

# Sustainability implications of artificial intelligence in the chemical industry

## A conceptual framework

Mochen Liao | Kai Lan | Yuan Yao 

Center for Industrial Ecology, Yale School of the Environment, Yale University, New Haven, Connecticut, USA

### Correspondence

Yuan Yao, Center for Industrial Ecology, Yale School of the Environment, Yale University, 380 Edwards Street, New Haven, CT 06511, USA. Email: [yao@yale.edu](mailto:yao@yale.edu)

Editor Managing Review: Jean-Marc Frayret

### Funding information

This work receives funding from North Carolina State University, Yale University, the Alfred P. Sloan Foundation through the contract with Environmental Law Institute (Prime Contract No. G-2018-10090, NCSU Contract No. 8012-01-NCSU) and U.S. National Science Foundation. This material is based upon work supported by the National Science Foundation under Grant No. (1847182 and 2038439). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

### Abstract

Artificial intelligence (AI) is an emerging technology that has great potential in reducing energy consumption, environmental burdens, and operational risks of chemical production. However, large-scale applications of AI are still limited. One barrier is the lack of quantitative understandings of the potential benefits and risks of different AI applications. This study reviewed relevant AI literature and categorized those case studies by application types, impact categories, and application modes. Most studies assessed the energy, economic, and safety implications of AI applications, while few of them have evaluated the environmental impacts of AI, given the large data gaps and difficulties in choosing appropriate assessment methods. Based on the reviewed case studies in the chemical industry, we proposed a conceptual framework that encompasses approaches from industrial ecology, economics, and engineering to guide the selection of performance indicators and evaluation methods for a holistic assessment of AI's impacts. This framework could be a valuable tool to support the decision-making related to AI in the fundamental research and practical production of chemicals. Although this study focuses on the chemical industry, the insights of the literature review and the proposed framework could be applied to AI applications in other industries and broad industrial ecology fields. In the end, this study highlights future research directions for addressing the data challenges in assessing AI's impacts and developing AI-enhanced tools to support the sustainable development of the chemical industry.

### KEYWORDS

artificial intelligence, chemical industry, conceptual framework, impact assessment, industrial ecology, machine learning, sustainability

## 1 | INTRODUCTION

The chemical industry plays a critical role in the global economy. In 2017, the contribution of the chemical industry to the global gross domestic product (GDP) was estimated to be \$5.7 trillion (ICCA & Oxford Economics, 2019). The chemical industry is one of the most energy-intensive manufacturing industries (IEA, 2020a; Yao et al., 2014) and a major source of greenhouse gas (GHG) emissions. In 2010, the chemical and petrochemical industry accounted for 14% of the direct GHG emissions of the global industry (IEA, 2020b). In addition, chemical production often involves hazardous materials and high-pressure/high-temperature conditions, which may lead to fire, explosion, and other types of chemical accidents. Those

chemical accidents could cause casualties, financial and social losses (Cui & Liu, 2017). To reduce the environmental burdens and enhance the energy efficiency and operational safety, many efforts have been made to develop and employ emerging technologies in the chemical industry (National Academics of Science Engineering & Medicine, 2016, 2018, 2019).

Artificial intelligence (AI) is one of the emerging technologies that have attracted increasing attention in recent decades. AI is a set of comprehensive frontier technologies that can perform activities as human intelligence (Ali et al., 2015; Mao et al., 2019). Symbolic AI, machine learning, and heuristics are different subsets of AI. Symbolic AI symbolizes cognition and logic deduction to reveal the process of human cognition (Haugeland, 1985). Typical symbolic AI technologies include expert system, fuzzy logic, and case-based reasoning. Machine learning is another type of AI that is able to learn and improve the performance of specific tasks from past experiences (Mitchell, 1997). Many machine learning techniques have been developed, such as artificial neural networks, support vector machines, and random forest. Heuristics are often used to solve high-dimensional problems by mimicking the natural biological evolution (e.g., genetic algorithm) or the collective behaviors of the animal societies (e.g., particle swarm optimization, ant colony optimization) (Tong et al., 2014). Other AI techniques include hybrid methods and agent-based modeling (Axtell et al., 2001; Bernhardt, 2007; Jennings, 2000; Wooldridge, 1997). In this study, the referred AI techniques exclude approaches in operations research (OR), such as optimization which is a mathematical process aiming at maximizing or minimizing the value of objective functions subject to constraints (Dantzig, 2016; Fang & Puthenpura, 1993). Although OR has been widely applied in the chemical industry (Micheletto et al., 2008; Wang et al., 2015; Wu et al., 2017; Zhang et al., 2018), OR is not equivalent to AI, and the differences between AI and OR have been discussed in the literature. For example, traditional OR relies more on prescriptive methods that are solved to identify the optimal solution under defined constraints, while typical AI techniques lean toward predictive methods that provide projections of system performance and answer the question of what will happen (Hazen et al., 2018). Another study discussed OR as mathematical programming modeling relations between constraints, while AI focuses on the relationships between symbolic variables and symbolic structures (Venkatasubramanian, 2019). Given the differences, this study does not include OR literature whose authors do not recognize their work as AI (see Section 2 for keywords used in literature search). However, it is noticeable that with the more applications of AI techniques in OR (e.g., predicting the values or probability distributions of constraints (Bertsimas & Kallus, 2020)) and OR in AI (e.g., training the predictive models (Sra et al., 2012)), the limits and boundaries between AI and OR become fuzzier (Hazen et al., 2018).

The chemical industry is increasingly interested in using AI to address challenges in process modeling, optimization, control, and fault detection and diagnosis (Hajjar et al., 2016). Many of those aspects are related to the environmental, economic, and social sustainability of the chemical industry. According to a survey conducted by Accenture (Accenture, 2014), 94% of the executives of companies in the chemical and advanced materials industry expect an industry-wide digitalization, and AI plays an essential role in enabling the digital revolution (World Economic Forum, 2017). A few studies reviewed AI applications in the chemical industry (Ali et al., 2015; Kadlec et al., 2009; Zerrouki & Smadi, 2017). However, these reviews focused on the technical aspects of AI applications without examining the sustainability implications of using AI in the chemical industry. One study indicated the potential of AI in achieving sustainable development goals, but industry-specific investigations, specifically for the chemical industry, have not been conducted (Vinuesa et al., 2020). A few studies reviewed the impacts of AI application on higher education (Ma & Siau, 2018), public administration (Reis et al., 2019), and policy-making (Vesnic-Alujevic et al., 2020). All three studies focus on social and policy implications, but none have developed sustainability assessment frameworks. This study reviewed the literature that explored various AI applications in the chemical industry and quantitatively/qualitatively assessed the sustainability-related impacts of AI technologies. Based on the review, we proposed a conceptual framework encompassing industrial ecology approaches and different modeling/assessment methods for a holistic evaluation of AI's impacts from environmental, economic, and social perspectives. In this paper, Section 2 reviews the AI applications in the chemical industry, Section 3 describes the conceptual framework, and Section 4 highlights the major conclusions and future research directions. The contributions of this work include:

- Performing the first comprehensive literature review focusing on the sustainability implications of AI applications in the chemical industry by different application types and impact categories.
- Identifying data and methodological gaps in understanding the environmental, economic, and social implications of AI applications in the chemical industry.
- Presenting a conceptual framework to guide the selection of methods and indicators for the impact assessment of AI applications in the chemical industry. This study also highlighted major data requirements and sources of each method.
- Highlighting future research directions for better assessing the impacts of AI applications and the potential integration of AI and industrial ecology approaches to support the sustainable development of the chemical industry.

## 2 | REVIEW OF AI APPLICATIONS IN THE CHEMICAL INDUSTRY AND THEIR SUSTAINABILITY

In this study, we collected and reviewed 63 AI applications based on the following criteria: (1) published within 15 years; (2) published in peer-review journals or conference proceedings; (3) conducted quantitative analysis or qualitative assessment for the impacts of AI applications. Studies were searched in the Web of Science (2021) and Google Scholar Search Engine (Google, 2021) based on the combination of keywords "artificial

intelligence” and “chemical industry,” and then manually screened by the selection criteria mentioned above. We categorized these studies based on the type of AI applications (Section 2.1) and their potential impacts related to different aspects of sustainability (Section 2.2), and the detailed summary of each study is presented in the Supporting Information Table S2.

## 2.1 | AI applications in the chemical industry

Based on the studies reviewed, we identified four different types of AI applications in the chemical industry:

- **Research & development (R&D).** R&D plays an essential role in industry innovation, especially for sustainability-related businesses (Hájek & Stejskal, 2018). AI has been used for predicting and optimizing chemical reactions (Marcou et al., 2015; Mohammadi & Penlidis, 2018; Zhou et al., 2017) and enhancing the chemical synthesis design (Segler et al., 2018). Machine learning has been explored for the screening and design of catalysts (Li et al., 2017; Li et al., 2017; Zahrt et al., 2019). Several studies highlighted the potential of AI in supporting the development of sustainable chemicals and materials (Doan et al., 2020; Gu et al., 2019). In addition to those technical aspects, one study investigated the use of artificial neural networks to evaluate and improve the job satisfaction of research labs (Azadeh et al., 2015).
- **Unit operations.** Unit operations (e.g., chemical synthesis and separation) are basic steps of chemical processes (Green & Perry, 2008). AI has been applied to improve the performance of specific unit operations, such as combustion (Zheng et al., 2009; Zhou et al., 2005), distillation (Ochoa-Estopier et al., 2013; Osuolale & Zhang, 2016, 2017), evaporation (Verma et al., 2017), compression (Qi et al., 2018), and reaction (Fernandes, 2006; Mosavi et al., 2019; Schweidtmann et al., 2018). Some studies focused on technical indicators such as yields (Fernandes, 2006; Geng et al., 2016; Keyvanloo et al., 2012; Schweidtmann et al., 2018), while the others focused on risk-related performance (Guo et al., 2009; Jaderi et al., 2019; Qi et al., 2018) and intelligent control of unit operations (Ji et al., 2016).
- **Processes and chemical plants.** AI has been explored in process system engineering for decades (Lee et al., 2018), for example, early AI applications in the 1990s for process control (Naidu et al., 1990; Saint-Donat et al., 1991; Ydstie, 1990). Recent studies explored different AI techniques such as deep neural networks, convolutional neural networks, and transfer learning (Wu & Zhao, 2018, 2020; Zhang & Zhao, 2017) to address process control problems in chemical plants that are much more complex than that in the 1990s (Luo et al., 2015; Sahebjamnia et al., 2016). A few studies integrated AI with risk assessment methods to improve the risk management of chemical plants (Aqlan & Mustafa Ali, 2014; Guo et al., 2019; Lavasani et al., 2015; Yazdi & Kabir, 2017). Another AI application is chemical process and plant design (Cecchini et al., 2012; Negny et al., 2012; Stéphane et al., 2010) that usually have direct impacts on the quality, cost, and environmental footprints of products (Stéphane et al., 2010). Several studies have explored the potential of AI in facilitating the eco-design of chemical processes (Robles et al., 2009; Ferrer et al., 2012; Negny et al., 2012). Other studies used AI to evaluate and enhance human factors such as health, safety, environment, and ergonomics (HSEE) in chemical plants (Azadeh et al., 2013; Azadeh & Zarrin, 2016).
- **Supply chain.** A supply chain is an integrated network where different entities such as suppliers, manufactures, and distributors work together to convert the raw materials into final products and deliver them to customers (Beamon, 1998). AI has been used to support the design, planning, and optimization of chemical supply chains with different environmental and economic aspects considered (e.g., genetic algorithm (Berning et al., 2004; Guillén et al., 2006), heuristic algorithm (Pozo et al., 2012)). Some studies focused on the supplier selection (e.g., case-based reasoning (Zhao & Yu, 2011), while others used AI techniques to forecast and manage disruptive events (e.g., agent-based modeling (Behdani et al., 2009, 2012, 2019; Ehlen et al., 2014)). Previous studies also integrated AI into traditional supply chain modeling techniques for renewable materials such as biomass (Castillo-Villar, 2014; Ghaderi et al., 2016; Lan et al., 2019).

## 2.2 | Sustainability implications of AI applications

This section presents studies with measured/estimated/indicated sustainability-related impacts of AI by four types of applications. Five types of impacts were identified (Table 1), including economic, energy, environmental, safety and human factor, and time. Energy and time are separated from the other three categories. Although reducing energy consumption and computational time could improve environmental and economic performance, such benefits need to be confirmed with additional assessments such as life cycle assessment (LCA) or techno-economic analysis (TEA). Therefore, those studies focusing on energy and time without analyzing environmental and economic performance were classified into different categories from environmental or economic categories.

Limited by the space, references were not shown in Table 1 but discussed in the following subsections. Table 1 shows in total 63 studies that are much smaller than the number of AI applications explored in the chemical industry (e.g., more than 180 studies based on previous reviews (Ali et al., 2015; Zerrouki & Smadi, 2017)). Furthermore, most studies shown in Table 1 only cover one or two impacts, and none of them have holistically assessed the impacts of AI from environmental, economic, and social aspects. Most studies (70%) in Table 1 include quantitative evaluation of AI's benefits, while the rest only qualitatively discussed the potential benefits. This study only includes peer-reviewed studies and does not include

**TABLE 1** The number of AI applications in the chemical industry by application types and impact categories

	R&D	Unit operations	Process and chemical plants	Supply chain
<b>Economic</b>				
Direct and indirect costs	6	3 <sup>a</sup> (3) <sup>b</sup>	6 (5)	N
Profits	N	3 (3)	N	6 (6)
Capacity and yields	N	4 (4)	3 (3)	N
<b>Energy</b>				
Energy efficiency	N	6 (6)	1 (1)	N
Specific energy consumption	N	2 (2)	4 (4)	N
<b>Environment</b>				
Emissions to air/water/land	Indirect reduction <sup>c</sup>	3 (3)	2 (1)	1 (1)
Life cycle environmental impacts		N	N	1 (1)
<b>Safety and human factor</b>				
Risk management	N	2 (2)	5	3 (3)
Process monitoring and fault diagnosis	N	2 (2)	7 (6)	N
Productivity	1(1)	N	3(3)	N
Simulation-based decision-making	N	N	N	2
Product safety	1 (1)	N	N	N
<b>Time</b>				
Time for chemical product and process design	4	N	N	N
Experimental time	4	N	N	N
Computation time	3	N	N	2(2)

N indicates "None of the studies have been identified."

<sup>a</sup>Total number of studies reviewed.

<sup>b</sup>The number within the parenthesis is the number of studies that quantitatively evaluated the impacts.

<sup>c</sup>Indicate reduction of environmental impacts by reducing the number of experiments needed.

unverified information online that qualitatively discussed the potential benefits of AI for the chemical industry. If they were included, the total number of studies with qualitative information of AI's impacts would be much higher than that in Table 1. Both observations indicate a strong need for quantitative and holistic assessments to better understand the sustainability implications of AI applications in the chemical industry.

### 2.2.1 | Economic aspect

The economic aspect in Table 1 refers to the direct or indirect impacts of AI on the economic gains of chemical production. Given that most chemical companies are for profit, it is not surprising to see the largest number of studies focusing on economic benefits in Table 1. Specific economic indicators evaluated in those studies are shown in Table 2.

Most studies focused on reducing the costs of chemical production through AI applications. Three studies assessed cost reduction using different indicators, as shown in Table 2 (Ochoa-Estopier et al., 2013; Osulale & Zhang, 2016, 2017). We identified six studies that applied AI to chemical processes and/or chemical plants. Two of them focused on reducing the economic penalty from the imbalance between the planned and consumed natural gas (Kovačič et al., 2016; Kovačič & Dolenc, 2016). Other studies applied AI to decrease the operating costs related to energy (Jahromi et al., 2018), capital costs (Cecchini et al., 2012), and raw material costs (specifically the cost of crude oil consumption) (Han et al., 2019). For AI applications to supply chains, one study proposed a genetic algorithm-based methodology that can optimize the different indirect cost components for the chemical supply chain (Berning et al., 2004), but relevant AI applications were not identified.

Several AI studies focused on improving the profits of chemical production, all of which used quantitative methods (e.g., TEA) and process data (e.g., mass and energy balance). Three studies applied AI to unit operations, and they used profit indicators such as profit rate (Ji et al., 2016) and annual operating profit (Ochoa-Estopier et al., 2013; Osulale & Zhang, 2017). The other three studies for supply chain used different indicators such as net present value (Pozo et al., 2012), expected profit (Ehrenstein et al., 2019; Guillén et al., 2006), and the average profit for scenarios with different supplier disruptions (Behdani et al., 2012, 2019), and other self-defined profit function (Cao et al., 2018). Note that this review does not

**TABLE 2** Summary of economic indicators assessed in AI applications reviewed in this study

Application types	Quantitative indicators
R&D	<ul style="list-style-type: none"> <li>No studies with quantitative indicators identified</li> </ul>
Unit operations	<ul style="list-style-type: none"> <li>Utility cost (Osuolale &amp; Zhang, 2016)</li> <li>Energy cost (Osuolale &amp; Zhang, 2017)</li> <li>Total annualized cost (Ochoa-Estopier et al., 2013)</li> <li>Annual operating profit (Ochoa-Estopier et al., 2013; Osuolale &amp; Zhang, 2017)</li> <li>Profit rate (Ji et al., 2016)</li> <li>Reactor productivity (Schweidtmann et al., 2018) and reaction yield (Fernandes, 2006; Geng et al., 2016; Pereira et al., 2020) that have direct impacts on costs and profits</li> </ul>
Process and chemical plants	<ul style="list-style-type: none"> <li>Raw material cost (e.g., crude oil consumption) (Han et al., 2019)</li> <li>The ratio of high-quality products (Sahebjamnia et al., 2016)</li> <li>Contract penalty (Kovačič et al., 2016; Kovačič &amp; Dolenc, 2016)</li> <li>Net present sink (Fahmi &amp; Cremaschi, 2012)</li> <li>Utility cost (Jahromi et al., 2018)</li> <li>Capital cost (e.g., sensor cost) (Cecchini et al., 2012)</li> <li>Reaction yield (Han et al., 2019) that has direct impacts on costs and profits</li> </ul>
Supply chain	<ul style="list-style-type: none"> <li>Expected profit (Ehrenstein et al., 2019; Guillén et al., 2006)</li> <li>Self-defined profit function (Cao et al., 2018)</li> <li>Average profit for 20/30 scenarios with different supplier disruptions (Behdani et al., 2012, 2019)</li> <li>Net present value (Pozo et al., 2012)</li> </ul>

include AI studies for bio-based chemicals as they have not been widely commercialized (Sharma et al., 2013), and readers are referred to a recent review of AI applications to biorefineries for more details (Liao & Yao, 2021).

In addition to costs and profits, some AI applications use indicators for plant capacity or product yields that directly impact the profits of chemical production. Some AI studies for R&D focus on improving the reaction yields (Mohammadi & Penlidis, 2018; Zhou et al., 2017) that could improve the profits if scaling up in the chemical production. However, none of these studies have provided unit-operation-level or process-level validations of potential economic benefits. Therefore, these studies are not included in Tables 1 and 2. Four studies used AI to increase the yields by developing predictive models for unit operations (Fernandes, 2006; Geng et al., 2016; Pereira et al., 2020; Schweidtmann et al., 2018) and employing heuristic-based yield optimization (Geng et al., 2016). Other studies developed AI-based predictive models for chemical products (Gong et al., 2017; Han et al., 2019), or used reinforcement learning to enhance the process control for optimizing the ratio of high-quality products (Sahebjamnia et al., 2016). These studies have quantitatively analyzed the improvements as these benefits are part of their modeling objectives.

In summary, many studies have quantified the economic benefits of AI applications in the chemical industry. They specifically focused on cost reduction, profits improvement, and capacity/yield increase, depending on the application types and specific AI techniques. All quantitative assessments need economic and process data (notably the data of energy and material flows), and many studies used economic analysis like TEA. These findings can be used as a reference for future economic assessment of different AI applications.

## 2.2.2 | Energy aspect

Similar to the economic benefits, most AI studies reviewed in this section include quantitative analysis of either energy efficiency or energy consumption as these indicators are parts of the goals of AI applications (and economic and energy aspects are exchangeable in some cases when the economic indicator is energy cost). Those quantitative analyses rely on the existing energy/exergy analysis methods and energy data. Table 3 lists specific energy indicators used in previous AI studies. For chemical processes and plants, most studies integrated AI with analytical tools such as exergy and energy analysis to model and optimize the energy consumption of chemical and advanced material production (Golkarnarenji et al., 2018; Jahromi et al., 2018; Zhu et al., 2018). They showed 8.82%–43.3% reduction of specific or total energy consumption of studied systems, and their analysis heavily rely on the historical energy data of the plants. In addition, one study used agent-based modeling to combine different models and blocks (e.g., process models, process control block, fault detection model, and optimization block) for the polyethylene terephthalate production, which approximately reduced 10% of the heat medium flow of the entire factory (Luo et al., 2015). Another study used machine learning to improve the energy efficiency of the purified terephthalic acid production (Gong et al., 2017), and they qualitatively discussed the improvement of the plant-wide consumption of fuels, water, steam, and electricity. Unlike those studies for chemical plants, all studies for AI applied to unit operations used technology/facility-specific indicators to assess the energy benefits of AI, such as indicators specifically for distillation columns (Osuolale & Zhang, 2016, 2017), boilers (Zhou et al., 2005), evaporators (Verma et al., 2017), a centrifugal compressor (Heinrich & Schwarze, 2017), and a gas

**TABLE 3** Summary of energy indicators assessed in AI applications reviewed in this study

Application types	Quantitative indicators
R&D	<ul style="list-style-type: none"> <li>No studies with quantitative indicators identified</li> </ul>
Unit operations	<ul style="list-style-type: none"> <li>Isoentropic efficiency (Heinrich &amp; Schwarze, 2017; Sun &amp; Yoon, 2018)</li> <li>Boiler efficiency (H. Zhou et al., 2005)</li> <li>Exergy efficiency (Osuolale &amp; Zhang, 2016, 2017)</li> <li>Steam economy (Verma et al., 2017)</li> <li>Steam consumption (Geng et al., 2016; Verma et al., 2017)</li> </ul>
Process and chemical plants	<ul style="list-style-type: none"> <li>Exergy efficiency (Jahromi et al., 2018)</li> <li>Energy-saving potential (Zhu et al., 2018)</li> <li>Total energy consumption (Golkarnarenji et al., 2018; Jahromi et al., 2018)</li> <li>Heat medium flow (Luo et al., 2015)</li> </ul>
Supply chain	<ul style="list-style-type: none"> <li>No studies identified</li> </ul>

cyclone separator (Sun & Yoon, 2018). Furthermore, two studies used AI to improve the steam consumption of unit operations (Geng et al., 2016; Verma et al., 2017).

Although no studies were identified for R&D, AI could bring energy benefits in reducing the energy consumption of R&D activities by reducing the number of trials, as shown in Table 2. For AI applications for the supply chain, some generic energy indicators such as energy consumption and energy-saving potential could be used to quantify supply-chain-wide energy benefits of AI. Note that the energy consumption of AI applications (e.g., energy consumption of information technology, IT, infrastructure needed by computing) also needs to be considered. García-Martín et al. (2019) reviewed power estimation models for machine learning. For example, Rouhani et al. (2016) estimated the energy consumption of the training phase of a feedforward neural network by counting the number of arithmetic operations and communications in the training process. Rodrigues et al. (2018) estimated the energy consumption of a convolutional neural network by accounting for the power used by IT components, such as the processor, memory, and other peripherals. Depending on the types of AI and related hardware, estimating the energy consumption of AI and machine learning could be very complex.

### 2.2.3 | Environmental aspect

Only seven studies (as shown in Table 1 and summarized in Table 4) have quantified the potential environmental impacts of AI applications in the chemical industry. AI can reduce the number of experiments in R&D, leading to a reduction of chemical usage and disposal from laboratories (that are considered as wastes to land or water) (Accenture, 2014; Choy et al., 2016). One study estimated a 19% reduction of chemical disposal by using the AI-based recursive operations strategy model for determining the optimal formula of product ingredients (Choy et al., 2016). AI may also reduce the life cycle impacts of conducting experiments. For example, all chemicals used in experiments have embodied impacts (e.g., embodied energy and carbon) that are impacts associated with the upstream production and transportation of chemicals (Yao & Masanet, 2018), reducing the number of experiments in R&D decreases the chemical usage, reducing the embodied impacts of chemical usage and as a result reducing the life cycle impacts of conducting experiments. The significance of such impacts will need to be quantified by systems tools such as LCA either for R&D activities (e.g., compare the life cycle impacts of experiments before and after AI implementation) or entire organization (e.g., conduct organizational LCA before and after AI implementation) (Martínez-Blanco et al., 2015). AI has been applied to unit operations and chemical plants to minimize the

**TABLE 4** Summary of environment indicators assessed in AI applications reviewed in this study

Application types	Quantitative indicators
R&D	<ul style="list-style-type: none"> <li>Chemical disposal (Choy et al., 2016)</li> </ul>
Unit operations	<ul style="list-style-type: none"> <li>NO<sub>x</sub> emissions (Zheng et al., 2009; Zhou et al., 2005)</li> <li>Naphtha generation (Geng et al., 2016)</li> </ul>
Process and chemical plants	<ul style="list-style-type: none"> <li>Reduced CO<sub>2</sub> emissions (Han et al., 2019)</li> </ul>
Supply chain	<ul style="list-style-type: none"> <li>Damage to human health/ecosystem quality/natural resources (Pozo et al., 2012)</li> <li>GHG emissions (Cao et al., 2018)</li> </ul>

**TABLE 5** Summary of safety and human factor indicators assessed in AI applications reviewed in this study

Application types	Quantitative indicators
R&D	<ul style="list-style-type: none"> <li>Safety and health indexes of chemical products (e.g., soil sorption coefficient and flammability) (Ng et al., 2014; Ten et al., 2016)</li> <li>Job satisfaction (Azadeh et al., 2015)</li> </ul>
Unit operations	<ul style="list-style-type: none"> <li>Feedback time (Ji et al., 2016)</li> <li>Sensor measurement deviation (Ji et al., 2016; Sriyakul et al., 2017)</li> <li>Criticality score (Guo et al., 2009; Jaderi et al., 2019)</li> </ul>
Process and chemical plants	<ul style="list-style-type: none"> <li>Fault detection and diagnosis indicators (e.g., fault detection rate, false positive rate, accurate classification rate) (Qi et al., 2018; Wu &amp; Zhao, 2018, 2020; Zhang &amp; Zhao, 2017)</li> <li>Sensor measurement deviation (Gonzaga et al., 2009)</li> <li>Failure probabilities of top events<sup>a</sup> (Aqlan &amp; Mustafa Ali, 2014; Guo et al., 2019; Lavasani et al., 2015; Yazdi &amp; Kabir, 2017; Yazdi &amp; Zarei, 2018)</li> <li>Reliability (Cecchini et al., 2012)</li> <li>Number of faults in a period of time (Sahebjamnia et al., 2016)</li> <li>Labor productivity indicators (e.g., job stress, staff efficiency, effectiveness, labor time) (Azadeh et al., 2013; Azadeh &amp; Zarrin, 2016; Jiang et al., 2018)</li> </ul>
Supply chain	<ul style="list-style-type: none"> <li>Supply-demand ratio (Ehlen et al., 2014)</li> <li>Cumulative late order and tardiness (Behdani et al., 2009, 2019)</li> <li>The similarity between the supplier qualification and the target qualification (Zhao &amp; Yu, 2011)</li> </ul>

<sup>a</sup>System-level failure events considered as the outcome of fault and event trees (e.g., the explosion of oil storage tanks) (Ruijters & Stoelinga, 2015).

NO<sub>x</sub> emissions from the boiler (Zheng et al., 2009; Zhou et al., 2005), the naphtha generated from the ethylene cracking furnace (Geng et al., 2016), and the CO<sub>2</sub> emissions from the ethylene production plant (Han et al., 2019). For the chemical supply chain, one study quantified and optimized supply-chain-wide GHG emissions by integrating a cyber-physical system (Cao et al., 2018). Another study that applied a nondominated sorting genetic algorithm in optimizing chemical supply chain design quantified the endpoint life cycle impacts of the supply chain (Pozo et al., 2012).

LCA has been used to evaluate the environmental impacts of emerging technologies in the chemical industry (Yao & Masanet, 2018). However, few studies have used LCA to quantify the potential life-cycle environmental impacts of AI applications, which could be caused by limited data availability (e.g., the lack of life cycle inventory (LCI) data of chemical plants, such as air emission data before and after AI implementation). Although the LCI data of some chemical production are available in databases such as Ecoinvent and USLCI (NREL, 2012; Wernet et al., 2016), the LCI data of specific facilities, unit operations, chemical plants, or supply chains before and after AI implementation are not available. Given that AI has not been widely adopted, how to acquire those data from either primary or secondary sources and integrate them into the traditional LCA framework is a challenge. Another critical issue is the acceptability of AI proposed solutions. The actual impacts of AI applications will depend on whether and how much those solutions generated by AI techniques can be accepted and feasibly implemented in the chemical industry. Addressing the uncertainty associated with the AI acceptability in qualitative assessment methods such as LCA is a research direction worth further investigation.

Although the LCAs of AI applications in the chemical industry are rare, AI has been used to facilitate the LCAs with limited LCI data. For example, one study has combined artificial neural network and process simulations to generate the LCI data of activated carbon produced from diverse biomass sources (Liao et al., 2019, 2020). Another study developed machine learning-based models to estimate the life cycle impacts of chemicals (Song et al., 2017), and a similar approach was used for predicting the life cycle impacts of sugarcane production (Kaab et al., 2019) and corn production (Romeiko et al., 2019). One study used LCA to estimate the environmental impacts of a chemical supply chain and integrated such impacts into their optimization models that utilized AI techniques (Pozo et al., 2012).

The LCA is needed for AI applications in the chemical industry to better understand AI's potential environmental impacts and identify the most sustainable pathways for large-scale, industry-wide AI adoption. Conducting LCAs for AI applications shares many challenges with LCAs for other emerging technologies, such as the large data gap. It also could be more challenging to identify and assess how physical processes and specific technical parameters will be changed after AI implementation. This is one of the challenges that we hope the conceptual framework proposed in this paper can address.

## 2.2.4 | Safety and human factor aspect

The safety and human factor aspect covers many factors from process safety to employee productivity, as shown in Table 5. AI applications for detecting abnormal conditions during chemical production can be traced back to the 1980s (Rich et al., 1989). Recent studies explored

different AI techniques and application types. One study developed a fuzzy logic integrated chemical product design framework to improve chemical product safety in early-stage chemical R&D (Ten et al., 2016). In another study, AI increased the reliability and accuracy in detecting abnormal conditions, improving the process monitoring and fault diagnosis, and enhancing the overall chemical production safety (Zhang et al., 2011). For AI applied to unit operations, AI-enhanced process monitoring has been developed for a rectification column (Ji et al., 2016) and a chemical reactor (Sriyakul et al., 2017). Other studies used AI to enhance the monitoring for polymerization processes (Gonzaga et al., 2009) and refineries (World Economic Forum, 2017) considered as AI applications for chemical plants. In addition, AI-based fault detection has been developed for reciprocating compressors (Qi et al., 2018) and Tennessee-Eastman process (Wu & Zhao, 2018, 2020; Zhang & Zhao, 2017). The safety impacts of those AI-based models can be quantified by indicators such as fault detection rate (Zhang & Zhao, 2017), and reliability (Cecchini et al., 2012).

Risk assessment is a critical method for safety improvement and management in the chemical industry (Lee et al., 2016). Previous studies have investigated the potential of AI in supporting risk assessment using different indicators and quantitative methods. Two studies used artificial neural networks to estimate the criticality score of petrochemical facilities (Guo et al., 2009; Jaderi et al., 2019). For processes and chemical plants, several quantitative risk assessment methods are available such as failure modes and effects analysis, fault tree analysis, and bow-tie analysis. Fuzzy logic and Bayesian network have been combined with fault tree analysis (Guo et al., 2019; Lavasani et al., 2015; Yazdi & Kabir, 2017; Yazdi & Zarei, 2018) and bow-tie analysis (Aqlan & Mustafa Ali, 2014) to analyze the petrochemical plants. AI significantly enhanced the capacities of traditional risk assessment methods, especially for complex systems with small datasets. In addition, agent-based modeling has been used to simulate the large-scale chemical supply chains and quantify the risks (using indicators such as reduced average profits) from homeland security events (Ehlen et al., 2014) and the effectiveness of different risk mitigation strategies (Behdani et al., 2012, 2019).

For the impacts of AI applications on the human factor aspect, two types of impacts were identified: improved labor/enterprise productivity and enhanced decision-making. AI-based models were established to estimate and enhance the staff productivity indicators (e.g., job stress and job satisfaction) for hazardous R&D laboratories (Azadeh et al., 2015), and chemical plants (Azadeh et al., 2013; Azadeh & Zarrin, 2016; Jiang et al., 2018). The productivity of individuals working at R&D laboratories and chemical plants was quantified by the HSEE and resilience engineering (RE) scores based on the data collected from questionnaires. For AI applications to chemical supply chain, AI can be used to enhance the supply-chain decision-making, such as supporting supplier selection (Zhao & Yu, 2011) and evaluating the effectiveness of different supply chain management strategies (Behdani et al., 2009; DeRosa et al., 2016). For example, Zhao and Yu (2011) adopted the case-based reasoning approach that was built on the AI technology (i.e., back propagation neural network) and developed a method to enhance the decision-making on supplier choices for the petroleum enterprise using the large amount of case data cumulated by a petroleum company in China (Zhao & Yu, 2011).

For chemical production, safety and human factors are highly correlated (Gordon, 1998). But few studies have evaluated the correlations between these two impacts (e.g., how the enhanced safety would improve HSEE-related scores or vice versa). Most studies that provided quantitative information of AI's impacts have included those impact indicators in their AI-based models. Those studies also have demonstrated the potential of AI in enhancing the traditional risk assessment from a methodology point of view and improving the employee productivity and supply chain decision-making from a practical point of view, although the latter improvement is much harder to be quantified than the former one.

## 2.2.5 | Time aspect

The time aspect is referred to the reduced time for the design, experiment, and computation by applying AI-based methods. Although time reduction is not directly related to sustainability, it could reduce the environmental, economic, and social impacts by reducing resource consumption and support the sustainable development of chemical processes/products, which is why we included this aspect in this review. For example, previous studies showed that computational time has direct correlations with the energy and carbon footprints of AI and machine learning, and thus training time should always be reported (Dhar, 2020; Henderson et al., 2020; Lacoste et al., 2019; Strubell et al., 2020).

In total, we identified four studies for accelerating chemical process and product design, three studies for reducing experimental time, and three studies for decreasing computational time in R&D. Although almost all studies mentioned the time reduction benefits of AI, few of them quantified such benefits. Two studies applied heuristic algorithms for supply chain optimization that found near-optimal solutions with a shorter computational time than traditional optimization methods (Ehrenstein et al., 2019; Pozo et al., 2012). It is noteworthy that besides the chemical industry reviewed in this study, AI technologies are widely reported to reduce the computational time in other industries and fields, including the power sector, food industry, transportation system, and other areas (Abduljabbar et al., 2019; Ahn et al., 2020; Ma & He, 2019; Ongsakul & Dieu, 2019; Zahraee et al., 2016). Another area is green supply chain design and management (GSDM), an emerging area that integrates environmental considerations into supply chain design and management (Srivastava, 2007). AI has been applied to supply chain management but mostly on the risk management

**TABLE 6** Summary of different AI adoptions in the chemical industry

	Traditional systems	Systems after AI adoption	Typical AI techniques <sup>a</sup>	Potential impact
1	TP <sup>Unknown</sup> → PI	TP <sup>AI-based</sup> → PI	<ul style="list-style-type: none"> <li>• Neural networks</li> <li>• Support vector machine</li> <li>• Random forest</li> </ul>	High
2	TP <sup>Unoptimized</sup> → PI	TP <sup>AI optimized</sup> → PI	<ul style="list-style-type: none"> <li>• Genetic algorithm</li> <li>• Particle swarm optimization</li> <li>• Differential evolution</li> </ul>	Medium
3	TP <sup>Traditional</sup> → PI	TP <sup>AI integrated</sup> → PI	<ul style="list-style-type: none"> <li>• Fuzzy logic</li> <li>• Case-based reasoning</li> <li>• Agent-based modeling (ABM)</li> </ul>	Low

TP, technical parameters that can be controlled; PI, performance indicators.

<sup>a</sup>Those AI techniques were identified through the literature reviewed in this study, this is not a comprehensive list of all applicable AI techniques.

domain (Baryannis et al., 2019). Liu et al. (2020) reviewed 36 studies that applied big data analytics to GSDM, and pointed out a few of them that have applied AI to green purchasing (Liu et al., 2020), although none of these are related to the chemical industry. Liao and Yao (2021) reviewed AI applications in the bioenergy field and discussed the potential benefits of AI in addressing computational barriers by providing near-optimal solutions for supply chain design problems (Liao & Yao, 2021).

### 3 | A CONCEPTUAL IMPACT ASSESSMENT FRAMEWORK FOR AI APPLICATIONS IN THE CHEMICAL INDUSTRY

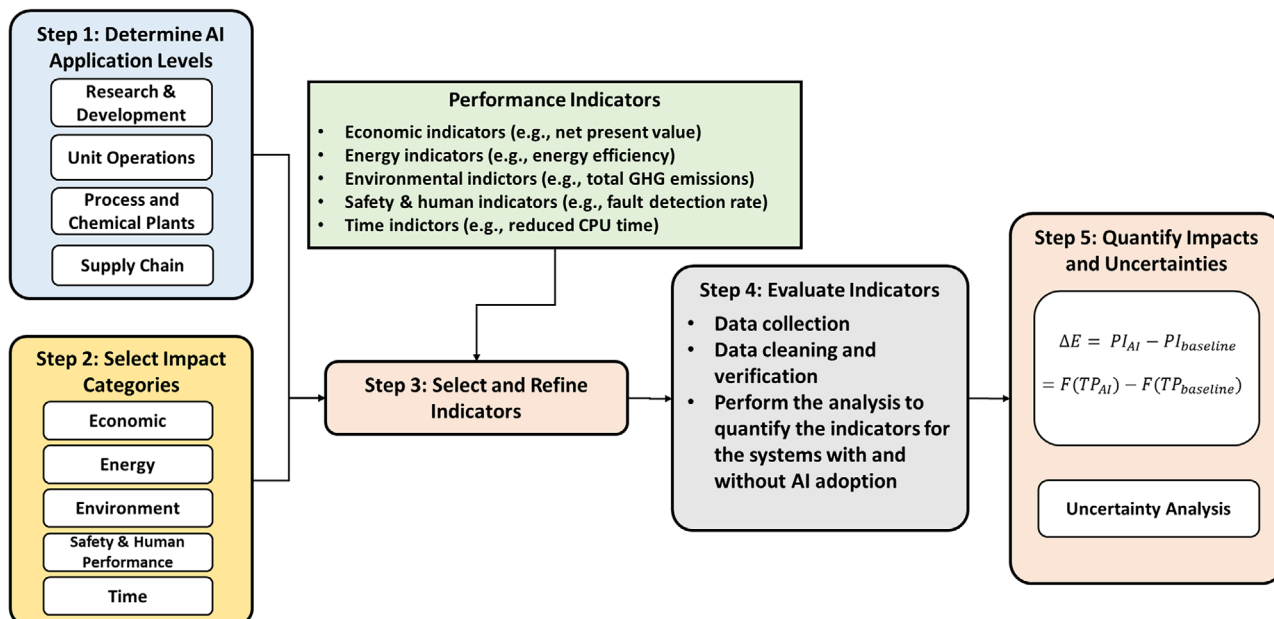
AI is in digital form, but AI applications in the chemical industry require interactions between AI and physical activities. To better quantify the potential impacts of AI applications, comprehensive understandings of how AI has been applied and interacted with existing models (digital systems) and chemical production (physical systems) are needed. By examining different AI applications and how AI interacted with chemical systems in the literature reviewed in Section 2, we identified three modes of AI applications, as shown in Table 6. Technical parameters (TP) are controllable parameters (e.g., temperature and material flow rates for unit operations). PI are performance indicators that depend on technical parameters (e.g., profits, energy consumption, and environmental emissions) and are related to five aspects discussed in the previous section. These three modes majorly differentiate in the relationships between TP and PI of the traditional systems, namely unknown relationships, known relationships but unoptimized, and known relationships but requiring enhancement.

In the first mode, the quantitative relationships between TP and PI of the traditional systems are unknown, thus improving PI mostly relies on trial and error or empirical knowledge. Powered by AI, PI can be directly predicted or estimated based on existing datasets. A few examples include the AI-based predictive models for improving the process monitoring of unit operations (Fahmi & Cremaschi, 2012; Gonzaga et al., 2009; Han et al., 2019). AI techniques that have been applied under this mode include artificial neural networks (Zhou et al., 2005), support vector machine (Golkarnarenji et al., 2018), and random forest (Marcou et al., 2015).

In the second application mode, the relationships between the TP and PI are known for the traditional system (the main difference between the first and second mode), but the system has not been fully optimized and AI-based optimization is used to improve the PI. For example, one study used differential evolution algorithms to reduce the utility cost of an ethylene plant by over 2 million \$/year compared with the baseline scenario (Jahromi et al., 2018). One study may use different application modes. For instance, besides using support vector machine to predict the process PI (AI application mode 1), Golkarnarenji et al. also used heuristic algorithms to optimize the energy consumption of a carbon fiber production line (AI application mode 2), and the optimized scenario showed ~40% reduction of energy consumption compared with the unoptimized traditional system (Golkarnarenji et al., 2018).

The third application mode used AI technologies to enhance the capabilities of traditional models for chemical production. For example, fuzzy logic has been used to enhance the fault tree analysis for the petrochemical industry (Lavasani et al., 2015; Yazdi & Zarei, 2018) by allowing for the estimation of failure probability with insufficient incident data. In this application mode, the relationship between TP and PI is also known as the traditional model, but the integration of AI can extend the capability of the traditional model.

The potential impacts of the first application mode may be the highest among the three since AI is used to establish the models that cannot be alternated by first-principle models (Venkatasubramanian, 2019). Such AI applications could potentially identify improvement opportunities that are very hard to be pinpointed without a comprehensive understanding of the relationships between TP and PI. The impacts of the second type of



**FIGURE 1** Schematic representation of the conceptual evaluation framework for the sustainability-related benefits of AI application in the chemical industry

AI applications could also be high given that the systems have not been fully optimized. The third application mode may have the lowest impacts given that the system may already be well optimized by traditional models.

Based on the three modes of AI applications, the impacts of AI adoptions can be calculated as:

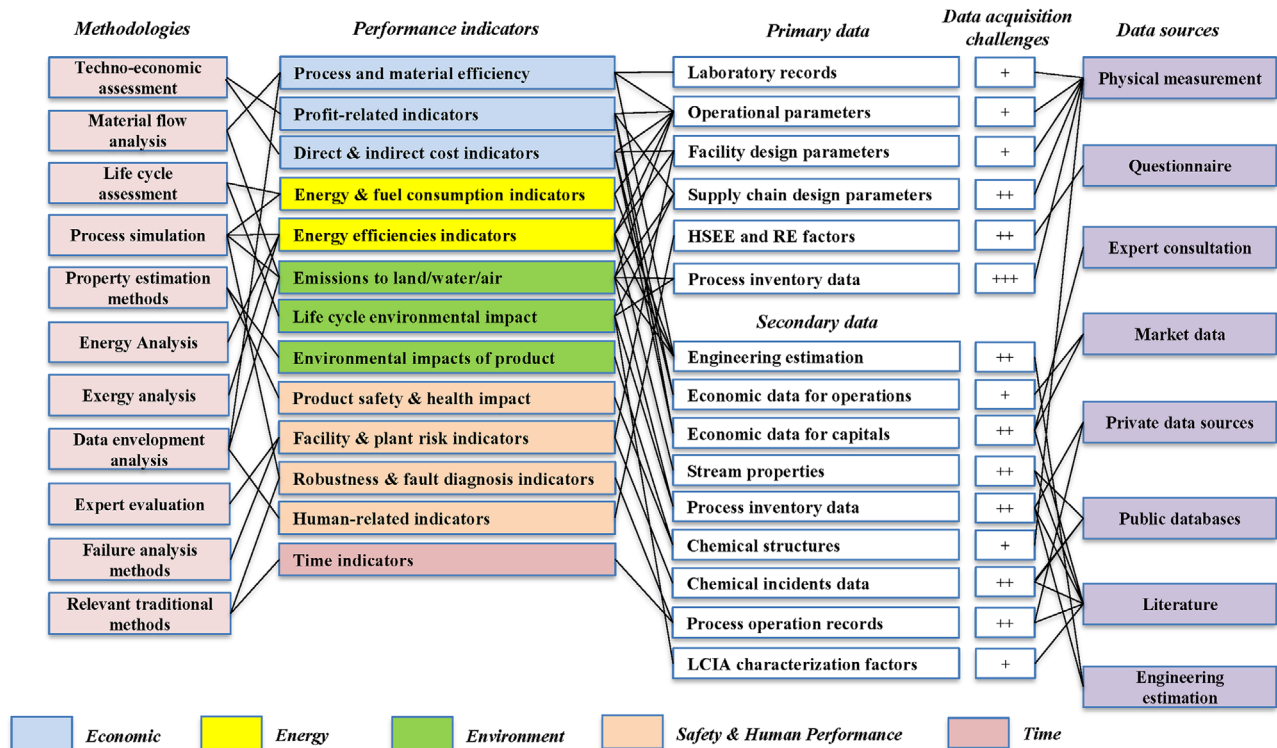
$$\Delta E = PI_{AI} - PI_{baseline} = F(TP_{AI}) - F(TP_{baseline}). \quad (1)$$

$\Delta E$  is the net impacts of the AI application, which is the difference between the PI after AI adoption ( $PI_{AI}$ ) and the PI before AI adoption ( $PI_{baseline}$ ). For those applications where the PI is quantitatively included in the AI model (as an objective function or parameter), such impact (or say PI difference) can be directly measured as demonstrated by studies reviewed in Sections 2.1–2.3 for economic, energy, and safety aspects. For those applications that do not include the PI in the AI models, such impacts can be estimated by parameterizing the PI by technical parameters TP(s) through a function  $F$  and evaluating the changes of TP caused by the AI adoption. Such an approach has been used to evaluate other emerging technologies in the chemical industry. For example, one study developed a process-based model for traditional ethylene production to parametrize the life cycle energy consumption of ethylene by energy efficiency and operational parameters so that the energy reduction enabled by the emerging technology can be estimated by changing the parameters affected by those technologies (Yao et al., 2016). A similar approach can be applied to AI applications.

The challenge then becomes the selection of PI and development of function  $F$  to perform the impact assessment. To address this challenge, we proposed a conceptual framework to guide the selection of PI and relevant quantitative assessment methods for assessing the sustainability impacts of AI, as shown in Figure 1. In this framework, the selection of the indicators is based on the AI application types and the major impact categories identified in the previous section. This study does not intend to develop a new impact assessment method. Instead, this work presents a conceptual framework to select appropriate indicators and qualitative assessment methods to understand system changes and relevant sustainability implications of AI adoption. As presented in Figure 1, five steps are included: (1) determine the AI application type; (2) select impact categories; (3) select performance indicators; (4) assess indicator; (5) quantify impacts and uncertainty of the AI application. The following subsections provide extended discussions for each step.

### 3.1 | Determine AI application types and impact categories

AI application type should be determined first. Four application types are included based on the review in Section 2. The application type can be determined based on where AI is applied or what TP(s) will be affected, and multiple application types may be included for the initial consideration. For example, if an AI technique can improve the yield of a unit operation, which will affect the mass balance of the entire chemical plant. Then both the “unit operations” and “process and chemical plants” should be considered.



**FIGURE 2** Data requirement and sources of PIs and evaluation methods

Based on the AI application type, potential impact categories need to be selected in the next step. Such a selection can be made based on the stakeholders' interest, preliminary assessment, engineering experience, or similar studies in the literature. Five major impact categories are included in the framework based on the review in Section 2, but additional impacts could be considered on a case-by-case basis. Furthermore, some impacts may be correlated and thus need to be considered together, for example, energy consumption (energy aspect) and energy costs (economic aspect). If one or multiple AI technique(s) can be implemented in different ways (e.g., three adoption methods as shown in Table 6) and conducting a full assessment for each of them is challenging, we suggest using Table 6 as a reference to determine assessment priority by having a qualitative assessment for the significance of the potential impacts.

### 3.2 | Indicator selection and refinement

Under each impact category by different application types, various PIs are available to assess the specific impacts of AI technologies (See Supporting Information Table S2). Figure 2 shows the major types of PIs under each impact category. A few additional aspects can be considered for indicator selection:

- **Data availability.** The data requirement of specific PIs and evaluation methods are shown in Figure 2. Primary data is obtained through direct measurement, and secondary data can be acquired from the literature, existing databases, or engineering estimations. The primary data of PIs or TPs by direct measurement should be used whenever available. Some data could be used to evaluate more than one indicator. For example, if the process data of energy and material flows are available, it is highly likely that different economic, energy, and environmental indicators can be estimated using TEA, LCA, and material flow analysis (MFA). A brief introduction of methods shown in Figure 2 and their data requirements are further discussed in the next section.
- **Analysis capability.** A variety of analytical methods for different PIs are provided in Figure 2. Most of those methods require specialized tools (e.g., engineering simulation software) and human resources (e.g., experienced LCA practitioners). Whether those resources are available for analyzing a specific PI in a reasonable timeframe is another factor to be considered.
- **Indicator applicability.** Some PIs are highly generic (e.g., yield and energy efficiency), while the others are limited to specific application types (e.g., isentropic efficiency for compressors and turbines). Generic PIs may be more suitable for comparisons across different

application types (for one or multiple AI techniques), while application-specific PIs will be more suitable for comparisons within the same application type.

### 3.3 | Indicator evaluation and impact assessment

This section provides a brief discussion of methods presented in Figure 2. Different economic indicators can be evaluated by TEA, a widely used economic analysis method to quantify the technical and economic feasibility (Scott, 2015). A TEA needs process data of all energy and material flows and relevant economic data (Lan et al., 2020; Liu et al., 2018) for operational activities and/or capitals (depending on the indicators). Such process data are also needed by MFA and LCA. MFA is a core method used in the industrial ecology area that quantifies and tracks materials being used, reused, and lost (Graedel, 2019). MFA has been used to support the circular economy in different industries (Johnson et al., 2020; Moriguchi, 2007; Wang et al., 2016) and track chemical emissions related to environmental impacts (Li & Wania, 2016; van Gils et al., 2020). Therefore, MFA could be suitable for AI applications that affect material efficiency (e.g., yields) and chemical products. Another core method of industrial ecology is LCA. As discussed in Section 2.2.3, few studies have conducted LCA for AI applications and one major barrier is data availability. Many methods have been explored for LCI estimation, such as process simulations (Montazeri & Eckelman, 2016; Smith et al., 2017), process design calculations (Parvatker et al., 2019; Yao & Masanet, 2018), stoichiometry, molecular structure-based models (Wernet et al., 2008), and machine learning-based method (Liao et al., 2020; Song et al., 2017). How to leverage those methods to fill the data gaps for AI evaluation, especially leveraging state-of-the-art machine learning and data analytics, is a research question to be explored. In addition to the LCI data of chemical production, the LCI data of background processes (e.g., upstream production of electricity and chemicals) and the characterization factors of life cycle impact assessment (LCIA) are available in many secondary data sources (see Supporting Information Table S1).

Process simulation is a powerful method to provide the process data needed by TEA, LCA, and MFA. Process simulation uses mathematical models to represent physical/chemical transformation processes in unit operations (Chaves et al., 2015). Various chemical simulation software are available, such as Aspen Plus (AspenTech, 2020) and gPROMS (Process Systems Enterprise, 2021). Process simulation requires detailed process information such as operating conditions and stream properties (considered as TP in Equation 1), therefore process simulation can be used to derive the function  $F$  in Equation (1), allowing for assessing AI's impacts by investigating the changes of TPs caused by AI.

Energy and exergy analyses are included in the framework. Energy analysis relies on the first law of thermodynamics, while exergy analysis relies on the second law of thermodynamics (Aljundi, 2009). Both analyses provide energy-related PIs, but exergy analysis is increasingly popular given its ability to analyze the energy quality and irreversibility aspects of thermodynamic processes, none of which can be analyzed by energy analysis (Aghbashlo et al., 2013). However, exergy analysis may require more data (e.g., the temperature profile of the environment). Therefore, the selection between energy and exergy analysis needs careful consideration of the analysis scope and data availability.

The environmental impacts and safety of chemical products are highly related to chemical structures. For example, the toxicity of chemicals is related to their properties and chemical structure (Manzetti et al., 2014). A large variety of first-principle or empirical methods are available to estimate different physical/chemical properties of chemicals based on their structure. Those methods are useful to assess the impacts of AI applications related to the design of chemical synthesis, especially new chemical products.

Empirical estimation and failure analysis methods (e.g., fault tree analysis as discussed in Section 2.2.4) can be used to evaluate risk-related PIs. Data envelopment analysis (DEA) is a nonparametric linear programming technique for evaluating the relative efficiency and productivity of decision-making units (Azadi et al., 2015), and it has been used to evaluate human/labor productivity (Hu & Cai, 2004; Mugeru et al., 2012), eco-efficiency (Zhang et al., 2008), and economic efficiency (Hoang & Alauddin, 2012) in other industries. DEA could potentially be used to evaluate the impacts of AI on PIs related to human, environment, and economic, but it needs extensive data, especially the process data that can reflect system changes over a period, which could be a challenge. In addition, other relevant methods such as confusion matrix (Xie et al., 2019) for fault diagnosis may be possible in evaluating different performance indicators.

Figure 2 lists major requirements of primary and secondary data and their acquisition challenges assessed by the authors. Figure 2 is not a comprehensive list of all data. Instead, we list major types and sources of data to provide high-level information for researchers and analysts to select appropriate methods and design the specific assessment. Some examples of secondary data sources are provided in Supporting Information Table S1. The impacts of AI application can be quantified by using the methods listed in Figure 2 to estimate the PIs' differences using Equation (1) discussed at the beginning of this section.

### 3.4 | Applications and limitations of the proposed framework

In this study, the proposed framework is based on the review of assessing the sustainability impacts of AI applications in the chemical industry. This framework could be tailored and used in other industries, or broad industrial ecology field (e.g., industrial symbiosis (IS)). AI applications are emerging in industrial ecology (Abduljabbar et al., 2019; Ahmad et al., 2021; Lütje et al., 2017; Ongsakul & Dieu, 2019; Rahmanifard & Plaksina, 2019).

For IS, AI has been applied to several topics, including identifying and simulating potential elements of an industrial ecosystem that could cooperate by using ABM and participatory modeling (Batten, 2009), simulating and assessing the potential economic benefits of companies adopting IS relationship by using integrated ABM and enterprise input–output model (Yazan & Fraccascia, 2020), simulating the mass and energy flows of the symbiosis relationship by using machine learning and ABM (Lütje et al., 2017), and filtering the IS opportunities by using concurrent epistemic game structures (Yazdanpanah et al., 2019). Unlike the AI applications in the chemical industry, AI applications in IS commonly involve with multiple companies or systems that seek symbiosis (Yazan & Fraccascia, 2020). This could lead to the integration of multiple AI technologies, the combination of AI application modes (see Table 6) and AI application levels (see Step 1 in Figure 1). For example, two studies used AI technologies (e.g., machine learning) to identify the symbiosis opportunities, which may belong to the first AI application mode and an application level of supply chain (Lütje et al., 2017; Yazdanpanah et al., 2019). AI technologies (e.g., ABM) can also be employed to simulate the symbiosis relationship between industrial entities that may be only optimized individually, which may belong to the third AI application mode and the application level of supply chain and process and plant (Lütje et al., 2017; Yazan & Fraccascia, 2020). Then Steps 2–5 in the proposed framework (Figure 1) can be applied.

One limitation of the proposed framework is the exclusion of IT infrastructure that is essential for AI applications in the chemical industry. The IT infrastructure may include computing facilities, data storage, sensors, and other devices (Ahmad et al., 2021). As discussed in Section 2.2.2., IT infrastructure has impacts such as energy consumption that can be complex and lack robust methods to assess such impacts. (Ahmad et al., 2021; Huang & Masanet, 2015; Shehabi et al., 2016). Hence, in this study, IT infrastructure is excluded but can be further investigated by future research.

## 4 | CONCLUSION

This paper reviewed a variety of AI applications in the chemical industry and highlighted five major sustainability-related implications of AI adoptions. Although AI is not new to the chemical industry, quantitative analysis for AI's impacts on the environmental, economic, and society is still limited. Most of the reviewed studies focused on the economic, energy, and safety aspects, while surprisingly, the environmental implications of AI have been rarely evaluated. Assessing the impacts of AI requires a comprehensive understanding of how AI interacts/affects physical and technical systems that generate economic, environmental, and social impacts. This review identified three modes of AI interactions with physical systems and highlighted the potential impacts for each mode. We then presented a conceptual framework based on the literature review and include methods from industrial ecology, economics, and engineering to guide the selection of performance indicators and evaluation methods for a holistic assessment of AI's impacts. A practical application of the framework requires real-world case studies with sufficient process information, which may be challenging for researchers like the authors, given the confidentiality of most AI projects announced by chemical companies. However, it could be a useful tool for the chemical industry to estimate the various impacts of AI technologies with different types of applications, supporting their decision-making related to technology/application selection and investment. For AI and chemical researchers, this framework could be used to quantify the big-picture impacts of AI and identify the most beneficial pathways of AI applications, which may foster more interdisciplinary research between the two fields to support the sustainable production of chemicals and advanced materials.

Industrial ecology methods LCA and MFA are powerful tools, although few studies have used these methods to evaluate the impacts of AI given the large data gaps. Machine learning has been used to fill the data gaps of LCA (Liao et al., 2020; Nabinger et al., 2019; Song et al., 2017), which is a promising direction to broaden the applications of industrial ecology approaches and address the data challenges of assessing AI's impacts. On the other hand, we identified AI applications in the industrial ecology field (e.g., potential AI application for an eco-industrial park (Zhang et al., 2017)). More AI case studies are needed to understand which AI technique should be used and how it can be used to support what specific industrial ecology practice.

## ACKNOWLEDGMENTS

The authors thank the feedback and support from Reid Lifset at Yale University and Dave Rejeski at Environmental Law Institute. The authors thank the funding support from the Department of Forest Biomaterials at North Carolina State University, Yale University, the U.S. National Science Foundation, and the Alfred P. Sloan Foundation through the contract with Environmental Law Institute.

## CONFLICT OF INTEREST

The authors declare no conflict of interest.

## DATA AVAILABILITY STATEMENT

The data that supports the findings of this study are available in the supporting information of this article.

## ORCID

Yuan Yao  <https://orcid.org/0000-0001-9359-2030>

## REFERENCES

- Abduljabbar, R., Dia, H., Liyanage, S., & Bagloee, S. A. (2019). Applications of artificial intelligence in transport: An overview. *Sustainability*, 11(1), 189. <https://doi.org/10.3390/su11010189>
- Accenture. (2014). *Accenture global digital chemicals survey*. [https://www.accenture.com/us-en/~media/accenture/conversion-assets/dotcom/documents/global/pdf/dualpub\\_6/accenture-insight-digital-chemical-survey-infographic.pdf](https://www.accenture.com/us-en/~media/accenture/conversion-assets/dotcom/documents/global/pdf/dualpub_6/accenture-insight-digital-chemical-survey-infographic.pdf)
- Aghbashlo, M., Mobli, H., Rafiee, S., & Madadlou, A. (2013). A review on exergy analysis of drying processes and systems. *Renewable and Sustainable Energy Reviews*, 22, 1–22. <https://doi.org/10.1016/j.rser.2013.01.015>
- Ahmad, T., Zhang, D., Huang, C., Zhang, H., Dai, N., Song, Y., & Chen, H. (2021). Artificial intelligence in sustainable energy industry: Status quo, challenges and opportunities. *Journal of Cleaner Production*, 289, 125834. <https://doi.org/10.1016/j.jclepro.2021.125834>
- Ahn, J. H., Kim, M. J., Cho, Y. W., & Kim, T. S. (2020). A quadruple power generation system for very high efficiency and its performance optimization using an artificial intelligence method. *Applied Thermal Engineering*, 168, 114861. <https://doi.org/10.1016/j.applthermaleng.2019.114861>
- Ali, J. M., Hussain, M. A., Tade, M. O., & Zhang, J. (2015). Artificial intelligence techniques applied as estimator in chemical process systems—A literature survey. *Expert Systems with Applications*, 42(14), 5915–5931. <https://doi.org/10.1016/j.eswa.2015.03.023>
- Aljundi, I. H. (2009). Energy and exergy analysis of a steam power plant in Jordan. *Applied Thermal Engineering*, 29(2–3), 324–328. <https://doi.org/10.1016/j.applthermaleng.2008.02.029>
- Aqlan, F., & Ali, E. M. (2014). Integrating lean principles and fuzzy bow-tie analysis for risk assessment in chemical industry. *Journal of Loss Prevention in the Process Industries*, 29, 39–48. <https://doi.org/10.1016/j.jlpi.2014.01.006>
- AspenTech. (2020). *Aspen Plus 11.1 user guide*. <https://www.aspentech.com/en/products/engineering/aspens-plus>
- Axtell, R. L., Andrews, C. J., & Small, M. J. (2001). Agent-based modeling and industrial ecology. *Journal of Industrial Ecology*, 5(4), 10–14.
- Azadeh, A., Bonab, N. A., Salehi, V., & Zarrin, M. (2015). A unique algorithm for the assessment and improvement of job satisfaction by resilience engineering: Hazardous labs. *International Journal of Industrial Ergonomics*, 49, 68–77. <https://doi.org/10.1016/j.ergon.2015.06.002>
- Azadeh, A., Saberi, M., Rouzbahman, M., & Saberi, Z. (2013). An intelligent algorithm for performance evaluation of job stress and HSE factors in petrochemical plants with noise and uncertainty. *Journal of Loss Prevention in the Process Industries*, 26(1), 140–152. <https://doi.org/10.1016/j.jlpi.2012.10.004>
- Azadeh, A., & Zarrin, M. (2016). An intelligent framework for productivity assessment and analysis of human resource from resilience engineering, motivational factors, HSE and ergonomics perspectives. *Safety Science*, 89, 55–71. <https://doi.org/10.1016/j.ssci.2016.06.001>
- Azadi, M., Jafarian, M., Saen, R. F., & Mirhedayatian, S. M. (2015). A new fuzzy DEA model for evaluation of efficiency and effectiveness of suppliers in sustainable supply chain management context. *Computers and Operations Research*, 54, 274–285. <https://doi.org/10.1016/j.cor.2014.03.002>
- Baryannis, G., Dani, S., Validi, S., & Antoniou, G. (2019). Decision support systems and artificial intelligence in supply chain risk management. In G. Zsidisin & M. Henke (Eds.), *Revisiting supply chain risk* (pp. 53–71). Springer.
- Batten, D. F. (2009). Fostering industrial symbiosis with agent-based simulation and participatory modeling. *Journal of Industrial Ecology*, 13(2), 197–213. <https://doi.org/10.1111/j.1530-9290.2009.00115.x>
- Beamon, B. M. (1998). Supply chain design and analysis: Models and methods. *International Journal of Production Economics*, 55(3), 281–294. [https://doi.org/10.1016/S0925-5273\(98\)00079-6](https://doi.org/10.1016/S0925-5273(98)00079-6)
- Behdani, B., Adhitya, A., Lukso, Z., & Srinivasan, R. (2012). Mitigating supply disruption for a global chemical supply chain-application of agent-based modeling. *Computer Aided Chemical Engineering*, 31, 1070–1074. <https://doi.org/10.1016/B978-0-444-59506-5.50045-6>
- Behdani, B., Lukso, Z., Adhitya, A., & Srinivasan, R. (2009). Agent based model for performance analysis of a global chemical supply chain during normal and abnormal situations. *Computer Aided Chemical Engineering*, 26, 979–984. [https://doi.org/10.1016/S1570-7946\(09\)70163-4](https://doi.org/10.1016/S1570-7946(09)70163-4)
- Behdani, B., Lukso, Z., & Srinivasan, R. (2019). Agent-oriented simulation framework for handling disruptions in chemical supply chains. *Computers and Chemical Engineering*, 122, 306–325. <https://doi.org/10.1016/j.compchemeng.2018.09.027>
- Bernhardt, K. L. S. (2007). Agent-based modeling in transportation. In G. Spring (Ed.), *Transportation research circular E-C113: Artificial intelligence in transportation*. Transportation Research Board of the National Academies.
- Berning, G., Brandenburg, M., Gürsoy, K., Kussi, J. S., Mehta, V., & Tölle, F. J. (2004). Integrating collaborative planning and supply chain optimization for the chemical process industry (I) - Methodology. *Computers and Chemical Engineering*, 28(6–7), 913–927. <https://doi.org/10.1016/j.compchemeng.2003.09.004>
- Bertsimas, D., & Kallus, N. (2020). From predictive to prescriptive analytics. *Management Science*, 66(3), 1025–1044.
- Cao, J., Mozaffar, M., Garcia, D. J., Ehmann, K., Ren, H., You, F., & Correa, J. E. (2018). Sustainable manufacturing with cyber-physical discrete manufacturing networks: Overview and modeling framework. *Journal of Manufacturing Science and Engineering*, 141(2), 021013. <https://doi.org/10.1115/1.4041833>
- Castillo-Villar, K. K. (2014). Metaheuristic algorithms applied to bioenergy supply chain problems: Theory, review, challenges, and future. *Energies*, 7(11), 7640–7672. <https://doi.org/10.3390/en7117640>
- Cecchini, R. L., Ponzoni, I., & Carballido, J. A. (2012). Multi-objective evolutionary approaches for intelligent design of sensor networks in the petrochemical industry. *Expert Systems with Applications*, 39(3), 2643–2649. <https://doi.org/10.1016/j.eswa.2011.08.119>
- Chaves, I. D. G., López, J. R. G., Zapata, J. L. G., Robayo, A. L., & Niño, G. R. (2015). *Process analysis and simulation in chemical engineering*. Springer. <https://doi.org/10.1007/978-3-319-14812-0>
- Choy, K. L., Ho, G. T. S., Lee, C. K. H., Lam, H. Y., Cheng, S. W. Y., Siu, P. K. Y., Pang, G. K. H., Tang, V., Lee, J. C. H., & Tsang, Y. P. (2016). A recursive operations strategy model for managing sustainable chemical product development and production. *International Journal of Production Economics*, 181, 262–272. <https://doi.org/10.1016/j.ijpe.2016.07.011>
- Cortes Robles, G., Negny, S., & Le Lann, J. M. (2009). Case-based reasoning and TRIZ: A coupling for innovative conception in chemical engineering. *Chemical Engineering and Processing: Process Intensification*, 48(1), 239–249. <https://doi.org/10.1016/j.cep.2008.03.016>
- Cui, H., & Liu, C. (2017). Applying industrial symbiosis to chemical industry: A literature review. *AIP Conference Proceedings*, 1864, 020090. <https://doi.org/10.1063/14992907>
- Dantzig, G. (2016). *Linear programming and extensions*. Princeton university press.
- DeRosa, S. E., Downes, P. S., Lentz, R., & Allen, D. T. (2016). Opportunities for chemical manufacturing using natural gas feedstocks in the San Juan Basin. *Industrial and Engineering Chemistry Research*, 55(30), 8480–8489. <https://doi.org/10.1021/acs.iecr.6b01370>
- Dhar, P. (2020). The carbon impact of artificial intelligence. *Nature Machine Intelligence*, 2(8), 423–425. <https://doi.org/10.1038/s42256-020-0219-9>

- Doan, H. A., Agarwal, G., Qian, H., Counihan, M. J., Rodríguez-López, J., Moore, J. S., & Assary, R. S. (2020). Quantum chemistry-informed active learning to accelerate the design and discovery of sustainable energy storage materials. *Chemistry of Materials*, 32(15), 6338–6346. <https://doi.org/10.1021/acs.chemmater.0c00768>
- Ehlen, M. A., Sun, A. C., Pepple, M. A., Eidson, E. D., & Jones, B. S. (2014). Chemical supply chain modeling for analysis of homeland security events. *Computers and Chemical Engineering*, 60, 102–111. <https://doi.org/10.1016/j.compchemeng.2013.07.014>
- Ehrenstein, M., Wang, C. H., & Guillén-Gosálbez, G. (2019). Strategic planning of supply chains considering extreme events: Novel heuristic and application to the petrochemical industry. *Computers and Chemical Engineering*, 125, 306–323. <https://doi.org/10.1016/j.compchemeng.2019.03.020>
- Fahmi, I., & Cremaschi, S. (2012). Process synthesis of biodiesel production plant using artificial neural networks as the surrogate models. *Computers and Chemical Engineering*, 46, 105–123. <https://doi.org/10.1016/j.compchemeng.2012.06.006>
- Fang, S. C., & Puthenpura, S. (1993). *Linear optimization and extensions: Theory and algorithms*. Prentice-Hall International, Inc.
- Fernandes, F. A. N. (2006). Optimization of fischer-tropsch synthesis using neural networks. *Chemical Engineering and Technology*, 29(4), 449–453. <https://doi.org/10.1002/ceat.200500310>
- Ferrer, J. B., Negny, S., Robles, G. C., & Le Lann, J. M. (2012). Eco-innovative design method for process engineering. *Computers and Chemical Engineering*, 45, 137–151. <https://doi.org/10.1016/j.compchemeng.2012.06.020>
- García-Martín, E., Rodrigues, C. F., Riley, G., & Grahn, H. (2019). Estimation of energy consumption in machine learning. *Journal of Parallel and Distributed Computing*, 134, 75–88. <https://doi.org/10.1016/j.jpdc.2019.07.007>
- Geng, Z., Wang, Z., Zhu, Q., & Han, Y. (2016). Multi-objective operation optimization of ethylene cracking furnace based on AMOPSO algorithm. *Chemical Engineering Science*, 153, 21–33. <https://doi.org/10.1016/j.ces.2016.07.009>
- Ghaderi, H., Pishvaei, M. S., & Moini, A. (2016). Biomass supply chain network design: An optimization-oriented review and analysis. *Industrial Crops and Products*, 94, 972–1000. <https://doi.org/10.1016/j.indcrop.2016.09.027>
- Golkarnarenji, G., Naebe, M., Badii, K., Milani, A. S., Jazar, R. N., & Khayyam, H. (2018). Support vector regression modelling and optimization of energy consumption in carbon fiber production line. *Computers and Chemical Engineering*, 109, 276–288. <https://doi.org/10.1016/j.compchemeng.2017.11.020>
- Gong, H. F., Chen, Z. S., Zhu, Q. X., & He, Y. L. (2017). A Monte Carlo and PSO based virtual sample generation method for enhancing the energy prediction and energy optimization on small data problem: An empirical study of petrochemical industries. *Applied Energy*, 197, 405–415. <https://doi.org/10.1016/j.apenergy.2017.04.007>
- Gonzaga, J. C. B., Meleiro, L. A. C., Kiang, C., & Maciel Filho, R. (2009). ANN-based soft-sensor for real-time process monitoring and control of an industrial polymerization process. *Computers and Chemical Engineering*, 33(1), 43–49. <https://doi.org/10.1016/j.compchemeng.2008.05.019>
- Google. Google Scholar Search Engine. (2021). <https://scholar.google.com>
- Gordon, R. P. E. (1998). The contribution of human factors to accidents in the offshore oil industry. *Reliability Engineering and System Safety*, 61(1–2), 95–108. [https://doi.org/10.1016/S0951-8320\(98\)80003-3](https://doi.org/10.1016/S0951-8320(98)80003-3)
- Graedel, T. E. (2019). Material flow analysis from origin to evolution. *Environmental Science and Technology*, 53(21), 12188–12196. <https://doi.org/10.1021/acs.est.9b03413>
- Green, D. W., & Perry, R. H. (2008). *Perry's chemical engineers' handbook* (8th ed.). McGraw-Hill Education.
- Gu, G. H., Noh, J., Kim, I., & Jung, Y. (2019). Machine learning for renewable energy materials. *Journal of Materials Chemistry A*, 7(29), 17096–17117. <https://doi.org/10.1039/c9ta02356a>
- Guillén, G., Mele, F. D., España, A., & Puigjaner, L. (2006). Addressing the design of chemical supply chains under demand uncertainty. *Industrial & Engineering Chemistry Research*, 45, 7566–7581. <https://doi.org/10.1021/ie051424a>
- Guo, C., Khan, F., & Imtiaz, S. (2019). Copula-based Bayesian network model for process system risk assessment. *Process Safety and Environmental Protection*, 123, 317–326. <https://doi.org/10.1016/j.psep.2019.01.022>
- Guo, L., Gao, J., Yang, J., & Kang, J. (2009). Criticality evaluation of petrochemical equipment based on fuzzy comprehensive evaluation and a BP neural network. *Journal of Loss Prevention in the Process Industries*, 22(4), 469–476. <https://doi.org/10.1016/j.jlp.2009.03.003>
- Hájek, P., & Stejskal, J. (2018). R&D cooperation and knowledge spillover effects for sustainable business innovation in the chemical industry. *Sustainability*, 10(4), 1064. <https://doi.org/10.3390/su10041064>
- Hajjar, Z., Tayyebi, S., Hosein, M., & Ahmadi, E. (2016). Application of AI in chemical engineering. In M.A. Aceves-Fernandez (Ed.), *Artificial intelligence – Emerging trends and applications* (pp. 399–416). <https://doi.org/10.5772/intechopen.76027>
- Han, Y., Wu, H., Jia, M., Geng, Z., & Zhong, Y. (2019). Production capacity analysis and energy optimization of complex petrochemical industries using novel extreme learning machine integrating affinity propagation. *Energy Conversion and Management*, 180, 240–249. <https://doi.org/10.1016/j.enconman.2018.11.001>
- Hazen, B. T., Skipper, J. B., Boone, C. A., & Hill, R. R. (2018). Back in business: Operations research in support of big data analytics for operations and supply chain management. *Annals of Operations Research*, 270(1), 201–211.
- Haugeland, J. (1985). *Artificial intelligence: The very idea* (1st ed.). The MIT Press.
- Heinrich, M., & Schwarze, R. (2017). Genetic optimization of the volute of a centrifugal compressor. *International Journal of Rotating Machinery*, 2016, 4849025. <https://doi.org/10.1155/2016/4849025>
- Henderson, P., Hu, J., Romoff, J., Brunskill, E., Jurafsky, D., & Pineau, J. (2020). Towards the systematic reporting of the energy and carbon footprints of machine learning. *Journal of Machine Learning Research*, 21(248), 1–43.
- Hoang, V. N., & Alauddin, M. (2012). Input-orientated data envelopment analysis framework for measuring and decomposing economic, environmental and ecological efficiency: An application to OECD agriculture. *Environmental and Resource Economics*, 51(3), 431–452. <https://doi.org/10.1007/s10640-011-9506-6>
- Hu, B. A., & Cai, L. A. (2004). Hotel labor productivity assessment – A data envelopment analysis. *Journal of Travel & Tourism Marketing*, 16(2–3), 27–38.
- Huang, R., & Masanet, E. (2015). *Data center IT efficiency measures*. <https://www.energy.gov/sites/prod/files/2015/01/f19/UMPCchapter20-data-center-IT.pdf>
- ICCA, & Oxford Economics. (2019). *The global chemical industry: Catalyzing growth and addressing our world's sustainability challenges*. <https://www.oxfordeconomics.com/recent-releases/the-global-chemical-industry-catalyzing-growth-and-addressing-our-world-sustainability-challenges>
- IEA. (2020a). *Chemicals*. <https://www.iea.org/reports/chemicals>
- IEA. (2020b). *Tracking industry 2020*. <https://www.iea.org/reports/tracking-industry-2020>

- Jaderi, F., Ibrahim, Z. Z., & Zahiri, M. R. (2019). Criticality analysis of petrochemical assets using risk based maintenance and the fuzzy inference system. *Process Safety and Environmental Protection*, 121, 312–325. <https://doi.org/10.1016/j.psep.2018.11.005>
- Jahromi, F. S., Beheshti, M., & Rajabi, R. F. (2018). Comparison between differential evolution algorithms and response surface methodology in ethylene plant optimization based on an extended combined energy - exergy analysis. *Energy*, 164, 1114–1134. <https://doi.org/10.1016/j.energy.2018.09.059>
- Jennings, N. R. (2000). On agent-based software engineering. *Artificial Intelligence*, 117(2), 277–296.
- Ji, X., He, G., Xu, J., & Guo, Y. (2016). Study on the mode of intelligent chemical industry based on cyber-physical system and its implementation. *Advances in Engineering Software*, 99, 18–26. <https://doi.org/10.1016/j.advengsoft.2016.04.010>
- Jiang, B., Zhao, Y., & Gu, W. (2018). Research and exploration on intelligent scheduling system in petrochemical industry. *Computer Aided Chemical Engineering*, 44, 2029–2034. <https://doi.org/10.1016/B978-0-444-64241-7.50333-5>
- Johnson, S., Echeverria, D., Venditti, R., Jameel, H., & Yao, Y. (2020). Supply chain of waste cotton recycling and reuse: A review. *AATCC Journal of Research*, 7(Special Issue 1), 19–31. <https://doi.org/10.14504/ajr.7.S1.3>
- Kaab, A., Sharifi, M., Mobli, H., Nabavi-Pelesaraei, A., & Chau, K. W. (2019). Combined life cycle assessment and artificial intelligence for prediction of output energy and environmental impacts of sugarcane production. *Science of The Total Environment*, 664, 1005–1019. <https://doi.org/10.1016/j.scitotenv.2019.02.004>
- Kadlec, P., Gabrys, B., & Strandt, S. (2009). Data-driven Soft Sensors in the process industry. *Computers and Chemical Engineering*, 33(4), 795–814. <https://doi.org/10.1016/j.compchemeng.2008.12.012>
- Keyvanloo, K., Sedighi, M., & Towfighi, J. (2012). Genetic algorithm model development for prediction of main products in thermal cracking of naphtha: Comparison with kinetic modeling. *Chemical Engineering Journal*, 209, 255–262. <https://doi.org/10.1016/j.cej.2012.07.130>
- Kovačič, M., & Dolenc, F. (2016). Prediction of the natural gas consumption in chemical processing facilities with genetic programming. *Genetic Programming and Evolvable Machines*, 17(3), 231–249. <https://doi.org/10.1007/s10710-016-9264-x>
- Kovačič, M., Šarler, B., & Župerl, U. (2016). Natural gas consumption prediction in Slovenian industry – A case study. *Materials and Geoenvironment*, 63(2), 91–96. <https://doi.org/10.1515/rmzmag-2016-0008>
- Lacoste, A., Luccioni, A., Schmidt, V., & Dandres, T. (2019). Quantifying the carbon emissions of machine learning. *arXiv:1910.09700*.
- Lan, K., Park, S., Kelley, S. S., English, B. C., Yu, T. E., Larson, J., & Yao, Y. (2020). Impacts of uncertain feedstock quality on the economic feasibility of fast pyrolysis biorefineries with blended feedstocks and decentralized preprocessing sites in the Southeastern United States. *GCB Bioenergy*, 12(11), 1014–1029.
- Lan, K., Park, S., & Yao, Y. (2019). Key issue, challenges, and status quo of models for biofuel supply chain design. In J. Ren, A. Scipioni, A. Manzardo, & H. Liang (Eds.), *Biofuels for a more sustainable future: Life cycle sustainability assessment and multi-criteria decision making* (pp. 273–315). Elsevier. <https://doi.org/10.1016/B978-0-12-815581-3.00010-5>
- Lavasani, S. M., Zendegani, A., & Celik, M. (2015). An extension to Fuzzy Fault Tree Analysis (FFTA) application in petrochemical process industry. *Process Safety and Environmental Protection*, 93, 75–88. <https://doi.org/10.1016/j.psep.2014.05.001>
- Lee, J. H., Shin, J., & Realf, M. J. (2018). Machine learning: Overview of the recent progresses and implications for the process systems engineering field. *Computers and Chemical Engineering*, 114, 111–121. <https://doi.org/10.1016/j.compchemeng.2017.10.008>
- Lee, K., Kwon, H. M., Cho, S., Kim, J., & Moon, I. (2016). Improvements of safety management system in Korean chemical industry after a large chemical accident. *Journal of Loss Prevention in the Process Industries*, 42, 6–13. <https://doi.org/10.1016/j.jlp.2015.08.006>
- Li, L., & Wania, F. (2016). Tracking chemicals in products around the world: Introduction of a dynamic substance flow analysis model and application to PCBs. *Environment International*, 94, 674–686. <https://doi.org/10.1016/j.envint.2016.07.005>
- Li, Z., Ma, X., & Xin, H. (2017). Feature engineering of machine-learning chemisorption models for catalyst design. *Catalysis Today*, 280, 232–238. <https://doi.org/10.1016/j.cattod.2016.04.013>
- Li, Z., Wang, S., Chin, W. S., Achenie, L. E., & Xin, H. (2017). High-throughput screening of bimetallic catalysts enabled by machine learning. *Journal of Materials Chemistry A*, 5(46), 24131–24138. <https://doi.org/10.1039/c7ta01812f>
- Liao, M., Kelley, S. S., & Yao, Y. (2019). Artificial neural network based modeling for the prediction of yield and surface area of activated carbon from biomass. *Biofuels, Bioproducts and Biorefining*, 13(4), 1015–1027. <https://doi.org/10.1002/bbb.1991>
- Liao, M., Kelley, S., & Yao, Y. (2020). Generating energy and greenhouse gas inventory data of activated carbon production using machine learning and kinetic based process simulation. *ACS Sustainable Chemistry and Engineering*, 8(2), 1252–1261. <https://doi.org/10.1021/acssuschemeng.9b06522>
- Liao, M., & Yao, Y. (2021). Applications of artificial intelligence-based modeling for bioenergy systems: A review. *GCB Bioenergy*, 13, 774–802. <https://doi.org/10.1111/gcbb.12816>
- Liu, G., Li, M., Zhou, B., Chen, Y., & Liao, S. (2018). General indicator for techno-economic assessment of renewable energy resources. *Energy Conversion and Management*, 156, 416–426. <https://doi.org/10.1016/j.enconman.2017.11.054>
- Liu, J., Chen, M., & Liu, H. (2020). The role of big data analytics in enabling green supply chain management: a literature review. *Journal of Data, Information and Management*, 2(2), 75–83. <https://doi.org/10.1007/s42488-019-00020-z>
- Luo, N., Zhong, W., Wan, F., Ye, Z., & Qian, F. (2015). An agent-based service-oriented integration architecture for chemical process automation. *Chinese Journal of Chemical Engineering*, 23(1), 173–180. <https://doi.org/10.1016/j.cjche.2014.09.047>
- Lütje, A., Willenbacher, M., Engelmann, M., Kunisch, C., & Wohlgenuth, V. (2017). Exploring the system dynamics of industrial symbiosis (IS) with machine learning (ML) techniques—A framework for a hybrid-approach. In V. Wohlgenuth, F. Fuchs-Kittowski, & J. Wittmann (Eds), *Advances and new trends in environmental informatics* (pp. 117–130). <https://doi.org/10.1007/978-3-319-44711-7>
- Ma, C., & He, R. (2019). Green wave traffic control system optimization based on adaptive genetic-artificial fish swarm algorithm. *Neural Computing and Applications*, 31(7), 2073–2083. <https://doi.org/10.1007/s00521-015-1931-y>
- Ma, Y., & Siau, K. L. (2018). Artificial intelligence impacts on higher education. *MWAIS Proceedings*, 42(5), 1–5.
- Manzetti, S., Van Der Spoel, E. R., & Van Der Spoel, D. (2014). Chemical properties, environmental fate, and degradation of seven classes of pollutants. *Chemical Research in Toxicology*, 27(5), 713–737. <https://doi.org/10.1021/tx500014w>
- Mao, S., Wang, B., Tang, Y., & Qian, F. (2019). Opportunities and challenges of artificial intelligence for green manufacturing in the process industry. *Engineering*, 5(6), 995–1002. <https://doi.org/10.1016/j.eng.2019.08.013>
- Marcou, G., Aires De Sousa, J., Latino, D. A. R. S., de Luca, A., Horvath, D., Rietsch, V., & Varnek, A. (2015). Expert system for predicting reaction conditions: The Michael reaction case. *Journal of Chemical Information and Modeling*, 55(2), 239–250. <https://doi.org/10.1021/ci500698a>

- Martínez-Blanco, J., Inaba, A., & Finkbeiner, M. (2015). Scoping organizational LCA—Challenges and solutions. *International Journal of Life Cycle Assessment*, 20(6), 829–841. <https://doi.org/10.1007/s11367-015-0883-x>
- Micheletto, S. R., Carvalho, M. C. A., & Pinto, J. M. (2008). Operational optimization of the utility system of an oil refinery. *Computers and Chemical Engineering*, 32(1–2), 170–185. <https://doi.org/10.1016/j.compchemeng.2007.05.013>
- Mitchell, T. M. (1997). *Machine learning* (1st ed.). McGraw-Hill.
- Mohammadi, Y., & Penlidis, A. (2018). Optimization in chemical reaction engineering: Oxidative coupling of methane as a case study. *Industrial and Engineering Chemistry Research*, 57(26), 8664–8678. <https://doi.org/10.1021/acs.iecr.8b01424>
- Montazeri, M., & Eckelman, M. J. (2016). Life cycle assessment of catechols from lignin depolymerization. *ACS Sustainable Chemistry and Engineering*, 4(3), 708–718. <https://doi.org/10.1021/acssuschemeng.5b00550>
- Moriguchi, Y. (2007). Material flow indicators to measure progress toward a sound material-cycle society. *Journal of Material Cycles and Waste Management*, 9(2), 112–120. <https://doi.org/10.1007/s10163-007-0182-0>
- Mosavi, A., Shamshirband, S., Salwana, E., Chau, K. W., & Tah, J. H. M. (2019). Prediction of multi-inputs bubble column reactor using a novel hybrid model of computational fluid dynamics and machine learning. *Engineering Applications of Computational Fluid Mechanics*, 13(1), 482–492. <https://doi.org/10.1080/19942060.2019.1613448>
- Mugera, A. W., Langemeier, M. R., & Featherstone, A. M. (2012). Labor productivity convergence in the Kansas farm sector: A three-stage procedure using data envelopment analysis and semiparametric regression analysis. *Journal of Productivity Analysis*, 38(1), 63–79. <https://doi.org/10.1007/s11123-011-0235-1>
- Nabinger, A., Tomberlin, K., Venditti, R., & Yao, Y. (2019). Using a data-driven approach to unveil greenhouse gas emission intensities of different pulp and paper products. *Procedia CIRP*, 80, 689–692. <https://doi.org/10.1016/j.procir.2018.12.001>
- Naidu, S. R., Zafiriou, E., & McAvoy, T. J. (1990). Use of neural networks for sensor failure detection in a control system. *IEEE Control Systems Magazine*, 10(3), 49–55. <https://doi.org/10.1109/37.55124>
- National Academies of Science Engineering and Medicine. (2016). *The changing landscape of hydrocarbon feedstocks for chemical production: Implications for catalysis: Proceedings of a workshop*. The National Academies Press. <https://doi.org/10.17226/23555>
- National Academies of Science Engineering and Medicine. (2018). *Data Science: Opportunities to Transform Chemical Sciences and Engineering: Proceedings of a workshop—In brief*. The National Academies Press. <https://doi.org/10.17226/25191>
- National Academies of Science Engineering and Medicine. (2019). Deployment of deep decarbonization technologies. In *Deployment of deep decarbonization technologies*. The National Academies Press. <https://doi.org/10.17226/25656>
- Negny, S., Belaud, J. P., Robles, G. C., Roldan Reyes, E., & Ferrer, J. B. (2012). Toward an eco-innovative method based on a better use of resources: Application to chemical process preliminary design. *Journal of Cleaner Production*, 32, 101–113. <https://doi.org/10.1016/j.jclepro.2012.03.023>
- Ng, L. Y., Chemmangattuvalappil, N. G., & Ng, D. K. S. (2014). A multiobjective optimization-based approach for optimal chemical product design. *Industrial and Engineering Chemistry Research*, 53(44), 17429–17444. <https://doi.org/10.1021/ie502906a>
- NREL. (2012). *U.S. life cycle inventory database*. <https://www.lcacommons.gov/nrel/search>
- Ochoa-Estropier, L. M., Jobson, M., & Smith, R. (2013). Operational optimization of crude oil distillation systems using artificial neural networks. *Computers and Chemical Engineering*, 59, 178–185. <https://doi.org/10.1016/j.compchemeng.2013.05.030>
- Ongsakul, W., & Dieu, V. N. (2019). *Artificial intelligence in power system optimization*. CRC Press.
- Osuolale, F. N., & Zhang, J. (2016). Energy efficiency optimisation for distillation column using artificial neural network models. *Energy*, 106, 562–578. <https://doi.org/10.1016/j.energy.2016.03.051>
- Osuolale, F. N., & Zhang, J. (2017). Thermodynamic optimization of atmospheric distillation unit. *Computers and Chemical Engineering*, 103, 201–209. <https://doi.org/10.1016/j.compchemeng.2017.03.024>
- Parvatkar, A. G., Tunceroglu, H., Sherman, J. D., Coish, P., Anastas, P., Zimmerman, J. B., & Eckelman, M. J. (2019). Cradle-to-gate greenhouse gas emissions for twenty anesthetic active pharmaceutical ingredients based on process scale-up and process design calculations. *ACS Sustainable Chemistry and Engineering*, 7(7), 6580–6591. <https://doi.org/10.1021/acssuschemeng.8b05473>
- Pereira, R. D., Badino, A. C., & Cruz, A. J. G. (2020). Framework based on artificial intelligence to increase industrial bioethanol production. *Energy and Fuels*, 34(4), 4670–4677. <https://doi.org/10.1021/acs.energyfuels.0c00033>
- Pozo, C., Ruiz-Femenia, R., Caballero, J., Guillén-Gosálbez, G., & Jiménez, L. (2012). On the use of Principal Component Analysis for reducing the number of environmental objectives in multi-objective optimization: Application to the design of chemical supply chains. *Chemical Engineering Science*, 69(1), 146–158. <https://doi.org/10.1016/j.ces.2011.10.018>
- Process Systems Enterprise. (2021). *gPROMS*. <https://psenterprise.com/products/gproms>
- Qi, G., Zhu, Z., Erqinhu, K., Chen, Y., Chai, Y., & Sun, J. (2018). Fault-diagnosis for reciprocating compressors using big data and machine learning. *Simulation Modelling Practice and Theory*, 80, 104–127. <https://doi.org/10.1016/j.simpat.2017.10.005>
- Rahmanifard, H., & Plaksina, T. (2019). Application of artificial intelligence techniques in the petroleum industry: A review. *Artificial Intelligence Review*, 52(4), 2295–2318. <https://doi.org/10.1007/s10462-018-9612-8>
- Reis, J., Santo, P. E., & Melão, N. (2019). Impacts of artificial intelligence on public administration: A systematic literature review. In 2019 14th Iberian conference on information systems and technologies (CISTI) (pp. 1–7). IEEE. <https://doi.org/10.23919/CISTI.2019.8760893>
- Rich, S. H., Venkatasubramanian, V., Nasrallah, M., & Matteo, C. (1989). Development of a diagnostic expert system for a whipped toppings process. *Journal of Loss Prevention in the Process Industries*, 2(3), 145–154. [https://doi.org/10.1016/0950-4230\(89\)80019-1](https://doi.org/10.1016/0950-4230(89)80019-1)
- Rodrigues, C. F., Riley, G., & Luján, M. (2018). SyNERGY: An energy measurement and prediction framework for Convolutional Neural Networks on Jetson TX1. In *Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications (PDPTA)* (pp. 375–382).
- Romeiko, X. X., Guo, Z., & Pang, Y. (2019). Comparison of support vector machine and gradient boosting regression tree for predicting spatially explicit life cycle global warming and eutrophication impacts: A case study in corn production. In *Proceedings of the 2019 IEEE International Conference on Big Data* (pp. 3277–3284). <https://doi.org/10.1109/BigData47090.2019.9005581>
- Rouhani, B. D., Mirhoseini, A., & Koushanfar, F. (2016). DeLight: Adding energy dimension to deep neural networks. In *Proceedings of the International Symposium on Low Power Electronics and Design* (pp. 112–117). <https://doi.org/10.1145/2934583.2934599>
- Ruijters, E., & Stoelinga, M. (2015). Fault tree analysis: A survey of the state-of-the-art in modeling, analysis and tools. *Computer Science Review*, 15, 29–62. <https://doi.org/10.1016/j.cosrev.2015.03.001>

- Sahebjamnia, N., Tavakkoli-Moghaddam, R., & Ghorbani, N. (2016). Designing a fuzzy Q-learning multi-agent quality control system for a continuous chemical production line – A case study. *Computers and Industrial Engineering*, 93, 215–226. <https://doi.org/10.1016/j.cie.2016.01.004>
- Saint-Donat, J., Bhat, N., & McAvoy, T. J. (1991). Neural net based model predictive control. *International Journal of Control*, 54(6), 1453–1468. <https://doi.org/10.1080/00207179108934221>
- Schweidtmann, A. M., Clayton, A. D., Holmes, N., Bradford, E., Bourne, R. A., & Lapkin, A. A. (2018). Machine learning meets continuous flow chemistry: Automated optimization towards the Pareto front of multiple objectives. *Chemical Engineering Journal*, 352, 277–282. <https://doi.org/10.1016/j.cej.2018.07.031>
- Scott, M. (2015). *Technical economic analysis guide - DRAFT*. [https://www.eia.gov/outlooks/documentation/workshops/pdf/tea\\_guide\\_071015\\_draft.pdf](https://www.eia.gov/outlooks/documentation/workshops/pdf/tea_guide_071015_draft.pdf)
- Segler, M. H. S., Preuss, M., & Waller, M. P. (2018). Planning chemical syntheses with deep neural networks and symbolic AI. *Nature*, 555(7698), 604–610. <https://doi.org/10.1038/nature25978>
- Sharma, B., Ingalls, R. G., Jones, C. L., & Khanchi, A. (2013). Biomass supply chain design and analysis: Basis, overview, modeling, challenges, and future. *Renewable and Sustainable Energy Reviews*, 24, 608–627. <https://doi.org/10.1016/j.rser.2013.03.049>
- Shehabi, A., Smith, S. J., Horner, N., Azevedo, I., Brown, R., Koomey, J., Masanet, E., D, S., Herrlin, M., & Lintner, W. (2016). *United States data center energy usage report*. <https://escholarship.org/content/qt84p772fc/qt84p772fc.pdf>
- Smith, R. L., Ruiz-Mercado, G. J., Meyer, D. E., Gonzalez, M. A., Abraham, J. P., Barrett, W. M., & Randall, P. M. (2017). Coupling computer-aided process simulation and estimations of emissions and land use for rapid life cycle inventory modeling. *ACS Sustainable Chemistry and Engineering*, 5(5), 3786–3794. <https://doi.org/10.1021/acssuschemeng.6b02724>
- Song, R., Keller, A. A., & Suh, S. (2017). Rapid life-cycle impact screening using artificial neural networks. *Environmental Science and Technology*, 51(18), 10777–10785. <https://doi.org/10.1021/acs.est.7b02862>
- Sra, S., Nowozin, S., & Wright, S. J. (Eds.). (2012). *Optimization for machine learning*. MIT Press.
- Srivastava, S. K. (2007). Green supply-chain management: A state-of-the-art literature review. *International Journal of Management Reviews*, 9(1), 53–80. <https://doi.org/10.1111/j.1468-2370.2007.00202.x>
- Sriyakul, H., Koolpiruck, D., Nuratch, S., & Songkasiri, W. (2017). Cyber-physical system based production monitoring for tapioca starch production. In *Proceedings of 2017 4th International Conference on Information Science and Control Engineering (ICISCE 2017)* (pp. 926–930). <https://doi.org/10.1109/ICISCE.2017.196>
- Stéphane, N., Hector, R., & Marc, L. L. J. (2010). Effective retrieval and new indexing method for case based reasoning: Application in chemical process design. *Engineering Applications of Artificial Intelligence*, 23(6), 880–894. <https://doi.org/10.1016/j.engappai.2010.03.005>
- Strubell, E., Ganesh, A., & McCallum, A. (2020). Energy and policy considerations for modern deep learning research. *Proceedings of the AAAI Conference on Artificial Intelligence* (pp. 13693–13696). <https://doi.org/10.1609/aaai.v34i09.7123>
- Sun, X., & Yoon, J. Y. (2018). Multi-objective optimization of a gas cyclone separator using genetic algorithm and computational fluid dynamics. *Powder Technology*, 325, 347–360. <https://doi.org/10.1016/j.powtec.2017.11.012>
- Ten, J. Y., Hassim, M. H., Chemmangattuvalappil, N., & Ng, D. K. S. (2016). A novel chemical product design framework with the integration of safety and health aspects. *Journal of Loss Prevention in the Process Industries*, 40, 67–80. <https://doi.org/10.1016/j.jlp.2015.11.027>
- Tong, W., Chowdhury, S., & Messac, A. (2014). A new multi-objective mixed-discrete particle swarm optimization algorithm. *Proceedings of the ASME 2014 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference* (pp. 1–10). <https://doi.org/10.1115/DETC2014-35572>
- van Gils, J., Posthuma, L., Cousins, I. T., Brack, W., Altenburger, R., Baveco, H., Focks, A., Greskowiak, J., Kühne, R., Kutsarova, S., Lindim, C., Markus, A., van de Meent, D., Munthe, J., Schueder, R., Schüürmann, G., Slobodnik, J., de Zwart, D., & van Wezel, A. (2020). Computational material flow analysis for thousands of chemicals of emerging concern in European waters. *Journal of Hazardous Materials*, 397, 122655. <https://doi.org/10.1016/j.jhazmat.2020.122655>
- Venkatasubramanian, V. (2019). The promise of artificial intelligence in chemical engineering: Is it here, finally? *AIChE Journal*, 65(2), 466–478. <https://doi.org/10.1002/aic.16489>
- Verma, O. P., Manik, G., Suryakant, J. V. K., Jain, D. K., & Wang, H. (2017). Minimizing of energy consumption in multiple stage evaporator using Genetic Algorithm. *Sustainable Computing: Informatics and Systems*, 20, 130–140. <https://doi.org/10.1016/j.suscom.2017.11.005>
- Vesnic-Alujevic, L., Nascimento, S., & Pólvara, A. (2020). Societal and ethical impacts of artificial intelligence: Critical notes on European policy frameworks. *Telecommunications Policy*, 44(6), 101961.
- Vinuesa, R., Azizpour, H., Leite, I., Balaam, M., Dignum, V., Domisch, S., Felländer, A., Langhans, S. D., Tegmark, M., & Nerini, F. F. (2020). The role of artificial intelligence in achieving the Sustainable Development Goals. *Nature Communications*, 11(1), 1–10. <https://doi.org/10.1038/s41467-019-14108-y>
- Wang, L., Agyemang, S. A., Amini, H., & Shahbazi, A. (2015). Mathematical modeling of production and biorefinery of energy crops. *Renewable and Sustainable Energy Reviews*, 43, 530–544. <https://doi.org/10.1016/j.rser.2014.11.008>
- Wang, W., Jiang, D., Chen, D., Chen, Z., Zhou, W., & Zhu, B. (2016). A Material Flow Analysis (MFA)-based potential analysis of eco-efficiency indicators of China's cement and cement-based materials industry. *Journal of Cleaner Production*, 112, 787–796. <https://doi.org/10.1016/j.jclepro.2015.06.103>
- Web of Science. (2021). <https://www.webofknowledge.com>
- Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., & Weidema, B. (2016). The ecoinvent database version 3 (part I): Overview and methodology. *International Journal of Life Cycle Assessment*, 21(9), 1218–1230. <https://doi.org/10.1007/s11367-016-1087-8>
- Wernet, G., Hellweg, S., Fischer, U., Papadokonstantakis, S., & Hungerbühler, K. (2008). Molecular-structure-based models of chemical inventories using neural networks. *Environmental Science and Technology*, 42(17), 6717–6722. <https://doi.org/10.1021/es7022362>
- Wooldridge, M. (1997). Agent-based software engineering. *IEE Proceedings-Software Engineering*, 144(1), 26–37.
- World Economic Forum. (2017). *Digital transformation initiative chemistry and advanced materials industry*. <http://reports.weforum.org/digital-transformation/wp-content/blogs.dir/94/mp/files/pages/files/dti-chemistry-and-advanced-materials-industry-white-paper.pdf>
- Wu, H., & Zhao, J. (2018). Deep convolutional neural network model based chemical process fault diagnosis. *Computers and Chemical Engineering*, 115, 185–197. <https://doi.org/10.1016/j.compchemeng.2018.04.009>
- Wu, H., & Zhao, J. (2020). Fault detection and diagnosis based on transfer learning for multimode chemical processes. *Computers and Chemical Engineering*, 135, 106731. <https://doi.org/10.1016/j.compchemeng.2020.106731>
- Wu, N. Q., Li, Z. W., & Qu, T. (2017). Energy efficiency optimization in scheduling crude oil operations of refinery based on linear programming. *Journal of Cleaner Production*, 166, 49–57. <https://doi.org/10.1016/j.jclepro.2017.07.222>

- Xie, Z., Yang, X., Li, A., & Ji, Z. (2019). Fault diagnosis in industrial chemical processes using optimal probabilistic neural network. *Canadian Journal of Chemical Engineering*, 97(9), 2453–2464. <https://doi.org/10.1002/cjce.23491>
- Yao, Y., Graziano, D. J., Riddle, M., Cresko, J., & Masanet, E. (2016). Prospective energy analysis of emerging technology options for the United States ethylene industry. *Industrial & Engineering Chemistry Research*, 55(12), 3493–3505. <https://doi.org/10.1021/acs.iecr.5b03413>
- Yao, Y., Graziano, D., Riddle, M., Cresko, J., & Masanet, E. (2014). Greener pathways for energy-intensive commodity chemicals: Opportunities and challenges. *Current Opinion in Chemical Engineering*, 6, 90–98. <https://doi.org/10.1016/j.coche.2014.10.005>
- Yao, Y., & Masanet, E. (2018). Life-cycle modeling framework for generating energy and greenhouse gas emissions inventory of emerging technologies in the chemical industry. *Journal of Cleaner Production*, 172, 768–777. <https://doi.org/10.1016/j.jclepro.2017.10.125>
- Yazan, D. M., & Fraccascia, L. (2020). Sustainable operations of industrial symbiosis: An enterprise input-output model integrated by agent-based simulation. *International Journal of Production Research*, 58(2), 392–414. <https://doi.org/10.1080/00207543.2019.1590660>
- Yazdanpanah, V., Yazan, D. M., & Zijm, W. H. M. (2019). FISOF: A formal industrial symbiosis opportunity filtering method. *Engineering Applications of Artificial Intelligence*, 81, 247–259. <https://doi.org/10.1016/j.engappai.2019.01.005>
- Yazdi, M., & Kabir, S. (2017). A fuzzy Bayesian network approach for risk analysis in process industries. *Process Safety and Environmental Protection*, 111, 507–519. <https://doi.org/10.1016/j.psep.2017.08.015>
- Yazdi, M., & Zarei, E. (2018). Uncertainty handling in the safety risk analysis: An integrated approach based on fuzzy fault tree analysis. *Journal of Failure Analysis and Prevention*, 18(2), 392–404. <https://doi.org/10.1007/s11668-018-0421-9>
- Ydstie, B. E. (1990). Forecasting and control using adaptive connectionist networks. *Computers & Chemical Engineering*, 14(4–5), 583–599. [https://doi.org/10.1016/0098-1354\(90\)87029-O](https://doi.org/10.1016/0098-1354(90)87029-O)
- Zahraee, S. M., Assadi, M. K., & Saidur, R. (2016). Application of artificial intelligence methods for hybrid energy system optimization. *Renewable and Sustainable Energy Reviews*, 66, 617–630. <https://doi.org/10.1016/j.rser.2016.08.028>
- Zahr, A. F., Henle, J. J., Rose, B. T., Wang, Y., Darrow, W. T., & Denmark, S. E. (2019). Prediction of higher-selectivity catalysts by computer-driven workflow and machine learning. *Science*, 363(6424), 1–11. <https://doi.org/10.1126/science.aau5631>
- Zerrouki, H., & Smadi, H. (2017). Bayesian belief network used in the chemical and process industry: A review and application. *Journal of Failure Analysis and Prevention*, 17(1), 159–165. <https://doi.org/10.1007/s11668-016-0231-x>
- Zhang, B., Bi, J., Fan, Z., Yuan, Z., & Ge, J. (2008). Eco-efficiency analysis of industrial system in China: A data envelopment analysis approach. *Ecological Economics*, 68(1–2), 306–316. <https://doi.org/10.1016/j.ecolecon.2008.03.009>
- Zhang, C., Zhou, L., Pan, M., Romagnoli, A., & Kraft, M. (2017). Towards intelligent thermal energy management of eco-industrial park through ontology-based approach. *Energy Procedia*, 105, 3295–3300. <https://doi.org/10.1016/j.egypro.2017.03.745>
- Zhang, H., Liang, Y., Liao, Q., Gao, J., Yan, X., & Zhang, W. (2018). Mixed-time mixed-integer linear programming for optimal detailed scheduling of a crude oil port depot. *Chemical Engineering Research and Design*, 137(18), 434–451. <https://doi.org/10.1016/j.cherd.2018.07.013>
- Zhang, P., Jeinsch, T., Ding, S. X., & Liu, P. (2011). Process monitoring and fault diagnosis – Status and applications. *IFAC Proceedings Volumes*, 44(1), 12401–12406. <https://doi.org/10.3182/20110828-6-IT-1002.03656>
- Zhang, Z., & Zhao, J. (2017). A deep belief network based fault diagnosis model for complex chemical processes. *Computers and Chemical Engineering*, 107, 395–407. <https://doi.org/10.1016/j.compchemeng.2017.02.041>
- Zhao, K., & Yu, X. (2011). A case based reasoning approach on supplier selection in petroleum enterprises. *Expert Systems with Applications*, 38(6), 6839–6847. <https://doi.org/10.1016/j.eswa.2010.12.055>
- Zheng, L. G., Zhou, H., Cen, K. F., & Wang, C. L. (2009). A comparative study of optimization algorithms for low NO<sub>x</sub> combustion modification at a coal-fired utility boiler. *Expert Systems with Applications*, 36, 2780–2793. <https://doi.org/10.1016/j.eswa.2008.01.088>
- Zhou, H., Cen, K., & Fan, J. (2005). Multi-objective optimization of the coal combustion performance with artificial neural networks and genetic algorithms. *International Journal of Energy Research*, 29(6), 499–510. <https://doi.org/10.1002/er.1070>
- Zhou, Z., Li, X., & Zare, R. N. (2017). Optimizing chemical reactions with deep reinforcement learning. *ACS Central Science*, 3(12), 1337–1344. <https://doi.org/10.1021/acscentsci.7b00492>
- Zhu, Q. X., Zhang, C., He, Y. L., & Xu, Y. (2018). Energy modeling and saving potential analysis using a novel extreme learning fuzzy logic network: A case study of ethylene industry. *Applied Energy*, 213, 322–333. <https://doi.org/10.1016/j.apenergy.2018.01.046>

## SUPPORTING INFORMATION

Additional supporting information may be found in the online version of the article at the publisher's website.

**How to cite this article:** Liao M, Lan K, Yao Y. Sustainability implications of artificial intelligence in the chemical industry: A conceptual framework. *J Ind Ecol*, 2021; 1–19. <https://doi.org/10.1111/jiec.13214>