Cyber-Physical Systems in Chemical and Energy Processes

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Abstract: Connectivity between physical and cyber systems has been dramatically invested over the last forty years, enabled by the advances of communication networks, computing power and automation. In this chapter, discuss the impact of such cyber-physical integration in chemical and energy processes, and how the advances in process monitoring, process modeling and digital twin, control and optimization, coupled with artificial intelligence (AI) and machine learning (ML) networks can play a key role in improving the safety, efficiency and productivity of cyber-physical systems (CPS). We also examine challenges and future directions in this field.

Keywords: Cyber-physical system, Data analysis, Smart manufacturing, Internet of things, Energy systems, Optimization, Control, Process safety management, Real-time monitoring

8.1 Introduction

Cyber-Physical Systems (CPS) refer to interconnected networks of physical components and computational algorithms that interact with each other and their environment. The term "Cyber-Physical Systems" (CPS) was officially introduced by Helen Gill at the National Science Foundation around 2006 [1,2]. This definition underscores the integration of computational and physical processes. The concept of CPS builds upon earlier ideas in fields like mechatronics, embedded systems, and pervasive computing. The term's roots can be traced back even further, linking to concepts from cybernetics, a term coined by Norbert Wiener to describe the control and communication between the animal and the machine [3]. As illustrated in Fig. 1, the general architecture of a CPS includes a physical system and a cyber system featuring the convergence of physical processing, sensing, computation, communication, and control [4]. The physical system comprises physical processes, sensors, and actuators. Typically, physical processes function as prototype units or plants, which are managed by the cyber system. On the other hand, the cyber system encompasses communication networks, computing, and control centers [5].

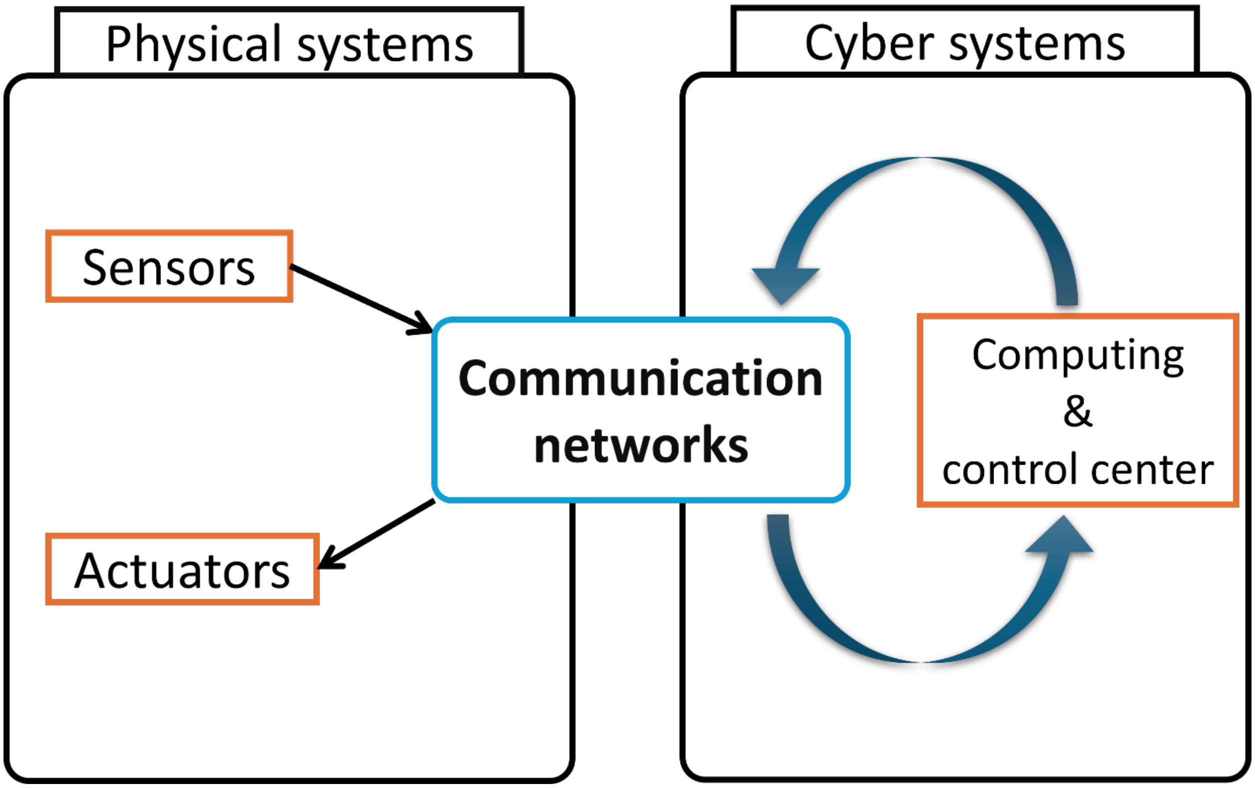

Figure 1. Typical structure of cyber-physical systems (CPS)

With the development of internet and data technology, CPS and related technologies have advanced, leading to a yearly increase in corresponding publications. In Figure 2, the number of publications on CPS has rapidly increased, from 1,336 in 2015 to 3,349 in 2023. CPS applications have expanded across various disciplines such as electrical and electronic engineering, computer science, automation control systems, energy and fuels, and chemical engineering, as illustrated in Figure 3. It's worth noting that CPS in the chemical and energy sectors represents a smaller portion of the total.

This chapter aims to provide a general summary of CPS in chemical engineering, focusing on process safety, control, and optimization. The remainder of the chapter is organized as follows: Section 8.2 discusses the components and architecture of CPS. Section 8.3 presents the applications of CPS in the chemical and energy sectors. Section 8.4 summarizes the challenges and future directions. Finally, Section 8.5 introduces a cyber-physical prototype for safer energy production, illustrated through a modeling and optimization framework.

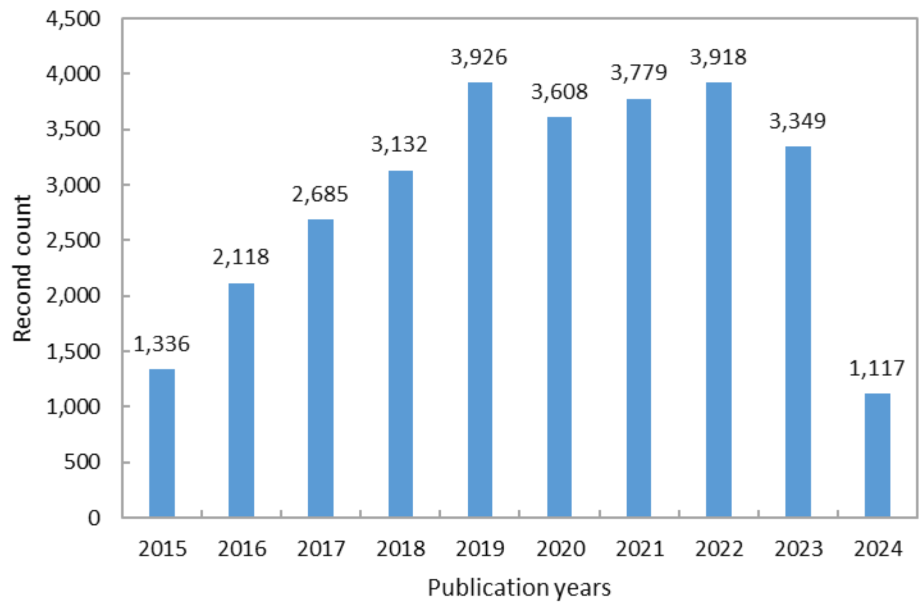

Figure 2. Analyses in the field of CPS by publication year

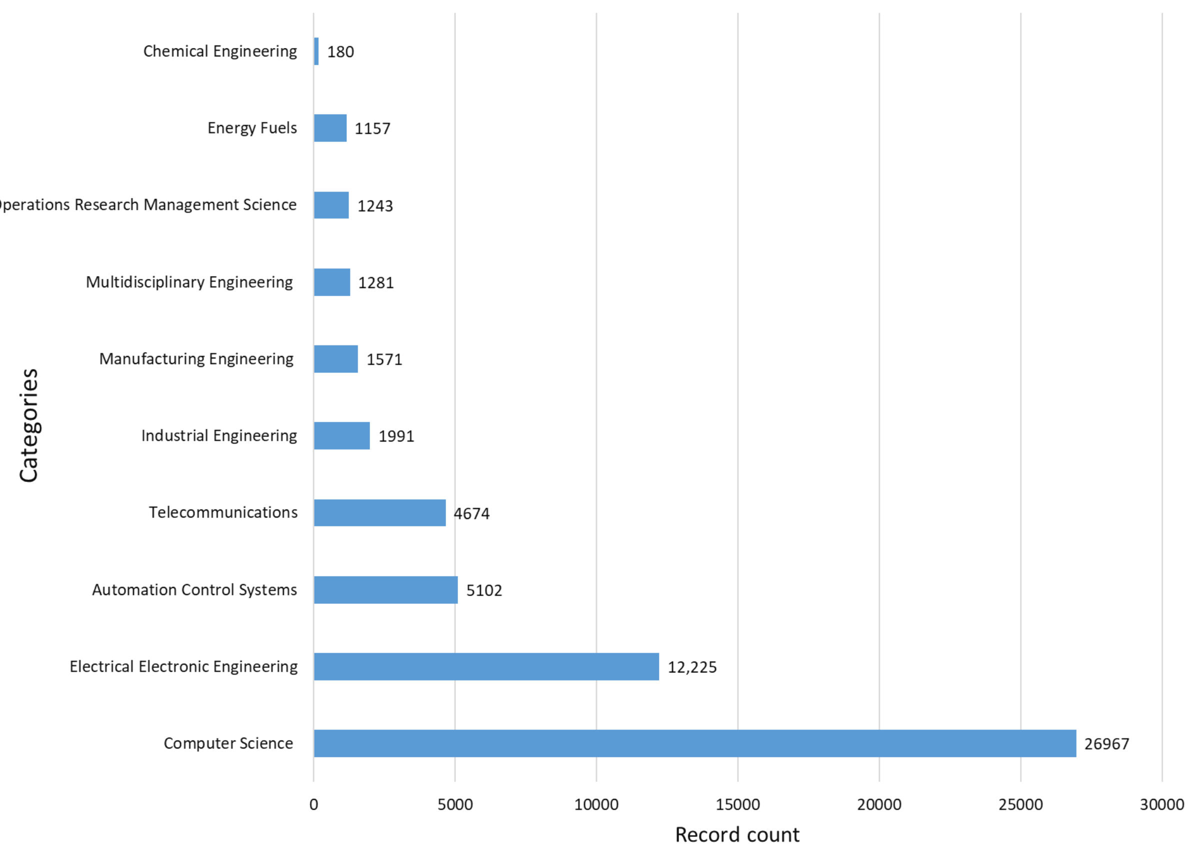

Figure 3. Analyses in the field of CPS - representative disciplines

8.2 Components and Architecture of Cyber-Physical Systems

8.2.1 Components of Cyber-Physical Systems:

a. Sensors and Actuators

Sensors in energy systems encompass a diverse range of technologies, including temperature sensors, pressure sensors, flow meters, and proximity sensors. Each type of sensor serves a specific purpose, capturing physical parameters crucial for monitoring and control. For instance, temperature sensors are employed in thermal power plants to monitor heat exchange processes, while flow meters measure fluid flow rates in pipelines and reactors. Sensors play a pivotal role in providing real-time data on process variables, equipment condition, and environmental parameters. This data serves as input for computational systems, enabling predictive analytics, fault detection, and adaptive control strategies. By continuously monitoring key parameters, sensors facilitate proactive decision-making and optimization of energy processes.

Actuators convert control signals from computational systems into physical actions, exerting control over various components and processes within energy systems. Examples of actuators include control valves, motorized dampers, variable frequency drives, and hydraulic actuators. These actuators modulate flow rates, adjust equipment settings, and regulate energy output to maintain desired operating conditions. Actuators are instrumental in implementing control strategies to optimize energy efficiency, enhance system reliability, and mitigate operational risks. By modulating process variables in response to feedback from sensors and computational algorithms, actuators enable dynamic adjustments and fine-tuning of energy processes. This dynamic control capability is essential for adapting to changing demand patterns, equipment failures, and external disturbances.

b. Computational Systems

Embedded control systems serve as the computational backbone of energy systems, executing control algorithms and decision-making logic in real-time. These systems integrate sensor data, process models, and control strategies to orchestrate the operation of energy processes. Examples include programmable logic controllers (PLCs) [6,7], distributed control systems (DCS)[8,9], and supervisory control and data acquisition (SCADA) systems [10-13]. Computational systems analyze sensor data, implement control algorithms, and optimize energy processes to achieve predefined objectives such as maximizing efficiency, minimizing costs, or ensuring safety. Advanced computational techniques such as model predictive control (MPC), adaptive control, and machine learning enable predictive maintenance, energy forecasting, and adaptive optimization in energy systems.

c. Communication Infrastructure:

A robust communication infrastructure is essential for facilitating seamless interaction between different components of CPS. This infrastructure encompasses wired and wireless networks, protocols, and standards for data exchange. Examples include Ethernet, Wi-Fi, and protocols like Message Queuing Telemetry Transport (MQTT) [14-16] and OPC Unified Architecture (OPC UA)[17-19], which enable data transmission and interoperability in energy management systems.

8.2.2 Architecture of Cyber-Physical Systems:

a. Layered Architecture:

CPS often adopt a layered architecture [20-22], dividing the system into distinct layers based on functionality and abstraction level. Common layers include physical layer, cyber-physical layer and cyber layer demonstrating perception, processing, communication, and actuation. Each layer interacts with adjacent layers and the cyber and physical environments to achieve system objectives. In energy systems, this architecture enables hierarchical control and optimization of energy generation, transmission, and consumption [20, 23, 24].

For example, Guzman et al. introduced a multi-layered CPS master diagram toward a combined safety and security risk analysis, as shown in Figure 4 [20]. The physical layer constitutes the lower level of the system, including the physical components, operators, and the physical dynamics that reflect their interactions. The middle layer, known as the cyber-physical layer, encompasses real-time communication functions. This involves data acquisition through sensors, transmission of data for processing, and further monitoring and control with the deployment of control actions by actuators. At the top level, the cyber layer incorporates SCADA, HMIs, and supervisory computers that utilize cloud platforms for data visualization and parameter adjustments, among other functions.

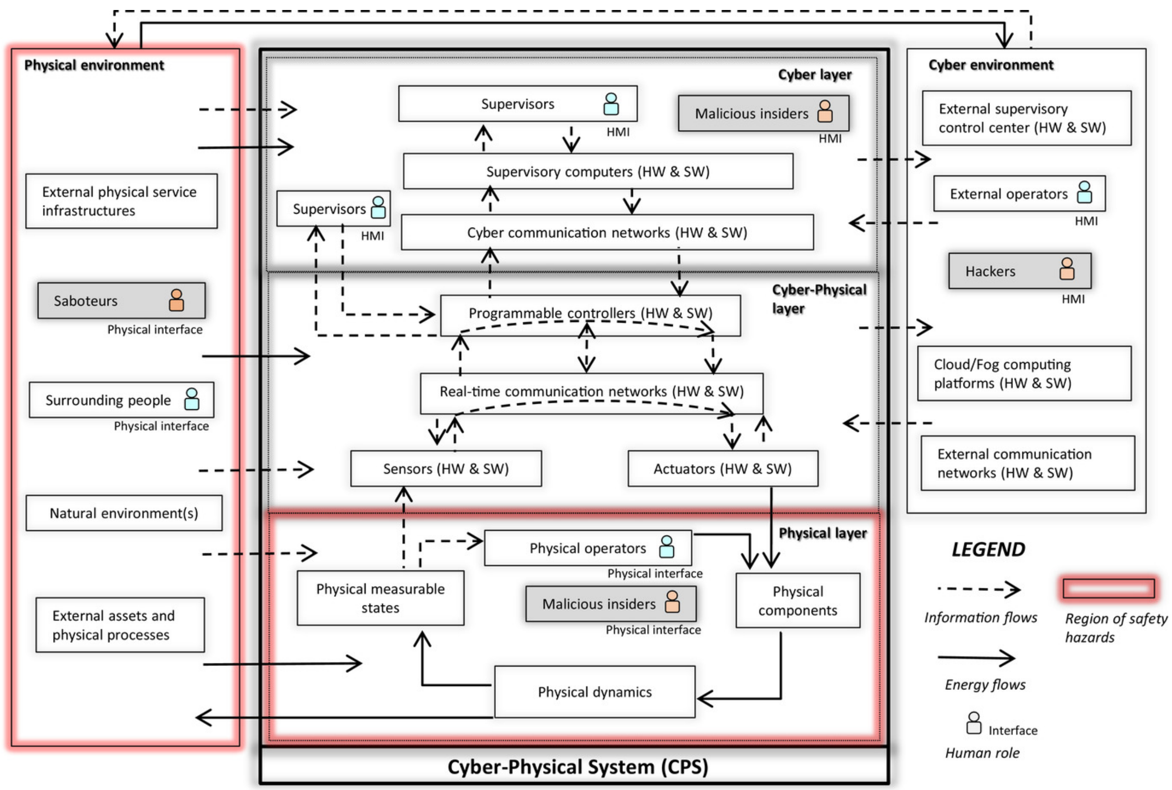

Figure 4. Multi-layered representation of CPS and environments with information and energy flows. [20] [https://doi.org/10.1002/sys.21509]

b. Distributed Control Systems:

Distributed control systems (DCS) decentralize control functions across multiple nodes within the CPS [25, 26]. This architecture enhances system resilience and scalability by distributing computational tasks and decision-making processes. In energy systems, DCS enables localized control of renewable energy sources, demand response mechanisms, and grid stability measures [26].

c. Edge Computing and Cloud Integration:

With the proliferation of Internet of Things (IoT) devices, edge computing has emerged as a critical component of CPS architecture [27-29]. Edge devices process data locally, reducing latency and bandwidth requirements, while cloud integration enables centralized storage, analytics, and management of data [30-33]. In chemical engineering, edge computing is deployed for real-time monitoring of processes, while cloud-based analytics enable predictive maintenance and optimization [34].

8.2.3 Integration of Sensors, Actuators, and Computational Systems

Actuators are closely integrated with computational systems, receiving control signals generated by higher-level algorithms based on sensor inputs and system objectives. This integration enables closed-loop control, where actuators continuously adjust process parameters to maintain desired operating conditions and respond to dynamic changes in the environment.

8.3 Applications of Cyber-Physical Integration in Energy Systems

The integration of Cyber-Physical Systems (CPS) in energy systems, particularly within the domain of chemical and energy industry, offers transformative opportunities for enhancing efficiency, sustainability, and resilience. In what follows, we explore various applications of CPS integration in energy systems, focusing on their implications for chemical processes. Through detailed analysis and case studies drawn from literature, we elucidate the role of CPS in optimizing energy utilization, improving process control, and enabling the transition towards sustainable energy solutions.

8.3.1 CPS Integration in Chemical Process Design:

a. Real-Time Optimization and Control:

CPS integration enables real-time optimization and control of chemical processes [35, 36], allowing for dynamic adjustments based on changing operating conditions and energy availability. Literature showcases examples of model predictive control (MPC) [37, 40, 41] and advanced process control (APC) strategies implemented through CPS to enhance energy efficiency and product quality in chemical plants [38,39].

b. Energy-Efficient Operation:

By integrating CPS, chemical processes can be operated more energy efficiently, with real-time monitoring of energy consumption and process variables [42, 43]. Advanced control algorithms, coupled with sensor networks and actuators, facilitate energy-aware decision-making, resulting in reduced energy costs and environmental impact [44,45].

8.3.2 CPS Integration in Renewable Energy Systems:

a. Integration of Renewable Energy Sources:

CPS plays a crucial role in the integration of renewable energy sources, such as solar and wind, into chemical processes [46, 47]. Literature highlights case studies where CPS-enabled smart grids optimize the utilization of intermittent renewable energy [46, 48], enabling chemical plants to adjust production schedules and energy consumption patterns accordingly[49]. For instance, this work discusses the use of advanced sensors, data analytics, and digital controls to enhance energy efficiency and real-time optimization, which highlights the importance of IIoT-enabled smart assets and data infrastructure for effective energy management [50]. Besides, Edgar et al presented a comprehensive framework for smart manufacturing that incorporates renewable hydrogen production. The paper introduces the Renewable Hydrogen Production and Utility Testbed (REHPUT), which integrates renewable power sources like solar and wind with a Proton Exchange Membrane (PEM) electrolyzer to produce hydrogen. This system includes hydrogen purification, storage, and electricity generation, demonstrating a complete cycle of renewable energy utilization [51].

b. Energy Storage and Grid Integration:

CPS integration enables efficient energy storage and grid integration solutions for chemical engineering applications [52-56]. Through the deployment of smart energy storage systems and demand response mechanisms [57-59], chemical plants can participate in grid balancing activities, contributing to grid stability and the integration of renewable energy. Kakodkar et al. proposed a framework that integrates renewable power generation, various energy storage technologies, and carbon capture, utilization, and sequestration (CCUS). This study explores the use of electrochemical storage, pumped storage hydropower, and compressed air energy storage for efficient energy storage solutions. Additionally, it addresses the integration of these storage solutions with the grid, considering factors like round-trip efficiency, discharge rates, and storage losses, thereby supporting the grid's resilience and stability [60].

8.3.3 CPS Integration in Process Safety and Reliability:

a. Predictive Maintenance and Safety Systems:

CPS integration enhances process safety and reliability through predictive maintenance and safety monitoring systems. By leveraging sensor data and machine learning algorithms, CPS-enabled systems can identify potential equipment failures and safety hazards, enabling proactive maintenance[61, 62] and risk mitigation measures [63]. EI-Kady et al demonstrated the use of digital twin (DT) models for predicting failures, enhancing system reliability, and enabling proactive maintenance. The paper also highlights the integration of IoT sensors for continuous monitoring and early warning systems to improve safety and reduce unscheduled downtimes [64]. Additionally, Amin et al developed a holistic framework that employs Bayesian Networks (BN) to model the probabilistic nature of safety and security events, facilitating real-time risk analysis and predictive maintenance [65].

b. Fault Detection and Diagnosis:

CPS integration facilitates fault detection and diagnosis in chemical processes, minimizing downtime and improving operational efficiency. Case studies demonstrate the implementation of CPS-enabled fault detection algorithms, which analyze sensor data to detect abnormal process behavior and diagnose root causes of equipment malfunctions [66,67]. Alauddin et al presents a robust neural network model for fault detection in the presence of mislabeled data. By incorporating data quality metrics based on Mahalanobis distances and trusted centers, the model enhances fault detection accuracy and robustness [68]. Wen et al. developed a risk model to distinguish between faults and cyberattacks, using game theory to explain conflicts, and applying the model to Continuous Stirred Tank Reactor (CSTR) systems. The proposed framework enhances fault detection and diagnosis by accurately identifying and mitigating the impact of cyberattacks [69].

8.4 Challenges and Future Directions

8.4.1 Advanced Modeling and Control Optimization Algorithms

CPS in chemical engineering has revolutionized the approach to process systems, particularly in energy systems. The intersection of physical processes with digital controls offers unparalleled precision, efficiency, and adaptability. A critical component of this integration is the development and implementation of advanced modeling and control optimization algorithms. These algorithms are pivotal in addressing the dynamic and complex nature of chemical processes, ensuring optimal performance, and adapting to changing conditions in real-time.

Advanced modeling techniques in CPS for chemical engineering encompass a range of methods designed to accurately represent the behavior of chemical processes. These include mechanistic models, data-driven models, and hybrid models. Mechanistic models are based on fundamental physical and chemical principles [70, 71]. They provide detailed insights into the process dynamics by incorporating equations derived from mass, energy, and momentum balances. An example is the use of computational fluid dynamics (CFD) to provide precise simulations of fluid behavior and enhancing manufacturing processes. By integrating CFD with Augmented Reality (AR), engineers gain improved cognitive abilities for problem-solving through interactive visualization. CFD's low cost, low risk, and meaningful insights offer competitive advantages in smart factories [72]. Additionally, CFD aids in optimizing ventilation, conditioning, and mitigating virus spread in industrial environments. The combination of CFD with cloud computing and big data analytics supports real-time decision-making and efficient system design and operation [73].

With the advent of big data and machine learning, data-driven models have gained prominence. These models utilize historical process data to predict future behavior without requiring explicit knowledge of the underlying physical phenomena. Techniques such as neural networks and support vector machines have been applied to model complex processes like distillation columns [74-76] and polymerization reactors [77,78].

Combining the strengths of mechanistic and data-driven approaches, hybrid models offer a balanced solution. They leverage mechanistic models to ensure physical plausibility and use data-driven methods to capture complex, nonlinear relationships that are difficult to model mechanistically [79]. An example is the hybrid modeling framework combining a nominal term, based on physicochemical principles, with a deviation term, which captures the effects of high-dimensional factors using machine learning. This approach enhances modeling accuracy by leveraging comprehensive state space (CSS) for real-time data and visualization. [80]

Control optimization in CPS involves developing algorithms that can handle the complexity and variability of chemical processes. These algorithms aim to achieve objectives such as maximizing efficiency, minimizing energy consumption, and maintaining product quality. Model predictive control (MPC) is widely used due to its ability to handle multivariable control problems with constraints. It predicts future process behavior using a dynamic model and optimizes control actions by solving a finite-horizon optimization problem at each time step. For example, the integration of stochastic MPC allows for handling probabilistic constraints, further improving CPS resilience and efficiency by allowing controlled violations of constraints when necessary [81]. Moreover, MPC in CPS enhances security and efficiency by leveraging cloud-edge computing. The MPCaaSS framework optimizes control parameters in the cloud and executes real-time control at the edge, ensuring robust performance against cyber threats and external disturbances through secure data transmission protocols [82]. The MPC strategy was employed to enhance CPS resilience by mitigating the effects of Denial-of-Service (DoS) attacks. It ensures stability and performance through optimization, even under constrained communication conditions [83].

Reinforcement Learning (RL) is an emerging approach in control optimization, where an agent learns optimal control strategies through trial and error interactions with the process environment. This method has been applied to coordinate actions among agents in dynamic environments, improving system robustness to changes. Specifically, RL applied to energy optimization in CPS, such as micro-grids with variable electricity prices, enhances the adaptive response of agents to environmental fluctuations, resulting in efficient energy usage and high productivity across interconnected systems.[84]. The parallel RL framework uses bidirectional LSTM networks for energy management in hybrid electric powertrains, optimizing control strategies in dynamic environments. This approach significantly improves fuel economy and system performance compared to traditional methods [85].

Robust and adaptive control techniques are designed to maintain optimal performance in the presence of uncertainties and disturbances, which ensure stability and performance across a range of operating conditions, while adaptive control methods adjust control parameters in real-time based on process feedback. Examples include adaptive control for mitigating sensor and actuator attacks.[86-88]. He et al summarized the role of robust control in addressing the challenges posed by multiple uncertainties, such as unknown disturbances, time-varying delays, and stochastic malicious attacks. By utilizing Lyapunov–Krasovskii functional (LKF) with advanced integral inequalities, robust control strategies ensure system stability with less conservatism. Applications, like load frequency control (LFC) in power systems, demonstrate the effectiveness of these methods in real-world scenarios.[89]

The future of CPS in chemical engineering relies heavily on the continued development and refinement of advanced modeling and control optimization algorithms. These tools are essential for addressing the challenges of complex, dynamic processes and unlocking new levels of efficiency and sustainability in energy systems. As these algorithms evolve, they will enable more intelligent, responsive, and resilient chemical processes, paving the way for significant advancements in the field.

8.4.2 Artificial Intelligence (AI) and Machine Learning (ML) for Data Analytics

The advent of CPS in chemical engineering has opened new avenues for optimizing process systems, particularly in energy systems. A pivotal aspect of this transformation is the application of AI and ML for data analytics. These technologies enable the extraction of valuable insights from vast amounts of process data, driving improvements in efficiency, reliability, and sustainability. This section delves into the advanced AI and ML techniques used in data analytics, their applications in chemical engineering, and future directions for research and development.

Supervised learning algorithms are widely used for predictive modeling in chemical processes. Techniques such as linear regression [90-92], support vector machines (SVM) [93,94], and neural networks [95,96] learn from historical data to predict future outcomes.

Unsupervised learning methods, including clustering [97] and principal component analysis (PCA)[98,99], are crucial for exploratory data analysis. These techniques help identify patterns and anomalies in process data without prior labels. Clustering algorithms like k-means have been used to segment operational states in chemical plants, facilitating better process monitoring and control [100,101].

Deep learning, particularly deep neural networks (DNN), has revolutionized data analytics by enabling the modeling of highly complex, nonlinear relationships in process data. For instance, convolutional neural networks (CNNs) has applied in CPS for detecting anomalies and cyber attacks in industrial control systems (ICS). They achieve this by extracting local features from time series data. Compared to traditional recurrent neural networks, CNNs offer faster training and execution, and they excel in handling complex multivariate time series prediction tasks [102]. Also, recurrent neural networks (RNNs) are essential in CPS for modeling dynamic, nonlinear processes in chemical engineering. They excel in handling high settling times and frequent interventions, making them suitable for system dynamics, real-time predictions, and optimizing control processes [103].

The future of AI and ML in data analytics for chemical engineering lies in several key areas. The integration of AI and ML with IoT devices will enhance real-time data collection and analysis. This synergy will enable more responsive and adaptive process control, improving efficiency and reducing waste [104]. As AI models become more complex, there is a growing need for explainable artificial intelligence (XAI) techniques aim to make AI decisions transparent and understandable, which is crucial for gaining trust and ensuring compliance with safety regulations in chemical engineering [105-106]. Besides, deploying AI algorithms at the edge, closer to the data source, can significantly reduce latency and improve real-time decision-making [107]. This approach is particularly beneficial for time-sensitive applications in chemical processes. In addition, combining mechanistic models with AI and ML techniques will enhance the robustness and accuracy of process models [108,109]. These hybrid models can leverage the strengths of both approaches, providing more comprehensive solutions for complex chemical engineering problems. In addition, AI and intelligence augmentation (IA) enable proactive monitoring and predictive maintenance, reducing downtime, optimizing operations, and improving safety, where IA collaborates with humans for decision-making, ensuring a balance between efficiency and safety [110]. Last but not least, AI and ML are transforming data analytics in chemical engineering, particularly in the context of cyber-physical systems in energy systems [111]. These technologies enable more efficient, reliable, and sustainable process operations by extracting valuable insights from data. As AI and ML continue to evolve, their integration with emerging technologies and methodologies will drive further advancements, addressing the challenges and unlocking new opportunities in chemical engineering.

8.4.3 Data Security and Privacy Concerns

The integration of Cyber-Physical Systems (CPS) in energy systems brings forth significant data security and privacy concerns. As these systems rely heavily on data collection, communication, and analysis, ensuring the confidentiality, integrity, and availability of sensitive information becomes paramount.

The proliferation of cyber threats poses a constant risk to CPS in energy systems [112,113]. Malicious actors may exploit vulnerabilities in communication networks or compromise sensor data, leading to potential disruptions or sabotage. The collection and storage of vast amounts of data raise concerns about data privacy [114]. Unauthorized access or disclosure of sensitive information could violate privacy regulations and undermine public trust. Establishing secure communication channels between components of CPS is essential to prevent unauthorized access and data tampering. Encryption, authentication, and access control mechanisms must be implemented to safeguard data in transit [113].

Blockchain technology offers a decentralized and tamper-proof approach to data management, enhancing security and transparency in CPS for energy systems [115-117]. By leveraging blockchain-based solutions, stakeholders can ensure the integrity and immutability of critical data [118,119]. Advancements in privacy-preserving techniques, such as homomorphic encryption and differential privacy, enable the analysis of sensitive data without compromising individual privacy [120]. By integrating these techniques into CPS, energy systems can mitigate privacy concerns while leveraging data for optimization and decision-making.

8.4.4 Interoperability and Standardization

Interoperability and standardization remain key challenges in the integration of CPS within energy systems. As CPS components are often sourced from different vendors and operate within heterogeneous environments, ensuring seamless communication and interoperability becomes complex.

CPS components, including sensors, actuators, and computational systems, may employ diverse technologies, communication protocols, and data formats. Integrating these components into a cohesive system requires addressing interoperability challenges [121, 122]. Legacy systems existing within chemical infrastructure may lack standardized interfaces or protocols, hindering their integration with modern CPS solutions. Retrofitting legacy systems to ensure interoperability presents additional challenges. The absence of universally accepted standards for CPS in energy systems complicates interoperability efforts. Without standardized interfaces and protocols, achieving seamless integration and communication between heterogeneous components becomes arduous [123].

Collaborative standardization efforts among industry stakeholders, regulatory bodies, and research institutions are crucial for defining common interfaces, protocols, and data models for CPS in energy systems. Standardization initiatives such as the Industrial Internet Consortium (IIC) [124] and IEEE P2413 [125] provide frameworks for interoperability and integration. Middleware platforms and middleware-as-a-service (MaaS) offerings provide abstraction layers and standardized interfaces to facilitate interoperability between diverse CPS components. By adopting middleware solutions, energy systems can achieve plug-and-play integration and scalability[126,127].

8.4.5 Scalability and Complexity Management

Scalability and complexity management pose significant challenges in the deployment and operation of CPS within energy systems. As systems expand in size and scope, managing complexity while ensuring scalability becomes increasingly critical.

CPS in energy systems exhibit inherent complexity due to the integration of diverse components, processes, and stakeholders. Managing this complexity requires robust design, modeling, and optimization techniques. As energy systems evolve and expand, accommodating growing volumes of data, devices, and users presents scalability challenges [128]. Ensuring that CPS architectures can scale efficiently to meet evolving demands is essential for long-term viability. Resource constraints, such as computational power, memory, and bandwidth, impose limitations on the scalability of CPS within energy systems. Balancing resource allocation and performance optimization becomes crucial to ensure efficient operation [129].

Distributed architectures, such as edge computing and fog computing, decentralize computational tasks and data processing closer to the source of data generation. By distributing workload and reducing reliance on centralized infrastructure, distributed architectures enhance scalability and alleviate resource constraints [130]. Model-based design methodologies enable the abstraction and modularization of CPS components, simplifying system design, analysis, and optimization. By employing model-based approaches, energy systems can manage complexity effectively while facilitating scalability and maintainability [131,132].

8.5 Cyber-Physical Prototype for Safer Energy Production – An Example via a Modeling and Optimization Framework

The parametric optimization and control (PAROC) framework proposed by Pistikopoulos et al. significantly contributes to the development and application of CPS by integrating various advanced methodologies and techniques [133-139]. Figure 5 shows a step-wise procedure that includes:

1. Developing and validating high-fidelity models to ensure accurate representation of the process system.
2. Simplifying complex models through system identification and model reduction techniques to make them computationally feasible for optimization.
3. Utilizing multi-parametric programming for optimization under uncertainty and developing explicit/multi-parametric model predictive control (mp-MPC) strategies.
4. Implementing model-predictive control and reactive scheduling to continuously update the optimization model based on real-time data.

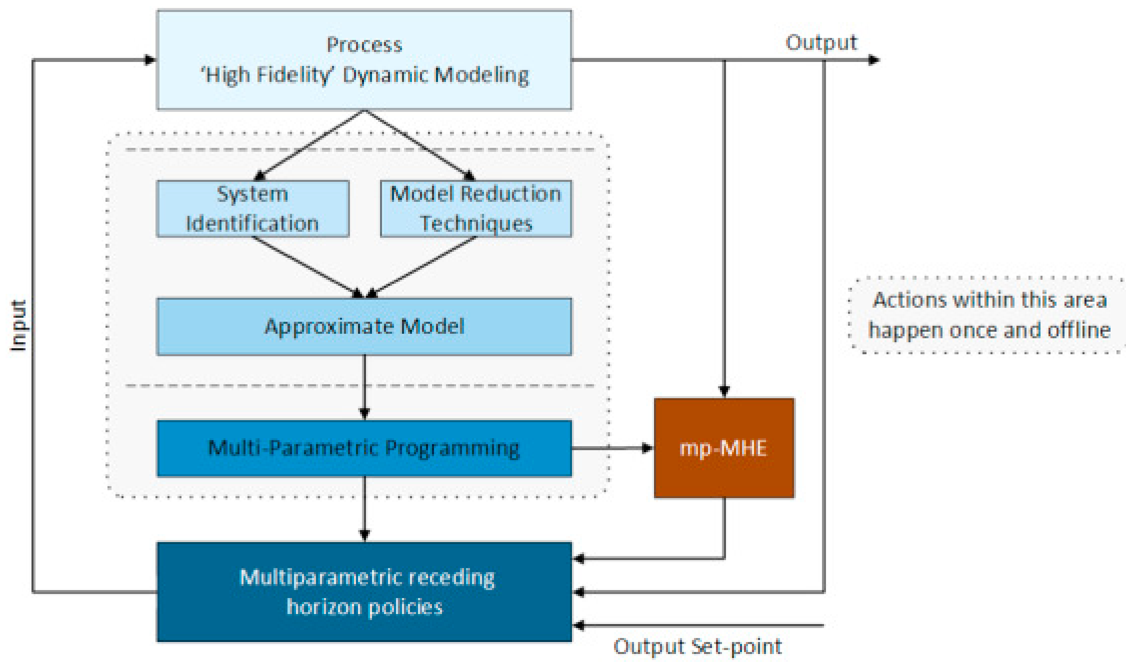

Figure 5. The architecture of PAROC framework [133] [https://www.sciencedirect.com/science/article/pii/S0009250915001451]

By combining these methodologies within the PAROC software platform, the framework supports the design, operational optimization, and advanced control of various process systems, enhancing their efficiency and adaptability in real-time scenarios.

In hydrogen energy systems, CPS enhances the efficiency, reliability, and safety of both hydrogen production and utilization processes. This integration is crucial for advancing hydrogen as a viable and sustainable energy source. Pistikopoulos et al. have been at the forefront of integrating CPS into hydrogen fuel cells and electrolysis cells. By deploying advanced sensors, they facilitate continuous real-time monitoring of key parameters such as temperature and electrical output. The data collected was processed in real-time, enabling adaptive control algorithms to dynamically adjust operating conditions. This ensures operational safety, enhances efficiency, and prolongs the lifespan of the stacks. For example, Ogumerem et al developed a smart metal hydride hydrogen storage (MHHS) system as shown in Figure 6 [40]. This system employs a high-fidelity dynamic model and an explicit model predictive control (eMPC) strategy, optimized through the PAROC framework. The approach ensures efficient thermal management and optimal refueling operations, maintaining safe operating temperatures and enhancing hydrogen storage efficiency. The integration of eMPC into a microcontroller allows real-time control, reducing energy consumption and improving the overall efficiency of the hydrogen storage process in fuel cell electric vehicles (FCEVs) [40]. Besides, Ogumerem et al proposed an optimal thermal management strategy, which was designed using the PAROC framework, effectively controls the operating temperature of the proton exchange membrane water electrolysis (PEMWE) system as depicted in Figure 7 [41]. By maintaining the differential water temperature across the electrolyzer within a safe range, the strategy prevents thermal degradation of the polymer membranes, thus enhancing system durability and efficiency [41]. Furthermore, Ziogou et al developed a combined approach by integrating nonlinear model predictive control (NMPC) with multiparametric programming [140]. The framework was applied to a PEM fuel cell in Figure 5, maintaining stable and efficient real-time operation under varying conditions by adjusting power, temperature, and gas flows.

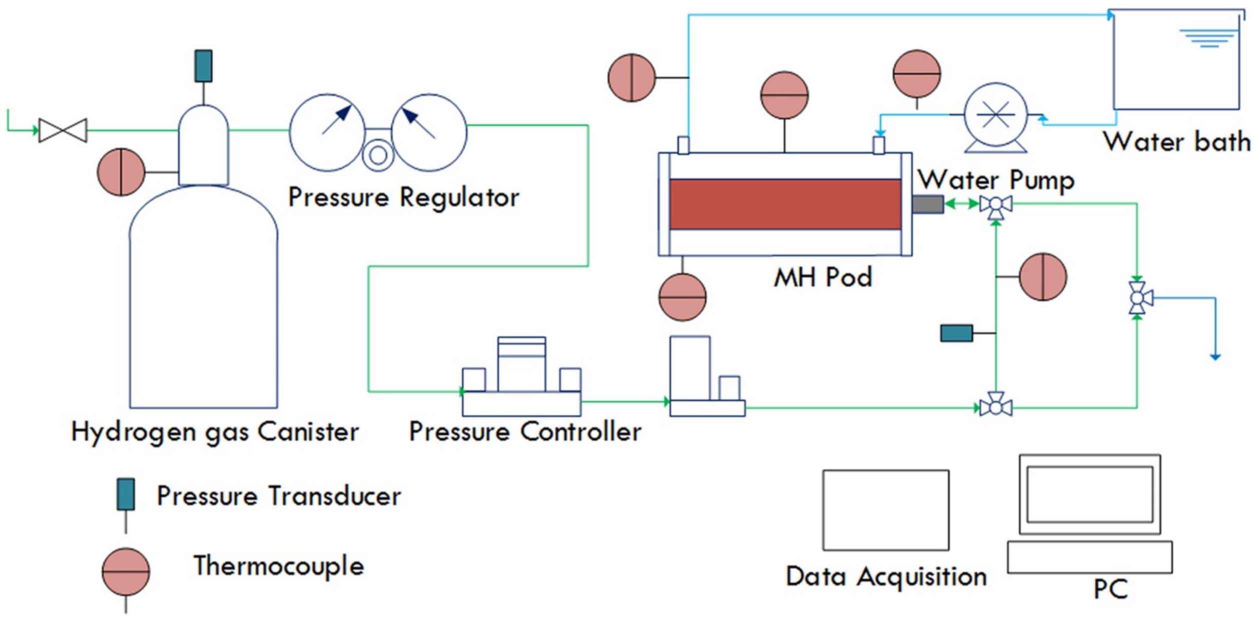

Figure 6. Process flow diagram of metal hydride hydrogen storage (MHHS) system [40] [https://aiche.onlinelibrary.wiley.com/doi/full/10.1002/aic.16680?casa_token=egfB_G1pDMYAAAAA%3AuV8Axbg82mvXjyRTdTGEFxqzpFiL0RbVgbPmtwrOKnA_lJPu2eCOQYL1Rsdg5PCWZDAgt4CY_60o9lk]

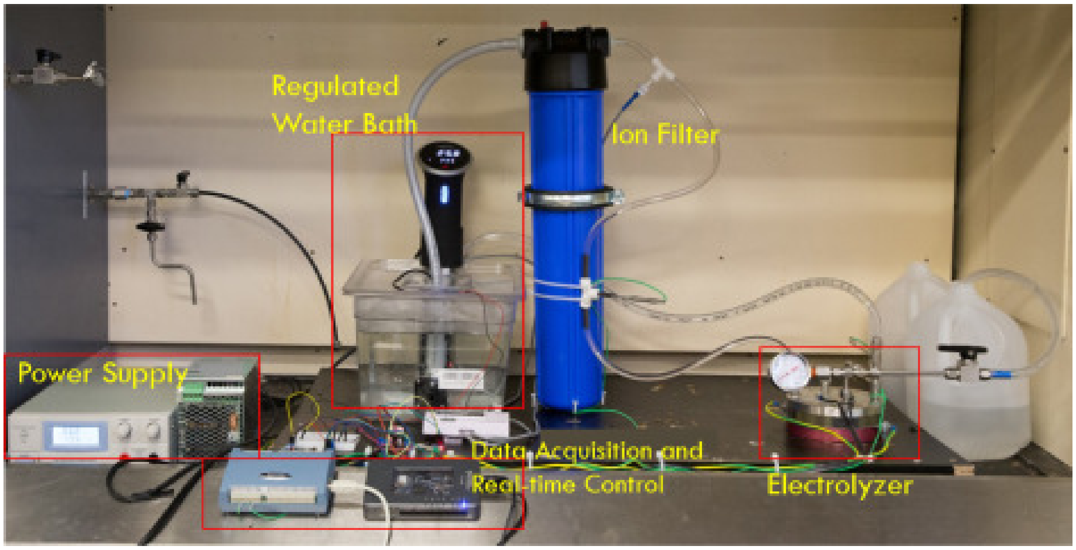

Figure 7. Experimental setup of proton exchange membrane water electrolysis (PEMWE)[41][https://www.sciencedirect.com/science/article/abs/pii/S0959152420302092]

8.6. Conclusion

This chapter has presented a brief overview of CPS in the context of process safety, with a focus on chemical and energy processes. We discussed how modeling, control, monitoring, and optimization can play a significant role in the advancement of such systems towards enhancing their efficiency, productivity, and real-time safety. We also presented a methodology framework applied to laboratory-based energy systems, to highlight some of the challenges in the future directions in this field.

ACKNOWLEDGMENTS

The authors acknowledge financial support from NSF RETRO Project CBET- 2312457, Mary O'Connor Process Safety Centre and Energy Institute at Texas A&M University, and Department of Chemical and Biomedical Engineering at West Virginia University.

DECLARATION OF AI AND AI-ASSISTED TECHNOLOGIES IN THE WRITING PROCESS

During the preparation of this work, the author(s) used ChatGPT 3.5 in order to improve readability. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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