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Review

Methodology for the Development of Virtual Representations within the Process Development Framework of Energy Plants: From Digital Model to Digital Predictive Twin—A Review

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Abstract: Digital reflections of physical energy plants can help support and optimize energy technologies within their lifecycle. So far, no framework for the evolution of virtual representations throughout the process development lifecycle exists. Based on various concepts of virtual representations in different industries, this review paper focuses on developing a novel virtual representation framework for the process development environment within the energy sector. The proposed methodology enables the continuous evolution of virtual representations along the process development lifecycle. A novel definition for virtual representations in the process development environment is developed. Additionally, the most important virtual representation challenges, properties, and applications for developing a widely applicable framework are summarized. The essential sustainability indicators for the energy sector are listed to standardize the process evaluation throughout the process development lifecycle. The virtual representation and physical facility development can be synchronized by introducing a novel model readiness level. All these thoughts are covered through the novel virtual representation framework. Finally, the digital twin of a Bio-SNG production route is presented, to show the benefits of the methodology through a use case. This methodology helps to accelerate and monitor energy technology developments through the early implementation of virtual representations.

Keywords: virtual representation; digital twin; process simulation; sustainability; process development

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1. Introduction

Digitization plays an essential role in everyday life. A continuous digital transformation can be observed since the early 1990s, especially in the economy and research sectors [1]. Thus, novel business models have emerged, and the vast potential for efficiency has increased as savings on energy, emissions, and cost in the manufacturing and energy sector have arisen [2]. Regarding the energy transition in the European Union, the climate goals should be reached by following the climate and energy framework 2030 [3], which will be executed by the Renewable Energy Directive (RED II) [4]. Therein, it is formulated that climate neutrality should be reached by rapidly reducing greenhouse gas emissions by integrating renewable energy carriers into the energy sector. Furthermore, the main targets are improving energy efficiency and reducing final energy consumption. Digitization can help support the energy transition process by speeding up the development of innovative renewable processes and optimizing energy efficiency. To enable a smart interconnected energy system [2,5], a horizontal and vertical cross-linking of energy producers, distributors and consumers has to be realized [6]. Borowski et al. [7] mentioned that digitization in the manufacturing and energy sector can lead to cost improvements of more than 25% compared to conventional productivity improvements [7]. Furthermore, digitization can increase the lifetime of energy plants by up to 30% [7]. Additionally, due to the increasing number of volatile energy technologies in the energy system, the supply security could be improved by advanced digital methods [2].

To achieve the proposed goals of climate neutrality by 2050 in the European Union, the development of novel environmentally friendly and innovative technologies must proceed quickly. The limited time leads to market competition within the renewable energy sector. On the one hand, the competition increases the efforts to develop novel technologies. On the other hand, the scale-up of novel, innovative energy technologies is often executed too early. Consequently, energy technologies that are not fully developed are scaled to the commercial and industrial scales without describing the full behavior of energy technologies with simulation models [8]. Since the physical plant is often better developed than the virtual representation, the same issues occur repeatedly. The solution to this problem can be the early evolution and implementation of virtual representations [9] within the process development, called frontloading [10]. Similar to virtual product development [10], early integration of virtual representations can help to save considerable time and money in the development process [10]. Furthermore, the virtual representations help to define ideal scale-up dates by determining and tracking milestones in the process development path. Figure 1 represents the cost reduction potential through frontloading and learning during process development. Therein, the theory of the increasing fixed production costs along the process development and the theory of learning and innovation in the technology rollout phase is combined [11]. By analogy with product development, it can be seen that about 65% of the production costs are defined in the conception phase [10,12]. Therefore, most of the energy production costs are determined within the conception phase by determining the input streams and process units. The early integration of virtual representations helps to compare different cost-effective process configurations [10]. Furthermore, development progress can be evaluated and validated by implementing virtual representations.

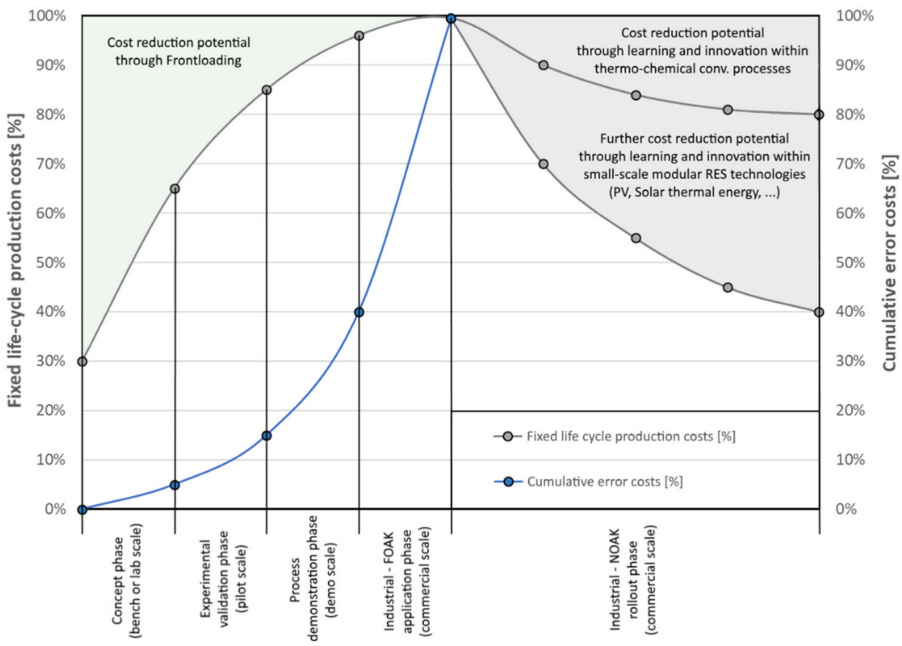

Figure 1. Cost reduction potential through frontloading and learning during process development [10–17].

In contrast to product development, developed processes are erected in lower quantities. Because the same process units are often used in different applications, advanced modeling techniques can help to lead the way towards a novel, cost-effective, renewable technology. Besides the acceleration of the development progress, virtual representations can also help to optimize the whole lifecycle of an energy plant from the early conception until the disposal phase [18]. Finally, the learning and innovation within the rollout phase of novel energy technologies can be supported by virtual representations through state-of-the-art knowledge transfer.

To exploit this cost reduction potential in the energy sector, methodologies, frameworks, and standards must be introduced to harmonize the heterogenous technology landscape [2]. Integrating standardized frameworks and methodologies within the process development sector can help to accelerate the development of novel environmentally friendly technologies.

So far, no framework for the evolution of virtual representations throughout the process development lifecycle exists. Therefore, this paper first reviews the existing literature in the area of frameworks, methodologies, properties, applications, and definitions for the development of digital twins in different industries. In Table 1, the review methodology is summarized. To improve the reliability and variety of the review process, three different databases were searched. Consequently, more than 130 papers were selected for the evaluation process. Within the evaluation process, the relevance of every paper was assessed by screening the title, abstract, introduction and conclusion. From the selected papers, more than half were excluded due to applications from non-comparable industries or misleading use of the terms "virtual representation" or "digital twin". Finally, a total of 53 papers were included in this review paper.

Table 1. Methodology of screening papers.

Databases	**ScienceDirect, Scopus, and Google Scholar**
Article Type	Scientific articles published in peer-reviewed journals or conferences, white papers, and books
Search Strings	"digital twin", "digital shadow", "digital model", "virtual representation", "product avatar", "cyber-physical equivalence", "cyber-physical production system", "virtual testbed"
Search Period	From January 2015 to June 2022
Screening Procedure	The relevance of the articles examined was determined by reviewing the title, abstract, introduction, and conclusion.
Exclusion Criteria	Several publications were excluded for the following reasons: ➢ Investigated industry is very different from the energy sector; ➢ Investigated application was misleadingly named as a digital twin or virtual representation.
Classification Scheme	The selected publications were divided into five groups: ➢ Frameworks and methodologies of virtual representations; ➢ Review articles about virtual representations; ➢ Definitions of virtual representations; ➢ Simulation models, emulation and Artificial Intelligence; ➢ Data communication.

Summing up the literature review, there are many ongoing investigations in the field of virtual representations around the world. Most of the screened methods and concepts focused on the manufacturing sector. As mentioned in several studies, no unified modeling framework for virtual representations exists [2,19–21]. One of the reasons for this lack of concepts and frameworks is the heterogenous landscape in terms of data communication and software tools [2,20]. In this context, there are many different requirements in several industries. Further, the digitization in the industry is strongly influenced by the considered sector [20]. In the energy industry, few digital twins have been developed. However, there is a high demand for digital twins, especially in dispatch optimization problems and operational control [19]. There is also significant potential in the virtual verification and monitoring of plants. In the energy sector, virtual representations are mainly used as a support instrument for the engineering process [20]. However, none of the mentioned studies deal with designing a new technology from scratch [20].

To enable the wide use of virtual representations in all phases of the energy plant lifecycle, a unified modeling framework for developing energy technologies has to be introduced. The interaction between the physical facility and the virtual model should be defined within every stage of process development. Furthermore, the scale-up of energy technologies could be supported by accompanying virtual representations to monitor development goals within each process development stage. The development of virtual representations is often costly and challenging due to the mismatch between the physical process and the models. A unified framework helps to determine the required granularity, accuracy, and complexity in every process development phase [22,23], which leads to appropriate models. These models could preserve the process knowledge of experts and scientists during the development cycle of novel energy technologies. In addition to the virtual representation of the physical process in the simulation model, data availability and quality [2] have to evolve during the process development path. Therefore, the need for smart sensors and advanced data communication tools [2] arises. Furthermore, the topic of data security [19] has become more and more important within the development cycle. Finally, a unified modeling framework helps to support the multidisciplinary approach of process development to generate state-of-the-art virtual representations of energy technologies with particular regard to multicriteria optimization to support the way towards climate neutrality.

The present review paper discusses the idea of providing a unified modeling framework in process development within the energy sector. Process development should be accompanied by high-fidelity virtual representations to optimize and accelerate the development progress. Therefore, the monitoring of the process development progress should be reached by introducing a model readiness level, which implies that the development progress of the physical energy plant and the virtual model are in line. Finally, the focus should be on the multicriteria optimization of energy technologies concerning sustainability in each process development stage. For the elaboration of this novel framework, the present review paper contains the following parts:

- The summary of existing concepts of virtual representations;
- The comparison of different definitions of virtual representations;
- The collection of possible applications, challenges and properties of virtual representations in the energy sector;
- The ascertainment of sustainable development goals and sustainability indicators concerning process development;
- The definition of process development stages with the introduction of the modeling readiness level;
- The development of a unified modeling framework for the optimized development of novel energy technologies with a particular focus on the interaction between the physical facility and the virtual model.

2. Concept and Methodology

For the conception of a process development framework based on the integration of virtual representations, some fundamental topics must be discussed. First of all, a summary of existing concepts and definitions of virtual representations in different fields of applications are investigated. Furthermore, energy plant lifecycle phases and hierarchy layers are discussed to obtain an overall picture of possible stakeholders of virtual representations in the energy sector. The properties, challenges and applications of virtual representations build the basis for possible usage settings. To obtain an overall picture of the technology's impact on the environment, sustainability indicators for the process development are summarized. Additionally, the technology scale-up levels and levels of process engineering are explained. Finally, the novel modeling readiness level is introduced as the basis for the following development framework.

2.1. Existing Concepts and Methodologies of Virtual Representations

In the last decade, numerous researchers and international institutions created reviews regarding the development and application of virtual representations of physical objects. First, Kritzinger et al. [9] mentioned that there is no common understanding of the term “digital twin” in manufacturing. Therefore, Kritzinger et al. [9] and Aheleroff et al. [24] introduced a definition according to the level of integration. This means that a virtual representation of a physical object can be classified as a digital model, digital shadow, digital twin, or digital predictive twin. Furthermore, Qi et al. [25] and Tao et al. [19] reviewed big data and digital twin approaches, focusing on manufacturing, product design, health management, and some energy-related sectors. Additionally, five digital twin dimensions were introduced [19]. The review papers from Liu et al. [20,26] are also strongly connected to the manufacturing industry. The literature review from Chen et al. [21] is focused on pharmaceutical and biopharmaceutical manufacturing. Further review works about the concepts and potential of digital twins in the industry can be found in [22,23,27–31].

In addition to literature reviews, several frameworks, methodologies, and concepts for digital twins have been published in the last decade. Most of the architecture models and frameworks in the literature are focused on the manufacturing sector. For example, Moreno et al. [32] proposed a concept for the manufacturing sector based on the example of a punching machine. Qi and Tao [25] and Lu et al. [33] introduced concepts for smart manufacturing which are focused on a big data approach. Experimental digital twins are created by combining virtual testbeds and digital twins, according to Schluse et al. [34,35] and Dahmen et al. [36]. The main idea is to establish digital twins as the core part of the development process and build all other parts around them [34]. Uhlemann et al. [37] and Trabesinger et al. [38] introduced concepts for generating cyber-physical production systems based on the optimization of the data acquisition approach. A novel architecture for large-scale digital twin platforms with a focus on flexible data-centered communication for the use in reliable advanced driver assistance systems was developed by Yun et al. [39]. Further information about the concepts and methodologies of digital twins can be found in [40–47].

The conducted research regarding concepts and methodologies for virtual representations in different industries represents the basis for the elaboration of a novel methodology for the development of virtual representations in process development.

2.2. Definitions of Virtual Representations

The first step towards a process development framework for the integration of virtual representations is the definition of the term “virtual representation” itself. In this paper, the term “virtual representation” refers to the overall expression of virtual objects mirroring a physical process using advanced digital methods. In the literature, the terms “digital twin”, “digital shadow”, and “digital model”, as well as “virtual representations”, are often used synonymously [9]. Furthermore, phrases such as “product avatar”, “cyber–physical equivalence”, “cyber–physical production system” and “virtual testbeds” are used in the literature for defining virtual representations in specific applications [28].

The first introduction of the term “digital twin” as a virtual representation was given by Grieves in 2003 [48] in the context of product lifecycle management (PLM). In the last two centuries, many definitions have evolved in different applications. Consequently, no unique definition for virtual representations has been reached yet [9,22,27]. One main reason could be the broad spectrum of virtual representation applications, making it difficult to find a unified definition. In Table 2, selected definitions from the literature are summarized to obtain an overview of the broad range of descriptions.

Table 2. Selection of virtual representation definitions in the literature.

No.	Year	Definition of Virtual Representation	Key Points	Field of Application	Ref.
1	2003	"The digital twin is a digital informational construct of a physical system, created as an entity on its own and linked with the physical system."	Digital and physical system linked	Product lifecycle management	[21,48]
2	2012	"A Digital Twin is an integrated multi-physics, multi-scale, probabilistic simulation of a vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its corresponding flying twin."	Best available physical models	Aeronautics	[27,49]
3	2012	"The digital twin 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. The topical role within Industry 4.0 manufacturing systems is to exploit these features to forecast and optimize the behavior of the production system at each life cycle phase in real time."	Different simulation disciplines, connected smart devices and real-time data elaboration, enabling forecasting and optimization of the system behavior within each lifecycle phase	Manufacturing	[27,50]
4	2015	"Very realistic models of the process current state and its behavior in interaction with the environment in the real world"	Realistic models to monitor the current state	Manufacturing	[27,51]
5	2016	"Virtual substitutes of real-world objects consisting of virtual representations and communication capabilities making up smart objects acting as intelligent nodes inside the internet of things and services"	Virtual substitutes with communication capabilities	Robotics	[34]
6	2016	"The simulation of the physical object itself to predict future states of the system."	Prediction of future states of the system	Manufacturing	[52]
7	2018	"The digital twin is actually a living model of the physical asset or system, which continually adapts to operational changes based on the collected online data and information, and can forecast the future of the corresponding physical counterpart."	Living model with continual adaptation to operational changes	Aircraft maintenance	[53]
8	2018	"A digital twin is a digital representation of a physical item or assembly using integrated simulations and service data. The digital representation holds information from multiple sources across the product life cycle. This information is continuously updated and is visualized in a variety of ways to predict current and future conditions, in both design and operational environments, to enhance decision making."	Multiple sources across the lifecycle deliver information, enhancing decision-making by predicting functions	Product lifecycle management	[54]
9	2019	"Themes related to the Digital Twin are the decoupling between physical and cyber entity, the presence and frequency of sensorial data flows, the use of computer simulation, the control of cyber over physical entity, the co-evolution of physical and cyber entity as well as the co-existence of physical and cyber entity."	Presence of sensorial data flows and co-evolution of physical and cyber entities	Manufacturing	[55]
10	2019	"A complete Digital Twin should include five dimensions: physical part, virtual part, connection, data, and service."	Five digital twin dimensions	Industry	[19]

Based on the summary of the selected definitions, it could be concluded that there is a broad consensus that a virtual representation is a digital reflection of a physical object. Additionally, the virtual representation is coupled with its physical counterpart and is an abstracted model description of the physical object. However, there are several inconsistencies in virtual representation characteristics in the literature. For example, there are different opinions about the data exchange, the real-time capability, the lifecycle perspective, and the fidelity level of the virtual representations.

For classifying virtual representations according to the data exchange between virtual and physical facility, the level of integration is discussed. Kritzinger et al., introduced the level of integration to differentiate virtual representations according to their data communication [9]. Figure 2 shows the integration levels of virtual representations. Therein, it can be seen that the digital model is characterized by two-way offline data communication between the physical and virtual components. The digital shadow is defined by one-way offline and one-way real-time communication between the two components. In the literature [9,24], the digital shadow is exclusively characterized by real-time data communication from the physical to the virtual component. Since there are also applications with a one-way real-time communication in the other direction, the term "digital shadow" is also valid for this approach. Digital twins are characterized by two-way real-time data communication between the physical and the virtual components [9]. Aheleroff et al. [24] extended the definition from Kritzinger et al. [9] using a predictive model approach, which is motivated by the work of Tuegel et al. [56]. The term "digital predictive twin" is introduced, which defines virtual representations with integrated predictive models.

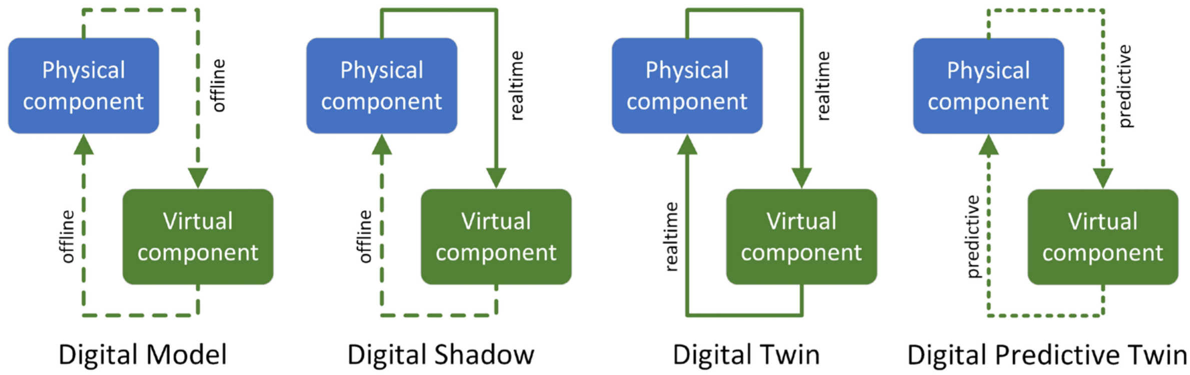

Figure 2. Virtual representation of integration levels concerning data communication. (Reprinted with permission from [24]. Copyright 2021 Elsevier).

In addition to the summarized definitions and levels of integration of virtual representations, the five-dimensional model, according to Tao et al. [19], is essential. As shown in Figure 3, the 5D model defines five mandatory parts for a complete virtual representation. The 5D model approach consists of physical and virtual components, data management, service, and connections. The physical component is the experimental or industrial facility to be investigated. The virtual component refers to all virtual models, flowsheets, and specifications, which serve as a basis for all virtual representation applications. The data management is responsible for the processing and storage of data. Within the service part, the investigated application is realized. The four mentioned parts are linked by connections responsible for the data transmission.

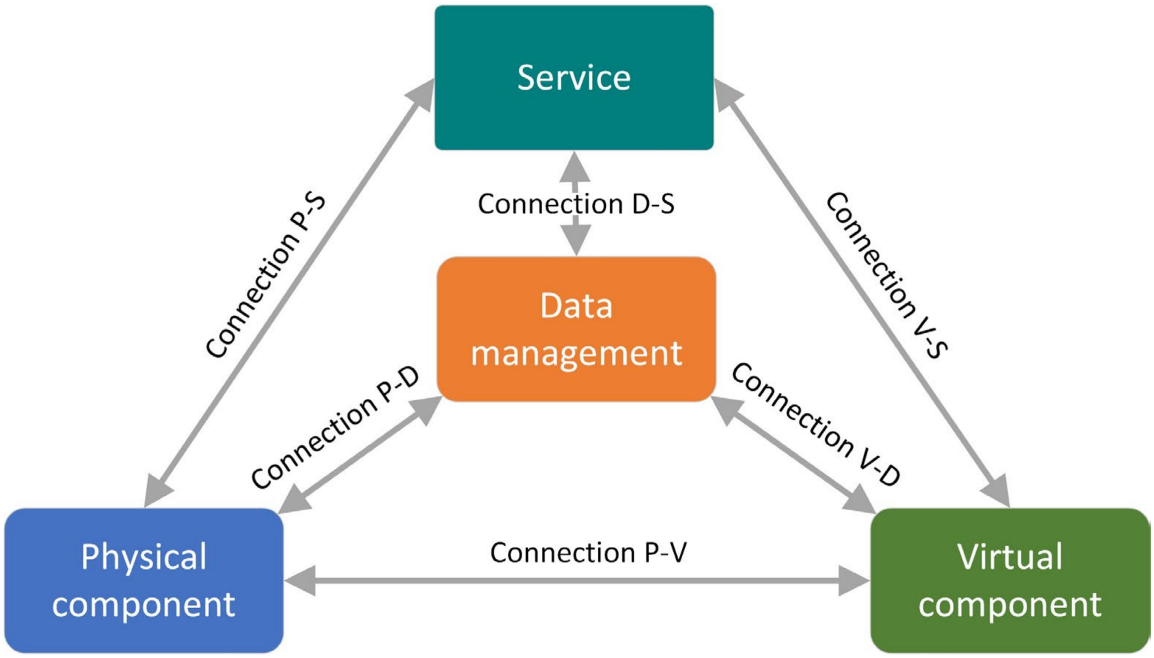

Figure 3. 5D model for virtual representations concerning a holistic approach. (Reprinted with permission from [57]. Copyright 2021 Elsevier).

Based on the summarized definitions in the literature, the level of integration approach, and the 5D model approach, a novel definition of virtual representations of energy technologies in the process development environment can be given:

Virtual representations in process development of energy technologies are digital reflections of physical facilities. The virtual component contains an abstracted model that is fitted as close as necessary to the physical component through the integration of measured values and domain knowledge.

Based on this definition, which emphasizes that the level of integration and model abstraction can differ in each process development and lifecycle phase, it is essential to develop a virtual representation by analogy with the physical facility with a clear overall development and engineering strategy [34]. This holistic approach requires the consideration of energy plant hierarchy levels [2] and energy plant lifecycle phases [54,58–60]. In the case of process development, the lifecycle perspective can be seen from two perspectives. On the one hand, the lifecycle perspective concerning the physical facility ranges from the design over the operation phase to the decommissioning phase [60]. On the other hand, the process development lifecycle perspective ranges from the lab-scale to the industrial-scale facility [61]. Each energy plant lifecycle phase is passed through in every process development phase, from lab to commercial scale. Therefore, the virtual representation architecture has to become more and more elaborate within process development. As well as the lifecycle perspective, the energy plant hierarchy layers have to be addressed to align the virtual representation framework with the foreseen user group. The energy plant hierarchy levels, according to IEC 62264 [62], range from the process level over the process control level to the enterprise level, and can be extended by the overarching energy system level. To conclude, the consideration of the lifecycle perspectives of energy plants and the energy plant hierarchy layers help to visualize the variety of players, which could be addressed within the development of a virtual representation. In addition to the discussion of the variety of virtual representation users, the planned applications and the associated properties, are discussed in the next section.

2.3. Applications, Challenges and Properties of Virtual Representations in the Energy Sector

There are many different applications in the process development framework in the energy sector [63] for the use of virtual representations. These applications are all confronted with different implementation types regarding energy plant hierarchy levels and lifecycle perspectives, as mentioned in Section 2.2. Furthermore, it is important to define virtual representation properties for developing a virtual representation framework. First, the Gemini principles [64] build a superordinate framework, which provides high-level guidelines for developing virtual representations regarding purpose, trust, and function. More detailed virtual representation properties can be defined based on these guidelines and principles.

Subsequently, the vast number of application possibilities within the energy sector must be discussed. Many literature reviews have summarized the possible applications of virtual representations in the industry in different fields [2,19–22,25–28,42,58,65,66]. Table 3 gives an overview of the possible virtual representation applications along the plant lifecycle phases, which are already discussed in Section 2.2.

Table 3. Possible virtual representation applications along the plant lifecycle phases.

Virtual Representation Applications	Conceptual Design and Engineering	Construction and Commissioning	Operation	Maintenance	Optimization	Decommissioning	Ref.
Collaboration	cooperation with suppliers, experts and inter-divisional coordination	coordination supplier	coordination logistics	coordination of spare parts supply and supplier	collaboration with external experts	coordination reuse and disposal	[2,20,58,65]
Documentation	process lifecycle management for the state-of-the-art documentation						[20,28,30,58]
Simulation and Monitoring	assistant for constructive and technical process design and construction		real-time performance	condition monitoring	reconfiguration and reconditioning	design of reuse	[2,22,27,58,66]
Evaluation and Verification	holistic evaluation of process design and construction		quality control	fault diagnosis/anomaly detection	holistic optimization	evaluation of reuse and disposal	[2,20,25,58]
Visualization	collision check and merchandising	construction assistant	support process understanding	visualization of 3D model or servicing plan	visualization of sustainability indicators	merchandising for reuse	[28,58]
Planning and Decision making	scheduling and support from design to commissioning		scheduling of operation and utility handling	proactive services	economic and ecologic dispatching	schedule for plant lifetime	[2,25,27,58]
Emulation	risk assessment	virtual commissioning	support and training of plant operators and maintenance engineers			virtual decommissioning	[22,30,42,58]
Orchestration	automation of process design and construction		process automation	automated maintenance services	advanced control strategies	-	[2,20,21,58]
Prediction	demand analysis and market prediction	stage of completion prediction	future performance	predictive maintenance	fault prediction of physical entities	prediction of a lifetime and residual value of physical entities	[20,21,25,58]

The given list of applications is incomplete and gives only an overview of the vast possibilities that arise with the development of virtual representations. The application possibilities can be categorized into nine groups, ranging from collaboration to prediction. Collaboration means the possibility of co-operation with different internal and external partners as well as the co-ordination possibilities arising from the virtual representation. The documentation aims to deliver state-of-the-art documentation of the energy plant throughout the whole lifecycle, often named “process lifecycle management”. The simulation and monitoring applications observe the process performance and support the design and commissioning. Several examples for simulation and monitoring applications can be found in [67–72]. The evaluation and verification stand for the information analysis, which helps to optimize the process from the design to the decommissioning phase by implementing sustainability indicators. The sustainability indicators are explained in detail in

Section 2.4. The visualization group stands for the use of a detailed 3D model, for example, as a design or maintenance assistant. Visualizing the sustainability indicators within the virtual representation can assist the plant operator in optimizing the process performance. The applications within the planning and decision-making group offer the possibilities that arise due to the implementation of virtual representations in terms of scheduling, economic and ecologic dispatching, and proactive action selection services. Emulation means nearly an exact duplication of the physical facility, consisting of the process behavior covered in the simulation and a detailed 3D model. Orchestration refers to the virtual control and automation tasks, which the implementation of a virtual representation could fulfill. Finally, the prediction services can range from market analysis to predicting the physical entities' plant lifetime and residual value.

In summary, there are many possibilities for the use of virtual representations in energy plants. Before developing a virtual representation framework, it is essential to define which applications in which energy plant lifecycle stage should be addressed. In addition to defining the applications, it is important to define which properties the virtual representation should fulfill to realize the foreseen applications. Beforehand, it is important to outline the challenges and problems which should be addressed during the evolution of virtual representation frameworks. As mentioned by Chen et al. [21], most challenges can be classified as time-, safety- or mission-critical. To enable stable real-time data communication between the physical and virtual components, it is important to decouple the control system from the virtual representation, which means that at any time the plant can be controlled manually via the control system. Additionally, cybersecurity safety measures against malicious attacks should be addressed. The data resolution, quality, and latency should be carefully checked and synchronized with the foreseen application. Furthermore, the heterogeneity of equipment for measuring components and control systems complicates the evolution of a standardized framework. Therefore, the use of standardized interfaces should be forced to realize exchangeable modeling blocks. The simulation models used should be robust and valid for a wide range of operations and applications to enable standardization. For advanced applications, hybrid or purely data-based models which have been parameterized for a specific application are often required. Consequently, a fast and user-friendly parametrization to other use cases should be enabled. Furthermore, a periodic recalibration of the simulation model must be considered to avoid model drifts. Finally, it should be pointed out that the results of virtual representations are all based on measurement values. Therefore, the continuous verification and recalibration of measurement equipment is indispensable. All these summarized challenges should be carefully addressed during the development of a virtual representation framework. The following discussion of virtual representation properties can assist with the development of an appropriate framework depending on the application [21].

In Table 4, an overview of possible virtual representation properties is listed. Therein, several property classes are defined to classify virtual representation approaches. The first property group has an overall focus. For example, the scalability indicates the implementation possibility of virtual representations within different energy plant hierarchy layers [73]. The interoperability specifies the equivalence between different model representations, which means the modeling tools are comparable, convertible or standardized [74]. The expansibility points out the flexibility of the used modeling techniques regarding the integration or replacement of models [74]. Finally, the functional safety represents the reliability and resilience of the virtual representation framework [73].

Table 4. Virtual representation properties in the energy sector.

Property Classes	Focus	Property Levels				Ref.
		Level 0:	Level 1:	Level 2:	Level 3:	
Scalability	Overall	Equipment level	Plant level	Enterprise level	Energy system level	[73,74]
Interoperability		Comparable	Convertible	Standardized		[73,74]
Expansibility		Fixed layout	Adaptable layout	Automated layout		[74]
Functional safety		Systematic capability	Implemented redundancies	Predictable failure analysis	Automated replacement	[73,75]
Technological scale-up possibility	Physical component	Modular	Partly scalable	Fully scalable		[76,77]
Degree of automation		Manual	Semi-automated	Fully automated		[78]
Physical safety		Primary safety measures	Secondary safety measures	Tertiary safety measures		[79]
Virtual representation capability	Virtual component	Static/Quasistatic	Dynamic	Ad hoc	Predictive	[45,63]
Virtual representation fidelity		Black box	Gray box	White box		[45,74]
Virtual representation intelligence		Human triggered	Automated	Partial Autonomous	Autonomous (self-evolving)	[45,63]
Connectivity mode	Data management and connection	Manual	Unidirectional	Bidirectional	Automatic	[45,63]
Data integration level		Manual	Semi-automated	Fully automated		[65]
Update frequency		Yearly/Monthly	Weekly/Daily	Hourly/every minute	Immediate real-time/event driven	[45,63,73]
Cybersecurity		Role-based access control	Discretionary access protection	Mandatory access control	Verified access control	[73,80–82]
Human interaction	Service	Smart devices	Virtual and Augmented Reality	Smart hybrid		[45,63]
User focus		Single	Multiple without interaction of energy plant hierarchy layers	Multiple with fully interaction of energy plant hierarchy layers		[65]

Furthermore, there are some individual properties listed for each virtual representation dimension. The physical component is classified by the technological scale-up possibility, the degree of automation, and the physical safety. For example, the technological scale-up possibility describes if all parts of the energy plant can be fully or partly scaled-up or if only a modular construction can manipulate the capacity. For example, the electrolysis of water is often not fully scalable due to technical limitations. The physical safety describes measures for preventing mechanical, electrical, chemical, biological, or explosion hazards and can be divided into primary, secondary, and tertiary safety measures [79]. Primary safety measures help to prevent hazard operation zones. Secondary safety measures include further precautions, e.g., the prevention of ignition sources, if hazard zones cannot be prevented. Tertiary safety measures describe structural hazard protection measures to limit the impact of incidents.

Additionally, there are several property classes for specifying the virtual component. The virtual representation capability implies the time dependency of the used models [45]. The fidelity stands for the degree of accuracy of the virtual component compared to the physical component [74]. Finally, the virtual representation intelligence indicates the ability of automatic decision-making, which ranges from human-triggered abilities over automated, rule-based approaches to autonomous full cognitive-acting approaches [45].

Moreover, data management and connection-focused property classes are mentioned. Therein, the connectivity mode refers to the integrated data exchange paths between the physical and the virtual component [45,65]. The data integration level represents the degree of automation of the data communication between the physical and virtual components [65]. The necessary update frequency of the virtual model depends on the application and ranges from weekly to real-time approaches [45]. Within the update frequency, the topics of latency, jitter, throughput, and bandwidth are important to note [73]. The cybersecurity property class represents the integrated protection features within the virtual representation against unauthorized access [80]. Besides the authorization and verification topic, cryptographic protection should also be considered [73].

The virtual representations deliver services which can be classified by human interaction and user focus. The human interaction implies the communication possibilities of the user with virtual representation [45]. The user focus indicates the extent to which users deal with the virtual representation service [65].The applications depend on different property levels of virtual representations, as discussed in Table 4, and deal with different plant hierarchy levels, as discussed in Section 2.2. Therefore, by developing virtual representations, it is essential to focus on the applications that must be addressed. Depending on the foreseen application, different property levels of virtual representations have to be implemented and different plant hierarchy levels considered. In developing novel energy technologies, it is crucial to develop the accompanying virtual representation so that as many applications along the energy plant lifecycle can be addressed. For the validation and evaluation of the virtual representation performance and the considered energy plant, it is essential to define key performance indicators (KPIs). These KPIs are even more important within the process development as a means of forming a holistic, optimized, sustainable energy process. Therefore, the KPIs are also named “sustainability indicators”.

2.4. Sustainability Indicators in the Energy Sector

Defining performance indicators is crucial for the development and optimization of energy processes. It is essential to link the performance indicators with sustainability to establish novel energy technologies and enable the energy transition towards climate neutrality. Therefore, the following performance indicators are called sustainability indicators. Successful development of novel energy technologies also implies compliance with legal, environmental, economic, and social requirements. Therefore, a multicriteria optimization of energy technologies regarding different aspects has to be fulfilled. The definition of sustainability can first be linked with the sustainable development goals (SDGs) [83]. They all highlight the global need for the sustainable development of the ecological, economic, and social environment. In terms of energy production, nearly all SDGs are relevant. Furthermore, the EU taxonomy [84] should be mentioned. This regulation provides a classification system, establishing a list of environmentally sustainable economic activities [84] exemplary in climate change mitigation. However, the EU taxonomy is controversial, because there is no common understanding of sustainability, especially in the energy sector.

Table 5 introduces the most important sustainability indicators for the energy sector to enable a method of quantifying sustainability. The sustainability indicators are classified into technical, environmental, economic, and social indicators according to [85]. Technical indicators are energetic and exergetic efficiency, which differ in considering the irreversibility of a process or lack thereof, when monitoring the performance of a process or plant. For carbon-based technologies, different conversion rates are also relevant to enable more detailed investigations. The plant lifetime and availability are essential indicators of supply reliability and economic aspects. The environmental indicators are classified into air, soil, ground, and water conditions, natural resources, utility consumption, and waste production. In terms of environmental indicators, it is essential to mention the lifecycle assessment methodology (LCA) to analyze environmental impacts. For detailed information regarding the fundamentals, requirements, frameworks, and guidelines of LCAs, refer to DIN EN ISO 14040 [86] and 14044 [87]. The assessment of environmental impacts is complex. However, developing and optimizing energy technologies regarding environmental requirements is important to enabling the energy transition towards climate neutrality. Besides technical and environmental indicators, economic indicators should be observed to enable affordable energy. The levelized production costs, which cover investment, fuel, operation, and maintenance costs over a lifetime, help to compare energy technologies with each other or the market value. The operating cash flow stands for the liquidity of a plant operator. To compare different investment scenarios or analyze specific investments in the energy sector, the net present value, payback time, and return on investment are all suitable indicators. The gross domestic and regional value is the value added created through energy production in a country or region within a certain period. For quantifying social impacts caused by energy production, the human toxicity potential and the job creation indicator can be named, for example.

Table 5. Selected sustainability indicators for the evaluation of energy technologies.

Sustainability Indicators			Unit	Description	Ref.
Technical indicators	Conversion rate **		%	Measuring the performance of a reactor or plant by observing the converted amount of a specific chemical compound during a reaction.	[76,88]
	Energetic efficiency		%	Measuring the performance of a technology by comparing the energy content of input and output streams.	[89]
	Exergetic efficiency		%	Measuring the performance of a technology by considering the irreversibility of a process.	[90]
	Plant lifetime		a	Measuring the usability period of a plant.	[89]
	Plant availability		FLH/a	Measuring the degree of utilization per year of a reactor or plant by referring to an operation at nominal power.	[89,91]
Environmental indicators	Emissions to air	Global warming potential (e.g., CO_2, CH_4, N_2O, etc.)	kg CO_2-eq/FU *	Measuring the insulating effect of greenhouse gases in the atmosphere preventing the earth from losing heat gained from the sun.	[85,92–97]
		Acidification potential (e.g., NO_x, SO_x, etc.)	g SO_2-eq/FU *	Measuring emissions resulting in acid rain, which harms soil, water supplies, human and animal organisms, and the ecosystem.	[85,92,94–96]
		Ground air quality (particulates, photochemical oxidants)	kg PM_{10}-eq/FU * kg NMVOC/FU *	Measuring gaseous and solid emissions which affect the ground level atmosphere.	[85,92,94–96,98]
		Ozone-depleting potential	kg R-11-eq/FU *	Measuring the depletion of the ozone layer in the atmosphere caused by the emission of, e.g., chemical foaming and cleaning agents.	[85,92,94–96]
	Soil, ground and water conditions	Eutrophication	g PO_4^{2-}-eq/FU *	Measuring concentrations of nitrates and phosphates, which can encourage excessive growth of algae and reduce oxygen levels within freshwater and marine water.	[92–96]
		Ecotoxicity	kg1,4-DB-eq/FU *	Measuring the potential for biological, chemical or physical stressors within freshwater, marine, or terrestrial ecosystems.	[94,96]
		Water consumption	kg H_2O/FU *	Measuring the amount of water consumed within a process.	[85,93,94]
	Natural resources, utility consumption and waste production	Primary energy consumption—fossil	MJ/FU *	Measuring the total fossil energy demand of a process.	[97,99]
		Primary energy consumption—renewable	MJ/FU *	Measuring the total renewable energy demand of a process.	[97,99]
		Electricity consumption	kWh_{el}/FU *	Measuring the total electricity demand of a process.	[85,97]
		Carbon utilization factor **	%	Measuring the amount of carbon converted from the fuel to the product within a process.	[88,100,101]
		Abiotic depletion	kg Sb-eq	Measuring the over-extraction of minerals, fossil fuels and other non-living, non-renewable materials which can lead to the exhaustion of natural resources.	[85,92,94]
		Wastewater amount	kg H_2O/FU *	Measuring the amount of wastewater produced within a process.	[85]
		Solid waste amount (disposal) **	kg ash/FU *	Measuring the amount of disposable waste produced within a process.	[85]
		Land use	m^2/FU *	Measuring the amount of land needed for the construction of a plant.	[85,94]

Table 5. *Cont.*

	Sustainability Indicators	Unit	Description	Ref.
Economic indicators	Levelized production costs	EUR/FU *	Measuring the price that would be charged per functional unit to achieve a net present value of zero for an investment.	[17,71,95,102,103]
	Operating cash flow	EUR/a	Measuring the profit/losses generated over a specific time period during regular operation.	[17,71,102,104]
	Net present value	EUR	Evaluates the technology investment by considering the time value of money.	[17,71,102,104]
	Payback time	a	Measuring the time required for return of the technology investment by revenues.	[17,71,105]
	Return on investment	%	Measuring the return of an investment by comparing profit and investment.	[104]
	Gross domestic/regional product (GDP/GRP)	EUR	Measuring the added value created through energy production in a country (GDP) or considered region (GRP) within a certain period.	[85,106]
Social indicators	Human toxicity	kg1,4-DB-eq/FU *	Measuring the quantity of substances emitted to the environment that harm humans.	[85,93–96]
	Job creation	-	Measuring the number of jobs created by the erection of a new plant.	[85,106]

* FU: functional unit (quantifiable description of the product function that serves as a comparable reference basis for all calculations) [86,87,107]. ** specific parameter for carbon-based technologies.

It should be noted that the overview of sustainability indicators in Table 5 introduces only selected quantifiable parameters. Of course, there are many more existing sustainability indicators. It is self-explanatory that not all of the presented sustainability indicators are applicable to all energy technologies. Depending on technology and location, these parameters also differ in importance and weighting. However, it should be clear that sustainable energy technologies can only be developed by considering a broad range of sustainability dimensions. Finally, the sustainable development and optimization of energy technologies shall always consider legal regulations, for example, emission and immission limits, or grid feed-in requirements. The definition of sustainability indicators forms the basis for quantifying development and optimization.

In summary, to develop a virtual representation framework in the process development environment, it is essential to define virtual representation applications and properties throughout the process development lifecycle. Furthermore, sustainability indicators have to be selected to ensure the evaluation and validation of the development's progress towards development goals. The following section introduces the novel model readiness level to link the sustainability indicators and virtual representation applications and properties with the process development lifecycle stages.

2.5. Introduction of the Modeling Readiness Level

Besides the technology performance evaluation via sustainability indicators, the definition of process development stages is essential for developing novel energy technologies. Therefore, the technology readiness level (TRL), which was first introduced by NASA [108], represents an important indicator for defining and monitoring the development progress. The TRL is also widely used within several national and international funding programs, such as EU Horizon 2020 [108], to classify research projects. In Figure 4, TRLs with the appropriate realized infrastructure, investigated process behavior, and the expected results within each process development lifecycle are visualized. Refer to [77,109] for further information on the TRL and related topics. To achieve the expected results in each process development stage, it is important to monitor and accompany the process development lifecycle with virtual representations. The virtual representation should combine all findings from the experimental test runs in each process development stage. To enable a successful framework for virtual representations, the definition of a modeling readiness level is important.

Figure 4. Modeling readiness level along the process development lifecycle of energy technologies [109–111].

After 10 years of investigation, Müller S. proposed the modeling readiness level (MRL) [109], by analogy with the TRL for the physical facility, to evaluate the development progress of virtual representations. Therefore, the virtual representation should evolve together with the physical experimental or commercial facility. Subsequently, the virtual representation capability, intelligence, and fidelity must increase throughout the process development lifecycle based on observations carried out within experimental test rigs. The mentioned key observations within each process development stage in terms of process behavior, operation mode, considered infrastructure, and expected results are listed in Figure 4. The MRL serves as a support instrument for tracking the development of virtual representations and should always be one step ahead of the TRL to enable forward planning.

In Figure 4, the MRL throughout the process development lifecycle of energy technologies is discussed. By analogy with the TRL, the same process development lifecycle stages are followed. In the concept and lab facility stage, TRLs 1–3 describe the way towards an experimentally proven core system. By analogy with the virtual representation in this process development stage, MRLs 1–3 are defined and range from the definition of operation and performance indication equations to the development of an integrated model library. During this first development stage, the temporal resolution is oriented towards the validation of the batch lab facility once per test run. The outcome shall be a virtual representation of the core process unit based on a steady-state simulation model with manual data management, service, and connection. For monitoring the sustainability and performance of the process in this development stage, first estimations of technical, environmental, and economic indicators based on the steady-state model are mandatory. Possible applications in this first stage for the virtual representation can be collaboration, documentation, simulation, or evaluation tasks as introduced in Table 3. Furthermore, the virtual representation types from digital model to digital predictive twin are linked with the process development lifecycle stages. In the concept and lab facility stage, all properties are connected to the virtual representation type of a digital model. The following pilot plant stage is covered by TRLs 4–5, validating the technology from laboratory to the real environment. Corresponding to the TRLs 4–5, the MRLs 4–5 define the creation and validation of a pilot plant model based on the main process units. Expected results in this stage are a virtual representation of the main process units based on a quasi-steady-state and dynamic simulation model with manual or semi-automated data management, service, and connection. The quasi-steady-state simulation model can observe and compare different operation points to find an optimum. Additionally, the dynamic model can display operation point changes and part-load observations to first consider monthly time-dependent operation behaviors caused by deviations of the input streams. The process performance analysis in this stage is based on the quasi-steady-state simulation model executed by reliable technical, environmental, and economic investigations. The virtual representation type in this stage is called "digital shadow", and it enables applications in collaboration, documentation, simulation, evaluation, and verification and visualization. The demonstration plant stage is covered by TRLs 6–7: the technology and system prototype demonstration in a relevant and operational environment. Simultaneously, the demonstration plant phase is accompanied by MRLs 6–7. Demonstration plants are characterized by the realization of the complete process chain, including utility and product logistics for the first time. Therefore, the complete evaluation of all utility streams and sustainability indicators becomes possible at MRL 6. Besides the technical, environmental, and economic indicators, social indicators can be analyzed due to the definition of a location. MRL 7 describes the completion of the 3D and simulation model consisting of all subunits of the whole process chain, including utility and product logistics. Therefore, the expected result in the demonstration plant stage is a virtual representation of the complete process chain based on a dynamic and ad hoc simulation model and virtualization with semi-automated or automated data management, service, and connection. The dynamic simulation model can analyze long-term process behaviors such as fouling and aging as well as start-up and shutdown scenarios. The ad hoc simulation model enables the real-time observation of the physical process. The virtual representation in this stage is named the "digital twin", and it enables most of the mentioned application fields according to Table 3, from collaboration to orchestration. The final commercial plant stage is characterized by TRLs 8–9, ranging from the complete and certified system to an approved market-ready competitive energy production plant in an operational environment. The corresponding MRL 8 describes the validation and evaluation of the virtual representation models by commercial energy plant facilities. Finally, MRL 9 is defined by the platform-based implementation, monitoring, and sharing of the virtual representation to enable a fast market penetration. The expected virtual representation in the final development stage includes the complete process chain based on a predictive simulation model and virtualization with automated data management, service, and connection. The expected results imply that the virtual representation, called the digital predictive twin, can deal with all kinds of short-term and long-term behaviors to enable applications from collaboration to prediction (see Table 3).

The definition of the MRL paves the way to introducing a virtual representation framework, which should help to develop appropriate models in each process development stage.

3. Virtual Representation Framework in the Process Development Environment

Subsequently, a virtual representation framework in the context of the process development environment is defined to provide a guideline for creating and developing appropriate virtual representations throughout the process development lifecycle. First of all, it should be mentioned that each virtual representation concept focuses on sovereignty, confidentiality, and reliability [109]. Furthermore, the virtual representation framework shall be based on standardized replaceable modules, called block modeling, to develop widely applicable virtual representations [66]. In Section 1, different framework approaches related to different fields of applications are summarized. These frameworks differ according to entities and properties as well as the architecture regarding information and network level. Different network architectures imply, for example, different data processing approaches. Therefore, defining an appropriate, generally accepted virtual representation framework is complex. For the development of a widely applicable virtual representation framework in the energy sector, the subsequently introduced framework addresses the development of virtual representations throughout the process development lifecycle.

The following 5D virtual representation framework is based on the 5D model as mentioned in Section 2.2. In Figure 5, the proposed 5D framework for developing virtual representations in the process development environment is visualized. Therein, it can be seen that every virtual representation consists of five dimensions. Every dimension is based on several subunits. The arrows in the background symbolize the order of the subunits.

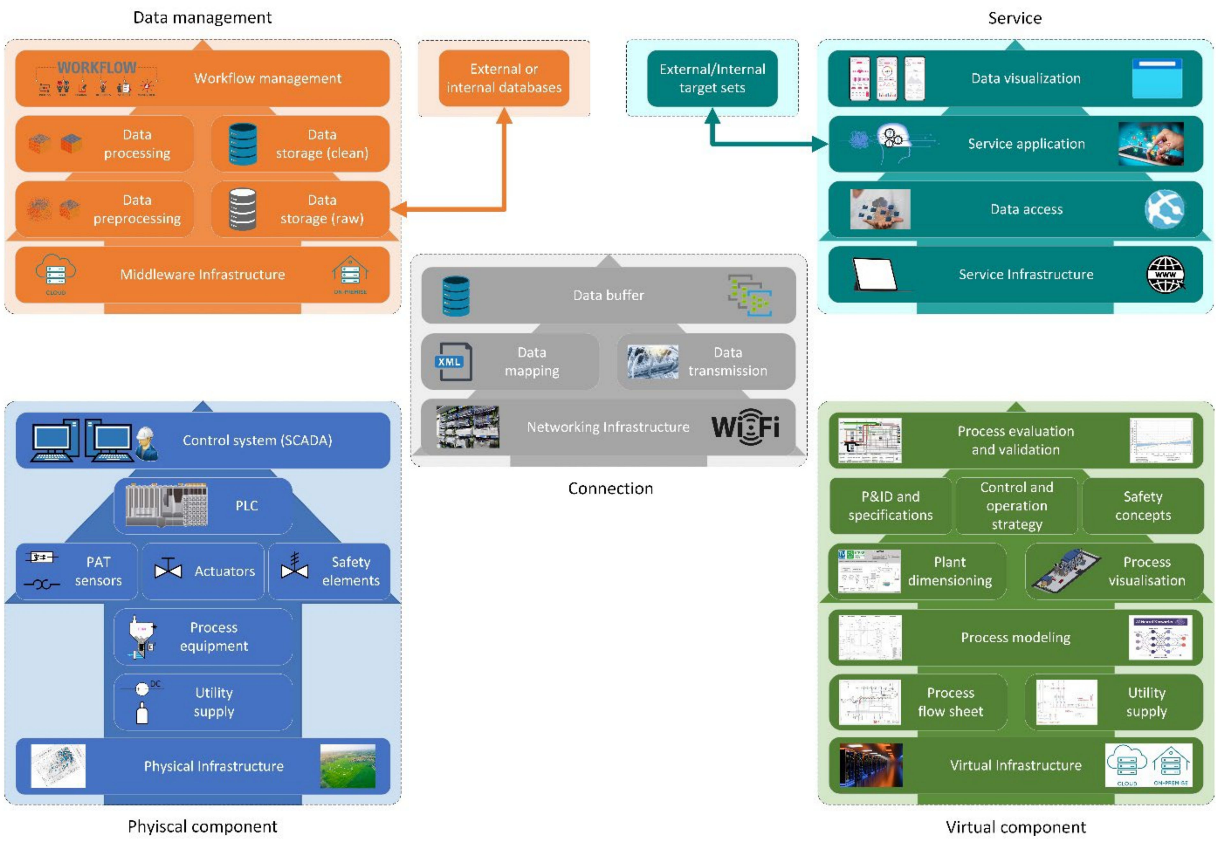

Figure 5. 5D virtual representation framework in the process development environment.

The physical component consists of the energy plant and the required physical infrastructure. This infrastructure includes the construction site and necessary utility supplies such as electricity, heat, or other process media. The most important part of the physical component is the process equipment, which is made up of the core energy production or conversion process units. Process analytical technology (PAT) sensors monitor the energy plant. PAT sensors comprise a wide range of analytical tasks, including thermocouples, pressure sensors, gas composition analytics, and orifice flowmeters for volume flow or other measurement applications. Actuators control the energy plant, for example, by manipulating valves. Safety elements are essential to prevent accidents and raise employee physical safety. To gather all the measuring and control signals from PAT sensors, actuators, and safety elements, one or more programmable logic controllers (PLCs) are used. The PLCs also form the interface between sensors, actuators, safety elements and the supervisory control and data acquisition system (SCADA). The data communication with other virtual representation dimensions can be realized by an interface to the SCADA system or directly from the PLCs.

The data management dimension is responsible for data handling. On the one hand, the data management is responsible for storing and processing the sensor data from the physical component out of the PLCs or SCADA system to feed the virtual component with appropriate datasets. On the other hand, data management also serves as an interface between the virtual component and service dimension to store and process modeling results. The data management dimension requires middleware infrastructure, which can be provided on premises via an edge device or cloud applications. The requirements of the middleware infrastructure are more or less driven by the desired services, the associated processing time, and the number of datasets. Data processing and data storage are often realized in two stages. Therefore, if the raw datasets from the physical component are large, the data preprocessing step is often set up on premises to realize a local filter to reduce the data size by condensing the datasets. The filtered datasets are stored in raw data storage, also often on premises, before the filtered data are transmitted to the cloud for a second processing step and to store the clean data properly. However, all these steps can also be realized exclusively on premises or within a cloud architecture. Additionally to the raw data from the physical component, further data from external databases such as analysis results from the laboratory can be merged with the filtered sensor values in the first storage stage. The last step within the data management dimension is workflow management. Workflow management systems are applied to arrange and streamline business processes [112]. Workflow management systems are mandatory in the case of complex workflow architecture.

Subsequently, the processed data from the data management are used in the virtual component to carry out the calculation, simulation, visualization, and specification tasks. All these subtasks are based on the virtual infrastructure, which can be analogous with the middleware infrastructure either on premises or based on cloud architecture or a mixture of both. In the first step, the process flowsheet and the utility supply build up the process layout, including all subunits and process media. The following process modeling is the core unit of the virtual component. Therein, physical-based or semantic data-based models describe the process behavior based on the defined process layout and media. In terms of physical modeling approaches, for example, mass and energy balances, kinetic approaches or computational fluid dynamics help to define input and output process flows as well as more detailed reaction and fluid dynamic behaviors [113]. Semantic modeling comprises all data-based approaches concerning machine learning, deep learning, ontology modeling approaches, and many more [20]. In terms of an engineering approach, the process simulation results serve as the input for plant dimensioning to define and optimize the geometry of all subprocess units. The following process visualization enables the illustration of the whole system. It should be mentioned that the engineering process is iterative. In terms of virtual representation applications, the process visualization (3D model) together with the process model can be seen as the core units to realize high-fidelity results and an immersive experience. On the basis of the 3D model, the piping and instrumentation diagram (P&ID), specifications, the control and operation strategy and safety concepts can be prepared. Refer to [76] for further details of engineering workflows and documents. Finally, the designed and optimized process should be validated based on sensitivity analysis, plausibility checks and domain knowledge. The process evaluation on the basis of the sustainability indicators helps assess the considered process and compare it with the best available competing technologies.

The service dimension is required to execute desired applications, ranging from data visualization for monitoring to process automation. By analogy with all the other dimensions, the service infrastructure delivers the architecture for developing the desired service. These can be local or web-based services hosted on premises or on cloud-based infrastructure. Provided services are physically separated within a multitier architecture. The most well-known framework for services is the three-tier architecture [114]. The three-tier architecture consists of a data access tier, the application tier and the data visualization or presentation tier. Within the data access layer, data from the data management and virtual component dimension are retrieved and processed to the service application layer. The service application layer builds up the logic of the service, where decisions and control take place. This can either be caused by internal or external target sets, which can be triggered through users or predefined functional units. The data visualization is the presentation layer, where services can be accessed through an appropriate user interface.

Finally, the connection layer represents the interface between the other dimensions. The data connection is based on networking infrastructure. The required networking infrastructure is driven by the desired service and can be, on the one hand, local networks such as fieldbus systems, wireless networks, or mobile networks [115]. On the other hand, global infrastructure such as the broadband internet via ethernet can be used [115]. The data connection is divided into data mapping and data transmission. The seven-layer ISO OSI reference model [116] describes the universal standard for data communication. Therein, each layer is required for particular tasks. The data transmission summarizes all transport-oriented layers from the physical to the transport layer [116]. The application-oriented layers are summarized as data mapping subunits, where the data structure is determined. For example, TCP IP data transport via ethernet protocol can be assigned to the data transmission [6]. Well-known data mapping protocols include FTP, HTTP, MQTT, and OPC UA [6,73]. The data buffer is responsible for intermediate storage or queuing data packets to supply the application with appropriate datasets.

The five dimensions of physical and virtual components, data management, service, and connection together form the 5D virtual representation framework in the process development environment. It should be mentioned that data sovereignty, confidentiality, and reliability are the overarching goals. The framework is be formed by interchangeable functional blocks based on standardized models, protocols, and guidelines. Additionally, the overall MRL level classified into the process development phases concept and lab facility, pilot plant, demonstration plant and the commercial plant can be linked with the five dimensions of virtual representations and the overall virtual representation properties. Table 6 gives an overview of mandatory dimension properties and overall virtual representation properties along the process development lifecycle. Therefore, each virtual representation dimension and subunit must evolve within each process development stage. Regarding the physical component, the physical infrastructure has to be extended from the core process unit in the concept and lab facility stage to the complete process chain in the commercial plant development stage. The decentral utility supply at the beginning of the development lifecycle must be replaced by fully integrated utility supply logistics at the end of the process development. The SCADA system shall be evolved from an automation system in the lab facility to a fully integrated process control system in the commercial plant. The virtual component steady-state simulation models have to be replaced stage-wise towards a fully predictive simulation model supplemented by virtualization of the complete process chain. The data management, service, and connection dimensions start with manual processes in the concept and lab facility stage towards fully automated processes in the commercial plant.

Table 6. Overall virtual representation properties within the 5D model approach.

Property Classes and Components	Focus	Concept, Lab Facility	Pilot Plant	Demonstration Plant	Commercial Plant
Scalability	Overall properties	Level 0: Equipment level	Level 1: Plant level	Level 2: Enterprise level	Level 3: Energy system level
Interoperability		Level 0: Comparable		Level 1: Convertible	Level 2: Standardized
Expansibility		Level 0: Fixed layout	Level 1: Adaptable layout	Level 2: Automated layout	
Functional safety		Level 0: Systematic capability	Level 1: Implemented redundancies	Level 2: Predictable failure analysis	Level 3: Automated replacement
Physical component	Virtual representation dimensions (5D)	Core process unit with decentral utility supply and automation system	Main process units with decentral utility supply and process control system	Complete process chain with central utility supply, product use and process control system	Complete process chain with fully integrated utility supply, product logistics and process control system
Virtual component		Steady-state simulation model of core process unit available	Quasi-steady-state simulation model of main process units available	Dynamic simulation model and virtualization of complete process chain available	Predictive simulation model and virtualization of complete process chain available
Data management		Manual data processing and storage approaches	Manual or semi-automated data processing and storage approaches	Semi- or automated data processing and storage approaches	Automated data processing and storage approaches with integrated workflow management
Service		Manual service application	Manual or semi-automated service application	Semi- or automated service application	Automated service application
Connection		Manual data communication	Manual or semi-automated data communication	Semi- or fully automated data communication	Automated data communication
Virtual representation type		**Digital Model (MRL 1–3)**	**Digital Shadow (MRL 4–5)**	**Digital Twin (MRL 6–7)**	**Digital Predictive Twin (MRL 8–9)**

Table 6 shows that the overall properties, as discussed in Section 2.3, namely scalability, interoperability, expansibility, and functional safety, are also linked with the MRL and development stages. The scalability indicates the possibility of evolution of virtual representations regarding the use within different energy plant hierarchy layers [73]. The virtual representation scalability in the concept and lab facility is on the equipment level because only the core process unit is available. The scalability reaches the energy system level in the commercial plant stage to connect the virtual representation with external stakeholders such as grid operators or suppliers. The virtual representation interoperability evolves towards standardized units, which means that all functional blocks are based on standardized models to enable cross-linking with other virtual representation environments. The expansibility refers to the flexibility of the used functional blocks to realize flexible layouts regarding replacing subunits or changes in the process streamline. Finally, functional safety should be evolved from systematic fault detection to the automated replacement of defective subunits.

The linkage of virtual representation properties with the MRL can also be enlarged to the dimension level, as outlined in Table 4. Not all proposed properties are mandatory for the desired services in the considered development stage. However, the virtual representation framework has to evolve to cover the proposed properties and requirements in each process development stage to ensure maximum freedom regarding possible services. In summary, each dimension has to evolve throughout the process development lifecycle. The physical component has to evolve from a core process unit in the concept and lab scale phase to a fully developed complete process chain in the commercial plant phase. Besides the development of the process equipment and utility supply, the physical safety and degree of automation has to evolve, and the possibility for scaling up must be approved along the process development lifecycle. The virtual component has to evolve from a steady-state simulation model to a predictive simulation model and virtualization of the energy technology to preserve the full knowledge of behavior. Consequently, the virtual representation capability, fidelity, and intelligence has to evolve. For realizing virtual representations for commercial plants, the manual data processing, storage, and communication approaches in the data management and connection dimension has to be replaced continuously by automated approaches throughout the lifecycle. The evolution of the data management and connection dimension can be evaluated by the virtual representation properties' connectivity mode, data integration level, update frequency, and cybersecurity. The foreseen services along the process development lifecycle will change. Therefore, the service dimension has to evolve as well.

Ultimately, a biomass-to-gas production route is utilized to explain the benefits of the virtual representation framework. The described technology is based on a dual fluidized bed gasification unit to convert biomass into product gas. Afterward, this product gas is cleaned in several steps to reach syngas quality. Within the methanation unit, the syngas is converted into raw Bio-SNG. After some upgrading steps, the Bio-SNG fulfills all requirements and can be fed into the gas grid system. The 1 MW Bio-SNG plant in Güssing, commissioned in 2008, represents the world's first synthetic natural gas production unit based on woody biomass at a demo scale [117]. In 2009, the Bio-SNG process was demonstrated successfully at a scale of 1 MW in Güssing [117]. The gasification unit in Güssing was operated for more than 10 years and had reached over 7500 operation hours by 2012. Based on this achievement, a 20 MW Bio-SNG plant in Gothenburg was planned, erected and operated. However, the 20 MW Bio-SNG demonstration plant could not reproduce the high number of operating hours in the gasification unit [102,118,119]. Several shutdowns occurred due to problems with the biomass feeding system, cooler clogging, and oscillating syngas quality [119]. Subsequently, this leads to the question of why the learned lessons from Güssing could not be transferred to Gothenburg. There could be several reasons, such as different utilities or other technical aspects. Furthermore, changing engineering companies might lead to a loss of domain knowledge.

All these problems can be improved by applying the raised 5D virtual representation framework. The quasi-steady-state simulation model from Güssing [117] was not suitable for condensing all lessons learned in a virtual model. Therefore, it is essential that the MRL is always one step ahead of the TRL to enable forward planning and anticipate future behavior. Furthermore, the virtual representation should always be able to process and reproduce gained knowledge from test runs. This would help to avoid recurring technology issues. To tackle the described issues, the research project ADORe-SNG [120] has been initiated to develop a virtual representation of the Bio-SNG route at a pilot scale. A digital predictive twin was developed to optimize the pilot-scale Bio-SNG production route. In

Figure 6, the virtual representation framework for the digital twin use case of the Bio-SNG production route is visualized.

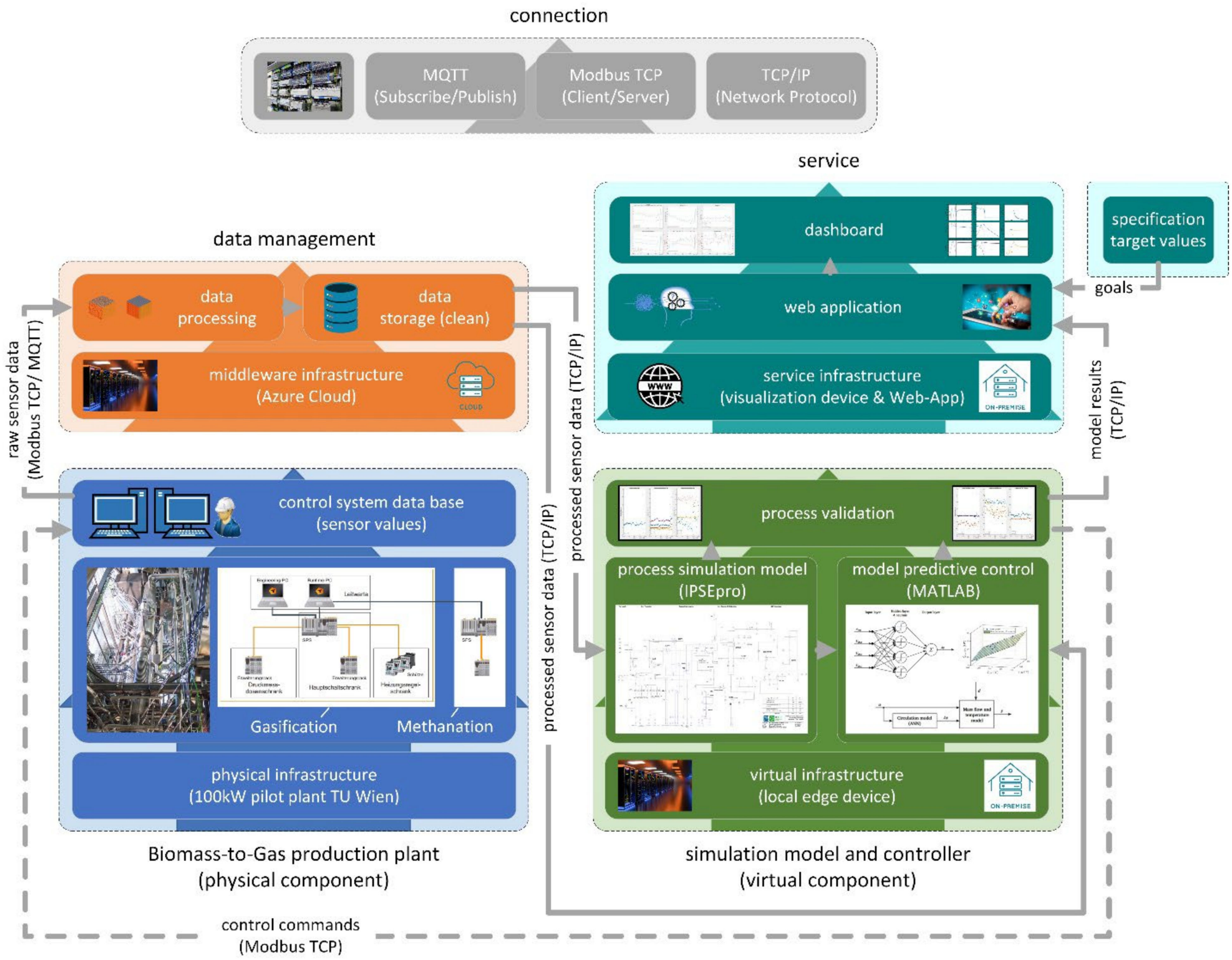

Figure 6. 5D virtual representation framework Bio-SNG route adapted from [121–123].

Within this project, a digital twin was implemented for the operation optimization of the 100 kW Bio-SNG pilot plant from TU Wien. The pilot plant is monitored and controlled via the APROL control system, which represents the top layer of the physical component. The raw sensor data are sent in real-time from the control system to the cloud-based data management. Afterwards, the real-time processed sensor data are sent every minute to the process simulation model in IPSEpro 8.0 and every five seconds to the model predictive control unit in MATLAB R2021b. The process simulation model helps to determine the present state of the process by the use of an overdetermined quasi-steady-state model. Furthermore, the consolidation of all measurement values as well as the determination of non-measurable variables is possible. The model predictive control unit helps to predict the plant's behavior as a function of the manipulated variables by the use of a gray-box-based dynamic model. With the help of the model predictive control unit, a full automation of the plant can be reached. The results from the process simulation model are used in the model predictive control unit to parametrize the dynamic model every minute. The results from the process simulation model and the model predictive control unit are validated in the final step from the virtual component dimension. Then, the model results are handed over to the service dimension, where finally a web application is used for the real-time data visualization. The results from the process simulation model are mostly sustainability indicators such as process efficiencies and yields. The results from the model predictive control unit are predictions for several manipulated variables to reach user-defined target values, which can be also defined within the web-application by the operator. Finally, the validated results from the model predictive control unit in the form of modifications of manipulated variables are returned to the control system to realize a fully automated closed-loop system [121–123].

The digital twin for the pilot plant of the Bio-SNG production route is already implemented and operational with real-time data. Moreover, an optimized operation point could be reached and held by the controller. Long-term operation of the digital twin is planned soon. The results from comparable control concepts showed that the fuel consumption could be reduced by 5%, while the product gas amount remained constant [124]. Furthermore, the number of operators can be reduced due the process automation.

Finally, the developed virtual representation framework can accompany further engineering and demonstration processes at a larger scale to gain better knowledge about process behavior and to gather this domain knowledge within the virtual representation. Based on these investigations, the concept should be validated at a 1 MW demonstration scale dual fluidized bed gasification plant in Vienna in Simmering. Further, a Bio-SNG plant in Güssing [125] and a 5 MW demonstration plant in Austria [102] are in the planning stage.

4. Conclusion and Outlook

The scope of this publication was the development of a virtual representation framework in the process development environment. The progress of process development can be monitored by introducing the novel modeling readiness level. Therefore, the modeling readiness level serves as a support for tracking the development of virtual representations and should always be one step ahead of the technology readiness level to enable forward planning.

Each virtual representation consists of five dimensions and should be based on the state-of-the-art models, which evolve along the process development lifecycle. The virtual representation framework is based on a novel definition, which implies that every virtual representation, independent of the process development and lifecycle phase, should fulfill the following statements:

- The virtual representation is a digital reflection of the physical facility;
- The virtual component contains an abstracted model that is fitted as close as necessary to the physical component through the integration of measured values and domain knowledge;
- The level of integration and model abstraction can differ in each stage, depending on the application.

The energy plant lifecycle perspectives and energy plant hierarchy layers are raised to obtain an overall picture of the different players and phases during a process development cycle. Virtual representation applications are summarized to show the variety of services that can be enabled due to the evolution of a virtual representation. Subsequently, possible virtual representation applications should always be defined to ensure a suitable framework. Challenges for the implementation of virtual representations are discussed to guide the development of frameworks. Additionally, properties of virtual representations are defined to address the evolutionary possibilities in each virtual representation dimension. Furthermore, the most common sustainability indicators are collected to enable a harmonized process evaluation through the integration of development goals in each lifecycle phase. The novel model readiness level is introduced to couple the virtual representation's evolution with the physical facility's process development. Therefore, the knowledge gained due to experimental test runs is preserved in the virtual component. Following the raised virtual representation framework, the final technology readiness level, which implies the proof of concept in a commercial environment, can only be reached if full knowledge of the behavior can be predicted with the accompanying virtual representation. Finally, the virtual representation framework determines the possible subunits for each dimension in the scope of the process development framework. The five virtual representation dimensions are also linked throughout the process development lifecycle phases with the modeling readiness level and accompanying overall properties.

Summing up, the presented virtual representation framework in the scope of the process development environment enables the standardization of the virtual representation development along the process development lifecycle. Therefore, the knowledge gained from the experimental test runs is preserved, the process development is always based on state-of-the-art models and the scale-up is not executed too early.

However, future research should focus on the validation of the novel virtual representation framework. Therefore, several process development cases of different energy technologies should be accompanied by the proposed methodology. Furthermore, it is essential to note that, independent of the virtual representation evolution stage, the sovereignty, confidentiality, and reliability of the monitored energy technology are prioritized. Finally, the virtual representation framework should be built on standardized, exchangeable block models in each dimension to enable fast adaptations depending on the addressed application. To conclude, the introduced virtual representation framework helps to enable smart interconnected energy systems. This is reached by accompanying the whole process development lifecycle with a suitable virtual representation from the beginning.

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Abbreviations

3D	three-dimensional
5D	five-dimensional
Bio-SNG	biomass-based synthetic natural gas produced via gasification and methanation
CH_4	methane
CO_2	carbon dioxide
CO_2-eq	carbon dioxide equivalent
DT	digital twin
EU	European Union
FTP	file transfer protocol
GDP	gross domestic product
GRP	gross regional product
ISO	International Organization for Standardization
H_2O	water
Horizon 2020	framework program funding research, technological development and innovation
HTTP	hypertext transfer protocol
KPI	key performance indicators

LCA	lifecycle assessment
MRL	modeling readiness level
MQTT	message queuing telemetry transport
N_2O	nitrous oxide
NASA	National Aeronautics and Space Administration
NO_x	nitrous oxide (general form)
OPC UA	open platform communications unified architecture
OSI	open systems interconnection
P&ID	piping and instrumentation diagram
PAT	process analytical technology
PLC	programmable logic controller
PLM	product lifecycle management
RED II	Renewable Energy Directive
Ref.	reference
SCADA	supervisory control and data acquisition
SDG	sustainable development goals
SO_2	sulfur dioxide
SO_2-eq	sulfur dioxide equivalent
SO_x	sulfur oxide (general form)
TCP IP	transmission control protocol/internet protocol
TRL	technology readiness level
Symbols	
%	percent
a	number of years
FLH/a	full load hours per year
FU	functional unit
g PO_4^{2-}-eq	grams of phosphate equivalent
g SO_2-eq	grams of sulfur dioxide equivalent
kg 1,4-DB-eq	kilograms of dichlorobenzene equivalent
kg CO_2-eq	kilograms of carbon dioxide equivalent
kg H_2O	kilograms of water
kg NMVOC	kilograms of non-methane volatile organic compounds
kg PM_{10}-eq	kilograms of particulate matter equivalent with a particle size smaller than 10 µm
kg R-11-eq	kilograms of trichlorofluoromethane equivalent
kg Sb-eq	kilograms of antimony equivalents
kWh_{el}	kilowatt hours of electrical energy
m^2	square meter
MJ	megajoule
MW	megawatt

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