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Energy digital twin technology for industrial energy management: Classification, challenges and future

Wei Yu [a], Panos Patros [b], Brent Young [a], Elsa Klinac [c], Timothy Gordon Walmsley [c,*]

[a] Industrial Information and Control Centre, Department of Chemical & Materials Engineering, The University of Auckland, Auckland, 1010, New Zealand
[b] ORKA – Cloud and Adaptive Systems Lab & Ahuora – Centre for Smart Energy Systems, Department of Software Engineering, University of Waikato, Hamilton, 3240, New Zealand
[c] Ahuora – Centre for Smart Energy Systems, School of Engineering, University of Waikato, Hamilton, 3240, New Zealand

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ABSTRACT

Digitalisation of the process and energy industries through energy digital twin technology promises step-improvements in energy management and optimisation, better servicing and maintenance, energy-efficient design and evolution of existing sites, and integration with locally and regionally generated renewable energy. This systematic and critical review aims to accelerate the understanding, classification, and application of energy digital twin technology. It adds to the literature by developing an original multi-dimensional digital twin classification framework, summarising the applications of energy digital twins throughout a site's lifecycle, and constructing a proposal of how to apply the technology to industrial sites and local areas to enable a reduction in carbon and other environmental footprints. The review concludes by identifying key challenges that face uptake of energy digital twins and a framework to apply the energy digital twins.

1. Introduction

The process heat and energy sectors are facing increasing pressure from global environmental challenges (e.g., climate change) to reduce energy consumption and greenhouse gas emissions while maintaining cost competitiveness through low operational and maintenance costs. Substantial research is currently underway to identify ways, such as new process technology, process systems integration, green fuels, and digitalisation, to minimise greenhouse gas emissions from the process and energy industries.

1.1. The industrial energy and emissions challenge

The industrial processing sector uses vast amounts of thermal energy in manufacturing processes and contributes 35.2% of estimated global CO_2-equivalent emissions (or 17.4 Gt CO_2-e), of which 69% are related to energy use in industry [1]. In New Zealand, the story is similar with industrial process heat accounting for 28% of gross CO_2-e emissions [2]. Even with considerable drivers for improvement, only 25% of sites in one study were reported to apply best practices regarding energy management and key performance indicators [3], which highlights a critical gap that needs to be closed to reduce energy and emissions from industry. The drivers, barriers and major factors for energy management systems were addressed by many researchers, for example, there is a need for an easy-to-handle and systematic method [4], energy efficiency KPI development [5], inclusion of long-term strategic targets [6], removal of barriers for energy management [7] and key pillars of successful energy saving projects [8]. Moreover, most current energy monitoring, control and management systems need major rethinking and upgrades to enable the rapid emissions reduction needed in the next decade, including new renewable energy technology implementation on existing processes [9]. Conceptually, DT technology shows great potential as a digital enabler for identifying the optimal physical solutions for both plant operations and assets to address the energy-emission crisis.

Industrial digitalisation through energy digital twins (EDT) is being considered to effectively manage and optimise site operations to minimise specific energy consumption, assist with energy-efficient design and evolution of their production processes and sites, and establish a green energy roadmap to switch to renewable fuels and better connect sites with locally generated renewable energy. As this review will demonstrate, EDT technology can be a paradigm shift that fundamentally changes the way a site operates to minimise specific energy consumption and increase renewable energy integration across all time horizons, including real-time control, production scheduling and

* Corresponding author.
E-mail address: tim.walmsley@waikato.ac.nz (T.G. Walmsley).

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List of abbreviations

AI	Artificial intelligence
ARIMA	Autoregressive integrated moving average
CAD	Computer aided design
CFD	Computational fluid dynamics
CRISP-DM	Cross industry standard process for data mining
DMD-c	Dynamic mode decomposition with control
DT	Digital twin
EDT	Energy digital twin
FPGA	Field Programmable Gate Array
IIoT	Industrial internet of things
IoT	Internet of things
KPI	Key performance indicators
ML	Machine learning
MPC	Model predictive control
PCA	Principal component analysis
RL	Reinforcement learning
RNN	Recurrent neural networks

planning, asset maintenance, and technology retrofit and upgrade.

1.2. A brief history of digital twin conception and development

Going back to 1970, NASA, faced with a crippled Apollo 13 spacecraft and stranded astronauts, employed high-fidelity simulations to virtually test a range of fix-it scenarios. The use of virtual simulation of a physical system enabled engineers to identify the best course of action to fix the spacecraft, which ultimately resulted in the safe return of the astronauts [10]. Three decades later in 2003, Grieves [11] coined the term digital twin (DT) to describe a system that contains: a physical part, a digital (or virtual) replica, and a connection between the two domains. Grieves [12] extended the definition to include a DT prototype, a DT instance, and a DT aggregate. Realising the similarities to the 1970 mission crisis, NASA connected the DT concept for application to space vehicles in 2010 [13] and 2011 [14]. After Grieves, most early papers defined DT as a high-fidelity simulation, without clearly specifying the connection between the virtual and physical parts. As DT research progressed, more researchers focused on the connection between virtual and physical parts, including seamless assistance [15], living models [16], updated virtual models [17] and bi-directional connections [18]. In addition, the concept of self-adaptation in DTs has started to be explored with ideas such as adaptivity [18] and self-evolution [19].

Since 2010, the topic of DT technology has experienced exponential growth in research activity and crossing into new fields, including renewable and sustainable energy. Fig. 1 presents a brief timeline of DT technology development emphasising definitional shifts. In particular, two studies helped to define and clarify different types of DTs. Kritzinger et al. [20] proposed to split the DT definition into three distinct categories according to the level of data integration (from least to most): digital model, digital shadow, and digital twin. The connectivity between the physical and digital twins was regarded as a critical and distinctive feature. As a result, a digital model, according to Kritzinger et al. [20] only contains non-automated data flow between the physical and digital twins; a digital shadow includes one-way automated data flow; while a digital twin requires two-way automated data flow. Written from a control engineering perspective, the study narrowed the definition of DT to fully automated applications while using the other terms for less-automated scenarios, including the Apollo 13 case. Madni et al. [17] proposed the classification of DT representations into 5 categories: model sophistication, physical twin existence, data acquisition from physical twin, machine learning of operator preferences and machine learning of the system and environment. In this definition, there is

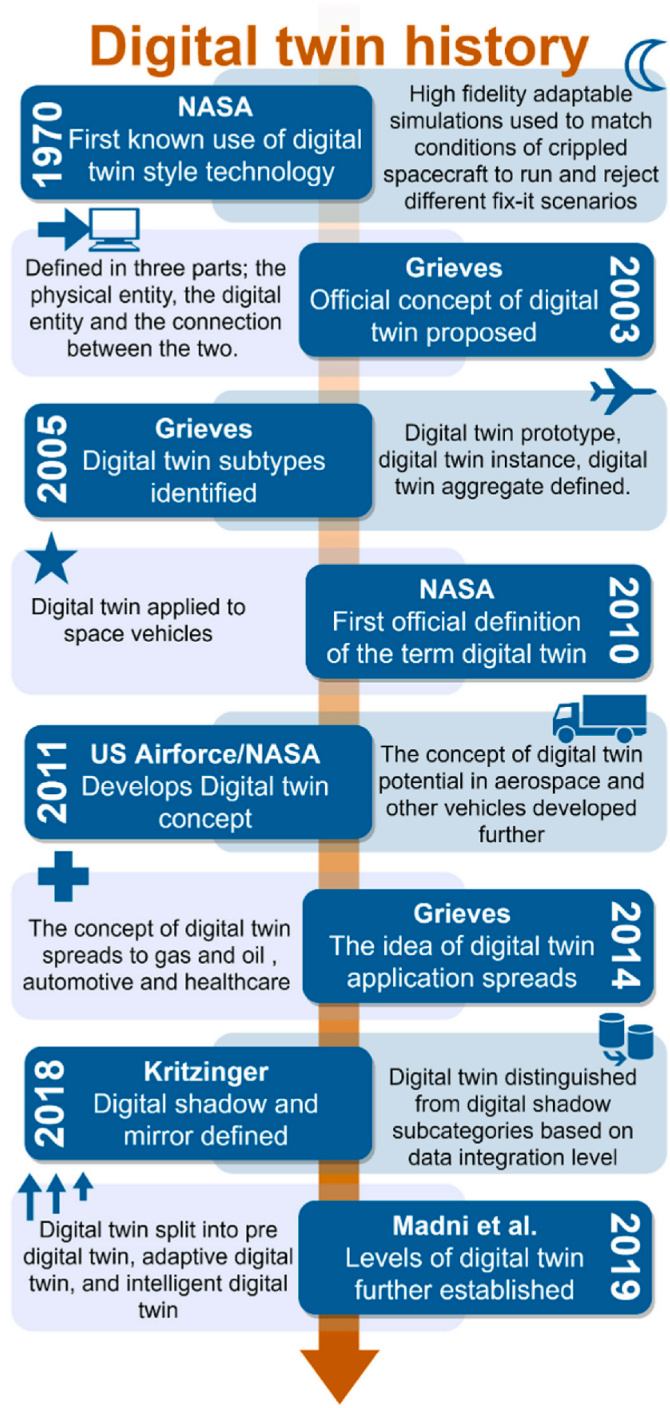

Fig. 1. A brief history of Digital Twin developments.

further discrimination of DT based on their connection to the physical twin and also introduces the sophistication or fidelity of the DT, while focusing only machine learning modelling approaches and not classifying DT modelling more generally.

1.3. Research and review gap

The usage of the term “digital twin” in academic and industrial literature has dramatically increased in the past five years. However, the DT research activities for different industries are not evenly distributed—the most popular areas are manufacturing DT (more than 1000 papers from Scopus since 2010) and building DT (400 plus papers from

Scopus since 2010). In contrast, only around 50 papers could be found for process or energy DT where the research focused on process heat and/or energy efficiency for the process and energy industries. Consequently, process and energy DTs are emerging areas in the field of digitalisation that need greater attention due to the pace and scale required to reduce greenhouse gas emissions in the face of global environmental challenges. The authors of this paper view the terms energy digital twin and process digital twin as synonymous and abbreviated to EDT, whereas the generic digital twin class is abbreviated to DT.

Given the emerging status of EDT, researchers need to coordinate ongoing efforts in delivering meaningful research outputs and impact on the industries to help with the immediate need for energy decarbonisation. The need for a systematic review of EDT technology is therefore warranted. In addition, there is a further need to develop a clearer definition of DT and EDT as terms, their attributes and how to classify the different DT fidelities. At present, definitions are often overly tailored to one specific application overlooking the fact that DT technology has become an overarching concept class that has value for many applications.

1.4. Review aim and novel contributions

This review aims to classify and discuss the design and application of energy (or process) digital twins to minimise lifecycle energy use and emission footprints and uptake renewable energy generation in the process and energy industries. To achieve this aim, this paper presents a thorough literature review that focuses on answering the following research questions:

- How does academic and industrial literature define DT technology and classify the various types of DT including EDT?
- What process and energy industries have interest in, or currently apply, EDT technology and what drives their implementation?
- What methods (e.g., algorithms, techniques, and frameworks) are reported as EDT developments and at what stage are the developments (e.g., research versus industrial implementation)?
- What are the key directions for future research in the EDT field for applications to the process and energy industries?

The review makes the following novel contributions to the literature:

- A novel multi-dimensional classification framework for DTs.
- Identifies current limitations to DT technology use in industrial energy management.
- A proposal of EDT application framework for industrial sites and local areas.

The remainder of this paper is structured as follows. Section 2 presents various definitions of DTs currently dominating the literature, contrasts and synthesises them, and proposes a novel and generalizable definition of DT as well as an associated classification framework. Section 3 outlines the method of the systematic literature review with focus on EDTs, and Section 4 presents its results with a focus on applications and methods of EDTs in the process heat and energy industries. Based on the review findings, Section 5 outlines key future directions for the research of EDT technologies and a framework for EDT application to industrial sites and local areas, and Section 6 concludes the paper.

2. Digital twin technology: definition and classification

This section compares and contrasts the various definitions of DTs currently used in both academic and industrial literature to propose a more generic DT definition that can be broadly applicable to all areas with interest in DTs. The novel definition is coupled with a classification framework for DTs that highlights the maturity level that a given DT has achieved on each of the proposed attributes of *looks-like*, *behaves-like* and *connects-to*, as well as the extra-functional dimensions of *problem-scale* and *time-granularity*. The section concludes by demonstrating how the new classification framework can help characterise EDTs.

2.1. Definitions in the literature

To provide a comprehensive literature review, 10 DT definitions from academic publications and 9 DT definitions from commercial and industrial companies, i.e., Microsoft, Siemens, IBM, PSE, KBC, Emerson, Ansys, Aspentech and Sight Machine, are listed in Table 1. The DT definitions can also be plotted as a word group cloud, as shown in Fig. 2. As a result, the root word terms: 'digital', 'physical', 'virtual', 'system', 'process' and 'product' are illustrated as the most common terms among all definitions.

Each of the definitions (Table 1) contain the same core elements as the original definition of Grieves [11] but were modified to suit a specific application area. Definitions from industry (e.g., by Microsoft and PSE) adapted their wording to highlight the strengths of the specific DT platform that they offer, as opposed to presenting a generalised definition. Some definitions reference the degree to which a virtual part contains the likeness of the physical part (often using the term fidelity), but the associated purpose was not often clearly stated. Additionally, the behaviour attribute of a DT is significantly different between the different applications and references.

The DT concept has grown in popularity and now crosscuts multiple research disciplines and industries. The weakness of many of the literature definitions is that they embed a distinct DT focus for a single discipline or application that does not translate well to others. Concurrently, there is a need to distinguish between the different types and fidelity of DT representations. To address these issues, this paper uses generic language to define and classify DTs for a broad range of disciplines and applications. The interested reader is referred to Jones et al. [21] and Liu et al. [22] for historical reviews of previous literature for the DT concept in the general manufacturing space.

Studying the variety of definitions presented in Table 1, highlights the breadth of expectations put on the concept of DTs. A general notion that can be extracted is that a DT is a digital representation of, and connects to something physical; however, what exactly is represented varies among product design, process design, asset operation, and system management, depending on the background and goals of the party proposing the definition. In general, a gap emerges in terms of the transferability of definitions beyond the proposed domain.

2.2. The proposed classification framework

As a generalised definition, a DT is a digital (or virtual) representation that looks-like, behaves-like, and connects-to a physical part or system with the goal of improving or optimising decision making for any time horizon. The combination of all three attributes defines the DT paradigm shift, setting DTs apart from traditional representations that capture either the likeness or the behaviour of a physical part or system but do not have a close connection to the physical system. Although all three attributes are necessary to achieve the best outcomes, the fidelity of each attribute varies depending on the purpose and application of the DT. In this light, DT is an overarching class that encapsulates many possible variations and provides freedom for researchers from different disciplines to progress the area of DT.

The following subsections discuss the individual DT attributes with examples that relate to the EDT area, the physical- and time-scale of DT application, and how to interpret the DT classification framework.

2.2.1. The looks-like attribute

Likeness is the attribute of a DT that expresses the appearance, structure, or architecture of a part or system. This attribute, from simplest to most detailed, can be classified into three categories:

Table 1
Definitions of digital twins (DT) in academia and industry.

No.	Refs.	Year/ Company	Definition (quoted from the reference)	Key points
1	[23]	2012	A DT is an integrated, multiphysics, multiscale, probabilistic simulation of an as-built vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its corresponding flying twin.	Integrated, mirror
2	[24]	2013	A cyber-physical model is a DT of the real machine that operates in the cloud platform and simulates the health condition with an integrated knowledge from both data-driven analytical algorithms as well as other available physical knowledge.	Cloud platform
3	[11]	2014	The DT concept model contains three main parts: a) physical products in real space, b) virtual products in virtual space, and c) the connections of data and information that ties the virtual and real products together.	Connection
4	[25]	2014	A DT is a life management and certification paradigm whereby simulations consist of the as-built vehicle state, as-experienced loads and environments, and other vehicle-specific histories to enable high-fidelity modelling of individual aerospace vehicles throughout their service lives.	Fidelity
5	[15]	2015	DT concept is the next wave in modelling and simulation, and the simulation is a core functionality of systems using seamless assistance along the entire life cycle, e.g. supporting operation and service with a direct linkage to operation data.	Seamless (connection)
6	[26]	2017	A DT is a computerised model of a physical device or system that represents all functional features and links with the working elements.	Representation
7	[16]	2018	A DT is 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
8	[27]	2018	A DT is a set of virtual information that fully describes a potential or actual physical production from the micro atomic level to the macro geometrical level.	Virtual information
9	[19]	2018	Based on previous literature, authors proposed characteristics of DT including: (a) real-time reflection; (b) interaction and convergence; and (c) self-evolution.	Adaptivity
10	[20]	2018	Classification of DTs into three subcategories, according to their level of data integration including digital model, digital shadow, and digital twins.	Data integration, connectivity
11	[17]	2019	A DT is a virtual instance of a physical system (twin) that is continually updated with the latter's performance, maintenance, and health status data throughout the physical system's life cycle.	Adaptivity
12	[18]	2019	DT can be regarded as a paradigm that uses selected online measurements, which are dynamically assimilated into the simulation world, with the running simulation model guiding the real world adaptively in reverse.	Dynamic, bi-directional, adaptive
13	[28]	2019	DT refers to a virtual object or a set of virtual things defined in the digital virtual space, which has a mapping relationship with real things in the physical space.	Mapping
14	[29]	Microsoft	Microsoft Azure DTs (proposed in 2018): This Internet of Things (IoT) platform provides the capabilities to fuse together both physical and digital worlds, allowing you to transform your business and create breakthrough customer experiences.	IoT platform
15	[30]	Siemens	The DT is the precise virtual model of a product or a production plant.	Precise virtual model
16	[31]	IBM	A DT is a virtual representation of a physical object or system across its lifecycle, using real-time data to enable understanding, learning and reasoning.	Real-time data
17	[32]	Emerson	Emerson's Digital Twin Starter Package (proposed in 2019) claims to be a first step towards a DT of an industrial production plant. It provides a virtual replica of the control system, non-intrusively mimicking operations.	Replica
18	[33]	Aspentech	DTs — virtualized copies of physical assets and their operating behaviours — will play key roles. They will also fundamentally change how humans work, interacting with intelligent systems, and virtual models ("twins").	Virtual copy
19	[34]	KBC	KBC introduced Petro-Sim 7 and Process Digital Twin in 2019, which can provide an integration with the OSIsoft's PI historian and Asset Framework.	Integration
20	[35]	PSE (Siemens)	PSE developed gPROMS Digital Application Platform in 2019 covering all key activities across the process design and operational life cycle through the creation of digital process twins.	Platform
21	[36]	Sight Machine	A DT is a dynamic, virtual representation of a physical asset, product, process, or system. It digitally models the properties, conditions, and attributes of the real-world counterpart.	Dynamic
22	[37]	Ansys	Ansys released ANSYS 19.1 (in 2018) containing the Twin Builder feature, which is an open solution that allows engineers to create simulation-based DTs–digital representations of assets with real-world or virtual sensor inputs.	Representation

1. 1-D representation, e.g., a process flow diagram.
2. 2-D representation, e.g., a process flow diagram with dimensions and coordinates.
3. 3-D representation, e.g., a virtual and augmented reality plant model.

EDTs often target low levels of the looks-like attribute because significant gains can be achieved through modelling the process behaviour (i.e., behaves-like attribute). With pressure to reduce energy and emissions, existing processes and sites have started to repurpose existing equipment and retrofit new upgrades, which naturally requires a deeper understanding of plant layout and space.

2.2.2. *The behaves-like attribute*

Behaviour is the attribute that mimics the outputs of a system for a given set of inputs with respect to time. This attribute, from simplest to most detailed, can be classified into three categories:

1. Single-state, static information, e.g., an average process system state.
2. Discrete, event-driven, multiple steady-states model, e.g., multiple equilibrium process system states.
3. Dynamic, time-driven, transient model, e.g., model predictive control.

In the process and energy industries, process simulation is a common tool to understand process behaviour and dynamics and to minimise site energy use and emissions. Global process systems engineering companies (e.g., Aspentech, KBC, and Siemens) provide well-known process simulation software programs, which are now becoming recognised as EDT's with high behaves-like fidelity but low looks-like fidelity.

2.2.3. *The connected-to attribute*

The connectivity between the DT and the physical system is an essential feature. It expresses how data flows between the physical and digital domains either in an automated, non-automated or mixed manner. This attribute, from simplest to most detailed, can be classified into three categories:

1. All indirect (e.g., non-automated) data flow between the physical part or system and the DT (also referred to as a *Digital Model*), e.g., CAD drawing based on a physical system.

Fig. 2. Digital twin definition word-root cloud.

2. Direct data flow (e.g., automated) from the physical part or system and indirect data flow from the DT in return (also referred to as a *Digital Shadow*), e.g., a plant operator's process data display.
3. Two-way direct data flow between the physical part or system and the DT (also referred to as a *Digital Manager*), e.g., a plant control system.

The proposed classification is a subtle shift from Kritzinger et al. [20], who described the three levels of the connected-to attribute using the terms Digital Model, Digital Shadow, and Digital Twin. Under their definition, a DT requires direct and automated data flow, which suits well the discipline of control engineering but not necessarily others (e.g., plant design and retrofit) that do not happen at runtime. Given the broad interest in DT, the term Digital Manager is introduced here to describe the essential feature of a DT's connected-to attribute while avoiding conflation with the overarching class of DT.

The connected-to attribute is critical for EDTs that seek to implement real-time dynamic optimisation to minimise energy use and emissions and maximise the product profit. For example, Leng et al. [38] implemented DT for parallel controlling of smart workshop with two way direct data flow. However, not all applications of EDTs rely on two-way, real-time data communication, e.g., plant evolution and retrofit, but should still be counted under the broad DT class.

2.2.4. Physical- and time-scale of the application

The physical scale of application of a DT is also useful to include in the classification process to demonstrate the range that various researchers have studied. This paper defines four scales for the classification process:

1. Nano, e.g., molecular level
2. Micro, e.g., single operation or part
3. Meso, e.g., collection of operations, including a factory or site
4. Macro, e.g., a community, local area, or region

The time-scale of the application is closely linked to the desired outcomes and required decisions over various time horizons.

In the case of EDTs applied to the process and energy industries, Fig. 3 presents some of the possible time-horizons and improvement opportunities, from seconds, e.g., process control, through to multiple decades, e.g., process design. DTs can enable improvements in all the time horizons to produce improved outcomes. To reiterate, different levels of DT fidelity are appropriate to deliver the desired outcomes. For example, process control that operates in real-time needs a high-fidelity DT that behaves-like and connects-to the process but does not require a high degree of looks-like. In contrast, a process design requires high fidelity in terms of looks-like and behaves-like, and less in the connects-to attributes. DTs used for new process designs, i.e., greenfield developments, are called pre-digital twins.

2.2.5. Interpretation of the classification framework for energy digital twins

Different applications require different types and fidelity of likeness, behaviour, and connectivity to be effective. Greater fidelity does not necessarily equate to a better EDT, rather it may just result in an over-engineered EDT. The simple classification approach is developed to help identify the types of EDTs in a more precise manner (Fig. 4) and to highlight research gaps. This review applies the classification approach to a subset of DT research that focuses on the process heat and energy industries, which are sometimes referred to as *process digital twins* or *energy digital twins*.

3. Review method

This systematic review focuses on the literature that discusses and applies EDT technology to the process and energy industries. This section summarises the review approach and recent, related work for the process and energy industries with a focus on EDT publications to identify gaps in the field. The proposed generic DT classification framework is applied to distil the essential features of current research directions and applications. This information will help other researchers to address the gaps in future needs of the process and energy industries.

3.1. Databases

To better cast a wider net, given the multidisciplinary nature of DT technology, the search included a variety of databases, including:

- Web of Science
- Scopus
- Google Search
- Google Scholar
- ScienceDirect

In addition, Google Search was used to find industry-oriented pieces of work that do not appear in strictly academic sources.

3.2. Inclusion and exclusion criteria

To ensure the selected papers met the needs of this study, the selected studies conformed to the following criteria:

- Originate in a scientific peer-reviewed venue or be technical reports and white papers produced by respectable industrial sources.
- Be written in English.
- Published between January 2010–April 2021.
- Must focus on DT concepts, key technologies, and industrial applications on process heat, energy, and decarbonisation.
- Not be a duplicate (search engines sometimes produce multiple links to the same work).

3.3. Search methodology

The review comprised the following three levels:

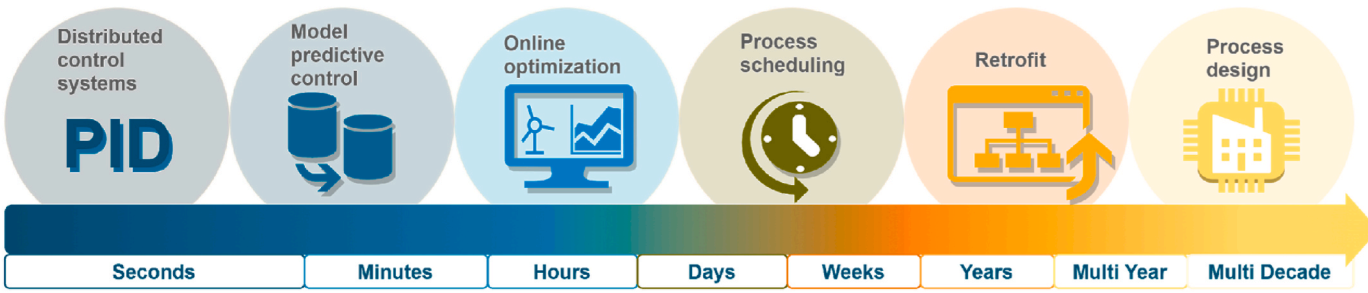

Fig. 3. Time-scales for different types of digital twin goals in the process and energy industries.

- Level 1: basic data collection from the designated databases to identify proper keywords by checking paper titles and abstracts.
- Level 2: automated search based on Level 1 search strings, followed by manual reading of the abstracts of the selected papers to filter the most promising papers.
- Level 3: full reading and analysis of the selected papers while also recursively including further studies via forward and reverse snowball sampling, with a stoppage criterion at 50 papers.

4. Results and discussion

This section first presents general statistics of the paper selected by the review methodology presented in Section 3, followed by a discussion on the discovered trends of EDT usage and implementation for the process heat and energy industries.

4.1. Review statistics

4.1.1. Keyword search

To better target the best keywords, the first step in the process was to skim through the top ten results on Google Scholar, in addition to leveraging the authors' experience in Process, Chemical and Software Engineering. The efficacy of these keywords was assessed via a level-1 search on Google Scholar focusing on recent papers published in 2021 to better capture cutting-edge trends. Table 2 counts the number of papers discovered per search string and per different level of filtering: full-text, abstract-only and title-only.

The results, which are sorted by most hits in full-text search, suggest that just using the terms "Digital Twin", "Smart Energy Systems", "Industry 4.0" and "Software Engineering" is not specific enough for a focused survey because of the large volume of papers being published recently. Consequently, and after skimming through the abstracts of the most promising papers, the following search terms were selected for the level-2 abstract screening part of the review, which not only focused on Digital Twins but also contained keywords that implied a technical focus on the process and energy industries (highlighted in Table 2).

4.1.2. Abstract screening

The basic search revealed a total of 2449 search hits, whose distribution per database is displayed in Table 3.

Next, the titles and abstracts of the first 30 search results per search string and database were manually examined to assess their relevance to process and energy systems. This resulted in a list of 53 papers that met the selection criteria of the study and were promoted for full-text reading.

4.1.3. Full-text screening

The final reading stage in the review process was to understand, classify and summarise the collective contribution of the 53 papers that pass through the previous filters.

Fig. 5 displays the primary and secondary drivers behind the studied papers. The primary motivator for EDT adoption in the process and energy industries are energy efficiency, closely followed by profit and decarbonisation. The secondary motivators are dominated again by energy/efficiency and then profit. This leads to the conclusion that the main objectives a successful process and energy EDT needs to fulfil are: (1) the optimisation of efficiency for energy usage reduction, to enable (2) a pathway for effective decarbonisation, while (3) the costs of the transition remain low.

Literature review statistics for publication type and applications for different industries for all publications are shown in Fig. 6(a) and (b) respectively. Journal papers and conference papers are 50% and 48% respectively of the source materials as shown in Fig. 6(a). The large fraction of conference papers (approximately half) indicates the research on EDTs is at an early stage compared to other industries such as manufacturing in general. In Fig. 6(b), regarding EDT applications for different industries, the dominant fraction is for generic processing (37%) which includes generic unit operations such as distillation columns, furnaces, and heat exchangers. And most of these applications are specific case studies. 30% of the applications were for the energy

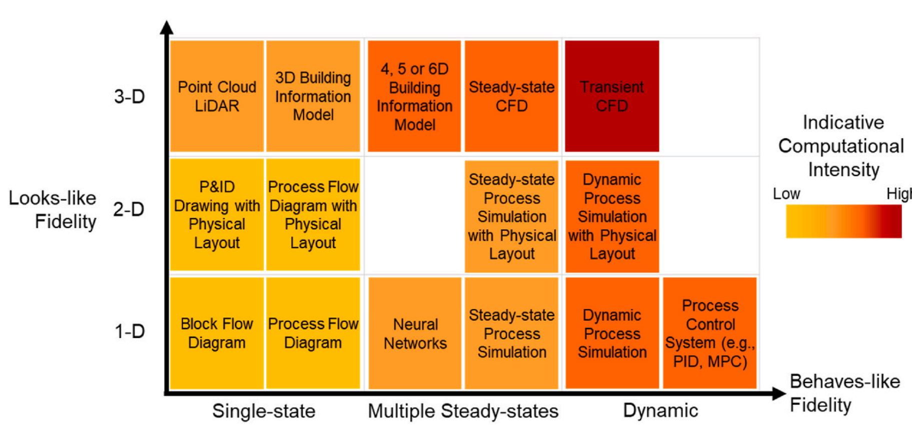

Fig. 4. Classifying EDT families using the proposed classification framework.

industry, but most of the applications focussed on EDT conceptual development and study of the EDT architecture instead of a real implementation.

4.2. Digital twin classification

A categorical review from 53 publications was conducted according to their content and different perspectives: type, DT class, specific research area, application scale, paper aim, and main technology used in the publication. Since some publications did provide clear categorical information mentioned above, 17 publications were selected for the categorical review, the results were listed in Table 4.

The classification uses DT_{ijk} ($i = 1\ldots3$, $j = 1\ldots3$, $k = 1\ldots3$) to represent each DT class defined in Section 2.2.1, the subscripts i, j, and k represent the DT looks-like, behaves-like and connected-to attributes, and the numbers of i, j and k indicate which of the 3 levels within each attribute is achieved. For example, DT_{131} represents a DT class having the 1-D representation look-like attribute, the dynamic, time-driven, transient model behaves-like attribute, and the mixed direct/indirect connected-to attribute. This classification method summarises DT complexity for ease of understanding, and aids in highlighting DT variations that are underdeveloped or under researched.

The distribution of results using the proposed classification framework are displayed in Fig. 7. These results highlight a general gap in the mid-level of likeness, i.e., 2-D representations. Additionally, most proposed EDT focus lack full two-way connectivity with the physical plant; thus, most studies fall primarily under the digital model or digital shadow grouping.

Considering the EDT likeness class: most papers (78%) use 1-D representation (e.g., block flow diagrams); few papers (5.5%) consider 2 D representation (e.g., researchers in one study found optimal reactor size design through a 2-D EDT [37]); and 14% papers used 3-D representation. Concerning the EDT behaviour class, the study of dynamic behaviour dominates current EDT studies for the process industries (~60% of papers). When it comes to the EDT connectivity class, the majority of the research focused on digital models (50%) and most of them were case studies; about 25% of papers concerned digital manager type connectivity, but most of them were pitched at the conceptual level.

Table 2
Number of papers discovered per search term/string during level-1 search.

Pilot Iteration Search Term/ String	Full-Text Hits (2021)	Abstract Hits (2021)	Title Hits (2021)
Digital Twin	9830	2430	728
Digital Twin & Industry 4.0	3490	320	8
Smart Energy Systems	1920	106	30
Digital Twin & Software Engineering	798	11	1
Digital Twin & Energy Systems	598	21	1
Digital Twin & Reactor	321	21	0
Digital Twin & process industry	232	13	0
Adaptive systems & Digital Twin	184	6	0
Digital Twin & distillation	138	5	0
Digital Twin & decarbonisation	136	4	0
Intelligent Digital Twin	128	11	6
Digital Twin & heat exchanger	124	2	1
Self-Adaptive Systems & Digital Twin	49	1	0
Knowledge-driven Digital Twin	46	0	0
Adaptive Digital Twin	29	1	1
Digital Twin & evaporator	29	0	0
Digital Twin & Process heat	26	0	0
Engineering Digital Twin	23	4	0
Digital Twin & reboiler	8	0	0
Personalised Digital Twin	6	0	0
Self-Adaptive Digital Twin	0	0	0

Table 3
Number of papers discovered per search term/string at first level.

Search String	Web of Science	Scopus	Google Scholar	ScienceDirect
"Digital Twin" AND "Process Heat"	0	61	59	17
"Digital Twin" AND "Process Industry"	10	780	544	159
"Digital Twin" AND ("Decarbonisation" OR "Decarbonization")	3	4	252	30
"Digital Twin" AND ("Reboiler" OR "Evaporator" OR "Heat Exchanger")	3	12	338	177

4.3. Application to product and asset life cycles

EDT applications in the literature cover all aspects of the product (or asset) lifecycle. The three categories or phases defined by Liu et al. [22] for all EDT applications are used in this paper, namely design, manufacturing, and service phases. The sub-categories for each phase were modified for the process heat industry based on the original definitions in Ref. [22] as follows.

Design phase

1) Optimisation: An EDT can help designers to determine all the design parameters for an optimally performing process to minimise energy use. An EDT can also be used for new process and plant design or can be used for retrofitting existing processes and plants to improve product quality, production rate and energy efficiency. A future application should the integration of renewable energy, both on-site and in the local area at the site-edge.
2) Data generation: For some processes, engineers may not have sufficient data for designing the process—for example, only lab-scale data may be available. An EDT may be used to generate needed data to rebalance a dataset and/or estimate untested operating states. Building accurate models from data using, e.g., machine learning has significant potential to feed into energy optimisation models.
3) Virtual evaluation, verification, and validation: An EDT can be an economical tool for testing the designed process/plant. A bottleneck

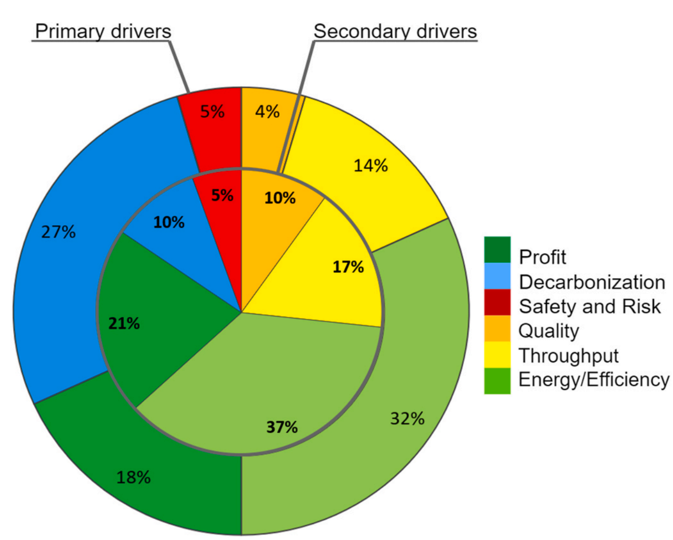

Fig. 5. Drivers underpinning research in process and energy digital twin technology.

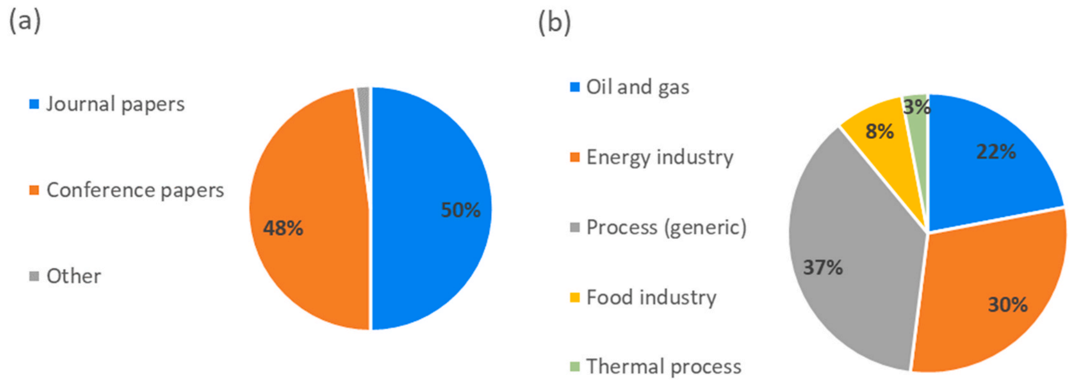

Fig. 6. Distribution of papers' venues and industrial domains.

unit can be identified in early-stage design, and extreme operating conditions can also be tested.

Operation phase

1) Process monitoring: An EDT may provide real-time monitoring in a better way compared to traditional monitoring technology. An EDT has the potential to integrate real-time data with a 3-D model virtually and provide a platform for analysing historical, current, and predicted data from both the virtual (digital) and physical twins. For example, a Kalman filter could be used to correct for sensor noise and dynamics.
2) Production control: Traditional production control heavily relies on measurements for the physical process/plant. Industrial engineers use models to help control, e.g., model predictive control (MPC), but the model only partially covers the process. The EDT can enhance current production control methods to reject disturbances and maintain a tight quality specification range through the data/information connection between virtual and physical parts.
3) Process prediction: All processes/plants face variation problems (e.g., raw material feed variation, utility system fluctuation). An EDT can provide predictions on how variations impact a physical process and plant. By implementing soft sensing technology e.g., by using machine learning methods, an EDT can also provide predictions of critical process variables which are difficult to be measured directly or expensive for direct measurement.
4) Process optimisation and production planning: Traditional process optimisation is commonly based on design information, and production planning is based on static information. These approaches show poor performance for dealing with disturbances and uncertainties. EDT can significantly improve process optimisation and production planning with rich monitoring and prediction information generated by an EDT.

Table 4
Categorical review of EDTs in the literature.

Paper	Type	DT likeness	DT behaviour	DT connectivity	Specific area	Application scale	Paper aim	Tools and/or Technology
[39]	Case study	2 D	Discrete event	Digital Model	Reactor	Meso	Process Design	AspenPlus
[40]	Case study	1 D	Discrete event	Digital Model	Thermal power plant	Meso	Optimisation	Thermoflow simulation
[41]	Case study	3 D	Discrete event	Digital Model	Glass product	Meso	Design	Multi-View synchronization
[42]	Concept	3 D	Static	Digital Model	Industrial process	Micro	Modelling	Simulation
[43]	Case study	1 D	Dynamic	Digital Shadow	Cooling tower	Meso	Prediction	Data-driven approach
[44]	Case study	2 D	Dynamic	Digital Shadow	Wind turbine	Meso	Prediction	ANSYS Fluent
[45]	Concept	1 D	Dynamic	Digital Model	Furnace	Micro	Modelling	Hybrid model
[46]	Case study	1 D	Dynamic	Digital Shadow	Multi-effect evaporation	Micro	Prediction	Simulation
[47]	Case study	3 D	Dynamic	Digital Shadow	Food refrigeration	Nano	Prediction	COMSOL
[48]	Case study	1 D	Discrete event	Digital Shadow	Furnace	Meso	Optimisation, Retrofit	UniSim Design, Matlab
[49]	Review, concept, case study	1 D	Dynamic	Digital Model	Energy	Meso	DT architecture	Hybrid model
[50]	Case study	1 D	Dynamic	Digital Manager	Steam turbine	Meso	Monitoring	Hybrid model
[51]	Concept	1 D	Discrete event	Digital Shadow	Petrochemical industry	Meso	Production optimisation	Machine learning
[52]	Case study	3 D	Dynamic	Digital Shadow	Solar Drying	Nano	Monitoring	COMSOL
[9]	Review	–	–	–	Processing	Meso	Data-driven energy saving	AI, IoT, Blockchain 3.0
[53]	Case study	1 D	Dynamic	Digital Model	Thermal process	Micro	Control design	Switched dynamic model
[54]	Concept	1 D	Discrete event	Digital Model	Process	Meso	Automatic model generation	BALAS

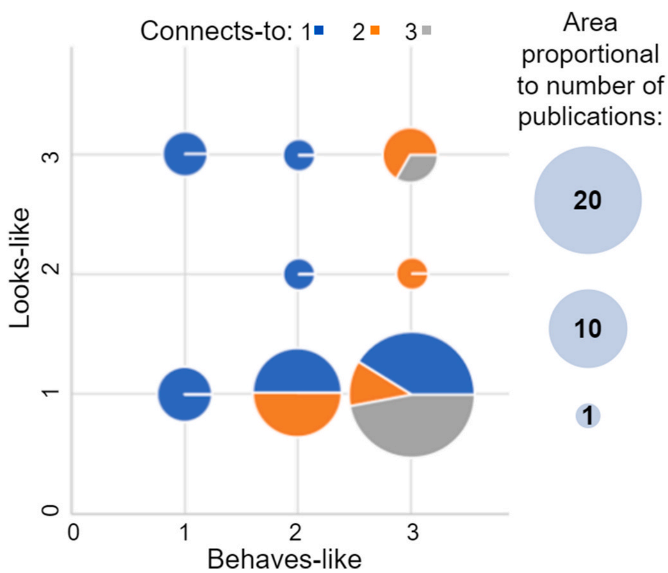

Fig. 7. Prevalence of different EDTs in process heat and energy literature.

5) Process training: Both industrial engineers and academic researchers have pointed out great potential for EDT implementation for training.

Service phase

1) Predictive maintenance: A similar idea to process prediction since an EDT can cope with disturbances and uncertainties, it can also provide more accurate maintenance times.
2) Fault detection and diagnosis: By comparing process variables from both virtual and physical processes, engineers can quickly identify fault locations. With the help of EDT, fault diagnosis can be also conducted to identify fault type/s or resource/s.
3) Virtual testing: Since a EDT is the digital representation of the physical twin, it can be used to test certain operations under situations in which the failure of the physical twin leads to great loss and damage.

The applications for design, processing and service listed in Table 5 reflect a fraction of the EDT technology applications in the process and energy industries: most of the applications (62%) are for the processing phase, around 35% of applications belong to the design phase, and only a few applications (3%) focus on service phase.

4.4. Software architecture

This section discusses software architecture models and methods proposed in the surveyed papers based on the methodology presented in Section 3. Overall, the development of EDTs is an interdisciplinary process. As such, with the growth of the DT sector, a number of lessons need to be drawn by the discipline of software engineering, which can inform how such software should be designed, tested and maintained. Software architecture provides this high-level overview by describing the main components DTs require and how they interact with each other and with the physical world. Eventually, the field needs to specialise into the software engineering of digital twins.

Several DT architectures have been proposed, such as a 3D-DT architecture [10], a 5D-DT architecture [58] and a 5C architecture [59]. A literature review about DT architectures can be found in Ref. [48]. A summary of DT architecture development relevant to EDTs is presented in Table 6.

A software engineering-oriented examination of these five papers indicates a high level of variance among the level of detail in the proposed software architectures and in certain cases, software processes to develop EDTs. The most comprehensive paper from a software engineering perspective, Steindl et al. [49], proposed a generic DT solution that could apply to EDTs, and included design diagrams for a layered software architecture spanning across six layers: Business logic; Functional; Information; Communication; Integration; and Asset. It also proposed ontology diagrams discussing the classification of software services to be exposed, as well as a RESTful API, a standard for HTTP connections over the Internet, to enable easier interoperability with existing software. The paper identified six domain-specific types of services: reconfiguration, control, prediction, diagnostic, monitoring, and simulation; as well as software management services. Lastly, the study defined an interface that all these services must implement comprising the following end points that: (1) retrieve service information, (2) retrieve model information, (3) train model, (4) inference using a model, (5) upload data, and (6) upload model.

Next in order of detail, Ors et al. [60] developed concepts for an AI-based operational EDT and presented a component diagram for the proposed architecture. Focusing on operations, the architecture inputs on-line measurements from the physical asset and various exogenous variables, while it outputs directly to the physical asset, updating its process and control data. The authors split the internal structure of their EDT into four main components: (1) an AI component responsible for performing surrogate & predictive modelling, optimisation and control using AI methods; (2) a traditional advanced process control component executing process-engineering oriented methods for scheduling, optimisation and control); (3) a data management and repository module; and (4) a process modelling component. The study also discussed that separate visualisation components need to be exposed to the human operator of the EDT and the deployment on the actual physical plant needs to be domain specific.

Focusing on the power industry, Huang et al. [61] presented a logical architecture diagram with four elements: physical entity, virtual entity, domain-specific services, and data. All these four elements were interconnected, which from a software engineering perspective might indicate a violation of the principle of separation of concerns. The study proposed that the virtual entity should contain six types of models, some of which appear to overlap, to meet the power industry requirements: geometric, physical, behaviour, unit, system, and complex system. Additionally, the paper proposed the usage of artificial neural networks as a method to perform data fusion for the various incoming data streams.

Min et al. [51] focused on the petrochemical industry and vaguely described processes operating in a continuous loop to regulate the plant's production plan, elements and controlling commands. Based on ML algorithms, they proposed concepts for model training, model evaluation, and online deployment, while maintaining connections with existing profit and market modelling and simulating/optimising software packages. It should be noted that this paper emphasised the reusability of existing modules over developing everything ground up.

The final paper with a strong software engineering angle, Blume et al. [43], presented a case study on cooling towers and, unlike the previous four papers, presented a software process to develop EDTs. In particular, the study described three EDT development steps: (1) business (and/or process) understanding; (2) data understanding, preparation and modelling, which included data selection, aggregation, feature selection, mining, hyperparameter tuning, transformation, outlier filtering; and (3) final evaluation and deployment.

Overall, these papers used software architecture diagrams and discussion primarily to represent, analyse and validate software requirements of EDT technology, rather than represent their actual implementation, which is a strong indication that this field has not settled yet. All of these papers assumed the process as a static system cut off from its environment and emphasised short-term operations. However, asset lifecycle improvement, including their retrofit, reconfiguring

Table 5
EDT applications for the process and energy industries.

Phase	Specific purpose	Ref.	Highlights
Design	Virtual testing	[41]	Iterative optimisation between static design and dynamic execution was implemented on a hollow glass production line.
	Optimisation	[39]	Design of a multi-tubular fixed bed reactor.
		[48]	Retrofit of methane reformer furnace system was proposed.
Processing	Process optimisation	[40]	Cost-effective impacts on plan operating economics were assessed for a 320 MW coal-fired thermal power plant based on its digital model.
		[51]	Production optimisation for the petrochemical industry was conceptually addressed using a machine learning-based EDT.
	Process prediction	[43]	The proposed data-driven EDT can provide power demand and cooling capacity predictions.
		[47]	Fruit inside temperatures in a fruit processing plant can be predicted by the proposed digital shadow.
		[52]	Fruit drying quality can be predicted by the proposed digital shadow.
	Process monitoring	[46]	Important variables were estimated from a digital model for monitoring purposes, and sensor miscalibration was identified by the proposed model.
		[50]	An on-line monitoring system for a steam turbine was developed based on hybrid models.
	Production control	[55]	MPC control was implemented on a EDT of cooling systems.
	Process training	[56]	The authors proposed a concept of a smart 3d viewer for the facility/asset.
Service	Fault detection and diagnosis	[57]	EDT concepts for forecasting emergencies in the oil and gas industry were discussed.

Table 6
Overview of DT architectures suitable for EDTs for the process and energy industries.

Architecture	Ref.	Proposed idea
AI-based operational EDT	[60]	Proposed a new framework of operational EDT by introducing three key components: surrogate modelling, predictive modelling and AI supported optimisation and control.
Data-driven EDT	[43]	A data-driven EDT framework was developed based on a cross industry standard process for data mining (CRISP-DM) concept. The framework was implemented for a cooling tower case study.
Machine learning-based EDT	[51]	A EDT architecture including IoT information and machine learning for petrochemical production control was proposed.
Power industry EDT	[61]	Different EDT structures for power plant control systems, online analysis of power grid and power system framework design were developed.
Generic EDT	[49]	A generic EDT architecture for industrial energy systems was proposed. The architecture was based on 5D-DT architecture and was aligned with the information technology layers of the Reference Architecture Model Industry 4.0 (RAMI4.0).

and retirement, will significantly contribute toward energy and greenhouse gas emissions reduction, for instance via retrofitting heat exchange networks [62]. Additionally, the integration of the site with its local renewable energy generation, industry, and community will be crucial, for instance by enabling it to benefit from exchanging heat and power [63]. As such, further research is needed to elicit software requirements and subsequently design EDT software that considers the industrial site as a constantly evolving system.

Besides software requirements elicitation and functional software design, this review also revealed a general lack of discussion around the satisfaction of non-functional requirements, such as performance, cyber security, and safety. Crucially, there was little discussion around EDTs being able to verify or the very least validate their operational decisions at run time before actuating them on a real plant. EDTs will be assisting in the operation of mission-critical systems where software failure can have catastrophic effects. Encompassing such quality assurance processes under uncertainty at the software level would de-risk the more rapid uptake of EDTs in the industry and make them safe and secure.

4.5. Modelling and simulation packages

Modelling and simulation play a crucial role within EDT technology. For a complex process, commercial process simulation software (e.g., Aspen HYSYS) is commonly used for building the EDT virtual plant. Their large user base, standardised approaches and technical support enables quality assurance in the application to large, complex processes. Such process simulators are usually examples of first-principles modelling (white-box modelling) with models relying on a fundamental understanding of physio-chemical phenomena. Researchers have also developed first principles-based models, but these are usually applied to small scale processes. Data-driven modelling (black-box modelling) has been implemented in many industries with new application technologies currently blooming, such as big data analysis, IoT and machine learning. Hybrid modelling (or grey-box modelling), which is a combination of white box and black box modelling, has also been used for EDT study. A summary is listed in Table 7. As mentioned previously in this review, most of these applications are of the 1D looks-like and dynamic behaves-like and indirect connects-to classes of DT and are proposals rather than industrial implementations.

5. Directions of future research

Many researchers have discussed DT challenges. For example, Fuller et al. [67] stated that the DT challenges were similar to data analytics, IoT and IIoT, and other researchers pointed out more DT challenges such as standardisation [20] (addressed in this paper), multidisciplinary cooperation [67], a consistent framework of DT [68], and complexity of implementation [69]. Comprehensive EDT development is inherently multidisciplinary, including fields such as chemical, mechanical, electrical, civil, and software engineering, data science. Because multidisciplinary research goals target different directions and focuses, there is a challenge in bringing together all the contributions into a DT framework.

5.1. Advancing energy digital twin technology

Based on the literature review and new classification framework, this review concludes with an overarching concept that defines how to implement EDT technology in the process heat and energy industries at a macro scale. The literature review showed that EDT technology can enable greater integration and optimisation within industrial (and commercial) sites leading to step increases in energy efficiency and renewable energy uptake. The implementation can also be extended to the “site edge” to further minimise resource consumption, waste, and emission footprints. The site edge refers to the community in the local area surrounding the site, such as other industrial sites, commercial and public operations, and residential housing. In many ways, EDT technology has the potential to help operationalise and synthesise the concepts of circular economy and circular integration [70], industrial symbiosis and industrial ecology [71], total site integration [72], and advanced site-wide control. Fig. 8 illustrates a new concept of how to envision an EDT’s interaction with an industrial site with a detailed description to follow.

Industrial sites often contain multiple operations and processes, which output signals, measurements and other data that form the basic inputs to the EDT. The EDT may also receive inputs from the site-edge (e.g., measurement of rooftop solar energy in the community) and from externalities (e.g., weather data and forecasts). The strategic, multi-objective goals of the EDT (e.g., minimisation of lifecycle cost, energy, and emissions) and constraints (e.g., 100% renewable energy) are set by the business owner, which is influenced and constrained by government regulation. The proposed framework of EDT provides one standard solution to achieve the decision making process from the government regulations to the plant units.

The outputs of the EDT include a wide range of effectors that enable the optimisation of site operations and assets. These effectors within the site may be automated or non-automated and include, for example, changes to control models and settings, plans to install new technology and retrofit existing technology, and information about the health of assets for predictive maintenance. An additional set of signals and effectors are also transmitted from the EDT to the site edge to influence the control, operation, and installation of relevant assets in the community. Assets in the community could be energy sources or sinks and have a range of ownership models with respect to the site, including non-site ownership, cooperative ownership with the site, and site-owned assets located outside the site limits. The ownership model, and any subsequent contract, dictates how the site can interact with the site edge asset. For example, a site may own rooftop solar panels in the residential estate, and therefore have complete control over their operation, and pay rent for the roof space to the individual owners. Or a site may send a price signal to the owners and operators of non-site assets to indicate the price level that the site is willing to pay for energy and services to influence the amount of flow sold to the site.

The EDT itself encompasses digital model, shadow, and manager components to accomplish the required exchange of information and complex computation. The framework also establishes a high-level relationship between the three levels of the connected-to attribute of DT technology. The Digital Model element contains the essential digital descriptions of each site assets' likeness and behaviour (either dynamic or non-dynamic). The Digital Shadow element encompasses and applies multiple instances of the digital models to mimic and predict how the site (and other) assets perform with time. The Digital Manager element uses multiple instances of digital shadows to test, question and optimise asset operations in the digital domain before outputting valuable information via the various effector signals to action change.

5.2. Critical research directions

Continuing from the overarching concept, urgent research directions in EDT technology that have been identified include the following:

1) Enhancement of EDT applications in service

EDT technology implementation on services has been reported in many systems and industries such as the automotive, manufacturing, building, and aircraft industries. A literature review about EDT implementation in services can be found in Ref. [22]. Based on the present literature review, only a few papers focus on EDT applications in service. As many researchers point out that the service and maintenance should be a major contribution area of EDT, this should be a direction of continued development for EDT applications in the process heat and energy industry.

2) Expansion of EDT to multiple application scales and the full lifecycle

Current EDT study and applications are targeted on micro and meso scales, e.g., a certain operation unit such as a furnace and a power plant. To obtain overall system optimisation and efficiency, there is a need to expand the EDT scale to the macro scale which can integrate different power supplies such as solar, hydro and wind power with different demands from both industrial and residential sectors together.

EDT developments for the process heat and energy industries commonly focus on one of three phases: design, processing, and service individually. In the future, EDT technology needs to cover the full lifecycle. For example, based on a current processing situation, a EDT could provide a suggestion on retrofitting the process to improve energy efficiency and an optimal maintenance service schedule simultaneously.

Taking account of the full lifecycle also means there is the opportunity to focus on lifecycle energy and emissions reductions. Many countries have set up target years to reach net-zero carbon-equivalent emissions, for example, 2050 for Europe, UK, New Zealand, and others. Researchers should use the EDT technology to help the process and energy industries to achieve net-zero-carbon targets by providing optimal process design using renewable energy, improving processing energy efficiency and obtaining optimal maintenance service schedule.

3) Development of adaptive EDT technology

It is well-known that processes change in performance with time (e.g., fouling), experience state transitions (e.g., cleaning), and operate in an ever-changing environment (e.g., external energy markets). There is

Table 7
A summary of modelling/simulation in EDTs.

Model basis	Software/Method	Ref.	DT class	Process	Units/Part
Commercial simulation software (first principles)	Thermoflow	[40]	DT121	Power plant	Boiler, steam turbine, scrubber
	ANSYS Fluent	[44]	DT231	Wind turbine	Wind turbine blade
	COMSOL	[47]	DT332	Food cooling	Mango fruit
	COMSOL	[52]	DT332	Food drying	Solar dyer, apple ring
	AspenPlus	[39]	DT221	Acrylic acid production	Multi-tubular reactor
	Modelica	[55]	DT131	Cooling system	Evaporator, tank, pump, heat exchanger
First principles	3D Java (visualisation)	[42]	DT311	Pipelines	Tank, connection pipes
	–	[45]	DT131	Industrial furnace	Burner, isolation, energy recovery
	–	[46]	DT131	Multi-effect evaporation	Evaporator
	Matlab	[48]	DT122	Reformer furnace	Furnace, heat exchanger
Data-driven	CRISP-DM	[43]	DT132	Cooling tower	Tank, pump, heat exchanger, cooling towers with fans
	Matlab/Simulink	[64]	DT132	Distillation (lab scale)	Distillation column, condenser, heat exchanger
	Statistical method	[65]	DT121	Rotary furnace	Furnace
	Machine learning	[51]	DT122	Catalytic cracking unit	Reaction/regeneration systems, distillation
Hybrid modelling	Updating model parameters	[50]	DT133	Steam turbine	Turbine, valve
	CFD (OpenSMOKE) + PCA	[66]	DT221	Combustion system	Combustion

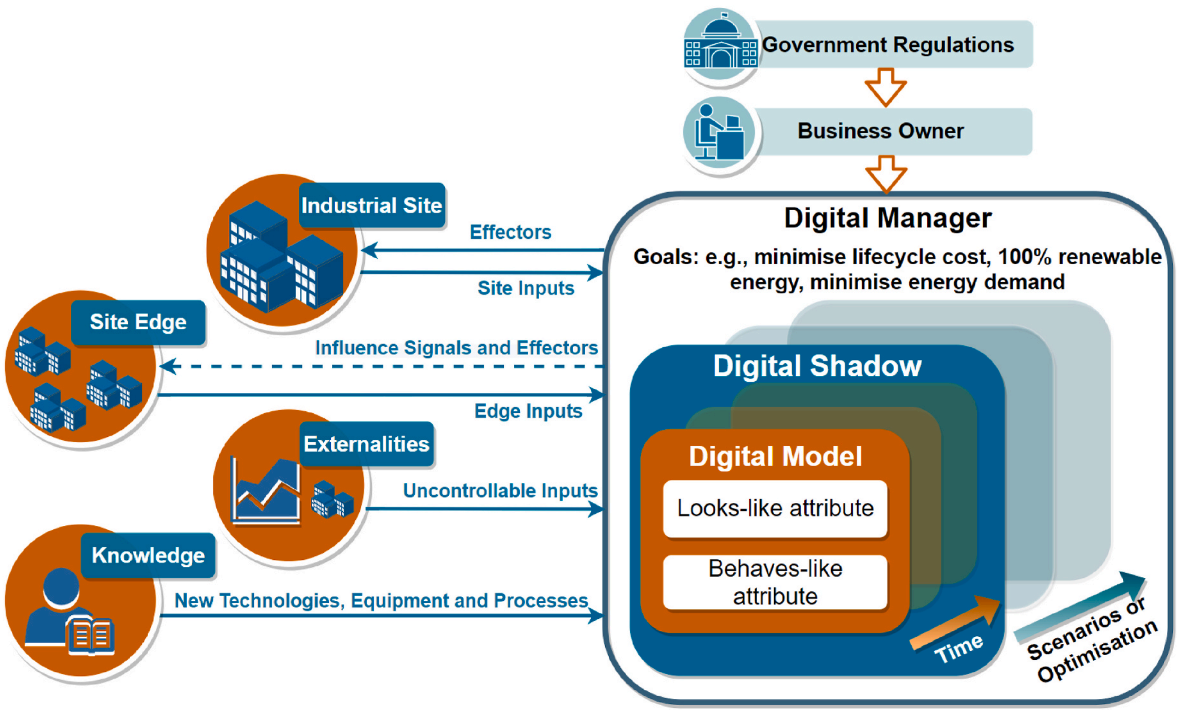

Fig. 8. A framework for the application of Energy Digital Twin technology (including Digital Model, Digital Shadow, and Digital Manager) to the process and energy industries.

a need to develop a new type of EDT technology that detects and adapts to these changes automatically. The attribute of self-adaptivity for an EDT adds the ability for the EDT to modify and recalibrate its behaviour and likeness under changing operating and external conditions, such that it satisfies operational goals and constraints (which may also vary with time) and accommodates possible future physical asset changes.

Further, adaptivity can be expanded to include hardware reconfigurability. Similar and perhaps inspired by Field Programmable Gate Arrays (FPGAs), which can be changed at runtime to represent any type of logic circuit, a digital-twin driven automated plant-control system will be able to rapidly reconfigure processes, such as manufacturing, while assuring the change management [73]. Additionally, FPGAs themselves could be incorporated as part of the computer hardware that operates a plant, which will allow the rapid deployment of new fit-for-purpose control algorithms that will have been first tested on the EDT. All these will require the establishment of a, hopefully open, architectural model, specification languages and optimised reconfiguration and planning algorithms. This research directly falls on the boundary between the fields of self-adaptive systems (software and computer engineering) and process systems engineering.

4) Enhancement of EDT platform security

The process and energy industries are critical infrastructure in global supply chains of commodity and advanced products. If EDTs participate directly in monitoring and actuating a site, it provides a large attack surface for cybercriminals and hostile nation-states with the intent to gain leverage over their target.

Research is needed to discuss what data can be monitored and how much of it should be sent to the cloud, which may risk greater system vulnerability. For instance, edge computing and federated learning could be used as a means to conduct first-pass training locally near the industrial plant before submitting a partially trained model, which would obfuscate raw-data, to a centralised location for further aggregation.

Additionally, research is needed to design active and multi-layered security for the EDT platforms. Active security means the EDT itself is looking for and mitigating threats through self-protection mechanisms. Multi-layered security allows the first security layer to be penetrated to trigger a response and stop an attack in subsequent layers.

5) Frameworks for EDT data ownership and sovereignty

EDTs will need access to an abundance of data from a variety of sources to make the best possible decisions. However, in a competitive market environment, industrial energy data is often viewed as highly confidential due to commercial sensitivities. As a result, there is a need to develop frameworks that enable data sharing while respecting the value of the data to the owner but also the wider value of the data to the country. Data sovereignty, for example, is a research field that seeks to define and understand how data can be subject to laws and governance structures within a country.

6) Specification of EDT software requirements

In consultation with stakeholders, further work is needed in EDT software requirements elicitation and analysis to better establish what exactly a EDT needs to be doing. This should be followed by the design of specification languages to describe the various components, interactions and goals the system would need to implement as well as the uncertainties it would operate under. Tools and methodologies should be developed to enable the design and verification of EDTs and potentially, automatically generate proven code artefacts. A standardised specification language for EDTs will also enable the automated interoperability of new and existing supporting software.

7) Engineering of AI-driven EDT

The usage of machine learning (ML) and other artificial intelligence (AI) algorithms for EDTs needs to mature by developing a clear understanding of what these methods can achieve for the process and energy industries. On the one hand, traditional AI optimisation techniques, such as simulated annealing and evolutionary optimisation, can dramatically reduce intractable search-spaces and have been widely applied to process optimisation and synthesis. On the other hand, data-driven techniques, such as recurrent neural networks (RNN) and dynamic mode decomposition with control (DMD-c), can computationally generate black-box models, or hybrid models, of systems that are too hard to model in first principles. In addition, time-series forecasting algorithms, such as autoregressive integrated moving average (ARIMA), could be used to model externalities and other uncontrollable events. Reinforcement learning (RL) techniques, including deep reinforcement learning, can be used to model advanced decision-making at a strategic level. In any data-driven case, however, research is required to automatically incorporate various AI engineering processes, such as feature engineering and training-validation-testing, into the system, while also leverage explainable AI models to enable quality assurance.

8) EDT computational requirements including benefit-to-power-use analysis

Since the main goal of EDT technology for the process industries is to reduce costs, energy, and emissions, a careful balance needs to be maintained to keep the computational requirements including the power, energy and emissions expended from operating EDT sufficiently low. For instance, contemporary deep learning algorithms are viewed as highly energy intensive, which is also exacerbated by the dramatically increasing network transmission volumes of the site and site-edge IoT data they would rely on. If computational requirements increases significantly, a trade-off may arise between the marginal benefit derived and the power consumed.

6. Conclusions

Digital twin (DT) technology and research were critically and systematically reviewed with a particular lens of application to the process and energy industries, i.e., Energy Digital Twin (EDT). Despite the process and energy industries being the flagship of many digital technologies, reports and publications on EDT technology applications and research studies were found to be relatively few compared to the manufacturing and building sectors.

Multiple, sometimes contrasting definitions of DT as a term and how to classify them were also found in the literature, and in use generally. To clarify and assist future researchers and practitioners in DT generally, the review developed a new multi-dimensional framework to classify DTs and applied it to EDTs. This framework classifies a DT according to its behaviour (static, multiple and transient state), connection (indirect, one-way direct and two-way direct), likeness (1-D, 2-D, or 3-D representation), and scale (*nano*, *micro*, *meso*, and *macro* physical scale and time scale) attributes. Applying this framework to the literature identified an EDT with 2-D likeness and able to model a process over multiple states as one potential research gap that could have significant benefits in assisting energy and emission reductions.

In terms of what the process and energy industries have interest in, EDT technology they currently apply, and primarily drives the implementation, applications feature most prominently in the energy related areas of energy generally, energy efficiency, or decarbonisation (59%); secondarily in the economically driven areas of profit, throughput or quality (36%); with the balance being in safety (5%). This leads to the conclusion that the optimisation of efficiency for energy usage reduction, to enable a pathway for effective decarbonisation, and ensure the associated costs remain low are the main objectives a successful EDT needs to fulfil.

EDT applications in the literature and public domain covered all aspects of the product or asset life cycle. However, there has been a focus on the design and operations phases predominately at the *nano* and *micro* scales. EDTs can unlock greater energy efficiency and renewable energy uptake through expanding the scale of application to include the *meso* and *macro* scales and covering the full life cycle, but this represents a challenging direction for future research.

CRediT authorship contribution statement

Wei Yu: Data curation, Investigation, Writing – original draft, Funding acquisition. **Panos Patros:** Methodology, Investigation, Writing – review & editing, Funding acquisition. **Brent Young:** Conceptualization, Writing – review & editing, Funding acquisition. **Elsa Klinac:** Visualization, Data curation. **Timothy Gordon Walmsley:** Conceptualization, Methodology, Writing – original draft, Funding acquisition, Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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