

Review

Artificial Intelligence and Cyber-Physical Systems: A Review and Perspectives for the Future in the Chemical Industry

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Abstract: Modern society is living in an age of paradigm changes. In part, these changes have been driven by new technologies, which provide high performance computing capabilities that enable the creation of complex Artificial Intelligence systems. Those developments are allowing the emergence of new Cyber Systems where the continuously generated data is utilized to build Artificial Intelligence models used to perform specialized tasks within the system. While, on one hand, the isolated application of the cyber systems is becoming widespread, on the other hand, their synchronical integration with other cyber systems to build a concise and cognitive structure that can interact deeply and autonomously with a physical system is still a completely open question, only addressed in some works from a philosophical point of view. From this standpoint, the AI can play an enabling role to allow the existence of these cognitive CPSs. This review provides a look at some of the aspects that will be crucial in the development of cyber-physical systems, focusing on the application of artificial intelligence to confer cognition to the system. Topics such as control and optimization architectures and digital twins are presented as components of the CPS. It also provides a conceptual overview of the impacts that the application of these technologies might have in the chemical industry, more specifically in the purification of methane.

Keywords: artificial intelligence; cyber-physical systems; industry 4.0; digital twins; chemical industry; methane purification



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1. Introduction

Technological advancements lead to several paradigm shifts in modern society. These advancements led to extremely fast computing capabilities, near-instant exchange of information at a global level, massive data generation, cloud data storage systems, etc. They also led to the emergence of novel cyber systems in which systematically generated data pipelines are used to perform specialized tasks [1–4]. For example, some countries employ artificial intelligence (AI) models to make use of video security imaging on the streets to identify criminals or potential crimes [5,6]. Furthermore, autonomous AI systems are used in healthcare [7], providing the identification of diseases in record time, such as the diagnosis of COVID-19. There are also several applications used in the chemical industry [8,9]. These new advancements are still very recent and have a high potential for creating critical changes in human society.

These new technologies are positioning the industry in a globalized context of intense renovation, where the system's performance is affected not only by their isolated operation but also by consumer demands, environmental, social, political, and worldwide financial situation. In this scenario, it becomes necessary to have an industry able to quickly respond,

adapt and reconfigure itself while constantly optimizing and controlling its processes. Those demands are starting to exceed the human capacity to efficiently cope and swiftly answer to all these situations simultaneously.

In this context, the current advances in distributed computing, communications, and embedded systems have been presented as an opportunity to propose a new kind of distributed, large-scale, cooperative, and flexible automation systems, referred to as cyber-physical systems (CPS). A CPS is usually defined as a system composed of a physical process integrated into a network and computing system [10–13].

In this review, we would like to present an overview of the CPS application in the chemical industry, and its potential to provide a disruptive breakthrough in this industrial field. The actual issues that limit the vast application of CPS technologies are pointed out. Artificial intelligence is identified as a key technology, not only within the CPS, as usually found, but as an element that can connect CPSs and provide cognition to the system. Therefore, allowing the system to achieve autonomy. Furthermore, some technologies that should be considered in the application of CPSs in the chemical industry are presented and scientific gaps are pointed out to better explore the potential of this emerging field, merging CPS and AI.

2. Methods and Literature Overview

A literature review is an essential methodological step. Thus, it must be developed in a systematic and explicit way in order to retrieve, select, and evaluate the results of retrospective and relevant studies. Within this context, a search strategy was developed to establish a careful analysis of what exists on the subject. A systematic literature review was done using the Web of Science database and stratified according to the Biliometrix procedures [14]. The terms used for this search form three groups, which are: “cyber-physical system” + “artificial intelligence”; “cyber-physical system” + “chemical engineering”; “cyber-physical system” + “artificial intelligence” + “chemical engineering”. The search of these terms were limited to the title, abstract and keywords of the references present in the Web of Science database.

Through the first search set, “cyber-physical system” + “artificial intelligence”, 447 articles were found between 2010 and 2021. In Figure 1, these articles are divided by year of publication and it can be seen that between the years 2019 and 2021 there was a significant increase in publications in this area, which represents 71% of the publications in this theme in the last 10 years. Therefore, demonstrating the increasing attention that the topic has been receiving in the last years. In view of the data presented in Figure 1, it is predicted that the interest in this area will continue to expand. However, it is important to mention that before 2015 the publications regarding CPSs are focused on either particular aspects or theoretical developments of the idea.

Complementarily, evaluating the state of the art for the group of words “cyber-physical system” + “chemical engineering” is strategic, since it allows the observation of the intersection between the cyber-physical system theme within the chemical industry, as is the focus of the present review. Figure 2 shows the search results for this group of words. In this case, only 17 documents were found, published between 2012 and 2021. Moreover, the records of scientific production with this theme arose from 2018 forwards. However, the number of publications in this search set is still far from the numbers presented in Figure 1. This demonstrates that it is a new theme for chemical engineering, still in its early phase of development.

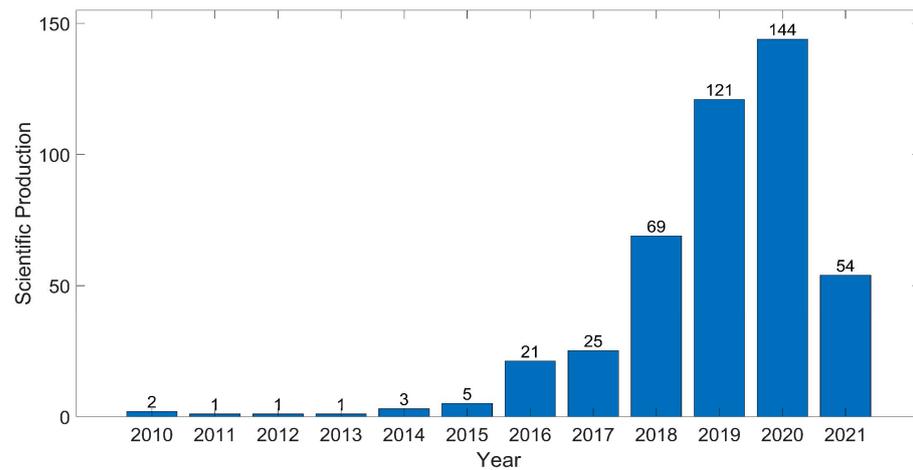


Figure 1. Number of scientific productions between 2010 and 2021 for the keywords “cyber-physical system” and “artificial intelligence”.

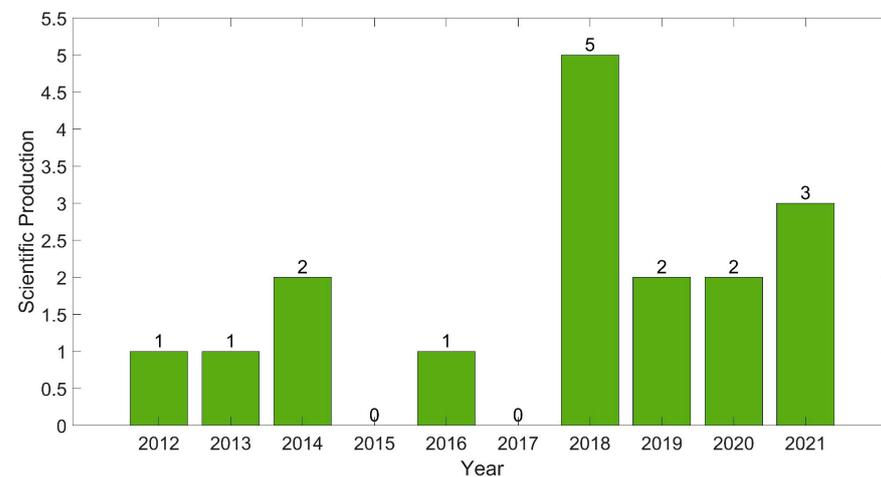


Figure 2. Number of scientific productions between 2012 and 2021 for the keywords “cyber-physical system” and “chemical engineering”.

Between the years 2012 to 2014, four scientific productions are found. The analysis of this specific period is of interest because this is when the concept of CPS was still forming. In Sangiovanni-vincentelli et al. (2012) [15], a manuscript with a very suggestive title “Taming Dr. Frankenstein: Contract-Based Design for Cyber-Physical Systems”, pointed out the complexity of cyber-physical systems. The authors considered CPSs as a system component from the controller point of view. The authors point out that CPS development will face a problem due to the inexistence of rigorous modelling, which considers the interactions between the physical and the cyber side, consequently making the system vulnerable. To address this early-stage problem, the authors proposed a methodology known as “enabling contract-based design (CBD)”, applied to some examples of “in controller design” in which contract-based design can be merged with platform-based design to formulate the system as a meet-in-the-middle approach. However, nowadays, this is still an open issue in the literature, mainly with the increasing complexity of the CPSs.

Still from the point of view of local components and not of CPSs as known nowadays, Basnight et al. (2013) [16] discuss techniques and procedures for inspecting, accessing, and manipulating an Allen-Bradley PLC (programmable logic controller) providing insights regarding system vulnerability while under attack, and about the accessibility and effectiveness of retrieving the PLC firmware for an investigation in view of a potential attack.

Lin et al. (2014) [17] address a resilient monitoring and control system (ReMAC) for resilient condition monitoring and assessment, along with Kalman filter based diagnostic methods integrated with supervisory systems of a chemical reactor with a water-cooling system. The ReMAC system is able to make correct evaluations of the units and performs well to achieve the best control actions despite sensor malfunction due to cyber-attacks. The referred work is still from the system control point of view. It is interesting to note the attention given by these two last works to the system security topic, which is another open issue in the modern CPS literature.

Squire and Song (2014) [18] is the first report in the literature that points to the potential of a more general application of CPS concepts in chemical engineering. The referred work presents a theoretical view about the emergence of CPSs, discussing the possibilities, precautions, and resolutions, for the chemical industry. In this industry, for instance, all the few publications about CPS, address it as a system component. For example, the work of Budiawan et al. (2018) [19] presents a distillation process, where the CPS is proposed as a component that promotes integration between physical process and cyber components. However, the work does not address the issue of cooperativity between CPSs. The bibliographic review made in this work did not find any publication in the field of chemical engineering that deals with the “CPS of CPSs” topic.

A cooperative system is defined as a system composed of several dynamic entities sharing information and coordinating tasks in order to perform a common goal [20]. Even though this concept has been presented in the last 20 years, it started to play a crucial role in today’s globalized society where production chains, supply chains and customers are linked worldwide. Although, it is a common idea in the fields of computer science, military armaments and transportation [20], it still requires greater attention in the field of process system engineering in order to broaden its concepts to an industrial operation. This is the concept that will revolutionize the CPS system, the cooperativity among CPS. In a way that they can perform common tasks synchronously. As in the example of the distillation column, this process is composed of several upper and downstream units. These units can have CPSs within them, and these CPS can communicate within the process, promoting autonomy. Furthermore, this process produces a product and will be inserted in a market, that also can communicate with the plant through the CPSs loop.

Day after day, it becomes impossible to deal with a production system separated from a global context. The cooperativity between systems is also a concept envisioned by the automobile industry to be used in autonomous vehicles, where the traffic is treated as a global system with vehicles in communication with the other, coordinating actions, and sharing information with the overall traffic and city [21]. In the same way, this characteristic is here proposed to be an important component of the proposed conceptual chemical unit.

Finally, the last keyword group, “cyber-physical system” + “artificial Intelligence” + “chemical engineering”, was searched. For this set of keywords, a single article was found—Dobrzański and Dobrzańska-Danikiewicz (2019) [22], which provides a literature review of the connection between human progress and development of materials science. Even though the searched keywords are mentioned in the text, the work does not explicitly address the topics. Therefore, to deepen the search, the group of words was sought in all searchable fields of the articles in the database. Using this approach, only seven documents were found, between the years 2015 and 2020, according to Figure 3. However, most of these articles present mentions about the topics and do not directly address the issue. However, in Gamer et al. (2020) [23] an overview about systems autonomy in chemical industry is presented, where the authors mention the importance of CPSs for this topic, pointing that the interaction between CPS and AI is a crucial factor to provide autonomy for large-scale systems. The referred work presents already the CPS as a macrostructure of integrated, distributed, and connected cyber and physical systems, which is presently the usual definition of CPS.

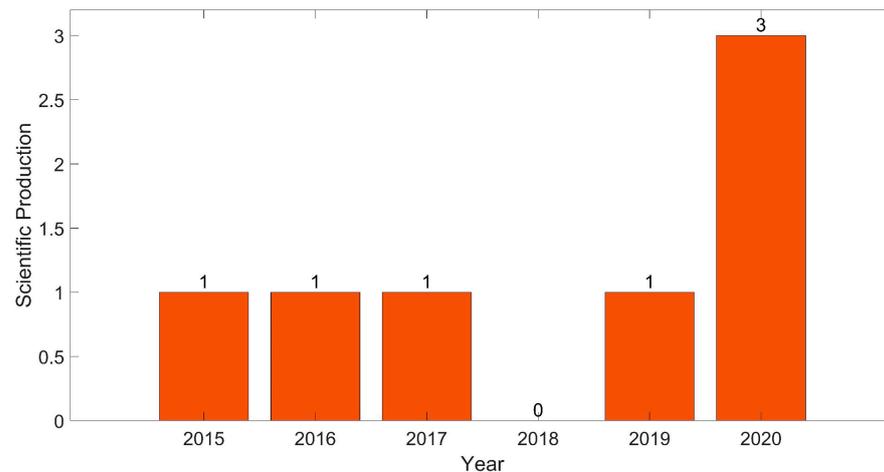


Figure 3. Number of scientific productions between 2015 and 2020, searched in all fields, for the keywords “cyber-physical system” and “artificial intelligence” and “chemical engineering”.

Finally, Figure 4 shows the overall result of the search methodology here followed. It points out a limited overlap between “cyber-physical system” + “chemical engineering”, suggesting that the application of cyber-physical systems in chemical engineering is still in an early stage of development. Furthermore, as mentioned, only one article with overlap between the three keywords was found in the search. Through Figure 4, it is possible to visualize the clear state of these topics in the literature.

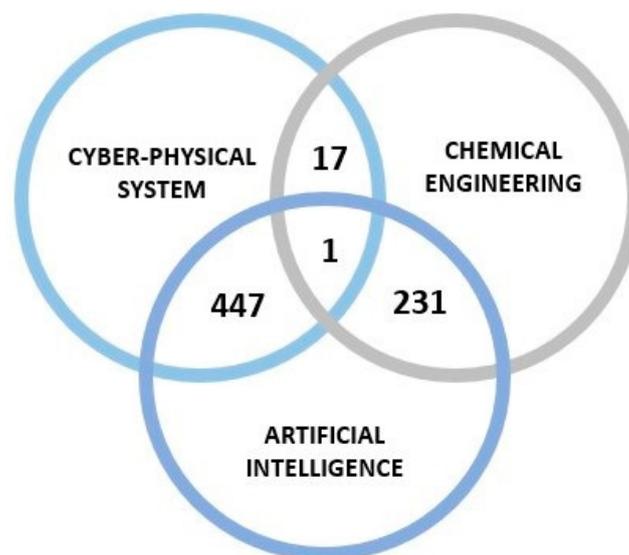


Figure 4. Venn diagram displaying the relationships between the searched keywords “cyber-physical system”, “chemical engineering” and “artificial intelligence”.

3. Cyber-Physical Systems

The CPS is a complex architecture that comprises several engineering levels, integrated with a physical process and working together. In view of the above search results it is possible to note the importance of CPS structures is rising, not only in research [13,24,25], but also in industry [26–28]. This can also be seen at the governmental level [13], where it is possible to see clear agendas focusing on the development of CPS to address modern social issues [11].

It is foreseen that through a concise integration of the new industry 4.0 technologies over the physical system, it will be possible to develop a more efficient, safer, environmentally friendly, and competitive system. In Park (2017) [24], the above potential is

summarized as: “The world economy has been confronting low economic growth for several years. Many experts agree that concepts such as openness, convergence, and creation of new market demand through new emerging technologies (e.g., Internet of Things, big data, and Artificial Intelligence) may solve the current economic crisis throughout the world”, thus enabling a series of social, environmental, political benefits as well.

In Suh et al. (2014) [19], a historical overview of CPSs is provided, throughout the referred work the cyber-physical systems are presented as a novel research field that makes an interception between several areas of knowledge: engineering, automation, informatics, and computer science. The referred work points out the increasing need of a new transdisciplinary engineering approach, which is not possible to find in nowadays universities.

The CPS is an emerging field of study; therefore, its aspects are still under development. In order to accommodate its potential into the already existing systems, studies have been developed addressing the concise integration of humans and CPS, the so called human-in-the-loop [29]. In Gil et al. (2020) [30], the tendency for increasing usage of CPSs structures to perform tasks is pointed out. However, the referred work also points out a barrier for these systems, that is, there are still tasks that are better-performed by humans. Therefore, in Gil et al. (2020) [30], the authors proposed a methodology for the design of CPSs that appropriately allocates human-in-the-loop solutions. This same concept of harmonic integration between human work and cyber-physical systems is presented in Sowe et al. (2016) [31].

As aforementioned, between 2010 and 2020 it was observed an increasing number of publications related to CPS components and issues. However, the existing CPS architecture is only dated from 2015 [32]. Therefore, it is an emerging and new field of study. Even though cyber-physical Systems are relatively novel and recent, there are increasingly prevalent studies related to CPS [32–36]. Furthermore, the integration of a cyber-physical system with other cyber-physical systems, in order to form a structure that can interact with physical systems, in an autonomous, self-managed and mutual way, is still a very new idea in both academic and industrial environments. The development of these cognitive cyber-physical systems is expected to bring revolutionary and disruptive changes to several sectors, such as transportation, energy, health, and production [13].

In this section of the work, an overview of the future perspectives of CPS integration in the chemical industry is presented. The AI is here introduced as an enabling component that can provide the essential cognition to the CPS, as aforementioned. Then, a connection between the CPS and the crucial topics, system control and optimization, found in chemical engineering. Finally, a link between another emerging topic, digital twins, and CPS is presented in the context of the chemical industry.

3.1. Cyber-Physical Systems Enabled by Artificial Intelligence

The focus of this work is to present and review the potential of AI application in an upper level of cyber-physical systems, enabling cognition to the system. On the lower level, within the system, AI can be an essential component within CPSs, for example, to perform faulty detection or real-time prediction of the system behavior [8,37–39]; to be used as a prediction model in control system architectures [40–42]; to perform process optimization [43–45]. This topic has been explored in the literature, as aforementioned. However, as the systems evolve, they become more and more complex. Nowadays, automatized systems tend to be composed of several components that should work harmonically in synchronicity. This requires refined tools at the decision level and at the operating management, which is a bottleneck in enabling large-scale CPS. Thus, AI is a crucial technology in enabling large-scale CPSs, making a bridge between the CPSs and providing them with real-time autonomous guidance.

AI can provide an essential ability for the system: cognition, which allows the modelling, representation and learning of complex behaviors and interactions between the system components and the system data. This can be achieved through the supervised or unsupervised training of AI models to perform these specific tasks. Moreover, AI models

are able to continuously learn from the system, conferring an adaptive ability to the CPS. As such, there is an increasing demand for research on the development and integration of large-scale AI networks. It is important to note that these comments refer to the application of AI in an upper level of CPSs to perform human tasks.

Therefore, through AI it might be possible to achieve a capacity where the chemical unit can vertically integrate several levels of management on itself, communicating with the CPSs structures and performing the management task with autonomy. As indicated by [23] the idea of systems that can operate themselves with reduced human assistance has become popular in the last years due to the recent development in the automotive industry, with self-driving transporting systems. This concept is based on a robust autonomous controllability and autonomous cordiality whose demands are modularity, discreteness, functional equality, data sharing, situation consciousness and self-management. Most likely due to a lack of technology, the idea was not thoroughly developed in the literature and no other author after Koshijima et al. (1997) [46] has mentioned it since then.

An enabling step towards the concept of large-scale CPS coordinated by AI is provided by the Internet of Things (IoT) [32]. An industrial IoT network already provides an extensive network of interrelated computing devices where information is exchanged constantly and made available in real-time. Therefore, the IoT can provide the necessary social environment for the AI models to exchange experiences and information and manage the system under their coordination. Radanliev et al. (2020) [32] provided a comprehensive review of the application of AI within cyber-physical systems.

Furthermore, the identification of AI for dynamic systems is still an open issue. Dynamic AI is one of the most important representations for chemical engineering dynamic systems, which are often highly nonlinear, have high settling times and need frequent intervention considering its future states. The most suitable approach in this situation is the recurrent neural networks (RNN). Among the RNN techniques, the deep neural networks (DNN) are highlighted by their successful application to address problems of several fields. However, there is a lack of new studies in the process engineering field in order to make use of the DNNs potential to solve a series of issues from the field [47]. Deep learning has not yet found many applications in the field of chemical engineering processes. Even though the AI/deep neural networks (DNN) field is currently in continuous growth, its capability to address problems concerning system dynamics is still under development [47–50]. In addition, techniques from distributed AI are also an enabling technology for self-managing, cooperation, and virtualization abilities desired for the development of large-scale cognitive CPSs.

3.2. Control, Optimization, Artificial Intelligence and Cyber-Physical Systems

In the chemical industry, process control and optimization are fundamental issues that always need to be addressed. Without them, even in their most rudimentary version of manual control and visual inspection, a process cannot operate. The control system and optimization literature applied to the chemical industry is robust, where it is possible to find several developments of these topics through time. It is not the goal of this work to perform a revision of these topics; however, as they play a fundamental role in the chemical industry, they should be addressed in any further development made in this field. Therefore, they are here presented as building blocks of the CPSs here envisioned.

In an Industry 4.0 environment, it is essential that a system be able to adapt to changes as quickly as possible, ensuring the best possible scenario in each different set of circumstances. To accomplish this, advanced control and optimization strategies must be designed in order to meet a balance between precise forecasting and representability of a complex process [14,15].

Due to the complex and dynamic nature of CPSs, conventional process control tools such as PID (proportional–integral–derivative controllers) are not up to the task of meeting their demands. Thus, more advanced control strategies must be developed. Model predictive control (MPC) is considered the standard method for application in complex industrial

systems [16]. In particular, according to several papers [17–22] nonlinear model predictive control strategies (NMPC) are known to perform better than linear MPC architectures.

However, there are several problems that prevent the practical implementation of NMPC techniques, such as the lack of strategies for a systematic tuning of the control parameters and restrictive conditions to guarantee stability and feasibility of the closed loop system. Moreover, the implementation of these methods requires high computational effort [14]. Thus, it is expected that research efforts will be focused on developing NMPC strategies to overcome the aforementioned challenges. These strategies should be able to guarantee closed-loop stability, with NMPC control laws that contemplate adaptive and active-learning formulations, yielding data-driven schemes for NMPC strategies.

Optimization of complex processes is, accordingly, a very complex task. An appropriate example of this can be observed in chemical processes due to the highly complex dynamics and interactions between the multiple process variables. Whereas the literature on off-line optimization of such systems is well established, based on detailed and rigorous models [15,23,24], real time optimization (RTO), which aims to dynamically provide the economically favorable and environment-friendly operating conditions, is still relatively unexplored. The main reason for this is the complexity of the optimization problem resulting from the use of stiff differential-algebraic system of equations (DAE)-based models. Substantial research efforts need to be invested in the use of RTO for on-line optimization strategies that are faster than DAE based models. In particular, RTO strategies based on DNN-type surrogate models are of particular interest to this topic. Deep Reinforcement learning [25] can also be used at this level to leverage the big data provided by CPSs. Deep reinforcement learning are strategies that present the potential to formulate a real-time optimization strategy that can learn gradually along the system lifetime. There are risks associated with implementing these optimization architectures, the main one being the increased computational burden that they entail. Similarly, to control strategies, striking a balance between computational burden and accurate representability of the CPS needs to be taken into consideration.

3.3. Digital Twins, Artificial Intelligence and Cyber-Physical Systems

The digitalization of a complete CPS in a virtual clone creates a virtual entity that is a mirror of both the cyber and physical systems, which can be a useful tool for system development, optimization, and monitoring. Allowing the existence of a virtual copy of the complete cyber-physical system can lead to several possibilities. This point involves the capacity to virtualize the cyber-physical system in a concise virtual environment, which can be used for real-time assessments of the physical environment, constantly learning from it, and providing reliable and precise information about the real scenario.

This process is called the twinning process or the building of a digital twin. The idea was originally proposed by Michael Grieves and John Vickers from NASA [26], which was, throughout the last decade, one of the first organizations to make use of the concept of digital twins, applying it to space exploration missions. A review of the literature shows that digital twins are claimed to be an essential technology for the new industrial revolution [51–54]. The number of publications focusing on digital twins [29] has been growing significantly since 2017, mostly originating from the areas of manufacturing and product life cycle assessment.

For instance, through the digital twin, it is possible to emulate and simulate in real-time the cyber-physical system behavior. The digital twin might be a key technology to provide an important tool to the system's robustness. Through the twin, the system can evaluate and predict the behavior of the physical system, while not compromising the operation of the physical system, drawing strategies to cope with the world dynamics. Furthermore, not only one twin can be built but several. Each twin might serve as a benchmark reference, with which the system will be able to check the CPS level and verify possible failures, malfunctions, or even digital threats. In summary, the digital twin can serve as a virtual and reliable laboratory for the system, through which it will be possible

to identify new operating modes, plan and schedule maintenance, predict, diagnose and isolate faults, constantly improving the system efficiency. The twins can be coupled to the upper artificial intelligence models. In this way this upper AI level can make use of the twins' potential to perform autonomous evaluations with robust information about the system.

Digital twins play an important role in the advent of large-scale and complex cyber-physical cognitive systems. Based on this technology, it is possible to explore several scenarios with precision and reliability without the need for a physical system. It is a breakthrough technology because it frees users from important traditional constraints.

4. Perspectives for Chemical Industry and Cyber-Physical Systems

The chemical industry is positioned in a globalized context of intense renovation, where the process performance is affected not only by plant operation and consumer demands, but also by environmental, social, political, and worldwide financial situation. The present social dynamics require an industry able to quickly respond to external changes, so as to defend itself from virtual threats (i.e., the flexibility to reconfigure itself), while constantly optimizing and controlling its processes. As aforementioned, those are demands that are starting to exceed the human capacity. It is foreseen that through a concise integration of the new industry 4.0 technologies over the physical system, it will be possible to develop a more efficient, safer, environmentally friendly and competitive system. The Davos Forum 2016 made clear the disruptiveness of these new technologies. Thus, the deployment of CPS in the chemical industry is a unique opportunity to cope with the current and future challenges of such an industry. Artificial intelligence techniques are often used in the chemical industry to address several daily basis problems, such as soft sensing [9,55–57], modelling [7,47,58,59], and control [40,42,60]. On the other hand, this application is limited to traditional tools of AI, such as feed forward neural networks and fuzzy logic. Intelligent systems are, nowadays, the main drive for the developments of AI tools. However, as aforementioned, these drives are mainly in the computer science and mechanical engineering fields. Thus, there is an increasing need in chemical engineering for translation of the novel achievements in the AI field into chemical systems tools [44,47,60].

For chemical processes, however, few authors have explored the potential of CPS (17 hits on Web of Science in the last 20 years). Ji (2016) [61] proposed a smart rectification column based on CPS. Budiawan (2018) [19] proposed a CPS-based automation on a mini-batch distillation column. Wang (2020) introduced a CPS for quality control in a pharmaceutical process. Moreover, the current works only consider CPS for automation purposes. There is a technological gap to be addressed to move from automation to autonomy. To fulfill this gap a cognitive capability is necessary. In this sense, AI is a potential key enabling technology [23], as it was presented in this work. Therefore, it is an issue that needs to be addressed, allowing the chemical industry to leverage the emerging technologies' potential. This can lead to a safer and more efficient chemical industry, in which systems can be operated without the need of human work. This last issue is a crescent problem in developed countries. It is expected a growth in the number of people aged 65 or older from 85 million today to more than 151 million in 2060, which will have an impact of less 20 million workers [62]. Developed countries' businesses are reaching a level where it is hard to compete with the eastern business, mainly due to the highly differentiated workforce, in number and cost, on those countries when compared with the workforce in developed countries [13]. To face this problem, the level of efficiency of the industries needs to be stretched up to its limit, keeping track of the safety and environmental constraints. This leads to a clear and crescent demand for improved technologies. In this scenario, on one hand, the new digital industrial revolution brings the potential of increased age-friendly work environments [63]. On the other hand, it brings the potential to make mechanical and repetitive work more efficient, which, instead of being done by humans, can be done by smart systems under human supervision.

On the other hand, the search for high-performance production systems, as a more efficient and economical way of production, is a necessary step to address these challenges the human population is growing, consequently so do the product demands. Hence, the production systems need to be able to ensure the necessary scale to attend to the demands. The urgent necessities for drastic changes in consumption and production are clearly expressed in the 2030 Agenda for Sustainable Development. Some authors point to the demand for more efficient and sustainable production systems as the most critical challenge for the future of humanity [64]. Therefore, in the chemical industry context, urgent studies that address this issue, from the perspective of chemical process systems and chemical plant efficient management, are required. In this scenario, it is clear the future potential that CPS systems enabled by AI cognition can have not only in the chemical industry but generally in society.

A Study Case, Upgrading of Methane, and the Potential Impact of CPS in the This Business

One example of an industrial application that could be benefited by cognitive CPSs is the upgrading of methane, more specifically, the separation of methane and nitrogen. The need for purified methane is ever-increasing, eventually leading to the depletion of conventional sources, meaning that unconventional sources must be exploited to overcome this issue.

Methane streams, when extracted from unconventional sources, such as shale formations, are diluted with several contaminants, including nitrogen. Due to the similarity in physical properties to those of methane, this separation is very challenging. With nitrogen being an inert, it lowers the calorific heat of the methane stream and, therefore, must be removed, generally when its content exceeds 3–4%, to meet pipeline gas specifications [65]. This is industrially achieved on a large scale through cryogenic distillation, being an extremely energy-intensive process, with high compression and capital costs associated, especially as the feed gas flow rate is decreased.

Being also utilized for domestic use and as a cleaner fuel alternative for transportation, in the industry, this resource is exploited for climatization, heating and cooling of process streams, in cogeneration processes and as feedstock in the steam reforming reaction for syngas production, being also applied in other industrial sectors (ceramics, textiles, food, metallurgic, pharmaceutical and fertilizers) [66].

This separation is usually done on a large scale through cryogenic distillation, being an extremely energy-intensive process, with high compression and capital costs associated, especially as feed gas flow rate is decreased. For this technology, the driving force is the volatility difference between the two gas molecules. At the intermediate stages of this process, at a pressure of 3150 kPa, their boiling points increase to 178.5 K and 124.5 K [67], which means that a distillation separation process can be effectively achieved by lowering the temperature to about 133 K. This system, called a nitrogen rejection unit (NRU), is usually implemented at the end of a natural gas purification process and can reduce the percentage of nitrogen present in a stream to values under 1%. Different process designs are implemented according to the N₂ content in the feed gas, inlet flow rate, presence of contaminants, product specifications. The most common cryogenic technology units are the single-column heat-pumped process, the dual-column process and the dual-column process with a pre-fractionation step [68]. Prior to the NRU, the inlet gas is compressed, and a pre-treatment of the feed stream is necessary to remove any contaminants that could freeze downstream in the cryogenic unit, such as water, CO₂ and heavy hydrocarbons. Excess H₂S and mercury are also removed upstream of the NRU. In the single-column process, the nitrogen is removed as an overhead product in the distillate with 99% purity and pure methane (99%) is produced at the base of the column. To provide the reboiler and condenser necessary duties, a closed-loop heat pump cycle is utilized [68]. For higher N₂ content in the feed gas (above 20%), the single-column process is no longer efficient, due to condensation problems in the upper trays of the distillation column. As such, a dual-column NRU can be utilized, allowing partial removal of the N₂ in a high-pressure column,

with the bottom product being fed to a low-pressure column for further nitrogen rejection. The dual-column system can be coupled to a prefractionation column, recovering a portion of the hydrocarbons present in the inlet stream at a higher temperature. Consequently, the stream is enriched in nitrogen, which is then processed in the main distillation columns. Figure 5 presents an overview of this process flowsheet.

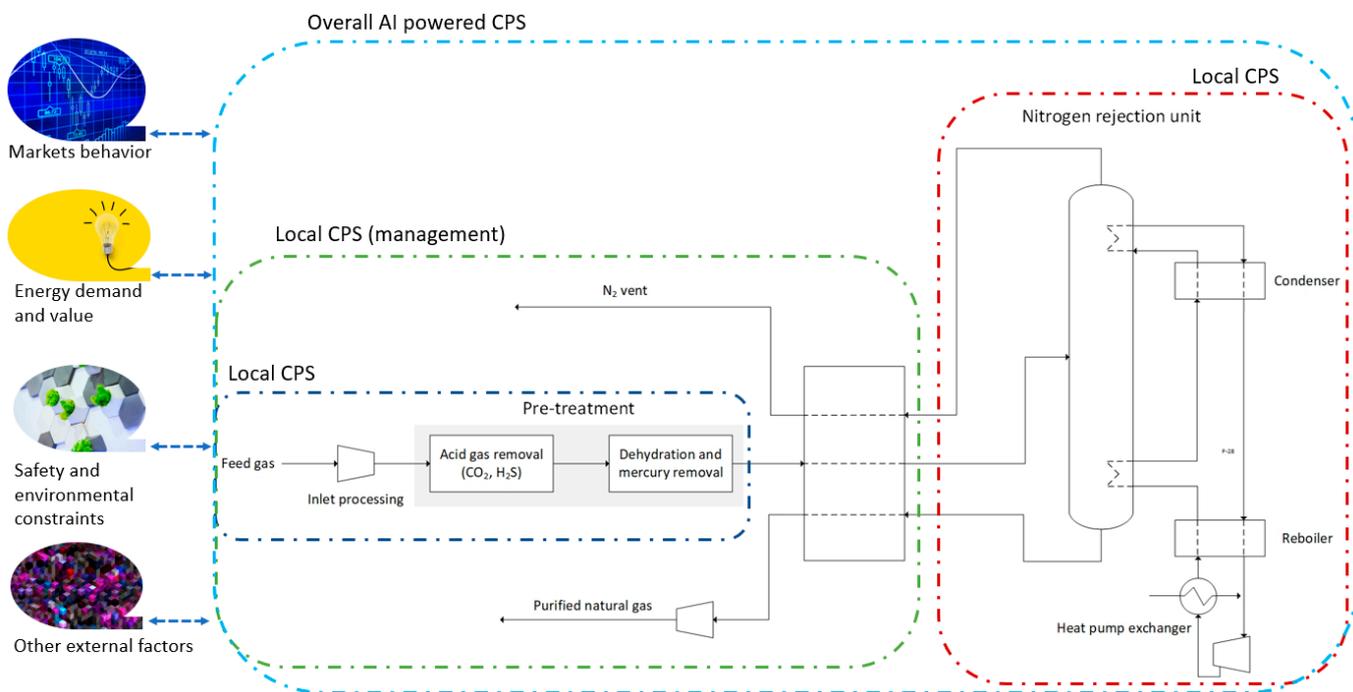


Figure 5. Process flowsheet of a single-column nitrogen rejection unit with a schematic representation of the possible local CPS of this process and the overall CPS powered by AI with its connection to the external environment.

It is worth highlighting that the concepts of CPS discussed in this work are not yet applied in the processes described in Figure 5. In this figure, the process flowsheet is presented with the possible local CPSs. Through the scheme depicted in Figure 5, it is also possible to envision the CPSs interaction between them and the overall CPS. These local CPSs can be built, following the actual CPS concepts, over the distillation column, over the pre-treatment units, and over the process input/outputs performing the system management. Each local CPS is composed of the process units and their sensors, actuator, controllers (PIDs and MPCs), and other hardware/software. Thus, the local Cyber-physical systems are a platform that interconnects these elements building an industry 4.0 environment over the physical system. The local CPS can increase the process robustness and reduce the system reaction time and the necessity for human intervention. A CPS of CPSs can then lead the gains to another level, to the whole system management. Furthermore, the AI-powered structure can process large amounts of data and convert it into information to provide effective and efficient decision making. This example makes clear the potential of this topic in the future of the chemical industry.

According to the 69th Edition of the BP Statistical Review of World Energy, the demand for natural gas has grown by 78 billion cubic meters (bcm), with a total of 3989.3 bcm being produced. The global natural gas consumption has achieved a 2% growth, reaching 3929.2 bcm in 2019, comprising about 24.2% of the global primary energy consumption [69]. This consumption leads to a global market for oil and natural gas separation equipment of approximately 8.3 billion dollars per year, expected to grow at a 4.5% CAGR (Compound Annual Growth Rate) until 2028 [68]. In the face of the value of this sector, and the complexity associated with its operation, this industry could benefit from more robust

cyber-physical systems that could optimally extract, process, and make methane available for the final consumers at lower operating costs.

This benefit is not only from the point of view of how the operation is processed, but also from the point of view that humans are limited beings, and several tasks are reaching our limits. This is clear when analyzing the data of human error in the industry. For example, in Moura et al. (2015) [69], it is presented an analysis of accidents in the industry provoked by human errors based on reports found in the literature. The authors have estimated a value of 28.67 billion dollars in material losses, a value updated to the 2013 inflation rate. It is easy to have an estimation of how much the CPSs benefit the industry operating with as little human intervention as possible. If one considers that several industrial sectors are still behind in these new industrial revolutions, for example, the chemical industry, and also considers that a significant perceptual of the human errors would be diminished by the autonomous operation of the system, one can find values around billions of dollars of savings by the usage of CPSs systems.

Of course, that to reach this level of savings, several studies need to be done to validate the operation of large-scale cyber-physical systems. However, it is possible to find several studies that have been published pointing out the economic potential of digital economy [70–72]. Nicolescu et al. (2018) [70] proposed a “functional model that aggregates these findings into a value-driven logic of the emerging global political economy enabled by digital technology in general and IoT in particular.” [71]. The referred work points out two critical issues, the potential value of digital technologies and the necessity for an interdisciplinary context to understand the potential value associated with these technologies. A study from NIST (National Institute of Standards and Technology, US) [72] provides the evaluation of the economic impact of new technologies in additive manufacturing. The study also points out the gaps and research needed to develop this emerging field better. Hence, the potential is clear. These systems can benefit the industry with billions in annual revenues. On the other hand, these systems can benefit human life, liberating humans from stressful, repetitive, and arduous tasks.

5. Conclusions

The modern industry finds itself in a paradigm of intense renovation, with issues concerning the integration of physical space with enabling the technologies from Industry 4.0. The dynamics of modern society are pushing humanity in the direction of an increasing necessity of complex CPSs with cognitive abilities, which grants these systems autonomy, without the need for human intervention. It is possible to catch a glimpse of a new industrial revolution, one that will assist in freeing humans from mechanical, repetitive, and stressful tasks, and even decision-making ones.

This review provides an overview of this newly emerging field, points out some scientific and technological gaps for the development and expansion of the potential of CPS in several human activities, with focus on the chemical industry. In the end, the potential impact in the chemical industry is discussed, with a special focus on methane purification. The technologies for that are mostly available already; they now require efforts to build a technological platform that allows their integration, intercommunication, and cooperation.

Through this review it is possible to see that the cyber-physical systems are in the imminence of achieving a large-scale application, since all the technological basis for it is already available. The challenges to conclude this new technological revolution are pointed out, one of these challenges is the connection of several CPSs within a concise environment to perform cooperative tasks autonomously. Artificial intelligence is then pointed out as a key technology to promote the integration of CPSs in a cognitive system that requires few human interventions.

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