Chapter 12

Artificial intelligence in process safety and risk management

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12.1 Introduction

The shift from dynamic risk management (DRM) to process safety management (PSM) represents a major advance in chemical engineering practice, focusing on exploiting the use of real-time data and adaptive safety strategies to mitigate ever-changing operational risks [1]. Conventional static risk assessment techniques are ineffective in managing contemporary chemical processes' dynamic and complex nature, where operating and environmental conditions dynamically alter risk profiles. The DRM model provides an active method by scanning real-time operational data and reviewing past incidents to update real-time risk assessments [2]. The transformation encourages a stronger safety culture within organizations and achieves tangible advantages, like lower incident rates, decreased downtime in production, and considerable cost savings. With improved operational efficiency and regulation adherence, digital risk management is emerging as a crucial investment in the industry's future.

One of the key elements of occupational risk analysis in advanced oxidation processes (AOP) laboratory activities is using a new risk level classification system that codifies risk assessments on a 0–10 basis. This enables a more numerical examination of laboratory risks, with a similar analysis of the financial costs of recommended preventive measures [3]. The S/C ratio ranks risks, so around 65% of identified risks are related to possible accidents, 30% to occupational diseases, and 5% to stress. Root cause analysis (RCA) methods enhance safety by defining the root causes of incidents, and several safety metrics, such as incident frequency and closure times, provide essential information for continuous improvement. These safety protocols align with the United Nations' Sustainable Development Goals (SDGs) 3, 9, and 12 and reflect the broader implications of systemic risk management in chemical laboratories.

Previous disasters, such as the Bhopal gas tragedy in 1984 and the Shiyan gas explosion in China, demonstrate the disastrous effects of the absence of appropriate safety measures in chemical engineering. Evidence-based process safety management (EBPSM) is a revolutionary technique, and studies have indicated that detailed risk assessment can minimize the risk of major accidents by up to 30% [4]. Applying systematic models, such as the systematic risk reduction framework (SRRF), has improved safety, for example, from 2.7 to 3.39 in a methanol plant through design modifications [5]. Methods such as the precedence table (CP) technique and fuzzy logic analysis have improved decision-making and safety. The integration of process safety and workplace safety enables a holistic approach to risk reduction and

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performance improvement. In a highly regulated sector, constant improvement in safety control is necessary to safeguard lives, property, and public confidence.

AI has radically changed chemical engineering, substantially enhancing safety and risk management through predictive maintenance, real-time monitoring, and data-driven decision-making. AI-based predictive maintenance reduced equipment breakdowns and unplanned downtime by approximately 50%. Real-time monitoring systems employ AI-based algorithms to identify process deviations and reduce the rate of events by 30%. AI-based risk assessment models improve hazard detection and prioritization, making decisions 40% more effective. In addition, AI improves operating parameters to increase production efficiency by 25% and ensure strict enforcement of safety protocols [6]. In addition to process optimization, AI enhances simulation-based training, emergency preparedness, and automatic compliance monitoring for improved workplace safety. Implementing AI-based security measures in organizations has helped achieve 50% of business goals. AI will account for 20% of the global workforce by 2028 and contribute 40% of economic output [7]. Applying AI in chemical engineering increases productivity and promotes proactive security through compliance with upcoming regulations. Companies using AI-based safety initiatives have improved their business objectives by 50%. AI solutions are expected to account for 20% of the total global workforce by 2028, and their share of economic productivity will be 40% [7]. Applying AI to chemical engineering improves operational efficiency and reinforces an active approach to safety, ensuring compliance with ever-changing regulatory standards.

With the development of PSM and integration of advanced risk assessment techniques, AI has emerged as a powerful tool for enhancing safety and operational efficiency in the chemical industry. As industries shift toward flexible, data-driven safety protocols, AI technologies are transforming risk detection, real-time monitoring, and emergency response systems. Unlike traditional AI studies that focus primarily on technological development, this chapter explores AI's practical applications in chemical engineering—such as supporting process hazard analysis, strengthening risk management, and enabling predictive maintenance through digital twin (DT) technology. Going beyond theoretical discussions, it critically evaluates current applications and identifies emerging trends, challenges, and the regulatory, interpretability, and data integrity concerns that must be addressed to fully leverage AI in process safety.

12.2 AI-driven hazard identification and risk assessment

12.2.1 Machine learning models for identifying potential hazards

Machine learning (ML) models are now integral to chemical engineering and have greater predictive ability than traditional hazard identification methods. ML approaches utilize dense data sets to enhance environmental monitoring, risk estimation, industrial safety, and disaster relief. One of the key strengths of ML is its ability to detect complex, nonlinear patterns in the identification of environmental hazards. This growing interest is reflected by the sharp growth in publications for ML applications in environmental science and engineering (ESE), of which 5855 publications were made between 1990 and 2020 (Fig. 12.1A). Artificial neural networks (ANNs) also performed better than the standard regression models, with an R^2 of 0.74 for particulate matter 2.5 (PM2.5) estimation and 0.83 for wastewater flow prediction [8]. Similarly, ML-based optimization models, such as Wang et al.'s multiobjective optimization (MOO) model, have been found to optimize chemical processes at high accuracy levels of $R^2 > 0.99$ while lowering the threats to the environment [9]. Such uses demonstrate how ML can be applied to improve decision-making and safety management.

ML is also crucial in predicting natural hazard-caused technological accidents (Natechs). Studies with XGBoost and Random Forest have reported receiver operating characteristic area under the curve (ROC AUC) scores higher than 0.8 in effectively distinguishing between high-risk and low-risk days based on climate predictors, such as precipitation and lightning [13]. Conformal prediction techniques also add to model credibility by controlling error rates and tuning sensitivity-specificity trade-offs, thus making ML models more trustworthy during hazard prediction. Deep learning (DL) advancements have also improved hazard categorization. The DL and gray model (DLGM) model outperformed traditional classifiers, like Random Forest and bidirectional encoder representations from transformers (BERT), with better accuracy and F1 scores. By applying a hierarchical feature fusion neural network (HFFNN), DLGM improves feature extraction by 7% in identifying risk themes [14]. The advancements suggest a growing role of hybrid ML approaches in industrial hazard identification.

ML has also been applied to emergency response planning for hazardous materials incidents. For instance, the Random Forest model achieved an F1-score of 0.95 for evacuation necessity prediction in railway hazardous material incidents, which outperformed decision trees (0.93) and logistic regression (0.77) [15]. The determinants for evacuation were incident type, existence of hazardous material, and phase of transport, demonstrating the importance of precise, data-driven risk determination. Despite these advances, issues persist. The "black box" nature of ML algorithms tests

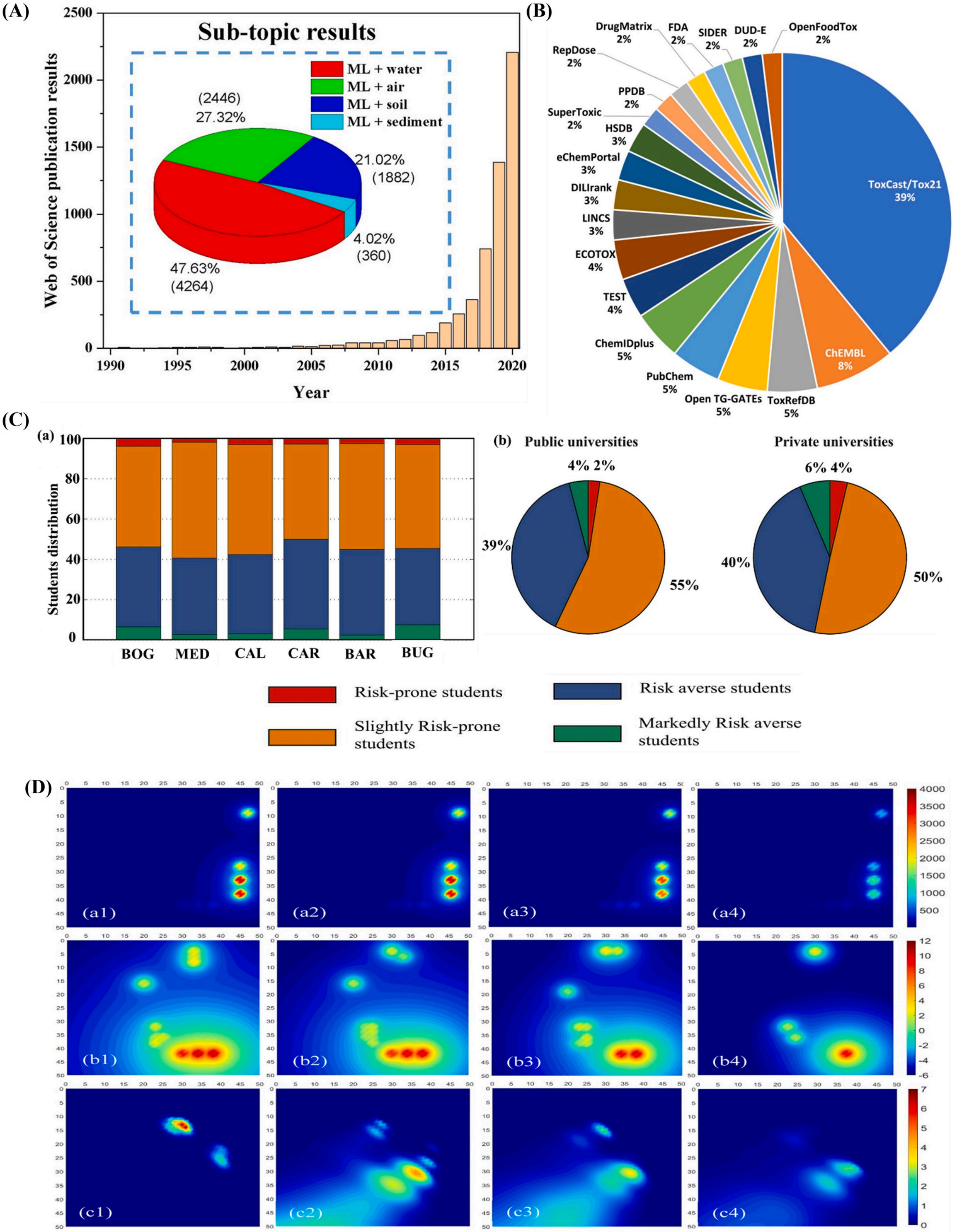


FIGURE 12.1 (A) Count of research papers on machine learning applications in environmental science and engineering (ESE) retrieved from the Web of Science (accessed on January 28, 2021) using the keyword "Machine Learning" alongside categories such as environmental science, water resources, public environmental occupational health, environmental engineering, and environmental studies. (B) Summary of the toxicity dataset utilized in building predictive toxicology models. (C) Displays risk perception analysis: (a) categorized by city and (b) comparing perceptions between public and private universities. (D) Illustrates the distribution of (a) thermal radiation (kW/m^2), (b) overpressure (log scale, MPa), and (c) toxic concentration (kg/m^3) at (1) 5 s, (2) 100 s, (3) 250 s and (4) 350 s following the initial accidents. The wind is blowing northeast at a speed of 1 m/s. The horizontal and vertical axes depict the spatial scale of the chemical plant at a 1:10 meter ratio [8,10–12].

interpretability, demanding rigorous validation and collaboration with subject matter experts [8]. Further, the effectiveness of models is heavily dependent on data quality—biases or errors in training data undermine predictive reliability. Incorporating ML into existing safety procedures introduces regulatory and logistical practicability questions, calling for cross-disciplinary strategies to implement pragmatic implementation.

12.2.2 AI algorithms for quantitative risk assessment

AI algorithms applied to quantitative risk assessment (QRA) have greatly improved predictive modeling, data analysis, and risk characterization in chemical engineering [16]. Various research studies have proven that AI would increase the validity and effectiveness of risk assessment in high-risk industrial processes. ML algorithms, such as gradient boosting (GB) and support vector machines (SVM), were used to improve an oil refinery's QRA techniques [17]. Two classifiers, ML1 to predict the probability of an accident and ML2 to estimate its severity, were trained with historical preliminary hazard analysis (PrHA) data. Their approach correctly identified and classified risk scenarios with an average accuracy of 96.40%. This study indicates the potential of AI to improve safety decision-making in complex industrial environments.

In addition, two dynamic risk models for transporting hazardous chemicals by vehicle have been proposed: the macro quantitative risk assessment (M-QRA) model and the rapid quantitative risk assessment (R-QRA) model. The M-QRA model considers accident probabilities, leakage risks, and domino risks [18]. However, the R-QRA model is marked by the need for speed and minimal data requirements regarding the number of vehicles and the weight of hazardous substances. They claim that the R-QRA model requires 70% of the data and half the computation time of the M-QRA model and is better suited for real-time assessment. The study also indicates the importance of safe parking distances between hazardous material trucks to avoid domino effects in the event of an accident. AI in QRA was also improved by developing a general regression neural network (GRNN) predictive model to predict explosion parameters, such as maximum overpressures and temperature, from eight input variables. The GRNN model calculated 1000 monitoring points within approximately 9.82 seconds to assist in emergency decision-making [19]. Second, fault tree analysis combined with the GRNN model to predict incident-induced fire and secondary explosion probability aided emergency response planning. The model's learning ability to use new data improves its predictability as time elapses, indicating AI's sensitivity to risk management.

Despite such advancements, AI-based approaches to air quality assessment are being experimented with. AI models are sophisticated and transparent to stakeholders, but it is difficult for them to understand the results. Furthermore, chemical engineering systems lack large datasets that reflect history and uncertainties [20]. AI models can also be challenged by epistemic uncertainties of chemical operations, leading to misleading results in the absence of adequate human intervention. Therefore, AI should be welcomed as an augmentation, not an alternative to traditional measurements by expert opinion. The future of work should be oriented toward developing AI models that combine human experience and field knowledge in decision-making with credible, explainable, and transparent results [21]. By addressing these concerns, AI can reformulate risk analysis approaches and optimize the safety performance of chemical engineering industries.

12.2.3 Risk ranking and prioritization using AI-based tools

Using AI-based computer software to categorize and prioritize chemical engineering risks significantly improves regulatory safety, process efficiency, and compliance. Using ML software and large toxicology databases, these computer programs can measure risks objectively and more accurately than traditional methods. Current research has shown that AI models can forecast as many as 30 different toxicity parameters, thus allowing for a large-scale assessment of chemical hazards, such as acute toxicity and environmental concerns [10]. This capability turns chemicals into a systematically ranked portfolio against multiple risk factors, enabling data-informed prioritization. A key benefit of AI-based risk ranking is that it provides access to large toxicology databases, with over 20 different sources used to develop predictive models. Curated databases, such as ToxCast and Tox21 (Fig. 12.1B), which undergo rigorous quality assurance processes, contribute to more accurate risk assessment [10].

Using ML methods, including deep neural networks and random forests, improved predictive precision and big data have been handled, allowing risk prioritization to be done more efficiently. The techniques allow for more efficient prioritization of the high-risk chemicals to allow mitigation strategies and regulatory interventions to tackle the riskiest chemicals first. In addition to chemical risk assessment, AI systems have also shown promise for operational risk management of wastewater treatment technologies, that is, membrane bioreactor (MBR) systems. AI techniques, such as ANN and genetic algorithms (GAs), optimized the operating parameters with a maximum chemical oxygen demand (COD) removal efficiency of 98% in hypersaline oily effluent and 91.57% in real ship wastewater with a hydraulic retention time of 8 hours [22]. These results validate the application of AI in predicting system failures, promoting environmental regulatory compliance and risk prevention in an early manner. Through appropriate modeling of system performance and optimization of the operating strategy, AI software improves decision-making and ensures the sustainability of chemical engineering processes.

In addition to operational efficiency and hazard recognition, AI-based risk ranking is applicable at an industrial scale in regulatory affairs and compliance, in general. For example, AI-based predictive analytics have improved regulatory decision-making, as evidenced by the 15–20% increase in european medicines agency (EMA) approvals, thanks to AI-based insights [23]. Roche and GlaxoSmithKline (GSK), to name a few, have achieved significant benefits; for example, Roche reduced clinical trial information review cycles by 30%, and GSK reduced regulatory dossier preparation time by 50% [23]. These innovations demonstrate AI's ability to automate compliance processes and accelerate the approval of new chemicals. AI applications allow risk assessment in real time, permitting fast reactions to evolving chemical engineering risks. Early pilot tests have indicated that AI-based systems can reduce the incidence rate by up to 40% using active monitoring and early detection of potential hazards [24]. Further, predictive maintenance software is more than 85% effective at predicting equipment failure, minimizing unplanned downtime and increasing plant security . Resource optimization through AI-based also resulted in up to 25% cost savings, since businesses are focusing their mitigation efforts on events with the highest potential for loss [24].

12.3 Advanced process hazard analysis with artificial intelligence

12.3.1 AI-based hazard and operability analysis and automation

Integrating AI in hazard and operability (HAZOP) analysis transforms risk assessment in chemical engineering by improving accuracy, efficiency, and automation. Conventional HAZOP techniques are based on expert judgments, frequently excluding systemic interactions and human factors that cause over 75% of industrial accidents [25]. AI-powered methods tackle these shortcomings by utilizing ML, predictive analytics, and system-theoretic techniques, enhancing hazard identification, automating risk evaluations, and refining safety measures. AI-driven system-theoretic process analysis (STPA) and fault detection algorithms have lowered accident rates by as much as 50% [26], while enhancements in diagnostic accuracy have reached 90%, resulting in a 25% decrease in incident occurrences [27]. AI-driven automated HAZOP tools reduce assessment periods by 30%, allowing safety teams to focus on key risks. This effectiveness results in significant financial advantages, allowing industries to save as much as $1 million per facility annually due to enhanced safety, decreased downtime, and reduced insurance expenses [28].

A case study of a styrene polymerization facility, which included 37,170 deviation simulations, indicated that single failures resulted in a significant severity of 45.45%, which increased to 72.65% for double failures and 93.13% for triple failures, underscoring the increasing risk of simultaneous deviations [29]. AI-powered ANNs streamlined the assessment process, quickly predicting risk severity and eliminating the need for extensive manual assessment. Aside from technical risks, AI enhances assessments of new materials, such as biodegradable plastics, where rapid degradation introduces unexpected risks. Predictive AI-driven models allow anticipatory measures, improving security by harmonizing evolving sustainability requirements. In addition, AI integrates aspects of human nature in evaluating risks. Research shows that 40% of individuals do not benefit from prior safety education, and the perception of risks differs based on proximity to industrial areas (Fig. 12.1C [a]) [11]. AI improves safety measures by integrating these behavioral insights into predictive analytics (Fig. 12.1C [b]), fostering a proactive safety culture [11]. Advanced DL models like extended deep process model analysis (EDPMA) have achieved 92.92% accuracy, 91.85% recall, and 92.38% F1 score, effectively tackling challenges associated with complex industry terminology and ambiguity in risk assessments [30]. However, AI's effectiveness depends on high-quality training data, and its limitations necessitate a collaborative AI-human approach, ensuring expert oversight in complex risk scenarios.

12.3.2 Dynamic hazard identification in real-time operations

AI-based dynamic risk identification enhances instantaneous risk estimation and chemical engineering optimization, overcoming the drawbacks of conventional periodic screening. Methods such as monte carlo simulation (MCS), computational fluid dynamics (CFD), and graphics processing unit (GPU)-based risk and operability analysis simulations provide instantaneous monitoring and forecast information, improving emergency preparedness planning and decision-making. For example, GPU-based HAZOP simulations analyze 100 times faster than traditional processes and examine 120,000 deviations in real time, making it possible for timely hazard examination and sensitivity studies [31]. Bayesian networks have significantly improved real-time risk assessment by offering crucial information about conditions of hazards. For vapor fire, the likelihood of occurrence was 72% for fire hazard, toxicity, and risk of explosion.

The sensitivity analysis revealed that severe confinement conditions raised the likelihood of an explosion by 49% [32]. As is evident through actual accident records, Bayesian networks' updating of the probabilities in real time ensures the right evaluation based on current operating data.

The dynamic process for off-normal scenario identification (DyPASI) combines traditional hazard identification methods with real-time data analysis, effectively uncovering underestimated risks in major accidents, such as the Buncefield oil depot explosion and the Toulouse fertilizer plant blast. Combining DyPASI with established methods, such as the Bow-Tie technique, improves hazard analysis by identifying failure points and human factors. Moreover, integrating DyPASI and dynamic risk assessment (DRA) improves hazard detection, fostering proactive safety measures in intricate chemical processes. A notable case study regarding the Xiangshui chemical explosion demonstrated the efficacy of AI-driven simulation for hazard recognition. Simulation of thermal radiation values at 9 kW/m^2 within seconds exposed staff and facilities to life-critical risks [12]. Using hazard simulations with AI can help upgrade evacuation plans, reduce exposure, and integrate emergency response systems for industries. Such thermal radiation levels are visually shown in Fig. 12.1D and reflect why real-time information must be considered in forecasting and evasion from hazards [12]. AI sensor networks enhance process anomaly early detection and act promptly before failure acceleration. AI incorporation into real-time risk monitoring generates a safety-oriented, proactive culture with constant observation and responsive risk determination [33]. Such advances enable extensive applications of AI-driven dynamic hazard identification (DHI) methods toward greater operating security and resilience for the chemical engineering sector.

12.3.3 Incorporating AI into bow-tie analysis for accident prevention

Integrating AI into Bow-Tie analysis enhances risk management, particularly within chemical engineering and high-risk sectors. Although Bow-Tie analysis outlines hazards and controls, conventional models depend on historical data and expert opinions, overlooking concealed risks. AI builds on this by facilitating real-time data analysis, dynamic risk assessment, and predictive modeling to improve safety controls and mitigation. A good case study in the healthcare sector illustrates the efficacy of AI in improving risk management. A cyber risk assessment in a hospital revealed major vulnerabilities, like poor staff awareness training on cybersecurity threats, poor employee selection processes, and poor monitoring systems. The hospital can detect and neutralize cyber threats in advance using AI-driven threat detection and risk management systems, reducing the likelihood of cyber risk from 0.45 to 0.39 [34].

Other improvements, like educating the employees on regulatory compliance and third-party risk management, reduced the cyber risk rating completely from 9 to 6 on the risk matrix. This case study shows how AI-enhanced Bow-Tie analysis can reveal essential gaps and offer data-driven insights to improve decision-making. Similarly, in chemical engineering, the integration of AI into Bow-Tie analysis provides significant benefits. Conventional risk identification techniques often fail to address significant safety concerns effectively. Research has found that risks like work at height (81%), equipment handling/storage (17%), and ergonomics (0.4%) are frequently overlooked during manual inspections [35]. AI-based risk assessment systems analyze vast amounts of data from incident reports, operational data, and safety analyses to identify underlying patterns and leading risk indicators. This proactive strategy allows organizations to tackle vulnerabilities before they escalate into incidents, greatly enhancing safety performance.

Furthermore, research illustrates the effectiveness of AI in risk management through a DRA approach that merges Bow-Tie analysis and Bayesian networks. This method was used for a 50,000 m^3 vertical external floating roof crude oil storage tank, focusing on the significant occurrence of a "major floating roof tank leak" [36]. The Bayesian network's probabilistic inference system continuously assesses risk levels in relation to operational conditions, ensuring the effective operation of safety barriers in real time. The findings indicated that using AI-driven risk evaluations lowered the probability of severe incidents by one to three orders of magnitude compared to traditional manual assessments. The method also enables ongoing updates of risk evaluations, boosting their capacity to enhance decision-making and risk management tactics in the petrochemical industry. Although AI improves Bow-Tie analysis, its success depends on the data quality, the robustness of the algorithms, and human supervision. The success of AI-based risk management relies on high-quality data, powerful algorithms, and appropriate validation of predictive models. Over-reliance on automation without human oversight can create significant gaps in decision-making, highlighting the need for a balanced approach where AI augments human capabilities rather than replaces them. By addressing these challenges, AI-powered tie analysis can significantly improve accident prevention, improve risk mitigation methods and encourage safer industrial operations.

12.4 AI for real-time process safety monitoring and emergency response

12.4.1 AI techniques for anomaly detection in process parameters

Integrating AI into real-time process safety monitoring has significantly improved chemical engineering risk identification and risk assessment (Fig. 12.2A). AI-driven models allow industries to examine data streams in real time, enhancing decision-making and reducing emergency response times by up to 30%. Sophisticated DL methods have improved the accuracy of risk assessment by more than 40%, allowing for better identification and prioritization of vulnerabilities in production systems [37]. One of the essential applications of AI is danger detection and alarm systems. These systems improve safety through real-time monitoring of potential dangers by interfacing AI with sensor networks. An example of a wireless sensor network for sensing drinking water quality (Fig. 12.2B) illustrates how internet of things (IoT) devices can detect vital parameters, such as pH and temperature, in real time [38]. This paradigm finds application in chemical processes where identical sensor arrays track signals of potentially hazardous states. AI code examines this sensor data to detect anomalies during normal operation and produces early warnings with an immediate response to prevent accidents.

Further, various AI methods have been applied across numerous industrial and environmental settings to identify hazards. These methods include wearable gas sensor networks for identifying toxic gases and DL algorithms for monitoring pollution and evaluating land cover. During emergency response scenarios, robotic inhaler devices and wireless sensors with AI have been highly accurate in detecting toxic gases like CO and NO_2 [40]. Furthermore, ML algorithms like MultiRocket are over 91% accurate in fire hazard detection, that is, flammability, toxicity, explosion, and corrosion [41]. These are extremely important in identifying impending threats so that grave accidents in chemical process plants are averted. Besides sensors, AI techniques also enable real-time observation through sophisticated tools like Fourier transform infrared spectroscopy (FTIR). FTIR spectroscopy is especially suited to examining combustion by-products and rapidly detecting toxic chemical reactions. For instance, chemicals like lithium-ion batteries have authenticated their rating as highly dangerous and recorded the necessity for cautionary security measures. For further risk assessment, Bayesian network analysis provides a probabilistic model for assessing likely failures and safety risks. For example, research that compared 8199 accident reports in the oil and gas industry revealed that asset reliability and integrity accounted for 50% of accident dependencies. This emphasizes the role of predictive maintenance and specific safety practices [42]. In addition, a cross-correlation analysis showed that asset integrity issues and overall accidents correlate with 0.73, implying the need for robust risk identification systems [42].

12.4.2 Predictive models for near-miss and incident forecasting

Integrating sophisticated predictive models has greatly improved accident and near-miss prediction in chemical engineering, where safety is crucial. The integration of grayscale neural networks with classical neural network techniques improved the prediction accuracy, outperforming GM(1,1) and backpropagation (BP) neural network models with a mean absolute error (MAE) ranging from 0.007 to 0.024% for the total number of near-misses and a relative error of $\pm 0.004\%$ for severe near-misses [43]. Nonetheless, depending on Chinese commercial aviation sector data restricts its applicability to chemical engineering since accident dynamics and reporting criteria differ. Future research should validate these findings across different sectors and enhance data collection methods. ML methods, such as text mining and natural language processing, have significantly transformed accident prediction.

Analysis of over 4000 inspection reports identified twelve major scenarios of near-certainty incidents associated with unsafe work and conditions, such as A1 (approaching restricted areas) with C2 (unprotected floor openings) and A5 (incomplete equipment inspection) with C8 (unsafely positioned ladders) [44]. Statistical tests, including chi-square analysis ($p < 0.01$) and lambda analysis (> 0.20), revealed strong relationships, validating automated near-certainty incident reporting and real-time data collection to reduce incident rates [45]. As illustrated in the styrene production study, Bayesian theory and event tree analysis were applied in risk assessment. The probability of emergency shutdown incidents increased to 0.15 over time, while severe ruptures were low (0.004) [46]. Real-time flow, pressure, and temperature data improve risk assessment and enable proactive safety measures. Generally, combining gray matter neural networks, ML, and Bayesian analysis improves chemical engineering accident prediction and safety management. Expanding these models to different industrial environments and improving data collection would further enhance operational safety systems.

12.4.3 Integration of AI with sensor networks for real-time safety insights

The fusion of wireless sensor networks (WSNs) and AI is revolutionizing real-time safety monitoring in chemical engineering, maximizing hazard detection, predictive maintenance, and operational performance. AI-driven algorithms,

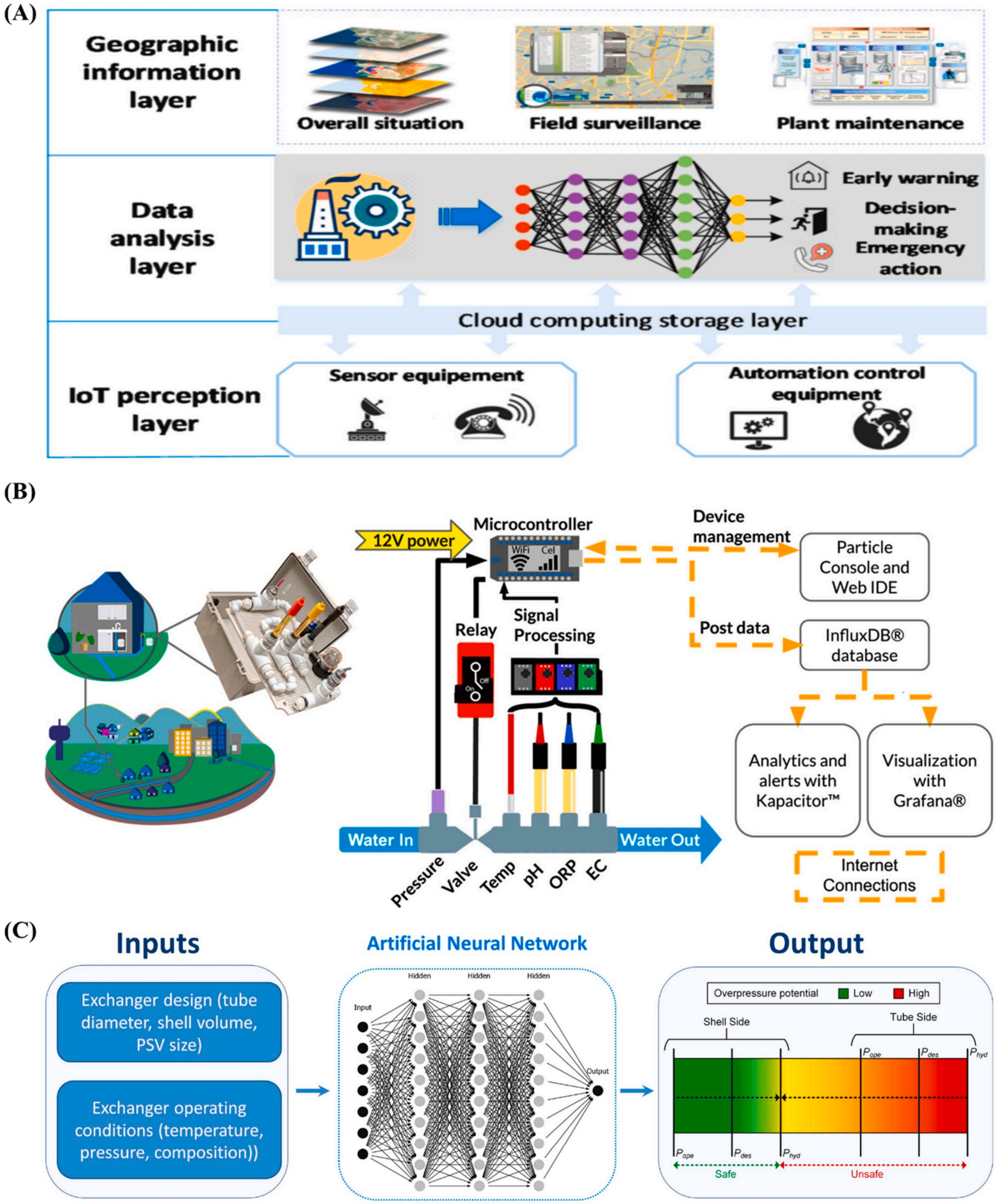


FIGURE 12.2 (A) A digital twin framework designed for emergency response planning. (B) A compact sensor module integrated with standard household plumbing, such as kitchen sinks and outdoor faucets. The sensing unit and electronic components are enclosed within a protective casing. The system architecture includes data acquisition, signal processing, and a cloud-based infrastructure for efficient data management and visualization. (C) Artificial neural network (ANN)-based consequence modeling approach for heat exchanger safety prediction. Design parameters and operating conditions serve as inputs to the ANN model, which generates a corresponding safety rating [37–39].

such as DL and ML, process voluminous and disparate sensor data to identify anomalies and hazardous situations promptly. This forward-thinking strategy enables rapid safety action, minimizes the risk of human error, and improves resource allocation. A significant benefit of AI-enhanced WSNs is their ability to boost energy efficiency and maintain data integrity through intelligent algorithms and energy-efficient routing techniques, ensuring reliable operation in energy-constrained environments [47]. In addition, digital twin systems (DTs)—virtual representations of physical processes—enable real-time observation and predictive maintenance, further improving process safety [48]. The combination of AI and automated detection systems has also demonstrated over 90% accuracy in anomaly detection, significantly improving chemical leak identification and process deviation monitoring [49].

Beyond safety, AI-based improvements bring significant economic and operational benefits. Companies such as badische anilin- und soda-fabrik (BASF) have reported a 2%–7% improvement in productivity, a 30% improvement in energy efficiency, and a 50% reduction in operating expenses, thanks to AI-driven sensor networks and additive manufacturing [50]. Automated sequential flow and injection technologies increase productivity by continuously examining hundreds of samples daily, are several times more efficient than conventional monitoring systems and less tiring than manual monitoring. Additionally, pairing AI with IoT enables remote monitoring and data analysis, allowing engineers to oversee operations globally and respond quickly in hazardous conditions. Nevertheless, as AI-based networks become increasingly central to chemical processing, robust cybersecurity measures are necessary to prevent threats like false data injection. Synergism between AI and sensor networks improves chemical engineering security systems and improves a stronger, more flexible, and efficient operating framework. The research highlights the need for scalable, affordable AI solutions tailored to the safety-critical requirements of such environments to ensure sustainable viability and better risk management. For example, Table 12.1 summarizes multiple real-time AI systems used for risk monitoring and emergency response, highlighting different models and their associated characteristics — including, based on indicative metrics, response time, types of hazards, and sensitivity — derived from concepts presented in the cited literature.

12.5 AI-enhanced emergency response and mitigation strategies

12.5.1 Intelligent systems for emergency scenario simulations

AI is the core of improving emergency response and proactive safety interventions. AI-driven applications chart outlined hazards to determine optimal response protocols, so safety personnel receive real-time recommendations for risk reduction. Such systems can detect hazardous gas leaks, building collapses, and overheating and provide automatic alarms and defensive measures that reduce emergency response times significantly. Predictive maintenance with AI has been determined to reduce industrial accidents by up to 30% through early anomaly detection and preemptive action [57]. Real-time monitoring through the IoT provides continuous temperature, pressure, and chemical concentration monitoring for proactive hazard detection before an incident escalates. One such safety readiness breakthrough is DT technology—a computer model of chemical processes that allows industries to simulate emergency response procedures in a safe environment. DTs help refine safety procedures by modeling real-time scenarios, minimizing operational risks, and improving response effectiveness.

Furthermore, ANNs enhance safety monitoring by delivering real-time predictions with over 99.56% accuracy in overpressure safety metrics [39]. These AI-driven frameworks align with established safety standards, such as API 521, significantly reducing the complexity of consequence modeling and enabling rapid risk assessment. For example, Fig. 12.2C demonstrates an ANN framework designed for predicting heat exchanger safety ratings, illustrating how the model can effectively assess safety in real time [39]. In emergency response and incident management, different AI methods are utilized to improve decision-making and speed up responses, as illustrated in Table 12.2, which outlines example systems and indicative performance characteristics based on concepts from the cited literature. These technologies enhance readiness, automate the decision-making processes, and sharply minimize response time. Lastly, this integration diminishes the threat of large incidents, provides additional security for humans and the environment, and fosters a culture of safety for chemical engineering operations.

12.5.2 AI tools for optimizing evacuation plans and resource allocation

Incorporating AI into humanitarian assistance logistics and emergency response functions significantly increases the efficiency of operations, especially in evacuation planning and asset allocation. AI technologies specifically decrease mean response time to as low as 2 hours, compared to 10.83 hours with traditional methods. In addition, AI-based resource allocation attains 85% accuracy, more than the 74.33% of traditional methods, while cost efficiency is increased to 90%, as opposed to 78.33% in traditional systems [61]. AI solutions are needed to enhance evacuation plans, strategies, and

TABLE 12.1 Real-time AI systems for risk monitoring and emergency response.

AI system	Real-time analysis model	Response time (ms)	Hazard type addressed	Alert sensitivity (%)	Data stream requirement (mb/s)	Sensor type	Decision-making speed (ms)	False alarm rate (%)	System cost ($)	Data latency (ms)	Coverage area (sq. Km)	References
Chemical leak detector	Dynamic thresholding	150	Chemical leak	92	2	Gas sensors	120	2	18,000	50	5	[51]
Toxic gas monitoring system	Multisensor fusion	100	Toxic gas exposure	95	3	Multigas analysers	110	12	22,000	40	10	[51]
Explosion risk assessment tool	Predictive analytics	250	Explosion scenario	90	4	Vibration sensors	200	3	16,000	60	15	[51]
Emergency response advisor	Machine learning	120	Chemical spill	94	3.5	Internet of things (IoT) devices	150	1.5	20,500	30	7	[51]
Hazardous material tracking	Real-time tracking	300	Hazardous movement	88	2.5	RFID tags	250	5	25,000	80	20	[52]
Environmental monitoring	Adaptive algorithms	180	Environmental hazard	91	2	Weather stations	130	2.5	19,000	20	12	[53]
Chemical storage surveillance	Continuous monitoring	160	Storage leak	93	2	Temperature sensors	140	2	21,000	45	8	[54]
Early warning system	Multiparameter Analysis	140	General hazards	96	3	Integrated sensors	125	1	23,000	35	18	[55]
Real-time risk assessment	Situational awareness	200	Various hazards	90	2	Multiparameter sensors	210	4	24,000	55	25	[56]

TABLE 12.2 AI in emergency response and incident management.

AI technique	Application area	Metrics for response effectiveness	Data sources	Tools/ software used	Accuracy	Precision	Speed	Response time	Model complexity	References
Machine Learning	Chemical process engineering	F1 Score	Simulation data	TensorFlow, R	90%	85%	High	2 s	Medium	[58]
	Earthquake prediction	Fast response alerts	GPS data, historical earthquake data	TensorFlow, Python	70%–85%	~75%	Seconds to minutes	< 1 min	High	[59]
Neural networks	Natural hazards management	Area under curve (AUC)	Remote sensing data	Keras, MATLAB®	92%	88%	Medium	1.5 s	High	[58]
Decision trees	Environmental monitoring	Recall	Sensor data	Scikit-learn	87%	80%	Fast	0.5 s	Low	[58]
Support vector machines	Disaster recovery	Precision-recall curve	Historical data	Weka, Python	85%	–	–	–	–	[58]
Neural networks	Social media monitoring	Disaster mapping	Social media feeds, location data	R, Python	Moderate	Moderate	Near real-time	Seconds	High	[59]
Geographic information systems (GIS)	Disaster response planning	Effectiveness of resource allocation	Geospatial data, satellite imagery	ArcGIS, QGIS	Moderate	High	Seconds to minutes	Short	Moderate	[59]
Convolutional neural networks (CNN)	360-degree monitoring	Collision prediction accuracy	Varied accident scenarios datasets	Custom AI models	90%	–	High	1.2 s	Medium	[60]
Reinforcement learning	Adaptive airbag deployment	Safety improvement percentage	Sensor fusion and real-time data	Custom AI frameworks	85%	–	Moderate	2 s	High	[60]

resource allocation, especially in dangerous situations, like chemical spills and hazardous material incidents [62]. These enhancements are supported in several studies. Krupka et al. [63] reported that AI-based evacuation simulation models save 20–30% of the evacuation time, compared to traditional methods.

Similarly, Higuchi et al. [64] also reported that AI algorithms enhanced emergency resource allocation in chemical spill scenarios and decreased response times by about 25% in simulation studies. Moreover, Chen et al. [65] showed that AI-based decision support systems increased the effectiveness of identifying the best evacuation paths, improving exercise safety results. Predictive models improved hazard prediction accuracy by 40%, improving chemical incident readiness. The systematic review illustrates that agent-based simulation (ABS) is the most frequent approach utilized in human behavior research in evacuations, occupying 43% of the literature in question. Routing optimization in evacuations mainly utilizes heuristic and metaheuristic methods, occupying 27% of the techniques used [66].

Further, the evacuation decision is the best-studied human behavioral parameter, accounting for 30% of research in this area, with some studies reporting clearance time reductions of as much as 30% compared to conventional methods. Human behavior identification during emergency response can enhance evacuation success by 25%, particularly if real-time dynamic route deviations are implemented [67]. Despite all these benefits, effective AI deployment requires cautious attention to data correctness and model integrity. AI model errors or biases may result in defective decision-making, which may even aggravate risks faced by chemical and humanitarian crises. That is why constant research, verification, and enhancement of AI tools become essential to assure their safety, effectiveness, and reliability in responding to emergencies. Incorporating AI-based approaches holds immense promise for revolutionizing evacuation planning and resource allocation, thereby enhancing the efficiency and effectiveness of emergency management strategies.

12.5.3 Adaptive response strategies powered by AI

Adaptive response strategies using AI have been shown to hold vast potential for maximizing complex chemical engineering processes and maximizing efficiency, profitability, and sustainability. AI-based strategies have immensely improved economic performance in process refining because traditional real-time optimization (RTO) systems are expected to make between 1 and 2 billion USD in annual profits [68]. Integrating AI and ML models into these systems has improved the management of nonlinear optimization challenges, including optimizing weighted average bed temperatures (WABTs) in hydrocracking units (HCUs). These AI-powered systems enable dynamic optimization, improve coordination between different units, and increase refinery margins by maximizing the production of high-value products while aligning production costs with market conditions. AI-supported adaptive response technologies also transformed water treatment. Creating an AI-based process controller (AIPC) for acid water treatment is a classic example of innovation beyond conventional techniques, one step ahead of traditional control by minimizing steam consumption and improving the precision of setpoint tracking. AIPC has enhanced operating reliability with fewer than 2% critical parameter errors. Such discoveries highlight AI's ability to make industrial processes more efficient and sustainable in resource usage [69].

In precision fermentation, AI-based approaches have shown encouraging outcomes, particularly employing model predictive control (MPC) and dynamic flow balance analysis (dFBA) in a way that fed-batch fermentation processes can be improved to a great extent. Gaussian process regression and SVMs have been utilized as ML algorithms to enhance fermentation and biomass concentration in Yarrowia lipolytica. Still, with all this, the issue of high computation costs and demands for data accuracy remains, pushing the development of AI implementation innovations. Life cycle assessment has also set up the environmental benefits of AI-fermentation by balancing greater yield against sustainability goals [70]. Adaptive response techniques based on AI have also revolutionized wastewater treatment. Studies indicate that AI technologies, such as those by Xylem Solutions, have reduced energy consumption by 30% and met regulatory requirements . MPC-based AI control methods have reduced energy consumption in pilot plants by at least 16% [71]. Despite this innovation, challenges such as the need for large training data sets and potential interpretability issues must be overcome. Robustness of models under unforeseen circumstances is required to avert operational failures. AI-based adaptive response methods possess enormous benefits in operations such as refining, water treatment, fermentation, and wastewater treatment, but their effective implementation calls for ongoing testing and tuning. Overcoming computing challenges and having the models validated is the precursor to completing the unlocking of AI potential in industrial operations. Appreciative respect for such approaches will determine their enduring impact on the chemical engineering sector's productivity, sustainability, and economic effectiveness.

12.6 AI integration in risk management and process safety

12.6.1 AI-driven risk management and predictive safety strategies

Integrating AI in chemical engineering risk management revolutionizes operational reliability, regulatory compliance, and risk prevention. AI-driven strategies, such as predictive analytics, advanced modeling, and smart automation, enable organizations to transition from reactive safety controls to proactive risk prevention. This AI-based approach reduces downtime, increases on-site safety, and supports compliance with upcoming regulatory requirements. One of the most significant benefits of AI risk management is that it utilizes data-driven predictive analytics to enable more effective risk identification. Predictive analytics from AI-powered risk models anticipate potential failures and process deviations, allowing engineers to address issues while they are still minor. Research has shown that AI-powered failure prediction models can reduce unplanned downtime by up to 40%, improving process stability and reducing financial losses through safety incidents [68]. Aside from real-time risk detection, AI facilitates compliance monitoring and streamlines regulatory processes. Intelligent automation reduces compliance-related administrative overhead by up to 60%, allowing safety professionals to focus on making important decisions and improving operations [72]. Table 12.3 overviews some data-driven AI techniques applied to emergency planning and risk management, presenting example methods and indicative performance metrics based on concepts from the cited literature. These techniques involve different applications, such as risk analysis, hazard identification, and resource allocation, all of which enhance safety strategies in chemical engineering.

The IoT and AI in chemical engineering work synergistically to enhance risk mitigation through a structured and harmonious platform. For example, as shown in Fig. 12.3A, a wireless sensor network continuously monitors critical parameters, such as pressure and temperature, in real time to ensure process safety and efficiency [83]. This data is then processed by a microcontroller-driven sensor system (Fig. 12.3B), which wirelessly transmits the collected information to central AI analytics platforms for further evaluation, enhancing predictive accuracy [83]. A user interface dashboard (Fig. 12.3C) graphically displays critical performance indicators and hazard warnings to support real-time decision-making, providing engineers with valuable information. As shown in (D) and (E), ML applications track historical patterns to predict deviations from normal working conditions [84]. Their predictive capability allows corrective actions to be taken in advance of hazards, reducing the number of accidents and system failures.

Anomaly detection software (Fig. 12.3F) alerts when parameters measured exceed prespecified limits, offering scope for intervention before accidents can be initiated. Additionally, a closed loop (Fig. 12.3G) continuously learns effective safety controls and near-miss accidents in ML algorithms, creating a culture of relentless improvement and operational excellence [84]. All these IoT- and AI-centric components combined form a top-level framework that enhances safety levels and optimizes the utilization of resources in chemical engineering. With AI-based predictive safety controls, industries can reduce risks to a great extent, improve sustainability, and ensure long-term efficiency in operations.

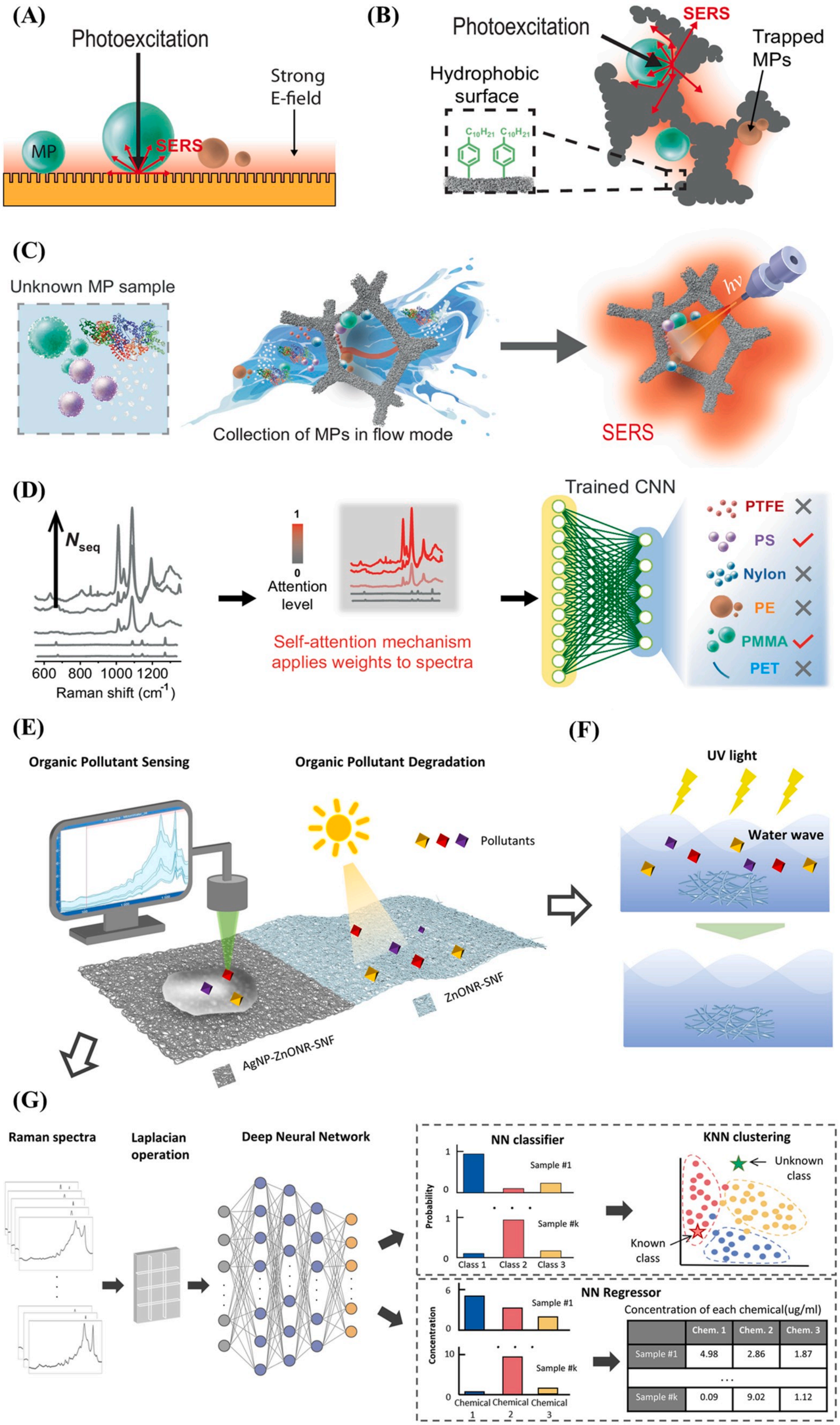
12.6.2 AI for process safety, workforce protection, and sustainability

AI is transforming PSM, the protection of the workforce, and sustainability using intelligent automation, real-time monitoring, and data-driven decision-making. Such technology enhances safety mechanisms and aids in environmental and operational sustainability. The workplace's safety and the workforce's protection are two of AI's most significant value additions. AI-driven safety simulations and scenario-based training create simulation-based learning experiences, augmenting worker preparedness for hazardous situations. Furthermore, applying robotics and automation in hazardous chemical processes minimizes humans' exposure to harmful or toxic environments. Research indicates that these technologies can reduce occupational hazards by more than 50% [85]. These systems are programmed to perform key tasks with increased accuracy and dependability, ensuring process efficiency and reducing risks to human labor.

Apart from safety, AI contributes significantly to sustainability initiatives. Optimization techniques of AI processes help industries save resources and reduce waste. The technologies can help reduce emissions and inefficiencies in operations by up to 15%, thus helping industries comply with global environmental standards and regulations [86]. Incorporating AI into safety measures helps ensure chemical processes are sustainable, safe, and meet modern industry standards. However, the blanket use of AI in risk management is confronted with numerous challenges. The major concerns are data integrity, transparency of algorithms, and regulatory adaptability. These must be addressed to facilitate the safe deployment of AI systems. Physics-informed machine learning (PIML) is one solution that enhances AI models' robustness by merging physical concepts with ML insights. PIML produces 25% more accurate predictions than conventional AI techniques and is valuable for process safety and risk management enhancement [87]. Continued investment in research, collaboration with industry, and standardization will be required to achieve the full potential of AI. AI data-sharing practices and adopting cross-industry collaboration could improve risk prediction by up to 30%.

TABLE 12.3 Data-driven AI techniques for emergency planning and risk management.

AI technique	Application framework	Detection accuracy (%)	Risk factors identified	Model complexity (high/ medium/low)	Training time (hours)	Data requirements (GB)	Computation time (ms)	Failure type detected	False positive rate (%)	False negative rate (%)	Scalability	Cost of implementation ($)	References
Deep learning (CNNS, HMMS)	Emergency planning framework	85	Evacuation routes, resource allocation	High	10	100	50	Risk assessments	5	10	High	20,000	[73]
Convolutional neural networks (CNNS)	Integrated AI systems	90	Monitoring behaviors, danger detection	Medium	6	75	25	Employee behavior anomalies	3	8	Medium	15,000	[74]
Bow-tie risk analysis	Cyber risk management	80	Cyber threats, vulnerabilities	Medium	12	60	30	Security incidents	10	15	Medium	25,000	[75]
Hidden markov model (HMM)	Dynamic risk assessment	82	Event occurrence likelihood	Medium	8	50	20	Critical incidents	4	12	High	22,000	[76]
Decision trees	Integrated risk monitoring	75	Hazard detection, anomaly monitoring	Low	5	30	15	Equipment failures	6	14	High	18,000	[77]
Monte carlo simulation	Simulation and modeling	78	Various emergency scenarios	Medium	12	120	40	Environmental impacts	8	11	High	30,000	[78]
Logistic regression	Risk evaluation framework	88	Fire hazards, environmental factors	Low	4	20	10	Fire incidents	7	9	Medium	10,000	[79]
Support vector machines (SVM)	Environmental monitoring	84	Toxic releases	Medium	7	40	22	Chemical leaks	5	6	Medium	14,000	[80]
Genetic algorithms	Crisis management framework	79	Optimal evacuation routes	High	15	150	55	Crowd control issues	9	13	Low	28,000	[81]
Reinforcement learning	Emergency logistics	86	Resource allocation, timing	High	–	–	–	–	–	–	–	–	[82]



	Chem. 1	Chem. 2	Chem. 3
Sample #1	4.98	2.86	1.87
...			
Sample #k	0.09	9.02	1.12

FIGURE 12.3 (A–D) Porous plasmonic substrates utilizing a self-attention-based neural network improve the SERS detection of MPs in water contamination by capturing MPs, boosting SERS signals, and employing SpecATNet to concentrate on key spectra for precise identification in complex mixtures.(E) Components of the AgNP-ZnONR-SNF system are designed to detect and degrade organic pollutants. (F) Diagram illustrating the photo- and piezo-catalytic degradation process. (G) Schematic representation of the machine learning models [83,84].

This would significantly enhance regulatory compliance and operational security. As AI keeps developing, it will be instrumental in the future of risk management and process safety, leading industries to adopt robust, new, and sustainable safety practices. The formal representation of chemical species in the OntoSpecies framework, as suggested by Fig. 12.4, also empowers AI applications in process safety, workers' protection, and sustainability in chemical engineering [88]. The ability of the ontology to bridge scattered chemical properties, classes, and uses allows for a more coherent and less confusing understanding of chemical relationships. This leads to improved development of AI models with improved accuracy in chemical behavior and interaction predictions, thus improving risk assessment and risk management processes. Furthermore, the OntoSpecies platform helps designers design safer chemical processes by enabling them to identify and evaluate the risks of a given substance before it is applied, thereby reducing the likelihood of accidents [88]. The inherent data relationships within the platform may also enable automatic compliance checking and reporting, ensuring conformity with safety standards and prevention of workers' exposure to unsafe substances. Lastly, the

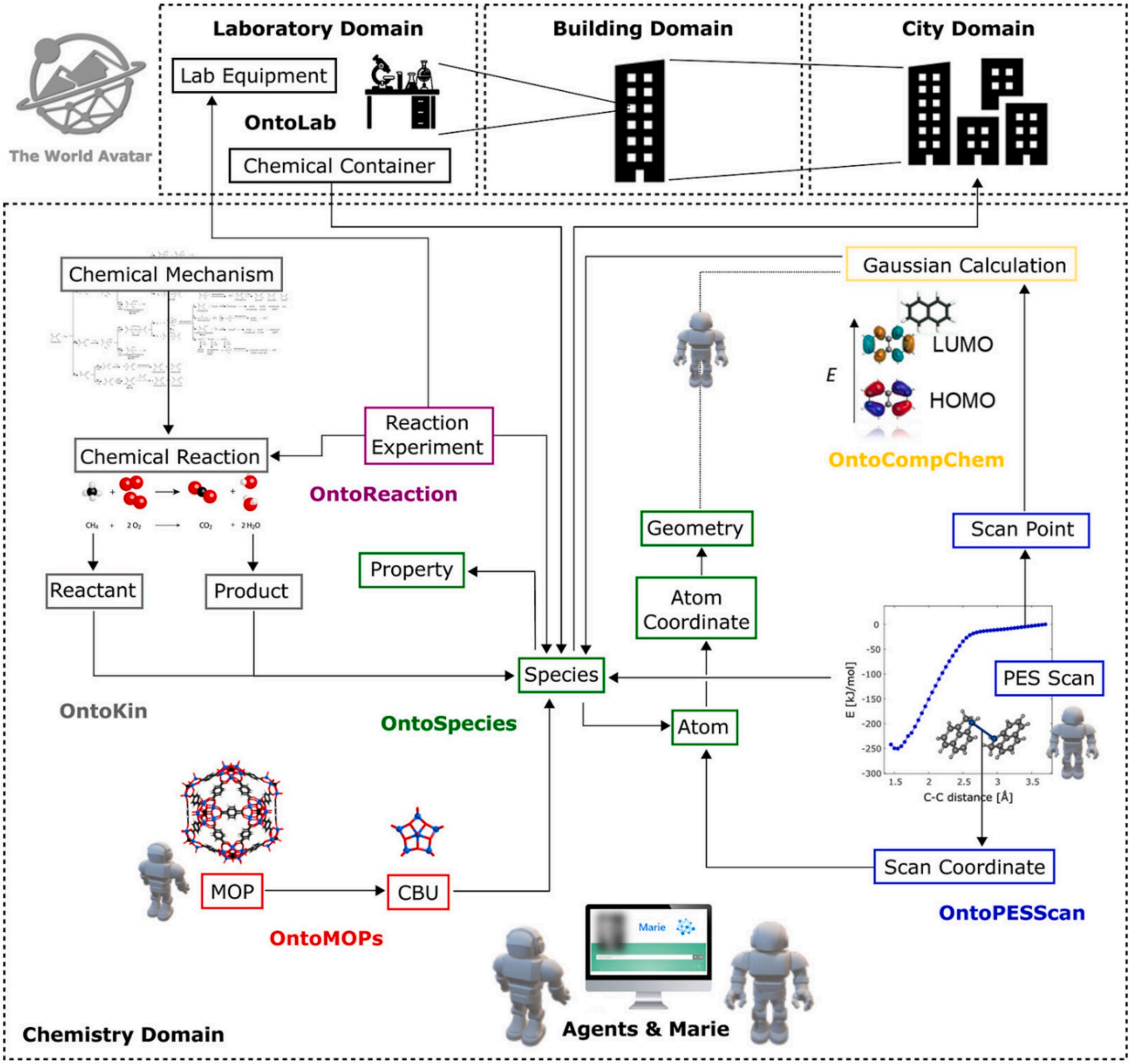


FIGURE 12.4 Integration of OntoSpecies with other TWA Knowledge Graph (TWA KG) components [88].

knowledge obtained through this structured data will guide more sustainable action through enhanced application of safer alternatives and optimization of resource use in chemical manufacture.

12.6.3 Data-driven approaches for improving safety culture

The use of AI in chemical engineering safety has improved risk assessment, anomaly detection, and accident prevention. ML-based AI models, such as deep reinforcement learning (RL) and unsupervised learning, handle big data to identify hazards and predict failures more efficiently than traditional methods [89]. Companies such as BASF use AI-based predictive maintenance to reduce unplanned shutdowns. In contrast, ExxonMobil uses anomaly detection algorithms to monitor sensor anomalies in real time, so that rapid intervention can be made [90]. DTs also help with process safety by simulating potential hazards without exposure to the real world, as Siemens has done for industrial processes [91]. It has been reported that firms, which have implemented AI-based safety interventions have reduced the rates of accidents by up to 30%, proving the effectiveness of AI in workplace safety and regulatory compliance [92].

Furthermore, Table 12.4 presents leading AI technologies and applications in industrial safety, depicting their expected impact, challenges, and readiness for implementation. For example, real-time learning enables flexibility in dynamic systems, while AI-supported equipment in automotive and industrial systems ensures compliance with rigorous safety standards. DL and neural networks continue to drive process monitoring and optimization, yet there are obstacles to making models interpretable and flexible [93]. In environmental safety, AI-powered risk analysis has also been shown to possess improved predictive power. ML-based algal bloom control research attaining over 85% accuracy [94], outperforming traditional automated models in managing complex and nonlinear environmental factors.

Whilst these advances have occurred, AI deployment in process safety is confronted at its very foundation with transparency, ethics, and regulation. The “black box” nature of AI choice can reduce stakeholder confidence, and bias in the training data can lead to inconsistency in risk analysis [102]. Moreover, existing regulatory frameworks like the international organization for standardization (ISO) and occupational safety and health administration (OSHA) provide safety-related guidelines that are not AI-specific, necessitating systematic policies for safe AI deployment [103]. A strategic roadmap is necessary to address challenges like needs assessment, data governance, pilot testing, and workforce training. Establishing clear regulatory guidelines and continuous monitoring mechanisms will enhance AI’s transparency and reliability. Collaboration among industry players, policymakers, and AI researchers will be necessary to develop safety assurance methods that keep pace with technological advancements. As AI continues to develop, achieving its full potential in chemical engineering safety is a careful balance of innovation, ethics, and regulatory compliance.

12.7 AI for fault diagnosis and failure analysis

12.7.1 Machine learning algorithms for root cause analysis

ML techniques have transformed industrial and chemical RCA in dealing with missing sensor data and nonlinearity issues. These issues typically derail traditional fault monitoring schemes, but AI-aided solutions, such as random forests and SVMs, dramatically improve fault diagnosis capability. The methods improve detection rates by as much as 25%, enabling faults to be detected early, before they become serious problems [104]. Recent studies confirm the effectiveness of advanced machine learning systems (AMLs) for RCA. For instance, a neural network (NN) classifier trained by GAs for fault diagnosis of power transformers resulted in a correlation coefficient of 0.9836 and a classification success rate of more than 98% in fault types [105]. This model outperformed traditional methods, like fast decision tree learner (FDTL), thereby solidifying that genetic diagnostic algorithms (GDAs) can enhance fault diagnosis accuracy and operational reliability. Domain-transfer diagnostic networks also provided up to a 30% increase in diagnosis accuracy, and some models resulted in a commendable overall accuracy rate of 97.3% [106].

Despite such development, there are hurdles still to be met. Decision tree AMLs, SVMs, and ANNs are also plagued by data shortages, nonlinearity, and difficulty with computing. SVMs, for example, offer greater misclassification than typical classifiers but become inefficient with a reduction in structural parameters unless properly calibrated [107]. Similarly, ANNs have extremely high accuracy but are frequently plagued with convergence and long learning time problems, particularly with increased model complexity. These problems point toward the need for robust methods to guarantee sound performance in actual use. Advanced probabilistic methods such as probabilistic principal component analysis (PPCA) and ID3 decision trees are being explored to address such limitations [108]. These methods enhance the efficiency of RCA by correctly detecting faults in intricate processes. When used on large sets of sensor and operation logs, ML methods can detect anomalies and patterns missed by traditional methods. However, to obtain the most benefit from these algorithms, one needs high-quality data, thoughtful model selection, and interdisciplinarity, such that the output is

TABLE 12.4 Emerging trends in AI technologies, industrial applications, and implementation readiness.

AI technology and techniques	Industrial applications	Expected impact	Key challenges	Proposed solutions	Implementation readiness	References
Offline embedded AI	Safety-critical systems (e.g., SIL4 railway interlocking)	Enhanced risk mitigation in safety functions, supporting safety integrity levels	Need for formal verification of all input/output combinations	Formal methods for safety verification (Class I) yielding high assurance	High, evidenced by safety compliance of existing systems (e.g., railway interlocking)	[95]
Runtime learning/ adaptation	Autonomous vehicles, robotic systems	Increased adaptability to dynamic environments and real-time decision-making	Challenges in runtime verification and handling high uncertainty	Use of safety bags for real-time safety assessments (e.g., safety envelope)	Medium, with ongoing developments in runtime checks and frameworks	[95]
AI-based safety functions	Advanced driver assistance Systems (ADAS)	Enhanced user confidence and safety in driving	Balancing human oversight with autonomous system actions	Developing trustworthiness standards and safety assurance cases	Medium to high, evolving as further standards are integrated	[96]
Autonomous systems	Drones, autonomous industrial vehicles	Efficiency gains and reduced operational costs through autonomous decision-making	Ensuring reliable decision-making in unpredictable environments	Standardization efforts in autonomous safety regulations (e.g., UL 4600, V-model structure)	Medium, contingent upon regulatory adoption and framework establishment	[95]
AI-integrated hardware	Application-specific integrated circuit (ASIC) and field-programmable gate array (FPGA) design in automotive	Increased production efficiency, reduced failure rates in hardware	Systematic error management and ensuring compliance with standards	Comprehensive auditing processes per existing safety standards (IEC 61508, ISO 26262)	High, due to established norms being followed in hardware manufacturing	[95]
Certification and assessment	Multidomain applications (e.g., automotive, industrial)	Higher trust in automated, AI-driven systems	Lack of universal testing frameworks and standards	Collaborative research to develop verification methods simulating existing requirements	Low to medium, ongoing standardization efforts	[97]
Deep neural networks (DNNS)	Image classification, process monitoring	Enhanced monitoring accuracy, better decision-making in process control	Reliance on large datasets and data quality	Develop robust data acquisition protocols and improve model interpretability.	High, established in industrial applications	[98]
Reinforcement learning (RL)	Optimizing large-scale industrial operations	Improved decision-making, optimized resource allocation	Ensuring safety and reliability of RL-driven decisions	Combine RL with traditional optimization methods to enhance reliability	Moderate to high, with ongoing research and integration	[98]
Hybrid modeling	Chemical process optimization	High accuracy in predictions and operational improvements	Integration of diverse modeling approaches (e.g., first principles and data-driven)	Use hybrid models combining traditional methods with AI/ML techniques	Moderate, needs more integration in industry	[98]

Data analytics	Chemometrics for monitoring and diagnostics	Better insights from historical operational data, predictive maintenance	Bridging gaps between different time scales and data complexities	Implement multiscale integrated decision-making frameworks	Moderate, evolving as more data is integrated	[99]
Generative AI	Process design, optimization	Increased productivity, enhanced design accuracy	Risks related to data privacy and intellectual property protection	Establish clear data usage policies, ensure transparency in data generation	Low to moderate, still emerging in industrial use cases	[98]
Education in data science	Curriculum development for chemical engineering programs	Better-prepared workforce for implementing AI techniques in industrial settings	Limited incorporation of data science in current curricula	Integrate statistical, ML, and programming concepts into the curriculum	Low, requires updates to education systems and curricula	[98]
Machine learning (ML)	Wastewater quality forecasting	Improved predictive maintenance, better water quality management	Data availability and quality challenges	Develop comprehensive data-collection strategies and model optimization	High, ongoing research and development	[100]
Artificial neural networks (ANNs)	Process optimization in wastewater treatment plants	Enhanced treatment efficiency, energy savings	Model interpretability and explainability	Create more transparent AI models and validation methods	Moderate, needs further transparency and validation	[100]
Deep learning (DL)	Monitoring and control systems	Automation and optimization of processes reduced manual intervention	Robustness, real-time decision-making, and model reliability	Conduct extensive testing, including edge-case scenarios	Moderate to high data conditions dependent	[100]
Integration with internet of things (IoT) and blockchain	Smart water management systems	Increased efficiency, data integrity, and traceability	Cybersecurity and data protection challenges	Implement robust cybersecurity measures to ensure secure data sharing	Variable depends on existing infrastructure and funding	[100]
Decision support systems	Operational decision-making (e.g., industrial plants)	More informed decision-making, improved operational outcomes	Regulatory, legal, and organizational challenges	Develop regulatory frameworks for AI applications and decision support	Low to moderate frameworks still evolving	[100]
Predictive modeling	Nutrient removal optimization in water treatment	Enhanced nutrient removal rates, compliance with environmental standards	Skill gaps in AI and water treatment knowledge	Develop capacity-building programs for operators and AI adoption	Low, requires training and skill development	[100]
Generative models (e.g., gans)	Molecular design, fault detection	Enhanced design accuracy, data augmentation for diverse datasets	Data heterogeneity, training data scarcity	Use generative models to augment and diversify datasets	Moderate, needs more domain-specific data and application	[101]

(*Continued*)

TABLE 12.4 (Continued)

AI technology and techniques	Industrial applications	Expected impact	Key challenges	Proposed solutions	Implementation readiness	References
Large language models (LLM)	Knowledge extraction, synthesis, planning	Improved decision-making, rapid prototyping, reduced time to insight	Trust, safety, and transparency concerns	Develop explainable AI techniques for model interpretation	High, LLMS already deployed in various domains	[101]
Autoencoders	Data compression, feature extraction	Efficient data representation, dimensionality reduction	Complexity in optimization problems and training stability	Implement hybrid models combining traditional and AI-based methods	Moderate, well-established techniques exist	[101]
Optimization algorithms	Process optimization, scheduling	Increased efficiency, reduced costs, improved profit margins	Uncertainty in problem parameters and environmental variables	Integrate AI-based optimization techniques for better decision support	Moderate, ongoing research in adaptive methods	[101]
Multimodal models (e.g., CLIP)	Multimedia data processing, diagnostics	Enhanced data analysis through diverse modalities (text, images, etc.)	Data integration and establishing universal evaluation metrics	Foster collaborative frameworks for data sharing and model integration	Low, requires more collaboration and infrastructure	[101]

explainable and valuable for providing insights. The success of machine learning algorithms (MLA) in the future for RCA depends on creating standardized data frameworks and models that explain the ability [109]. Solving these issues will improve the integration of ML knowledge into current real-time analysis (RTA) methods, leading to improved operational efficiency, reduced downtime, and safer industrial practices.

12.7.2 Predictive modeling for failure modes and effects analysis

AI-powered fault diagnosis has transformed predictive maintenance by greatly minimizing unplanned downtime, with sectors like manufacturing and energy experiencing up to a 25% reduction in unforeseen equipment failures [110]. Methods such as self-supervised learning, anomaly detection, RL, and DL are applied on a large scale in sectors such as automotive manufacturing, smart farming, oil refining, and pharmaceutical manufacturing sectors. For example, Tesla Gigafactories use contrastive predictive coding based on multisensory data such as temperature, vibration, and pressure to improve fault detection quality and reduce operating expenses. In addition, explainable AI methods (XAI), such as shapley additive explanations (SHAP), increase transparency, provide more trustworthy AI-based maintenance models, and make them more suitable for industries where reliability and safety are paramount. In petrochemicals, a new method integrating failure mode and effects analysis (FMEA) with a weighting method to analyze risk factors has improved project cost estimate accuracy from 43 to 44% [111].

Nevertheless, the model's performance depends on professional judgment and subjective weightings of risk and complexity, which may lead to bias in less formalized project environments. In addition, model effectiveness is also dependent on the continuous provision of valid, up-to-date information from stakeholders, which is difficult in dynamically changing project environments. Thus, additional empirical trials in different operational environments are crucial to verify the model's applicability and ensure that it brings value to cost management and enables project sustainability. AI-powered tools have also revolutionized conventional failure modes, effects, and criticality analysis (d-FMECA) procedures. An AI-enhanced tool has reduced the manual effort required for these processes by around 50%, dramatically speeding up risk assessment [112]. Case studies show that the neural network aspect of the tool achieves an exceptional error rate of just 5.78% when it comes to predicting the failure parameters of critical components [112].

This accuracy enables the tool to consistently produce risk priority numbers (RPNs) and provide users with visual representations of risk information via 3D plots, facilitating decision-making and enhancing predictive maintenance approaches. The integration of statistical modeling of failure distributions into these AI tools enhances predictive capabilities, enabling more accurate predictions of possible failures in complex systems such as chemical engineering. For example, risk assessments in gas chlorination facilities at water treatment plants have recognized that hazardous substances, such as ammonia (NH_3) and hydrocarbons, were significant factors leading to high RPNs for chlorine cylinders. Operational elements, such as inadequate cylinder management and ineffective airflow regulation, exacerbated safety problems as RPNs exceeded critical limits [113]. These results highlight the strength of AI-powered FMEA tools in maximizing reliability and safety through early and effective risk detection, encouraging proactive mitigation. Table 12.5 contrasts some AI techniques for predictive maintenance and failure prevention, presenting representative applications and indicative performance metrics based on concepts from the cited literature and their application in industry. These AI-capable applications maximize the reliability and accuracy of predictions, minimize downtime, and encourage overall system reliability, which is visible in the manufacturing, aerospace, and energy industries.

12.7.3 AI applications in reducing downtime and equipment failure risks

AI has emerged as a helpful resource in minimizing downtime and reducing the likelihood of equipment failure in chemical engineering. AI can predict breakdowns before they happen by analyzing vast amounts of data from equipment sensors, past maintenance histories, and current operating conditions [117]. The predictive approach vindicates maintenance planning, streamlines resource allocation, and improves overall performance. Predictive maintenance is well-suited for ML and DL algorithms. A comparative analysis of more than 20 fault detection models indicated that deep forest and GB algorithms achieved an average accuracy above 90% [118]. Multinomial logistic regression and long short-term memory models (LSTM) achieved reassuring levels of over 80% accuracy. These results reflect the potential of AI for early machine breakdown detection, reducing costly downtime, and improving system reliability.

AI-powered decision-making tools, including real-time monitoring and anomaly detection, increase the system reliability of predictive maintenance systems to the next level. AI facilitates real-time detection of anomalies from normal behavior, allowing instantaneous remedial action to prevent catastrophic failures. Tests on industrial process fault detection, as in wastewater treatment, demonstrate the resilience of such models as UMAP-SVDD, which couples dimensionality reduction with fault detection. It can deal with high-dimensional nonlinear data to enhance fault detection accuracy and eliminate false alarms. Fig. 12.5A presents some oscillation detection methods [119]. In contrast, Fig. 12.5B demonstrates that the UMAP-SVDD model surpasses conventional approaches regarding fault detection rates and

TABLE 12.5 Predictive maintenance and failure prevention with artificial intelligence.

AI technique	Application area	Metrics for failure prediction	Data sources	Tools/ software used	Accuracy (%)	Precision (%)	Recall (%)	Uptime improvement (%)	Processing time	Model complexity	References
Machine Learning	Manufacturing	Remaining useful life (RUL)	Sensor data	Python, R	> 85	> 80	> 75	15	10 s	Moderate	[114]
	Predictive maintenance	Mean time between failures (MTBF)	Sensor data, historical failures	Python, R, TensorFlow	95	90	85	20	2 h	High	[115]
Deep learning	Automotive	Fault diagnosis	Internet of things (IoT) data, historical logs	TensorFlow, Keras	> 90	> 85	> 80	20	30 s	High	[114]
	Anomaly detection	Root cause analysis	IoT data, logs	Keras, PyTorch	92	88	80	15	3 h	High	[115]
Regression analysis	Energy sector	Prediction of failures	Operational data	MATLAB®	> 80	> 75	> 70	10	5 s	Low	[114]
Support vector machine	Aerospace	Anomaly detection	Telemetry data	Weka, Scikit-learn	> 88	> 82	> 78	18	15 s	Moderate	[114]
	Predictive analytics	Anomaly scores	Vibration data, temp data	Weka, Scikit-learn	90	85	–	–	–	–	[115]
Neural Networks	Industrial robotics	Health status assessment	Real-time monitoring	PyTorch	> 92	> 87	–	–	–	–	[114]
	Predictive maintenance	Usage patterns	Time-series data	MATLAB®, TensorFlow	94	91	82	25	4 h	High	[115]
Decision trees	Condition monitoring	Failure rate	Machine operating data	Scikit-learn	89	87	78	10	30 min	Moderate	[115]
Random forest	CNC machine wear	AUC, ROC, Precision, Recall	Sensor data	Python (scikit-learn)	94	92	90	15	5 min	Medium	[116]
XGBoost	Motor vibration	Cross-entropy, F1 Score	Vibration sensors	R, Python	95	93	89	20	3 min	High	[116]
Support Vector Machines (SVM)	Turbine performance	AUC, PRC, TPR, TNR	Time-series data	MATLAB®	92	90	88	10	4 min	Medium	[116]

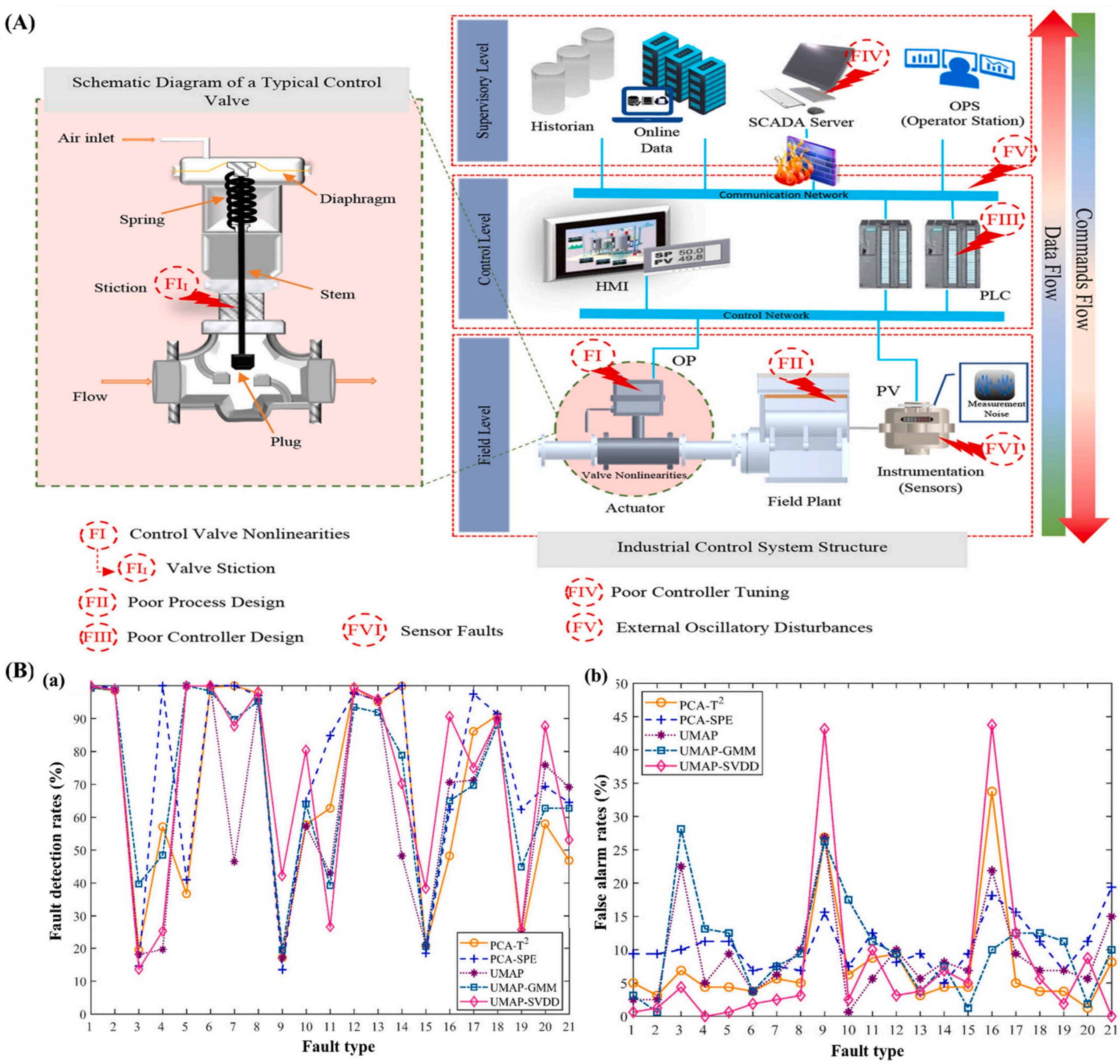


FIGURE 12.5 (A) The framework structure of industrial control systems and fundamental degradation processes. (B) (a) rates of fault detection in the TE process employing various methods and (b) rates of false alarms in the TE process utilizing different methods [119,120].

minimizing false alarms, significantly improving predictive maintenance systems [120]. Data quality is critical to the effectiveness of AI in predictive maintenance. The model created by Kang et al. [121] highlights the importance of data management in assessing equipment failure risks. Proven in oil well drilling operations, this framework uses a decision tree model to evaluate data quality, ensuring that only relevant, high-quality information contributes to risk assessment.

This approach resulted in an average decision accuracy of 79.17% [121]. AI-based systems have the capability to provide more accurate predictions by placing utmost importance on data integrity, accuracy, and quantity, lowering equipment failure and minimizing downtime strategies. Despite these advances, incorporating AI in maintenance planning adds a chain of issues. Effective data management is essential, yet most industries are confronted with massive amounts of operational data. To this, resistance from employees in the form of those hired using traditional means can stifle the application of AI. To address such challenges, it is necessary to prioritize staff training, expand data management procedures, and decipher AI models, which play crucial roles. Explainable AI allows engineers to comprehend and trust the results produced by AI, thereby facilitating improved decision-making.

12.8 Digital twins for process safety and risk management

12.8.1 Creating digital replicas of chemical processes for safety analysis

DT technology has revolutionized operational effectiveness and safety in the chemical industry by delivering dynamic, real-time representations of physical processes. These virtual models enable predictive maintenance, quick detection of inefficiencies, and automatic correction of errors, significantly decreasing the chances of accidents and promoting smoother operations. For instance, BASF has leveraged DTs to foresee equipment failures beforehand, minimizing unexpected downtime and maintenance costs. Moreover, by optimizing essential process variables like temperature, pressure, and flow rates, BASF enhanced energy efficiency and minimized waste generation [122]. DTs in chemical process safety have facilitated early identification of hazards and regulatory compliance. It requires less time to build DTs, Dow Chemical informs, accelerating product innovation through the ability of cross-functional teams to collaborate. Fig. 12.6A shows that bioprocess DT platforms integrate physical operations with

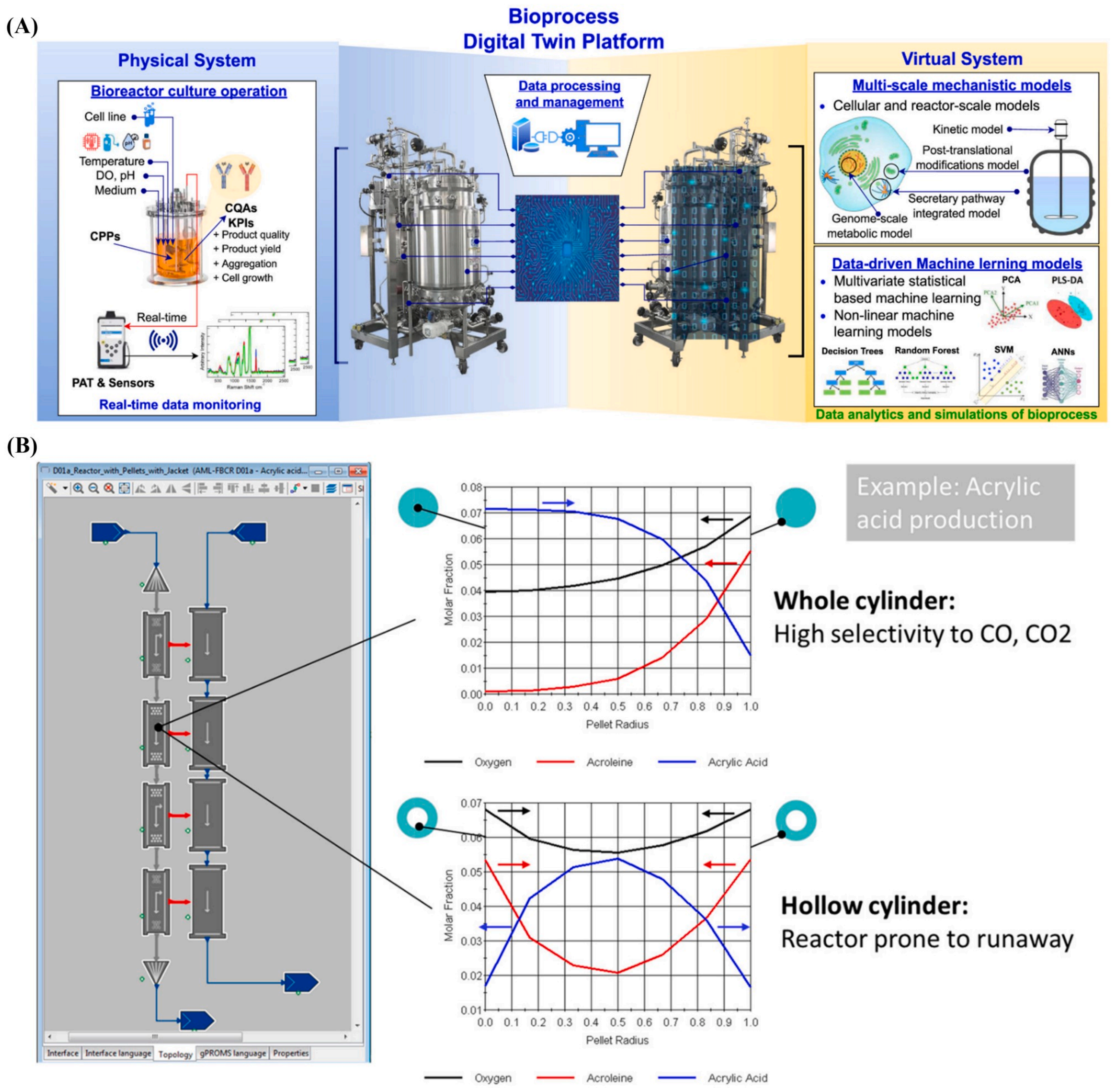


FIGURE 12.6 (A) A bioprocess digital twin platform concept consisting of physical system components, data processing and management, and virtual system modules. (B) Using the reactor digital twin to make catalyst decisions [123,124].

virtual modeling, enabling engineers to simulate and enhance chemical processes within a controlled digital setting [123]. This aligns with Industry 5.0 principles, which focus on human-centered design and sustainability by facilitating data-driven decisions while following stringent safety regulations.

Yet, DT implementation is difficult, mainly with regard to the accuracy of the base models and the smooth combination of data from various sources. They are successful with accurate simulations and continuous updates to reflect real-time conditions. In addition, interoperability between varied DT systems requires adherence to standardized communication protocols, such as ISO 15926, to support easy data sharing and collaboration among engineering teams [125]. DT simulation errors can lead to serious safety oversights without authentic data and validated models. DT technology has been applied outside chemical processes with great promise to maximize battery performance. Advanced simulations have proved the effects of microstructural properties, such as porosity and tortuosity, on the efficiency of rechargeable batteries. These assessments enabled performance to be improved by up to 30% in a specific capacity by optimizing particle shape and size [126]. In addition, numerical twin simulations have shown that electronically isolated active materials and ionically disconnected electrolyte regions are crucial in decreasing conductivity, underlining the importance of microstructural connectivity for optimal performance. Dynamic simulations show that mechanical changes caused by internal stresses during use can reduce battery life, as phase transitions and lithium deposition can lead to a 15% decrease in efficiency under certain circumstances [126].

12.8.2 Real-time simulations for accident scenario prediction and prevention

Combining DT and AI has greatly improved the prediction and anticipation of accident scenarios. By generating real-time dynamic digital models of the vehicle, the driver, and the traffic environment, AI-powered DTs continuously calculate real-time inputs to mimic several driving scenarios to detect possible risks before accidents happen [127]. These simulations offer an active traffic safety idea with which it is possible to determine potential risky situations beforehand and implement preventive measures. The new monitoring technology is the most critical element of such simulations, that is, IoT sensors, providing correct and continuous input data. For example, piezoelectric vibration sensors were claimed to have a 96.3% detection rate for mechanical failure causes, suggesting their presence in on-board monitoring [128]. Furthermore, the customization of driver behavior models improved prediction accuracy by 27.8% over generic models, proving the importance of simulation customization [129].

The precision of AI-based DT simulation in predicting driver behavior, as evidenced by the six-second prediction of lane-change intention, shows the accuracy of AI technology in simulation. Unlike crash forecasting, traffic management, and resource planning are also simplified by DTs. DTS improves transportation system decision-making by understanding what has already happened and refining predictive models through learning. For instance, the DT of Chattanooga (CTWIN) utilizes low-level data from 114 cameras to provide real-time traffic observation [130]. Employing an AI-based signal control algorithm, CTWIN reduced traffic congestion and energy use by 20%, thereby demonstrating the use of DTs in the transportation management of cities [130]. However, with all the advantages, reliability in DT simulations relies on data quality and predictive algorithm strength. To improve the accuracy of simulations, it is crucial to tackle problems such as integrating data between various platforms, variations in the real world, and data imbalances in diagnosing defects. In addition, data and data security problems must be meticulously processed because these technologies gain solid ground in transport systems.

12.8.3 Role of digital twins in optimizing process safety lifecycle

The heightened interest in DT studies clearly stems from the sharp increase in publications, from 17 in 2021 to 30 in 2022. The increase reflects dedication across sectors to improve operational effectiveness through innovative technologies. As the DTs fed by AI progress, the sectors gradually use these technologies to enhance defect detection, failure assessment, and predictive maintenance. Many industries are targeting 10–15% cost reductions by adopting DTs, showcasing their potential to drive significant operational improvements [110]. DTs provide a precise virtual model of physical assets in real time. By combining data from different sensors and working conditions, DTs can model possible failures and dangerous situations. This forecasting capacity allows organizations to recognize and cope with risks before their emergence, improving risk assessment and proactive security measures. These models provide important information throughout the life cycle of complete processes—design and execution to operation and maintenance organization—assisting to improve their safety measures. For example, Fig. 12.6B displays a simulation analysis of an acrylic acid reactor [124], emphasizing the impact of design decisions on performance measures and presenting the capacity of DTs to guide operational strategies.

The effect of DT on process safety is evident in sweeping, quantifiable results. In subway tunnel excavations, for instance, research has indicated that with better predictive analysis and real-time monitoring, safety-related incidents are minimized by 30%. Moreover, the potential for modeling and assessing scenarios before implementation has enhanced decision-making performance by 25%, enabling safer construction [131]. Apart from promoting safety, DTs have also contributed to time and cost savings, with firms attaining 40% of time saved on safety inspections and risk assessment, reducing project lifecycles and reducing downtime. DTs have also been attributed to 30% less unplanned downtime and 25% enhanced operational efficiency, with response time to safety issues enhanced by 40% [132].

Furthermore, the agility of DTs allows for instant modification of safety procedures based on operational feedback. The agility makes safety procedures relevant and responsive to a changing environment, minimizing risks and enhancing overall safety results. With ongoing monitoring of systems and simulating risks that can potentially occur, DTs provide a proactive approach to safety risk management. Yet, effective deployment of DTs is not easy, particularly in data integration and periodic model validation. To survive, DTs must enable companies to validate and ensure the reliability of their models, including ongoing technology enhancement and adjustment. In brief, DTs transform the process safety lifecycle by improving risk management, maximizing operational efficiency, and saving significant amounts of money. Their ability to mimic actual situations, foretell failures, and instantaneously revise protocols makes them a great value addition to improving safety and performance. As industries increasingly embrace DTs, their contribution to PSM will increase manifold, revolutionizing the approach to safety management across industries.

12.9 Conclusion

The integration of AI and ML has transformed hazard identification and risk assessment in chemical engineering, significantly revolutionizing safety protocols to a great extent. AI-based technologies such as predictive modeling, real-time monitoring, and data analysis have greatly improved hazard detection, emergency response, and the speed and accuracy of decision-making. For example, AI models have reduced emergency response times by 30% and increased risk assessment accuracy by more than 40%, fostering a proactive safety culture and enabling industries to identify and mitigate risks before they lead to incidents. Additionally, AI's role in optimizing safety management controls, QRAs, and regulatory compliance has contributed to a reduction in operational risks. AI -powered sensor networks have achieved over 90% accuracy in detecting chemical leaks, while predictive models have improved near-miss predictions, leading to more effective resource allocation than conventional methods. However, the widespread adoption of AI presents challenges. Issues such as data integrity, model interpretability models, and regulatory compliance remain significant obstacles. The open nature of most AI architectures necessitates transparency, rigorous testing, and expert oversight to ensure trustworthiness. Moreover, human intelligence remain remains essential for integrating AI into adaptive systems, providing sound judgment and enhancing security. Combining AI with DT technology has also proven invaluable, enabling real-time simulation of ongoing events to improve emergency preparedness and operational efficiency. For example, DTs have reduced safety accidents by 30% and operational expenses by 10%–15%, highlighting such technologies' cost and safety benefits. Lastly, while AI and DTs have already transformed safety procedures, addressing ongoing concerns related to data integrity, cyber-attacks, and regulatory frameworks will be crucial to their continued success. These efforts will pave the way for future innovations that will make the chemical engineering industry more secure, sustainable, and efficient.

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