensor). However, the procedure for making the adjustment is described in some detail, which is not the case with the majority of the reviewed research discussed next.

Wang et al. (2021) developed a digital twin of an autoclave for fabricating fiber reinforced plastic composite at a high temperature and pressure. Equipment failures can have significant consequences, motivating investments to predictive fault detection. Data driven methods such as machine learning could be used, but there is limited data on failure conditions, as the process operator endeavors to keep the autoclave in a healthy and safe state. To obtain such data, the authors use a high-fidelity digital twin to drive a virtual replica of the process to abnormal operating regions. The twin is constructed as a combination of geometric, physical, behavioral and rule-based models. The geometric model corresponds to the 3D process CAD models discussed previously. The physical and behavioral models correspond to a dynamic simulation model. The rule-based model covers the process control system, but also the failure modes of the process equipment. The digital twin is driven to a state that is very close to the current state of the physical process, after which a fitting procedure is applied. The fitting adjusts operating rules, boundary conditions, mesh partitioning, initial conditions, and component mesh relationships. The magnitude of the fitting is determined by the deviation between the state of the digital twin and corresponding measurements from the physical process.

Kender et al. (2021) developed a digital twin of an air separation process to investigate the frequent transients that process is expected to undergo. The process extracts N_2 and O_2 from the air intake. Whereas many researchers are content to synchronize the twin with the operational process, Kender et al. (2021) consider the evolution of the twin throughout the lifecycle phases of (pre-) sales, equipment and process design, commissioning, and operation optimization. Steady state simulation is used in the first two phases and high-fidelity dynamic simulation in the latter two to accurate capture the nonlinear process behaviour. However, the system is decomposed to subsystem, and it is possible to substitute lower fidelity linear models when such fidelity is acceptable with respect to the objectives of the investigated being carried out with the digital twin. The ability to vary the level of fidelity would make it possible to avoid the use of many separate simulation models throughout the plant lifecycle, which is contrary to the digital twin philosophy. With respect to the method for adjusting the dynamic simulation model to the current state of the physical system, the authors state that it is possible to connect to either historical or live operating data, without elaborating further. Using this digital twin, the authors perform simulations to determine the fastest possible safe startup and shutdown of the process. Other applications of the twin include real-time monitoring and verification of the accuracy of sensor measurements.

Koulouris et al. (2021) consider the special characteristic of food processing industry, which involves batch processing. Due to the highly seasonal nature of raw ingredients production and rapidly changing market demand, the scheduling of the production is a critical task, involving a combination of make-to-order and make-to-stock. The authors define a digital twin as a synchronization of plant-floor simulations and the scheduling function. The recipe-based representation is identified as a good starting point for the synchronization, which is not yet implemented in practice. It is assumed that a human performs the scheduling function, so the role of the digital twin is to ensure that this work is being carried out against a real-time synchronized model of the situation at the plant floor. The case study shows examples of rescheduling done in response to unexpected occurrences at the plant floor.

Aversano et al. (2021) develop a digital twin on top of physics-based reduced-order-models for a furnace operating in flameless combustion conditions. This is an example of a process in which the installation of physical sensors throughout the process is difficult or impossible due to the harsh conditions. The digital twin can be used to predict the state of the process in a three-dimensional space, functioning as a soft sensor. Real-time data from the available sensors is an input to the digital twin, thus synchronizing it with the physical process and enabling it to predict the process state in locations in which there are no physical sensors.

Yu et al. (2020) develop a digital twin for steam turbines in a thermal power plant. As the penetration of renewable generation in the power grid increases, thermal power plants often need to be driven to operating regions in which they were not originally designed to operate, also known as off-design operating modes. In particular, the rapid changes in power generation required from the turbines poses challenges to the operation of the high-pressure control valve systems that govern the steam flow to the turbine, impacting both the turbine as well as the combustion process. The operation of these control valves is of crucial importance to ensure safety, optimize the energy efficiency and minimize emissions in the off-design mode. The purpose of the digital twin is to enable accurate online performance monitoring. A physics-based steam flow model for the subsystem has been created, corresponding to an as-designed system. Due to factors such as aging of the valve components, the parameters are adjusted based on operating data to obtain an as-is system.

Maksim et al. (2020) model a process for producing yellow phosphorus from apatite-nepheline ore waste. The objective is to reduce energy consumption. A neural network model of the process is run in parallel to the physical system, and its energy consumption output is compared to the energy consumption measurement of the real system. The error between these is used to train the neural network until the error is below an acceptable threshold. After this, the neural network can be used to investigate combinations of process parameters to identify the best combination for the purpose of energy consumption minimization. It is notable that this approach differs from the other approaches that were reviewed previously, in which operating data was used to adjust an as-built simulation, thus achieving an as-is model. In this case the physics-based model is not adjusted, but the operating parameters are optimized.

Table 1 Overview of state-of-the-art applications of digital twins in process industries

Reference	Process	Use case
Martínez et al., 2018C	Water process in Figure 1	Predict future state of the process under specific operating conditions
Wang et al. (2021)	Autoclave	Generate training data for predictive fault maintenance
Kender et al. (2021)	Air separation process	Determine fastest possible startup and shutdown
Koulouris et al. (2021)	Beverage process	Rescheduling in response to disturbances at plant floor
Aversano et al. (2021)	Furnace operating in flameless combustion conditions	Soft sensor
Yu et al. (2020)	Valve subsystem of steam turbine in a thermal power plant	Online performance monitoring
Maksim et al. (2020)	Producing yellow phosphorus from apatite-nepheline ore waste	Minimize energy consumption

The state-of-the-art works that have been reviewed in this section are summarized in Table 2, which shows a breadth of different types of processes as well as different use cases for the digital twin, indicating a high potential for this technology in process industries. Further research is required to develop digital twins that can realize several use cases. Further research is also needed to ensure that digital twins are accurate throughout an entire process or subprocess, rather than in specific regions of the process. Although safety has been considered in some works, the existence of safety functions or safety instrumented systems has not been included in the scope of the modelling of digital twins, so the real process may behave very differently than the digital twin in abnormal operating regions, if the safety functions are activated.

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