DIGITAL TWINS

Terms & Definitions

TASK XVIII

DIGITALIZATION, ARTIFICIAL INTELLIGENCE AND RELATED TECHNOLOGIES FOR ENERGY EFFICIENCY AND GHG EMISSIONS REDUCTION IN INDUSTRY

SUBTASK 2

METHODS AND APPLICATIONS OF DIGITAL TWINS

June 2022

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About IETS Task XVIII Subtask 2

In IETS Task XVIII *Digitalization, Artificial Intelligence and Related Technologies for Energy Efficiency and GHG Emissions Reduction in Industry* we are working on identifying technologies that can be applied in industry to increase the energy efficiency and ultimately reduce the emission of greenhouse gases.

Subtask 2 of IETS Task XVIII focuses on Methods and Applications of Digital Twins (DT) to promote the application of DTs in industry, in order to improve energy efficiency and reduce GHG emissions. Subtask 2 has the following sub-objectives:

- Overview of methods and applications of DTs and their requirements for different industry sectors
- Analysis of the potential benefits of these methods, focusing on the impact on energy efficiency and GHG emissions reduction
- Creation of an international, interdisciplinary network of research and industry

Digital Twins have the potential to improve industrial energy systems considerably. Not surprisingly, there has been quite a hype around digital twins during the last years. Though, successful implementations of digital twins in industry are rare and the actual return-on-investment is hard to estimate. For this reason, many companies are still hesitant to employ digital twins. As different definitions of DT exist and potential applications are often indistinct, a uniform description and definition for them is required.

Within Subtask 2, an overview of this extensive topic is presented in the form of a Glossary. A literature review was conducted and findings from previous work were collected to clarify the terms and definitions around the topic digital twin.

Glossary

The aim of this report is to provide much needed definitions and a glossary of terms for this emerging field that can be used as basis for future publications and work. A glossary is provided below, which also reflect the structure of this report.

Table 1 - Glossary

Term	Description
Digital Twin	A Digital Twin is a virtual representation that matches the physical attributes of a "real world" entity*, through measured values and domain knowledge and features automated bidirectional communication with that entity.
***Physical Entity**	A physical entity is an abstraction of a "thing" persisting in the real world, which has to be mirrored or twinned in the virtual world. Josifovska et al. (2019).
Digital Model	A Digital Model is a digital representation of an existing or planned physical object that does not use any form of automated data exchange between the physical entity and the digital entity. Kritzinger et al. (2018)
Digital Shadow	Based on the definition of a Digital Model, if there further exists an automated one-way data flow between the state of an existing physical entity and a digital entity, one might refer to such a combination as Digital Shadow. (Kritzinger et al. (2018))
Cyber-Physical System	Cyber-Physical Systems are autonomous and cooperative elements and sub-systems across all levels of production, able to communicate with each other in situation-dependent ways. Monostori (2014)
Cyber-Physical Production System	When Cyber-Physical Systems are connected to perform smart manufacturing, we have a Cyber-Physical Production System. Rojas & Rauch (2019)
Industry 4.0	Industry 4.0 represents the technological evolution from embedded systems to cyber-physical systems. In Industry 4.0, embedded systems, semantic machine-to-machine communication, Internet-of-Things and Cyber-Physical System technologies are integrating the virtual space with the physical world. In addition, a new generation of industrial systems, such as smart factories, is emerging to deal with the complexity of production in cyber-physical environment. GTAI (2014)

Energy 4.0	In analogy to Industry 4.0, Energy 4.0 stands for the transition to energy systems of the fourth generation, sometimes also referred to as smart energy systems. These energy systems will be based on renewable, volatile energy carriers, a high amount of flexibilization, and interconnection between different industry sectors and feature extensive application of digital technologies. Lund et al. (2017); Robison et al. (2015)
Key Performance Indicators	In general, the interaction of digital twins and key performance indicators can be understood in two ways: • The digital twin receives key performance indicators regarding the performance of the process as input information from physical entity and bases operation on these KPIs (can be e.g., aggregated / calculated data from processes). • Furthermore, key performance indicators can also be defined for the digital twin itself.
Optimization	Optimization is generally understood to be the search for the best possible solution in the sense of a certain goal in a decision-making area, whereby frame conditions can be taken into account. Floudas & Pardalos (2008)
Digitization	Digitization is the process of changing data into a digital form that can be easily read and processed by a computer. Oxford Online Dictionary (2021)
Digitalization	In the context of industrialization, digitalization describes the transition to new, disruptive business cases driven by evolving Information and Communication Technologies, the automation and flexibilization of business operation and the interconnection of information, things and operatives. Hanschke (2018)
Services	To solve the problem of interoperability between a digital twin and different users / stakeholders and to enable innovative business models, the functions of the digital twin can be encapsulated into standardized services with user-friendly interfaces for easy and on-demand usage. Tao et al. (2019)
Modeling approaches	In the context of digital twins modeling is understood as the task of creating a virtual representation of some real system in order to compute certain properties or make predictions of the behavior. Different modeling approaches can be applied. Relevant characteristics of models are performance, real-time capability, level of detail, resolution of the entity in time or process level etc.

Big Data	Big data is high-volume, high-velocity and high-variety information assets that demand cost-effective, innovative forms of information processing for enhanced insight and decision making. Gartner (2021)
Information and communication technology	The term "Information and Communication Technology" is generally accepted to mean all devices, networking components, applications and systems that combined allow people and organizations (i.e., businesses, nonprofit agencies, governments, and criminal enterprises) to interact in the digital world. Pratt (2021)
Sensors	A device that responds to a physical stimulus (such as heat, light, sound, pressure, magnetism, or a particular motion) and transmits a resulting impulse (as for measurement or operating a control). Merriam Webster (2021)
Internet of Things	The IoT is a concept, in which basically any device - mechanical or digital - is connected in a network with the ability to transfer data without the requirement of human interaction. Hofmann et al. (2020)
Knowledge representation	Ontologies are knowledge representations of a domain that contain explicit descriptions of concepts, properties, attributes or features of those concepts and logical restrictions on the classes and properties. They are explicit conceptualization of objects, concepts, and their relations that form a knowledge base as well as the basis of what "exists" in a "universe of discourse" for AI systems. (Hofmann et al. (2020))
Simulation	Simulation is the prediction of a real-world process or system with given parameters over time.
Optimization method	Optimization is generally understood to be the search for the best possible solution in the sense of a certain goal in a decision-making area, whereby frame conditions can be taken into account. (Floudas & Pardalos (2008))
Virtual reality	Virtual reality is a technology where the user can immerse into a virtual environment and can roam and interact with it. Zhou & Deng (2009)
Augmented reality	A system that supplements the real world with virtual (computer-generated) objects that appear to coexist in the same space as the real world. Azuma et al. (2001)

Condition Monitoring	The assessment of the current condition of a physical entity by employing measurement data.
Predictive Maintenance	The main objective of predictive maintenance is to employ the information gathered from condition monitoring to predict the point of time at which maintenance activities are the most cost-efficient and before the physical entities optimal performance deteriorates. Sinha et al. (2010)
Preventive Maintenance	Preventive maintenance is performed periodically. It is meant to prevent the physical entity from sudden failure and/or deterioration in efficiency by inspecting, servicing and replacing critical parts of the physical entity on a predetermined frequency.
Reactive Maintenance	Also known as breakdown maintenance, reactive maintenance is the type of maintenance which is performed at a point of time at which a critical failure of a significant deterioration in efficiency already occurred in a certain part of the physical entity.
Predictive Control	Typically, advanced control methods involve more complex calculations than the conventional PID controller algorithm. Advanced control has the following features: • Process modeling and parameter identification (off-line or on-line) • Prediction of process behavior using process model • Evaluation of performance criterion; subject to process constraints • Optimization of performance criterion • Matrix calculations (multi-variable control) • Feedback control Airikka (2004)
Forecasting	Forecasting is a common statistical task in business and is about predicting the future as accurately as possible.
Decision Making Support	A decision support system is a computer-based application that collects, organizes, and analyzes business data to facilitate quality business decision-making for management, operations and planning. A well-designed decision support system aids decision makers in compiling a variety of data from many sources: raw data, documents, personal knowledge from employees, management, executives and business models. Decision support system analysis helps companies to identify and solve problems and make decisions. Techopedia (2021)
Flexibility	Flexibility is the capacity to adapt. Golden & Powell (2000)

Abbreviations

AI	Artificial Intelligence
DT	Digital Twin
CPPS	Cyber-Physical Production Systems
CPS	Cyber-Physical Systems
E4.0	Energy 4.0
GHG	Greenhouse gas
ICT	Information and Communication Technology
IT	Information Technology
I4.0	Industry 4.0
KPI	Key Performance Indicator
LCOE	Levelized Cost of Energy
LCOH	Levelized Cost of Heat

1. Introduction

Digitalization has become an integral part of daily life. Similarly, in Industry, digitization can provide a number of benefits, such as higher productivity, lower costs and flexibility of industrial processes, thus improving efficiency and saving energy. Furthermore, digitalization can support the integration of renewable sources and sustainable production; specifically for energy intensive industries. This can further reduce greenhouse gas emissions (GHG) in industry. However, digitalization poses several challenges, including data management and data security issues. The availability and quality of big data, which is dependent on available sensors, acts as a critical element and enabler for a successful implementation.

As part of a project of the International Energy Agency (technology program "Industrial Energy Technologies and Systems" - IEA IETS Task XVIII), an international consortium is addressing the issues associated with digitization along the value and development chain in industry. In particular, the project is dedicated to digitization, artificial intelligence (AI) and related technologies for increasing energy efficiency and the reduction of GHGs in industry.

The overall objective of this work is to increase the knowledge, development and application of digitalization, AI and related technologies to improve the economic and environmental performance of energy and GHG intensive industries. In addition, it aims to create the necessary foundation and framework conditions for improving the digital twins (DTs) implementation in industry. To address this, the methods and applications of digital twins, challenges and solutions in connection with digitization, as well as roadmaps for the implementation of digitization measures in energy-intensive industry, are examined.

The project specifically addresses these challenges by bringing together experts and initiating joint research and work. The international project is led by Mouloud Amazouz, CanmetENERGY, Natural Resources Canada, who is coordinating an 11-country consortium including Austria, Canada, Denmark, Finland, France, Germany, Portugal, Netherlands, Italy, Sweden and Switzerland. The Austrian consortium is led by the Institute for Energy Systems and Thermodynamics at the Vienna University of Technology, in partnership with AEE INTEC, the Austrian Institute of Technology and the Montanuniversität Leoben. Background

Within ***IEA IETS Task XVIII Subtask I*** Whitepaper on "Digitalization in Industry"[1] (Hofmann et al. (2020)) was elaborated by the Austrian participants covering the following issues:

- A brief overview of energy consumption and GHG emissions in Austria, focusing on digitalization applications for industry and related projects in Austria
- An overview of technologies, including the Digital Twin (DT), and applications
- Explicit definitions
- Barriers, gaps, needs and future potentials

The definitions and terms were addressed in Subtask 1 of Task XVIII. The document can be accessed here: [Whitepaper_TaskXVIII_Subtask1]. Although several definitions for DT applications have been covered, there remains a lack of detail regarding the background of DTs. (Hofmann et al.) (2020) provide several useful definitions that can be built on to analyze digitalization methods and applications. This report thus focuses on a more detailed review of possible existing definitions and their analysis in the context of DTs.

[1] https://www.energieforschung.at/assets/project/downloads/White-Paper-Digitalization-in-Industry.pdf or White-Paper-Digitalization-in-Industry.pdf (tuwien.ac.at)

1.1 Framework

The work presented in this document is part of the ***IEA IETS Task XVIII Subtask 2.***

The scope of the work in this Task is to analyze, describe and show potential applications of DTs in (energy-intensive) industrial energy supply systems to contribute to environmental protection measures, particularly the reduction of GHG emissions.

However, the European Commission does not only address the reduction of GHG emissions within the regulatory framework of its climate goals, it also emphasizes the importance of reducing primary energy consumption, which corresponds to increasing energy efficiency, as well as increasing the share of renewable energies. Within this Task, methods and the application potential of DTs contribution to climate protection measures are addressed for industrial energy supply systems.

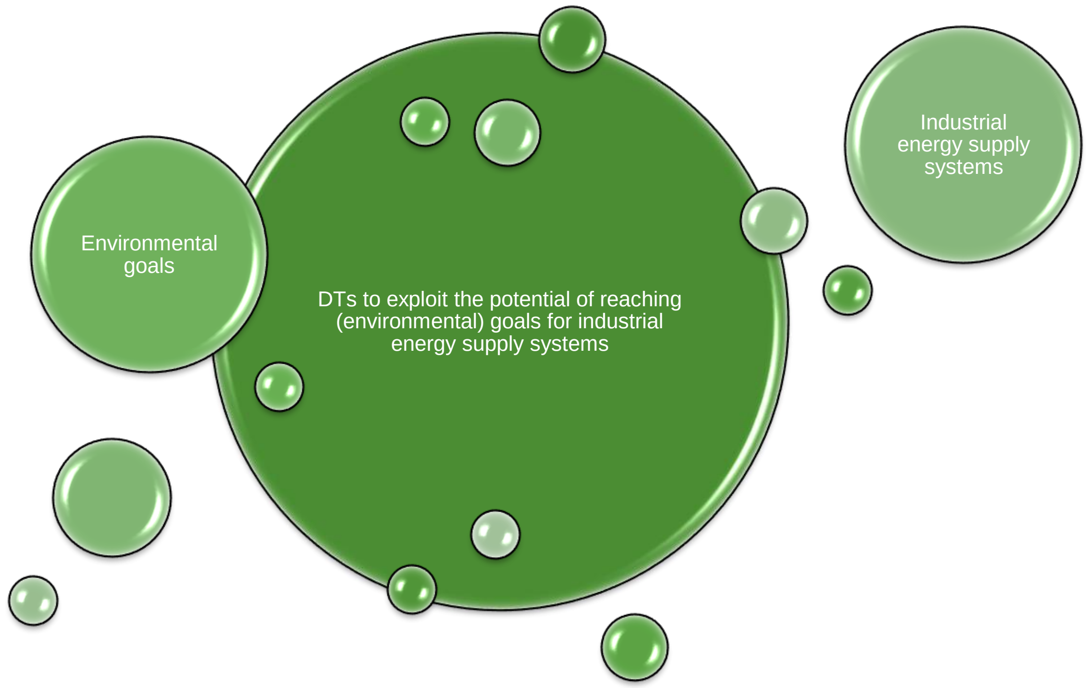

Figure 1 – Within IEA IETS Task XVIII Subtask 2, methods and the application potential of DTs contribution to climate protection measures are addressed for industrial energy supply systems.

However, this subtask does not seek to evaluate the DTs of industrial production facilities itself. Nevertheless, the work in this subtask requires the analysis of interfaces from the production process with industrial energy supply and its impact / relevance for DTs. Examples for such interfaces, considered in this subtask are:

- Sensors (are essential for data collection as basis for DT formulations)
- Prediction of load / demand profiles (are essential for a certain set of DT applications especially in the context of e.g. decision support)
- Application of controllers (are essential to build the connection from the DT to the physical entity again)
- Analysis of flexibility

Different questions and application cases of the DT will be defined in further activities of this Task. For these applications / use cases, the objects and transferred data shall be defined, as outlined in Figure 2 below. Additional information required, includes the following:

- Inputs and forecasts
- Requirements for the generation units and the operation (temperatures, observation of wear and tear, etc.)
- Control structure

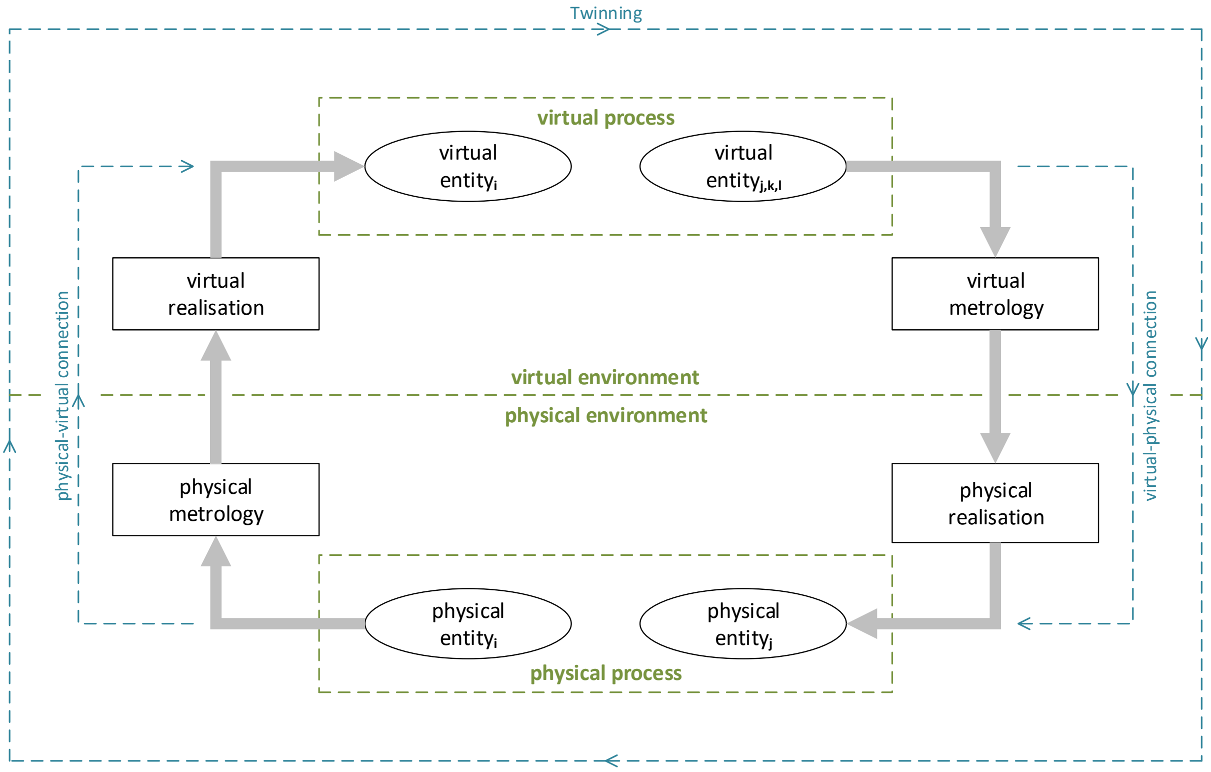

Figure 2 – Visualization of a DT according to Jones et al. (2020)

1.2 System Definition and Boundaries

1.2.1 Multi Energy Systems

In this ***IEA IETS Task XVIII*** we assess DTs in different contexts or systems, with a combination of different primary energy sources, final energy carriers, and energy vectors. These systems are further defined as multi energy systems.

1.2.2 Interfaces

Different types of interfaces become relevant when it comes to DTs. The business unit “Automation and Digitalization” at the Fraunhofer Institute of Optronics, System Technologies and Image Exploitation (IOSB), describes the relevance/role of standardized interfaces for DTs as follows:

> Models from different phases of the life cycle should interact. Due to the well-known heterogeneity of interfaces, this is a big challenge today. Standardized syntax (protocols) and semantics (information models) provide a remedy. Industrie 4.0 components interact with each other via submodels contained in their administration shells (Asset Administration Shells).
>
> Fraunhofer IOSB (2021)

In general, several interfaces have to be clearly defined when it comes to DT implementation and application to ensure usability and successful usage. Examples are machine-machine interfaces, human-machine interfaces, and interfaces between single components.

1.3 Method and Organization of this report

This report was developed along the following lines. Firstly, a literature review was performed to provide a comprehensive knowledge base and background information for Chapter 2. This Chapter gives an overview of derived definitions that can be used in the form of a glossary in the future. This glossary is summarized in the beginning of this document and is the main output of this report. Please refer to ***Table 1 - Glossary***. Furthermore, the results the literature review and the basis for this report were presented in a Task Meeting at the international level in October 2021. This was followed by a survey for the Annex members and interested partners. The relevant findings from this survey regarding definitions and understanding for DTs can be seen in the document "***EXISTING DIGITAL TWIN SOLUTIONS – Report on questionnaire***".

2. Relevant Terms and Definitions – Literature review

The following chapter is organized as follows. Section 2.1 outlines the general terms relevant to DTs. The most relevant technologies and methods regarding DT applications are discussed in Section 2.2, followed by Section 2.3, which outlines how DT can be applied and and its value creation potential.

2.1 General Terms

2.1.1 Digital Twin

A definition of the term DT was already presented in ***IEA IETS Task XVIII Subtask 1***. However, compared to that, the present document gives a much more detailed view. This is because, firstly, the DT is of great importance in ***IEA IETS Task XVIII Subtask 2*** and, secondly, the exact definition of DT is still vigorously debated in today's scientific literature.

IEA IETS Task XVIII Subtask 1 Definition in Whitepaper (Hofmann et al. (2020))

> A Digital Twin is a virtual representation that matches the physical attributes of a "real world" factory, production line, product, or component in real-time, through the use of sensors, cameras, and other data collection techniques. In other words, DT is a live model that is used to drive business outcomes, and can be implemented by manufacturing companies for multiple purposes:
>
> - DT of an entire facility
> - DT of a production line process within a facility
> - DT of a specific asset within a production line
>
> Richter (2019)

As part of ***IEA IETS Task XVIII Subtask 1***, the definition presented in this whitepaper already gives a very detailed view of the DT. However, in addition to many similar definitions, partially contradictory aspects can also be found in the published definitions in literature, some of the most notable of which are outlined below.

Further Definitions

While some state that the first definition of the DT concept was made as early as 2002 in the context of product lifecycle management (Kritzinger et al. (2018)); Grieves (2014), the first actual definition of the DT was given by NASA in 2012 as:

> …an integrated multi-physics, multi-scale, probabilistic simulation of a vehicle or system that uses the best available physical models, sensor updates, etc., to mirror the life of its corresponding twin.
>
> Glaessgen & Stargel (2012)

This early definition, which is until today widely recognized in the field of DT research (Kritzinger et al. (2018)), has given rise to many more , for example Boschert & Rosen (2016) refer to the DT from a "simulation viewpoint" as:

> a description of a component, product or system by a set of well aligned executable models with the following characteristics:

- The DT is the linked collection of the relevant digital artefacts including engineering data, operation data and behavior descriptions via several simulation models.
- The DT evolves along with the real system along the whole life cycle and integrates the currently available knowledge about it.
- The DT is not only used to describe the behavior but also to derive solutions relevant for the real system.

(Boschert & Rosen (2016))

These characteristics very much align with a definition given by Negri et al. (2017) and reported, amongst others by Cimino et al. (2019) and (Kritzinger et al.) (2018):

The DT consists of a virtual representation of a production system that is able to run on different simulation disciplines that is characterized by the synchronization between the virtual and real system, thanks to sensed data and connected smart devices, mathematical models and real time data elaboration.

(Negri et al. (2017))

(Negri et al.) (2017) even went so far as to present a table of 16 separate definitions of the DT in literature.

In a recent review paper (Jones et al.) (2020) summarize a list of key concepts surrounding the DT:

DT	A complete virtual description of a physical product that is accurate to both micro and macro level.
DT Prototype	The virtual description of a prototype product, containing all the information required to create the physical twin.
DT Instance	A specific instance of a physical product that remains linked to an individual product throughout that products life.
DT Aggregate	The combination of all the DT Instances.
DT Environment	A multiple domain physics application space for operating on DTs. These operations include performance prediction, and information interrogation.

(Jones et al. (2020))

Browsing through this literature, one can find that there are some common elements or wording in all of these definitions:

- The DT features (or is in itself) a **virtual representation** of a **real-world asset.**
- This virtual representation is **coupled with** its **physical counterpart** (uni- or bi-directional) and,
- it is based on measured values.

Notwithstanding the above, some aspects are still used inconsistently, for example:

- **(Bi-)directional communication** (See the distinction of Digital Shadow and Digital Model below)
- **Real-time capability** (and if so: What is real-time?)
- **Information** representation **vs.** AI/**model based** computations as virtual representation

IEA IETS Task XVIII Subtask 2

To facilitate greater clarity for future work, we propose the following definition of the DT, as it should be understood throughout Subtask 2:

> A Digital Twin is a virtual representation that matches the physical attributes of a "real world" entity*, through measured values and domain knowledge and features automated bidirectional communication with that entity.

* (Josifovska et al.) (2019) noted that throughout DT definitions, the DT is often seen es either the digital / virtual representation of a ***physical object*** Wagner et al. (2018) or a ***physical entity*** and further raised the very justified question as to what the difference between the two terms is. They state that a *physical entity is an abstraction of a "thing" persisting in the real world, which has to be mirrored or twinned in the virtual world* (Josifovska et al. (2019)).

This is also the general view of the definition here presented DT definition for ***IEA IETS Task XVIII Subtask 2***. As such, the physical entity of a considered DT could be a single process unit or even part of that unit, but also a whole energy system including boundary conditions (e.g. external energy supply systems/grids).

It should be noted however, that this viewpoint should not be seen as a rejection of differing definitions, rather, the authors note that other definitions might also be valid in specific domains and application scenarios.

2.1.2 Categorization: Digital Model / Shadow / Twin

In a recent categorical literature review, (Kritzinger et al. (2018)) introduced a categorization into **Digital Model, Digital Shadow and the Digital Twin**. According to their work, these three terms are often used synonymously in DT literature. However, the given definitions differ in the level of data integration between the physical and digital entity (Kritzinger et al. (2018)) and are sometimes even contradictory Stecken et al. (2019). Definitions for the DT have been stated above.

(Kritzinger et al. (2018)) thus defined the Digital Model as follows.

> A Digital Model is a digital representation of an existing or planned physical object that does not use any form of automated data exchange between the physical entity and the digital entity.
>
> (Kritzinger et al. 2018)

Digital data of existing physical systems might still be in use for the development of a Digital Model, but all data exchange is done manually. According to the definition, a change in state of the physical entity has no direct effect on the digital object and vice versa.

For clarification on the different types of digital models, please refer to Section 2.2.1.

> Based on the definition of a Digital Model, if there further exists an automated one-way data flow between the state of an existing physical entity and a digital entity, one might refer to such a combination as Digital Shadow.
>
> (Kritzinger et al. 2018)

Thus, according to the definition, a change in state of the physical entity leads to a change of state in the digital entity, but not vice versa. This definition is already widely recognized in literature Julian Franzen et al. (2019); Santolamazza et al. (2020); Sepasgozar (2021). The Digital Shadow is also often seen as part or core component of a DT Ladj et al. (2021).

2.1.3 Cyber-Physical System

Similar to the very basic concept of a DT, defined by three different elements(the physical space, the virtual space, and the connection between them to exchange data and information) (Grieves (2014)) a comparable concept from the industrial domain is known as Cyber-Physical System (CPS), or sometimes more specifically as the Cyber-Physical Production System (CPPS).

(Monostori (2014)) describe CPS as

> autonomous and cooperative elements and sub-systems across all levels of production, able to communicate with each other in situation-dependent ways.
>
> (Monostori (2014))

The goal of CPS is to have several elements that can acquire and process data, allowing them to self-control certain tasks and interact with humans Steindl et al. (2020) and achieve collaborative and real-time interaction between the real and digital worlds through feedback loops and the interaction between computational and physical processes Cheng et al. (2016). Hence, a certain kind of virtual representation of the production system must be available, thus enabling a characterization of a CPS by a physical entity and its cyber counterpart, which is also a prerequisite for the DT (Negri et al. (2017)). Therefore, some researchers see a DT as only the digital model inside a CPS Lu et al. (2020),this conversely implies that a DT is the prerequisite for a CPS (Jones et al. (2020)); (Steindl et al. (2020)). This aligns with Negri et al. (2020), who found that papers in the manufacturing field mention the use of the DT to simulate a CPS. Zheng et al. (2019) state that the DT in the broad sense belongs to the CPS but has a higher fidelity degree focusing more on data and models with ultra-high-fidelity simulations.

2.1.4 Cyber-Physical Production System

Cyber-Physical Production Systems (CPPS) also often stand as a synonym for the future factory environment, often also called Smart Factory Weyer et al. (2016). In such a smart factory or CPPS, all field devices, tool machines, production modules and product will turn into CPS allowing for autonomous information exchange and triggering of actions within an CPPS Lee et al. (2015).

One proposed definition is:

> The application of the generic concept of Cyber-Physical Systems to industrial production systems is known as Cyber-Physical Production Systems.
>
> (Perez et al. 2015)Perez et al. (2015)

(Rojas & Rauch (2019)) put it even more plainly and stated:

> When Cyber-Physical Systems are connected to perform smart manufacturing, we have a Cyber-Physical Production System.
>
> (Rojas & Rauch (2019))

2.1.5 Industry 4.0

The term Industry 4.0 (I4.0) was first introduced in an article published by the German government in November 2011, referring to the fourth industrial revolution Zhou et al. (2015). However, there is no widely accepted definition for the term Industry 4.0 (Stecken et al. (2019)). According to (GTAI (2014)),

> Industry 4.0 represents the technological evolution from embedded systems to cyber-physical systems. In Industry 4.0, embedded systems, semantic machine-to-machine communication, Internet-of-Things and Cyber-Physical System technologies are integrating the virtual space with the physical world. In addition, a new generation of industrial systems, such as smart factories, is emerging to deal with the complexity of production in cyber-physical environment.
>
> (GTAI (2014))

I4.0 can also be characterized by Manzei et al. (2016):

- The dynamic connection of internal and external data sources and
- the automated analysis and processing of thereby generated information
- for demand-driven preparation or control of processes,
- located at different points in the value chain of an industrial company,
- to make them faster, cheaper, customer oriented, more efficient, resource-saving and flexible.

2.1.6 Energy 4.0

The declared goal of Energy 4.0 (E4.0) is to exploit efficiency- and flexibilization-potentials in processes to optimize the conversion, distribution and consumption of energy Rehtanz (2015).

> In analogy to Industry 4.0, Energy 4.0 stands for the transition to energy systems of the fourth generation, sometimes also referred to as smart energy systems. These energy systems will be based on renewable, volatile energy carriers, a high amount of flexibilization, and interconnection between different industry sectors and feature extensive application of digital technologies.
>
> (Lund et al. (2017)); (Robison et al. (2015))

2.1.7 Key Performance Indicators

In general, the interaction of DTs and key performance indicators (KPIs) can be understood in two ways:

- The DT receives KPIs regarding the performance of the process as input information from physical entity and bases operation on these KPIs (can be e.g., aggregated / calculated data from processes).
- Furthermore, KPIs can also be defined for the DT itself.

In the following, interesting process-related KPIs, regarding the performance and sustainability (aligned to the overall topic of this IEA IETS Task XVIII) of an energy supply and conversion system are listed:

- Levelized Cost of Heat (LCOH) / Levelized Cost of Energy (LCOE): estimating the average cost of electric power generation over the lifetime of power plants
- Payback period: indicating how much time is needed to recover the initial investment. It can be calculated by dividing the initial investment in € by the yearly savings in €/a
- Long-term economic evaluation: consideration of the yearly costs over a long period of time and the calculation of the accumulated costs. A good approach is to calculate the net present value (NPV)
- CO_2 emissions: environmental indicator, the CO_2 emissions associated with the fuels are estimated by using pre-calculated emission factors on the primary energy consumption.
- Primary and final energy consumption: The primary energy consumption (PE) is directly associated with the cost of operation of heat and power, and with the CO_2 emissions, depending on the type of fuel that it is used. The final energy consumption, as a performance indicator, helps to analyze the impact on the consumer side
- Share of renewables: represents the share of energy produced by renewable energy sources out of the total energy produced. Notice that Internal use of waste heat is in general not to be considered since it has already been produced from one of the main energy production units (or grid)
- Energy flexibility and stability: extent to which a power system can modify energy (electricity and heat) production or consumption in response to variability, expected or otherwise
- Autarky degree: indicates the degree of self-sufficiency. We calculate it based on the energy produced by the different energy production units, dividing the self-production by the total energy produced/imported
- Surface needed: amount of area needed for the technical solution is indeed a relevant KPI, especially for solar technologies

2.1.8 Optimization

In general, “optimization” is often understood as improvement of a system, a process or a unit without a systematic consideration to what extent of the best possible solution (for a specific optimization criterion) this improvement was done. Within this work and further activities in the project “optimization” is used for systematic approaches to determine the best solution for a previously defined criterion (objective function) under given frame conditions or without violating defined limitations (constraints).

Here, optimization is the selection of “the best” solution. In terms of industrial systems, optimization can be understood as the adjustment of a process or system to optimize some specified set of parameters (KPIs) without violating any constraints including the product quality. In this context, often applied goals are:

- maximizing energy, resource efficiency and the share of renewable energy or
- minimizing CO_2 emissions, cost (CAPEX and OPEX), losses, etc.

> Optimization is generally understood to be the search for the best possible solution in the sense of a certain goal in a decision-making area, whereby frame conditions can be taken into account.
>
> (Floudas & Pardalos (2008))

Further insights in different application fields of optimization are given in sections 2.2.8 and 2.3.5

2.1.9 Digitization

The term digitization generally refers to the conversion of analogue data into a digital form. Within this scope, "digitization" is considered as a primarily technical term, contrary to "digitalization", which is often used with a different meaning (see 2.1.10).

> Digitization is the process of changing data into a digital form that can be easily read and processed by a computer.
>
> (Oxford Online Dictionary (2021))

2.1.10 Digitalization

Digitalization is sometimes used synonymously with the term Digitization (see 2.1.9), i.e., the practice of converting information into a digital form that can be processed by a computer. However, from a socio-economic perspective, the aim of digitalization is not only to convert analogue to digital signals but also to create value using digital content Kemmerich & Storch (2016). The following definitions have been found:

> In the context of industrialization, digitalization describes the transition to new, disruptive business cases driven by evolving Information and Communication Technologies, the automation and flexibilization of business operation and the interconnection of information, things and operatives.
>
> (Hanschke (2018))

> Digitalization, enabled by Industry 4.0 technologies allow a remotely sense, real-time monitoring and control of devices and cyber physical production elements across network infrastructures.
>
> (Negri et al. (2017))

To emphasize this fundamental change, the term "digital transformation" is also often used, especially if the change is happening on multiple levels, including the process level, organization level, business domain level and society level Parviainen et al. (2017).

2.1.11 Services

In Industry 4.0, services in general and especially services related to physical products play an increasingly important role Tao & Qi (2019).

> To solve the problem of interoperability between a digital twin and different users / stakeholders and to enable innovative business models, the functions of the digital twin can be encapsulated into standardized services with user-friendly interfaces for easy and on-demand usage.
>
> (Tao et al. (2019))

Services are a main part of a DT and one of five dimensions of DT modelling in the 5D-concept proposed by (Tao et al. (2019)). A DT without services just copies a real physical entity without further evaluation. Services can be grouped into (Negri et al. (2017)); (Jones et al. (2020)); Padovano et al. (2018):

(1) functional services,
(2) enterprise services,
(3) application services, which are confined to specific application content and
(4) infrastructure services

Due to the important role of services inside a DT, ontology-based smart service architectures for DT are recommended, often based on RAMI4.0[2] Adolphs et al. (2015), acting as foundation for data integration and data exchange between various applications as part of the DT functionality Koschnick (2020); Steindl et al. (2019); (Steindl et al. (2020)).

[2] RAMI 4.0 defines a service-oriented architecture. Application components provide services to other components via a communication protocol over a network. The basic principles are independent of providers, products and technologies. The aim is to break down complex processes into easily understandable packages, including data protection and IT security.

2.2 Basic Technologies and Methods (Requirements)

2.2.1 Modeling approaches

The following definition has been found in a whitepaper within the project "Industrial internet consortium" by Malakuti et al. (2020).

> A digital twin should contain computational or analytic models that are required to describe, understand and predict the twins' operational states and behaviors, and models that are used to prescribe actions based on business logic and objectives about the corresponding real-world object. These models may include models based on physics or chemistry, engineering or simulation models, data models based on statistics, machine learning and Artificial Intelligence. It may also include 3-D models and augmented reality models for aiding human understanding of the operational states or behaviors of real-world objects.
>
> (Malakuti et al. (2020))

Here, we use modeling in the sense of the task of creating a virtual representation of some real system (or a process, a component, an entity, etc...). The model can then be used to compute certain properties or make predictions of the behavior. There is a vast number of different modeling approaches. Generally speaking, the best suited modeling approach for a given modeling task is determined by the available information and the purpose of the model. Further relevant characteristics of models are:

- Performance
- Real-time capability
- Level of detail
- Resolution of the entity in time, process level etc.

Therefore, the following definition can be derived.

> In the context of digital twins modeling is understood as the task of creating a virtual representation of some real system in order to compute certain properties or make predictions of the behavior. Different modeling approaches can be applied. Relevant characteristics of models are performance, real-time capability, level of detail, resolution of the entity in time or process level etc.

The following classifications and distinctions of models can be made:

Dynamic vs. (quasi-)stationary models

Dynamic models can reproduce the time-dependent behavior of a system, including the dynamic transition between two (quasi)-stationary states. (Quasi-)stationary models, on the other hand, are only valid if the system is in a stable state. This is an acceptable simplification, if the system is operated in a stable state most of the time and state-transitions are not of interest.

White Box, Grey Box & Black Box modeling

Modeling approaches can be distinguished based on the type of information that is required for the modeling. On the one extreme, models can be built based exclusively on analytical knowledge about the system - i.e., equations that describe the physics of the system. This is usually termed as *White Box* or *physical* modeling, because we know exactly what is going on inside the model. On the other extreme, models can be derived from empirical data with virtually no knowledge about the system. These approaches are called *data-driven* or *Black Box* modeling, because the model output is computed by some algorithm, but the inner working of the model remains obscure.

Most modeling approaches cannot be classified as either *Black Box* or *White Box*. Rather they use a combination of physical knowledge and empirical data. In that sense, it is useful to think of this classification as a continuum with White Box models on one end and Black Box models on the other. In-between, there are various shades of *Grey Box* modeling.

Adaptive vs. static models

Traditionally, modeling was a laborious task done by experts. Once a model was set up, it could not be adapted without a big effort. With the advent of data-driven modeling, this is no longer the case. With the right strategies, models can be adapted automatically based on real-time data. This is especially valuable for systems that change over time (due to wear, degradation, etc....). With adaptable models, accurate predictions of the system behavior can be computed, where static models would yield inaccurate results.

Stochastic vs. deterministic modeling

Stochastic modeling defers from deterministic modeling in that it features at least one random variable. The uncertain variables are usually modeled by means of statistics and probabilistic constraints, through probability density functions Li & Dong (2019). Typical stochastic modeling approaches include scenario representation, stochastic modeling and chance constrained stochastic modeling Alqurashi et al. (2016).

Causal vs. acausal models

In causal modeling, the modeled system is, directly or indirectly, described by a system of ordinary differential equations (ODE) in explicit form Schweiger et al. (2020). Simply speaking, causal models feature direct equations, where it is clear how the unknown quantities are derived from the known ones, hence “causal”. However, the development of such models becomes difficult especially for large scale systems François E. Cellier, Hilding Elmqvist, Martin Otter (1996). This led to the development of the acausal approach where models essentially are expressed in terms of undirected equations (Schweiger et al. (2020)).

2.2.2 Big Data

In general, the term "big data" became established when huge amounts of digital data sources and storage abilities became possible. This field deals with data processing faced with increasing and rapidly growing data availability. Three characteristic traits of big data, proposed by Doug Laney in 2001 are: volume (enormous data quantity), velocity (created in real-time) and variety (being structure, semi-structured and unstructured) (Hofmann et al. (2020)).

> Big data is high-volume, high-velocity and high-variety information assets that demand cost-effective, innovative forms of information processing for enhanced insight and decision making.
>
> (Gartner (2021))

2.2.3 Information and Communication Technology

Information and Communication Technology (ICT) is a very broad field extending the information technology (IT) domain. Due to powerful technological developments in this field, it is considered as a key driver for digitalization and encompasses essential enablers for DTs.

> The term "Information and Communication Technology" is generally accepted to mean all devices, networking components, applications and systems that combined allow people and organizations (i.e., businesses, nonprofit agencies, governments, and criminal enterprises) to interact in the digital world.
>
> (Pratt (2021))

2.2.4 Sensors and data acquisition

Sensors are technical components measuring certain physical or chemical properties qualitatively or quantitatively. These measured variables are recorded and converted into further processable electrical signals. In general, the following classifications for sensors are used (Hofmann et al. (2020)):

- active & passive sensors (they either generate an electrical signal based on the measuring principle or require auxiliary energy supplied from outside to generate an electrical signal)
- based on the measuring principle (e.g. mechanical, resistive, piezoelectric, capacitive, optical, acoustic, magnetic sensors) Hoffmann (2015)
- Smart sensors represent a new classification category. They process data in an intelligent way, provide additional information about their environment or about themselves and can communicate within a sensor system (e.g. to improve measurement accuracy) Wollert (2015).

Especially this last category gains importance due to a new development in computing and communication/ IT, the Internet of Things (IoT), see section 2.2.5.

> A device that responds to a physical stimulus (such as heat, light, sound, pressure, magnetism, or a particular motion) and transmits a resulting impulse (as for measurement or operating a control).
>
> (Merriam Webster (2021))

2.2.5 Internet of Things (IoT)

In general, the Internet of Thing (IoT) is understood as connection between physical devices on the basis of internet technology. Mentioning of IoT started around 2005, e.g. in a report by the International Telecomunications Union (ITU):

> Machine-to-machine communications and person-to-computer communications will be extended to things, from everyday household objects to sensors monitoring the movement of the Golden Gate Bridge or detecting earth tremors. Everything from tires to toothbrushes will fall within communications range, heralding the dawn of a new era, one in which today's internet (of data and people) gives way to tomorrow's Internet of Things.
>
> International Telecommunications Union (2005)

In subtask 1 of this IEA IETS Task XVIII the following definition was presented in the whitepaper:

> The IoT is a concept, in which basically any device - mechanical or digital - is connected in a network with the ability to transfer data without the requirement of human interaction.
>
> (Hofmann et al. (2020))

2.2.6 Ontology/ Knowledge representation

Knowledge presentation and reasoning, sometimes also referred to as knowledge engineering, is a promising field of AI and IT. This discipline attempts to integrate knowledge into computer systems to develop solutions for complex problems.

> Ontologies are knowledge representations of a domain that contain explicit descriptions of concepts, properties, attributes or features of those concepts and logical restrictions on the classes and properties. They are explicit conceptualization of objects, concepts, and their relations that form a knowledge base as well as the basis of what “exists” in a “universe of discourse” for AI systems.
>
> (Hofmann et al. (2020))

Data analysis methods in combination with domain knowledge from ontologies can be used to analyze and semantically enrich the time series data, i.e. to add certain metrics to the data and to automatically identify and label inconsistencies (Steindl et al. (2019)). Therefore, ontologies are considered a key enabler for digital twins.

2.2.7 Simulation

Simulation is a key aspect for digital twins and energy systems modelling. Within the meaning of computer science, we consider its definition as follows.

> Simulation is the prediction of a real-world process or system with given parameters over time.

Simulations require the use of models, which represent the key characteristics and behavior of the given process of system, and which are executed by computers to produce a simulation.

2.2.8 Optimization method

Depending on the set optima criteria, a process or system can be optimized. In many cases the step of the optimization is a mathematical optimization (mathematical programming) and addresses the selection of the best element (Elements), with regard to set criterion, from a set of available alternatives INFORMS (2014).

Optimization problems of sorts arise in all quantitative disciplines from computer science and engineering to operations research and economics, and the development of solution methods has been of interest in mathematics for centuries Du et al. (2008).

Applying digitalization, an industrial system is modelled and simulated, consisting of mathematical functions and the optimization problem is maximizing or minimizing one or more of these functions. Again, the optimization can be done for decarbonization of a system, exergetic optimization, economic optimization, etc.

2.2.9 Virtual reality (VR)

In general, virtual reality can be understood as a simulated experience in the fields of entertainment, education and business, including e.g. virtual meetings. Augmented reality in comparison is a "more extended" aspect of the experience. A general definition of virtual reality is the following one:

> Virtual reality is a technology where the user can immerse into a virtual environment and can roam and interact with it.
>
> (Zhou & Deng (2009))

2.2.10 Augmented reality (AR)

Augmented reality is a technology which aims to blend a virtual and the real world. E.g., virtual images are added to the real environment or elements of the real environment are removed. Jetter et al. (2018)summarize that augmented reality does not necessarily create a new artificial reality but overlays additional virtual information on real objects or surroundings. This technology can be extended to all senses Azuma (1997). (Azuma) (1997) identified potential for application in many fields such as medical treatment, entertainment, or industry and divided augmented reality in three important components: virtual reality fusion, real-time interaction, and 3D registration. An early definition for augmented reality is

> A system that supplements the real world with virtual (computer-generated) objects that appear to coexist in the same space as the real world.
>
> (Azuma et al. (2001))

Further definitions on the topic can be found e.g. by Billinghurst et al. (2015). However, lately augmented reality has been mentioned as visualization tool for DTs to improve different aspects of manufacturing. Thus, the range of applications and the relevance of augmented reality for DTs is expected to grow in the future.

2.3 Applications and value creation based on services by Digital Twins

On a DT platform multiple services can interact with each other and have access to various interfaces and data sources. A benefit is that the data is managed in one central place. Data pre-processing has only to be done once and this also ensures that all services have the same information. Certain functionalities, like a specific simulation model, can be encapsulated as a service and then be used by various other services.

2.3.1 Condition Monitoring

Similar to the definitions in Álvarez Tejedor et al. (2011) and Chaulya & Prasad (2016), Condition Monitoring (CM) can be described as

> The assessment of the current condition of a physical entity by employing measurement data.

By preprocessing the raw data (normalization, PCA, Feature Extraction, sensor fusion, soft sensors, …) valuable information about the current state of the physical entity is gathered and further utilized in several CM-related Services like *Fault Detection and Classification* or *Predictive Maintenance*.

Fault Detection and Classification

The goal of fault detection and classification in the context of a DT is to automatically detect and classify faulty conditions of the physical entity based on the information provided from condition monitoring in order to enhance the safety and reliability of industrial process operations Shokry et al. (2016). For complex classification tasks, machine learning methods (e.g. Support Vector Machines, Decision Tree, k-Nearest Neighbor, Artificial Neural Networks, …) often come into use.

Soft sensors

Soft sensors, sometimes also technically denoted as inferential estimators, represent an attractive approach for estimating primary process variables, especially when conventional hardware sensors are not available, too expensive or when technical limitations hamper their on-line use Zamprogna et al. (2005). They typically use models and measured secondary process variables to provide additional information on the state of the process.

2.3.2 Types of Maintenance

Predictive Maintenance

As stated by (Sinha et al. (2010)), the main objective of predictive maintenance is to employ the information gathered from condition monitoring to predict the point of time at which maintenance activities are the most cost-efficient and before the physical entities optimal performance deteriorates.

Preventive Maintenance

In contrast to predictive maintenance, preventive maintenance is performed periodically. It is meant to prevent the physical entity from sudden failure and/or deterioration in efficiency by inspecting, servicing and replacing critical parts of the physical entity on a predetermined frequency. Similar definitions can be found in Mokhatab et al. (2019), (Álvarez Tejedor et al. (2011)) and Papavinasam (2014).

Reactive Maintenance

Reactive maintenance, also known as breakdown maintenance, is the type of maintenance which is performed at a point of time at which a critical failure of a significant deterioration in efficiency already occurred in a certain part of the physical entity. Due to higher downtime and maintenance cost compared to predictive and preventive maintenance, reactive maintenance only plays a minor role in the context of DTs.

2.3.3 Predictive control

Basic process control systems, e.g. PID-based control schemes, are integrated in the process components to ensure basic requirements for operation and automation. Advanced process approaches are usually integrated in higher layers, often later than basic PIC controllers. Their aim is to consider performance or improvement and optimization potentials in the process. Advanced process control systems combine process knowledge with control techniques in an intelligent way. They enable considering coupled, multi-variable system dynamics. Lately, developments in this field focused on model-based control, e.g. adaptive or model predictive control. Examples are: fuzzy control, robust control, neural network-based control, optimal control, etc. (Hofmann et al. (2020))

> Typically, advanced control methods involve more complex calculations than the conventional PID controller algorithm. Advanced control has the following features:
>
> - Process modeling and parameter identification (off-line or on-line)
> - Prediction of process behavior using process model
> - Evaluation of performance criterion; subject to process constraints
> - Optimization of performance criterion
> - Matrix calculations (multi-variable control)
> - Feedback control
>
> (Airikka (2004))

2.3.4 Forecasting

> Forecasting is a common statistical task in business and is about predicting the future as accurately as possible.

Therefore, all available information including historical data and knowledge of any future events that might impact the forecasts are needed to achieve a precise forecast. There are different things which can be forecasted. Some can be easier forecasted than others. Several factors affect the predictability of an event or a quantity including:

- How well do we understand the factors that contribute to it
- How much data is available
- Whether the forecasts can affect the thing we are trying to forecast

Forecasts can be classified in the three different groups short-term, medium-term, and long-term forecasts. This classification describes how long the prediction horizon is. Another way to classify forecasts is to separate them qualitative and quantitative forecasts. For the DT quantitative forecasts are in focus. In the field of the DT various objects are interesting for a forecast. Some of them are energy demand, production capacity, redispatch potentials, downtimes, remaining useful lifetime etc.

2.3.5 Decision Making Support

Decision support systems for industrial systems gain attractiveness due to raising complexity, competition and challenging requirements from legal and regulatory frameworks.

> A decision support system is a computer-based application that collects, organizes, and analyzes business data to facilitate quality business decision-making for management, operations and planning. A well-designed decision support system aids decision makers in compiling a variety of data from many sources: raw data, documents, personal knowledge from employees, management, executives and business models. Decision support system analysis helps companies to identify and solve problems and make decisions.
>
> (Techopedia (2021))

In the context of industrial applications, often optimization methods are applied to support decision making regarding both, strategic decisions such as investments and pricing decisions and operational decisions. The following two optimization approaches are partly already used in real tools and applications.

- **Design Optimization**: Optimization of the technical specifications of an entity (e.g. capacities of machines, plants, ...).
- **Operational Optimization**: Optimization of the usage of given units (time schedule and operation mode), optimal scheduling of production, storage management, ...

DTs have the possibility to offer the service of decision support when applied in industrial environment.

2.3.6 Flexibility

In general, “flexibility” is used to characterize different properties for industrial systems. A rather general approach is to define flexibility as opportunity to achieve a specific outcome in different ways or the sensitivity of manufacturing systems to change Chryssolouris (1996). This is summarized in the following definitions. A very short, but rather comprehensive definition was given by (Golden & Powell) (2000).

> Flexibility is the capacity to adapt.
>
> (Golden & Powell (2000))

A more extensive definition can be found in Wikipedia.

> In the context of engineering design one can define **flexibility** as the ability of a system to respond to potential internal or external changes affecting its value delivery, in a timely and cost-effective manner. Thus, flexibility for an engineering system is the ease with which the system can respond to uncertainty in a manner to sustain or increase its value delivery.
>
> Wikipedia (2020)

(Chryssolouris) (1996) distinguishes between the following types of flexibility:

- Machine flexibility – ability to make a change required for specific production processes
- Process flexibility – ability to produce in different ways with different materials
- Routing flexibility – ability to handle breakdowns and continue operation
- Volume flexibility – ability for economic operation for different volumes

- Expansion flexibility – ability to expand system easily or in modular way
- Operation flexibility – ability to interchange ordering of operations for each part type
- Production flexibility – universe of part types a system can produce

In the following examples different meanings for the term flexibility are given. A more detailed overview of different types of flexibility and their rather low correlation is analyzed for pulp and paper factories by Upton (1995).

Flexibility in production

Regarding the product-related view the following understanding of flexibility could be detected:

- Flexibility of product type (often considered as lot size 1), e.g. 3-D printers but also large production units which can easily change between different types of products (e.g. same paper machines for specific papers)
- Flexibility in the actual production amount (often mentioned as examples for flexible processes in "scheduling" or demand side management analysis)

Flexibility of energy supply

Here, two main contributions how flexible unit operation can be distinguished:

- Flexibility regarding how energy is provided
    - Using more than one energy-carrier in one energy supply, conversion of storage unit (e.g. hybrid-fired units)
    - Fulfilling one demand level with more than one energy supply unit and thus more than one energy carrier (e.g. heat-only-boilers and power-to-heat units to supply steam)
- Flexibility regarding how fast the energy supply schedule can be changed in order to react to changing circumstances (prices, production changes, failures, etc.)
    - This can be realized by fast ramping and fast starting energy supply units (often understood as "flexible units")
    - Another option is to operate storage units or combinations of storage and production units in such a way (decouple supply and consumption time) that flexibility can be provided by them

By combining the flexibilities mentioned above another aspect comes along: the importance of **when** energy is provided ("be flexible in the planning"). Not only flexible units but also the respective planning tools can help to provide flexibility. Here, above-described concepts of operational optimization of energy supply systems can help to take advantage of the flexible components in industrial production and energy supply systems.

Another important concept often mentioned in related discussions is "Demand Side Management". The target of Demand Side Management is a flexible load control to enhance energy efficiency and cost optimization. Examples for demand side management can be

- Peak shaving
- Valley filling
- Load shifting

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