

Digital Twin and AI Powered Optimization Framework for Smart Petrochemical Operations under Saudi Vision 2030

SYED ARIF ALI BUKHAREE
ORCID: 0009-0003-1612-8383

Abstract- Digital transformation is reshaping petrochemical value creation as producers seek higher reliability, lower energy intensity, safer operations, and stronger environmental performance under increasingly volatile market conditions. Within this shift, digital twins and artificial intelligence have moved from isolated pilots to an integrated capability that can synchronize plant data, process models, asset histories, and optimization logic across the full operating lifecycle. This review examines how digital twin architectures, AI techniques, and industrial connectivity can be combined into an optimization framework for smart petrochemical operations aligned with Saudi Vision 2030. The study has three objectives: to synthesize the technological foundations of digital twins for petrochemical plants; to assess how AI supports prediction, diagnosis, control, maintenance, and decision optimization; and to develop an implementation framework tailored to Saudi industrial priorities, including productivity, localization, sustainability, and workforce capability. A structured review methodology inspired by recent review designs in chemical engineering and future industrial systems was used to organize evidence published between 2020 and 2025. The analysis indicates that the strongest operational value emerges when physics-based process knowledge is fused with machine learning, historian data, IIoT streams, and enterprise systems rather than when AI or digital twins are deployed as stand-alone tools. Across the literature, high-value applications include soft sensing, abnormal situation detection, energy optimization, predictive maintenance, production scheduling, emissions monitoring, and operator decision support. Yet the review also finds persistent barriers in model governance, cyber risk, data quality, semantic interoperability, and organizational readiness. To address these gaps, the paper proposes a layered framework linking sensing, contextualization, hybrid modelling, AI analytics, prescriptive optimization, and human-in-the-loop governance. The framework is discussed in relation to petrochemical complexes in Saudi Arabia, where integration with process simulation, SAP-like enterprise workflows, reliability systems, and sustainability reporting

can accelerate both operational excellence and Vision 2030 outcomes.

Keywords: Digital Twin, Artificial Intelligence, Petrochemical Operations, Hybrid Modelling, Predictive Maintenance, Energy Optimization, Saudi Vision 2030

I. INTRODUCTION

Petrochemical operations are among the most data-rich and optimization-sensitive industrial environments. They involve tightly coupled reaction, separation, heat integration, utilities, logistics, and safety functions that must remain stable despite feedstock variability, catalyst ageing, market uncertainty, and strict environmental limits. Traditional process control and planning systems remain essential, but they are often fragmented across distributed control systems, historians, computerized maintenance platforms, laboratory information systems, and enterprise resource planning layers. As a result, many plants still struggle to convert operational data into coordinated action across reliability, energy, throughput, and sustainability objectives. Recent work in sustainable chemical engineering shows that AI is increasingly being used to connect these layers by enabling predictive, prescriptive, and adaptive decision support across production systems (Ali et al., 2026). In parallel, digital twins are evolving from static engineering replicas into living virtual counterparts that update with plant conditions and support optimization through the full asset lifecycle (Redchuk et al., 2025; Karkaria et al., 2025).

For Saudi Arabia, this transition has strategic significance. Vision 2030 places strong emphasis on industrial diversification, digital transformation, energy efficiency, environmental stewardship, and local capability development. The petrochemical sector is central to these goals because it links

hydrocarbons to higher-value manufacturing, export competitiveness, and industrial services. Smart petrochemical operations therefore require more than automation upgrades; they require integrated intelligence that can improve plant economics while reducing downtime, flaring, emissions, and unplanned maintenance. Digital twins offer a natural organizing concept because they can align engineering models, operational states, and business objectives. AI strengthens this capability by learning nonlinear relationships, detecting latent patterns, estimating hidden variables, and recommending decisions under uncertainty (Banafaa et al., 2024; Das et al., 2023). When these capabilities are implemented in a governed and interoperable manner, they can support a move from reactive to anticipatory plant management.

The literature, however, remains dispersed. Some studies focus on digital twins as process representations in chemical manufacturing, others on AI-enabled optimization or predictive maintenance, and others on broader Industry 4.0 and Industry 5.0 transitions. Review studies often analyze one domain, such as membrane systems, energy, mobility, or manufacturing hierarchies, rather than providing an integrated petrochemical operations perspective (Ali et al., 2026; Ullah et al., 2025). Moreover, many publications emphasize technical promise but say less about deployment logic in complex petrochemical enterprises where model fidelity, cybersecurity, change management, and human trust shape performance. This review responds to that gap by synthesizing the evidence into a sector-specific framework for Saudi petrochemical systems. Rather than treating digital twins and AI as separate concepts, it examines how they can function as a combined optimization stack.

Accordingly, the review addresses four questions. First, what digital twin capabilities are most relevant for petrochemical operating environments? Second, which AI methods generate the highest value when embedded within those twins? Third, what implementation barriers repeatedly appear in the 2020–2025 literature? Fourth, how can these findings be translated into a practical framework for smart petrochemical operations under Saudi Vision 2030? By answering these questions, the paper contributes a

structured review, two synthesizing tables, and a staged implementation model for industry and research.

II. REVIEW METHODOLOGY

The review adopted a structured narrative methodology informed by contemporary review designs used in industrial AI, chemical engineering sustainability, and future network surveys (Ali et al., 2026; Ullah et al., 2025). The aim was not to produce a meta-analysis of identical experiments, which is rarely feasible in this domain, but to systematically organize convergent evidence from peer-reviewed journal articles, selected conference papers, and authoritative industry-linked studies published between 2020 and 2025. Search strings were built around combinations of “digital twin,” “process digital twin,” “petrochemical,” “chemical process industry,” “AI,” “machine learning,” “optimization,” “predictive maintenance,” “energy management,” “smart manufacturing,” and “Saudi Vision 2030.” Screening emphasized studies that addressed operational use cases rather than purely conceptual discussion. Sources were retained when they met at least one of five relevance filters: hybrid process modelling, plant-wide monitoring and optimization, asset and maintenance analytics, sustainability and energy optimization, or implementation governance. Studies focused on unrelated domains without transferable process or asset logic were excluded.

After screening, the literature was coded into thematic clusters: digital twin architecture, data infrastructure, AI methods, operational applications, sustainability outcomes, and deployment barriers. The coding approach was influenced by scientometric and thematic grouping strategies used in recent broad reviews of AI for sustainable chemical engineering and digital twin-enabled industrial systems (Ali et al., 2026; Redchuk et al., 2025). This enabled comparison across heterogeneous studies while still preserving domain specificity. The synthesis was interpretive rather than statistical, but it remained evidence anchored: repeated claims were only emphasized when they appeared across multiple clusters of studies, and deployment arguments were linked to reported use cases in refining, chemical processing, manufacturing,

or analogous continuous industries. The final framework was then derived by combining recurrent technical layers with organizational requirements observed across the reviewed literature.

III. DIGITAL TWIN FOUNDATIONS FOR PETROCHEMICAL OPERATIONS

A digital twin in petrochemical operations can be defined as a dynamic, data-connected virtual representation of process units, assets, utilities, or whole sites that updates with physical-system behavior and supports monitoring, simulation, diagnosis, prediction, and optimization. In petrochemicals, the twin can exist at multiple scales. At equipment level, it may represent compressors, pumps, heat exchangers, furnaces, or reactors for condition monitoring and maintenance. At process-unit level, it can capture reaction, separation, and energy interactions for control and yield optimization. At site level, it can integrate utilities, emissions, production planning, logistics, and business constraints to support enterprise-wide decisions. Recent industry and academic work stresses that value increases when these scales are linked hierarchically rather than developed in isolation (Meng et al., 2023; Jiao et al., 2021; Redchuk et al., 2025).

The literature consistently describes three twin foundations. The first is data connectivity. Industrial historians, IIoT devices, laboratory systems, maintenance records, and enterprise platforms provide the time-series and contextual data needed to keep the twin live. The second is modelling fidelity. Petrochemical twins often rely on first-principles models because mass transfer, reaction kinetics, thermodynamics, and equipment constraints remain central to trustworthy process representation. The third is intelligence augmentation. AI and machine learning compensate where mechanistic models are incomplete, too slow, or weak in uncertainty handling. Hybrid twins therefore dominate the most promising use cases because they combine physical meaning with adaptive learning. Reviews of AI in manufacturing and sustainable chemical engineering repeatedly show that hybridization is more robust than purely data-driven modelling in high-consequence

operations where extrapolation and explainability matter (Ali et al., 2026; Zhang et al., 2025).

In smart petrochemical contexts, digital twins are not only simulation mirrors. They act as operational coordination systems. They can reconcile plant measurements with expected process states, provide soft sensors for variables that are expensive or slow to measure, estimate remaining useful life for assets, test what-if operational scenarios, and expose decision trade-offs across energy, throughput, safety, and emissions. This is particularly useful in integrated complexes where local optimization can unintentionally degrade plant-wide performance. A furnace may be optimized for one objective, for example, while downstream separation or utility consumption worsens. The digital twin helps maintain system perspective, while AI accelerates pattern recognition, forecasting, and prescriptive analysis.

IV. AI CAPABILITIES WITHIN THE PETROCHEMICAL DIGITAL TWIN

The AI layer within a petrochemical digital twin generally performs six functions. First, it supports data quality assurance by detecting missing values, drift, sensor anomalies, and inconsistent tags before analytical models are executed. Second, it performs estimation through soft sensing. Machine learning models such as random forests, support vector regression, gradient boosting, and deep networks can estimate quality variables, composition indices, fouling rates, or catalyst activity from more accessible signals. Third, AI supports diagnosis by classifying abnormal situations, identifying likely root causes, and ranking risk patterns. Fourth, it enables prediction through failure forecasting, demand estimation, utility consumption forecasting, and emissions projection. Fifth, it supports optimization by identifying control setpoints, maintenance priorities, scheduling actions, and resource allocations under multiple constraints. Sixth, it can support interaction through explainable dashboards, operator assistants, and natural language interfaces for maintenance and operations workflows.

Among these functions, predictive maintenance is one of the most mature. Studies across manufacturing and process operations show that AI-driven twins can infer

degradation patterns from vibration, temperature, flow, pressure, and maintenance history, allowing interventions before catastrophic failure occurs (Ali et al., 2026; Ullah et al., 2025). For petrochemical plants, this is important because failures in rotating equipment, fired heaters, compressors, and exchanger networks often cascade into production losses, energy inefficiency, and safety exposure. When the twin embeds maintenance logic alongside process dependencies, maintenance decisions become economically richer. The relevant action is not simply “repair the asset,” but “optimize the timing and scope of intervention relative to production commitments, utility margins, and spare parts availability.”

Energy optimization is another major AI contribution. Petrochemical complexes are highly energy intensive, and small improvements in steam, fuel, refrigeration, compression, or heat recovery can produce significant financial and environmental gains. AI models can learn the nonlinear interaction between operating conditions and utility intensity, then feed optimization routines that recommend lower-energy operating windows without violating process safety or product quality. In recent optimization-centric reviews of digital twins, this prescriptive function is identified as one of the defining advances beyond visualization and monitoring (Karkaria et al., 2025). In Saudi Arabia, where industrial decarbonization and efficiency improvement are strategic priorities, this capability aligns directly with Vision 2030’s emphasis on sustainable competitiveness.

The literature also points to advanced AI techniques with growing relevance. Reinforcement learning is increasingly discussed for adaptive control and scheduling, although full industrial deployment remains limited because safety constraints, exploration risk, and trust requirements are high. Explainable AI is gaining importance for regulated and high-risk environments because operators and engineers must understand why a model recommends a shutdown, setpoint change, or maintenance action. Federated and privacy-preserving learning, though more visible in cybersecurity and distributed systems research, may become useful in petrochemical groups that want to train models across multiple plants without centralizing all raw data. Generative AI and large language models are beginning to appear as

operator-support interfaces, but their industrial value is strongest when constrained by verified process knowledge rather than used as free-form autonomous agents.

V. OPERATIONAL APPLICATIONS IN SMART PETROCHEMICAL PLANTS

Across the 2020–2025 literature, six application clusters repeatedly emerge for petrochemical and adjacent process industries. The first is process monitoring and soft sensing. Here the digital twin combines first-principles calculations with data-driven estimators to reconstruct unmeasured process conditions, infer product quality in near real time, and flag deviations before laboratory confirmation is available. This reduces analytical delay and enables tighter operational correction. The second is abnormal situation management. AI-enhanced twins can compare real behavior against expected trajectories and identify incipient disturbances such as fouling, instability, feed drift, control valve malfunction, or heat-transfer deterioration. Because petrochemical operations are strongly coupled, early detection is more valuable than perfect diagnosis after the fact.

The third application cluster is predictive maintenance and reliability optimization. Instead of relying on preventive maintenance intervals alone, the twin can estimate condition and consequence, then connect this information to maintenance workflows and spare-part logic. When integrated with enterprise systems, this supports better work-order timing and resource planning. The fourth cluster is production and planning optimization. By linking process twins to market, inventory, utility, and feedstock information, plants can simulate production plans under alternative constraints and optimize economics more holistically. This is where the integration of AI into ERP-like workflows becomes useful; real-time analytics should not stop at the control room if the objective is enterprise optimization. Studies on AI in SAP-like real-time data environments, although not petrochemical-specific, reinforce the importance of integrating predictive analytics, workflow automation, and cloud scalability in enterprise decision loops (Jampani et al., 2023).

The fifth cluster is energy and emissions management. Here, digital twins support fuel and steam

optimization, flare minimization, carbon-intensity tracking, and utilities balancing. AI improves performance by identifying patterns not easily observable through rule-based approaches, such as interactions between ambient conditions, equipment degradation, and utility demand. The sixth cluster is operator decision support and training. Twin environments can simulate disturbances, test optimization recommendations, and improve procedural readiness. This human-centered use case is critical because the best reported outcomes in the literature generally occur when human expertise is augmented, not displaced. Industry 5.0-oriented discussions of digital twins in the chemical sector similarly emphasize the need to preserve human judgement while expanding the speed and granularity of digital decision support (Redchuk et al., 2025).

A useful way to understand the operational value of the framework is to view it through a typical petrochemical decision cycle. In steady-state operation, the twin ingests process and asset data, reconciles them against expected unit behavior, and updates quality and health estimators. If the analytics layer detects an emerging anomaly, such as a heat-exchanger fouling trend or compressor performance loss, the system should not only trigger an alert but also calculate probable economic, safety, and energy consequences under different response options. It may compare immediate intervention, controlled derating, or continued monitoring, then recommend the action with the best plant-wide outcome. This is where digital twins outperform isolated dashboards: they connect abnormal signals to future operational scenarios and business consequences. In integrated Saudi complexes, where upstream feed conditions and downstream commitments interact continuously, such scenario-aware decision support can reduce costly local optimization and improve coordination across operations, maintenance, and planning teams.

The same logic applies to sustainability management. Petrochemical firms increasingly face pressure to quantify and reduce emissions, water use, waste generation, and indirect energy losses. A conventional reporting architecture often measures these outcomes after the fact, while a digital twin architecture can intervene during operation. For example, a twin can estimate the carbon and steam implications of

alternative furnace strategies, identify flare-risk patterns during grade changes, or compare production plans using combined economic and environmental objective functions. AI then improves responsiveness by learning where deviations typically arise and by forecasting likely deterioration before it becomes visible in lagging indicators. Such capability is important for Saudi industrial policy because Vision 2030 is not only concerned with output expansion but also with higher-value, more sustainable industrial performance. A twin that can quantify operational trade-offs in near real time therefore becomes a management instrument for both productivity and compliance, supporting stronger environmental governance without compromising competitiveness.

VI. SAUDI VISION 2030 RELEVANCE

Saudi Vision 2030 provides a compelling strategic frame for smart petrochemical operations because it links industrial upgrading to broader national goals: economic diversification, digital leadership, sustainability, local content, human capability development, and globally competitive manufacturing. Digital twins and AI contribute to each of these dimensions. Economically, they improve margin protection through reduced downtime, yield improvement, energy savings, and faster decision cycles. Environmentally, they support emissions visibility, resource efficiency, and better control of flaring, waste, and maintenance-related losses. Institutionally, they encourage the integration of operational technology, information technology, and engineering knowledge, building a more modern industrial capability base. Socially, they create demand for data engineers, reliability analysts, process data scientists, and digitally enabled operators, supporting high-skill employment and localization.

The Saudi petrochemical context also offers enabling conditions. Large integrated industrial sites generate the process scale, data density, and optimization complexity necessary for digital twins to produce material value. At the same time, these complexes are increasingly connected to energy-transition expectations, including lower carbon intensity, circularity, and smarter asset utilization. The literature suggests that site-wide twins create the most sustainable value when they connect operations, maintenance, and business systems rather than

optimizing single equipment items in isolation (Hydrocarbon Processing, 2024; Aramco Careers, 2026). For Saudi Arabia, this means that deployment strategies should move beyond disconnected pilot projects. The twin should become part of industrial architecture, with clear ownership, model governance, cybersecurity controls, and workforce integration.

VII. DEPLOYMENT CHALLENGES AND GOVERNANCE

Despite strong promise, the literature documents several persistent deployment barriers. Data quality is the most repeated issue. Many process plants still contain noisy tags, inconsistent naming conventions, missing context, sparse failure labels, and weak synchronization between historian, maintenance, and laboratory systems. AI models trained on such data may produce unstable or misleading recommendations. Semantic interoperability is another barrier. A digital twin requires not just signals but meaning: equipment hierarchies, process relationships, maintenance taxonomies, alarm contexts, and operating regimes. Without contextualization, AI outputs remain fragmented and difficult to operationalize. Recent reviews in sustainable chemical engineering emphasize that AI success depends as much on data architecture and domain framing as on algorithm choice (Ali et al., 2026).

Cybersecurity and governance are equally important. A live twin connected across industrial and enterprise layers expands the attack surface and raises questions about access control, model updates, and decision authority. High-value optimization recommendations can also become liabilities if traceability is weak. Engineers and operators may distrust a system that cannot explain why it recommends a throughput increase, a shutdown deferment, or a change in recycle ratio. This is why explainability, validation, and human-in-the-loop approvals appear repeatedly in the literature as prerequisites for industrial adoption. Model drift is another concern. Process conditions, feedstocks, catalyst states, and maintenance histories change over time; AI models that are not monitored and recalibrated can degrade silently. For petrochemical plants, this is especially risky because incorrect confidence can be worse than explicit uncertainty.

Organizational readiness also shapes outcomes. Digital twin projects frequently start as technology programs rather than operational transformation programs. This leads to underinvestment in change management, workflow redesign, and capability building. The literature suggests that the strongest implementations are cross-functional: process engineers, data scientists, operations teams, maintenance planners, cybersecurity specialists, and enterprise architects work from a shared value case rather than from isolated technical objectives. Saudi projects seeking Vision 2030 alignment should therefore treat digital twins as capability-building initiatives, not just software deployments. Governance should specify model ownership, validation routines, retraining rules, escalation boundaries, and links to key performance indicators such as energy intensity, downtime, throughput stability, and emissions.

VIII. PROPOSED OPTIMIZATION FRAMEWORK

Based on the literature synthesis, a practical optimization framework for smart petrochemical operations can be organized into six layers. The first is the sensing and connectivity layer. It includes plant instrumentation, analyzers, laboratory data, historians, condition-monitoring systems, maintenance records, and enterprise data feeds. Its purpose is to ensure reliable, timestamped, and secure access to operational data. The second is the contextualization layer. Here, tags are mapped to equipment hierarchies, process units, maintenance objects, and business contexts so that data becomes decision-ready. This layer is essential because it converts isolated signals into structured operational knowledge.

The third layer is the hybrid modelling layer. This combines first-principles process models, equipment models, and reduced-order digital replicas with data-driven estimators. In petrochemicals, this hybrid form is superior to purely black-box modelling because it preserves physical meaning and improves extrapolation outside the training envelope. The fourth layer is the AI analytics layer. It includes anomaly detection, soft sensing, predictive maintenance, forecasting, and diagnostic classification. The fifth layer is prescriptive optimization. This layer translates predictions into decisions through optimization solvers, rule-constrained recommendations, or

scenario ranking. Its outputs may target control setpoints, cleaning schedules, utility configurations, production plans, or maintenance timing. The sixth layer is human and governance integration. It includes dashboards, explainable recommendation logic, approval workflows, cybersecurity controls, retraining governance, and performance review routines.

This layered structure matters because many failed initiatives jump directly from data acquisition to dashboards or from machine learning to automated recommendations without building contextual and governance foundations. The reviewed evidence suggests that sustainable value emerges when each layer is deliberately linked. For example, predictive maintenance should not only estimate failure probability; it should be connected to consequence weighting, work-order systems, and production impacts. Energy optimization should not only recommend lower-fuel operation; it should also account for product quality, constraints, emissions, and operator workload. The proposed framework therefore supports a controlled path from descriptive visibility to diagnostic intelligence, predictive awareness, and finally prescriptive optimization.

9. Phased Implementation Roadmap and Future Directions

Implementation should be phased. Phase one should establish data readiness and use-case prioritization, focusing on high-value and technically feasible targets such as rotating-equipment health, exchanger fouling prediction, utility optimization, or soft sensing for quality variables. Phase two should develop the hybrid twin and associated analytics, with clear validation against process-engineering benchmarks and maintenance outcomes. Phase three should integrate prescriptive recommendations into workflows, including work orders, control-room support, and management dashboards. Phase four should expand from unit-level to plant-level or site-level coordination, connecting utilities, production planning, sustainability metrics, and enterprise systems. At each stage, governance should define approval rights, retraining cycles, cybersecurity controls, and value realization metrics. This staged pathway is consistent with lessons from industrial AI and digital twin research more broadly: organizations that scale from validated use cases while preserving

model transparency and human trust are more likely to obtain durable value than those pursuing large, undifferentiated transformation programs from the outset.

Several future directions are especially relevant for Saudi petrochemical operations. One is site-wide orchestration. Most current twins remain unit-centric; future value will come from linking process units, utilities, storage, maintenance, and planning into coordinated site twins. A second direction is closed-loop sustainability optimization, where energy, water, emissions, and reliability indicators are optimized together rather than in separate reporting systems. A third direction is industrial foundation models constrained by process knowledge. Instead of generic generative AI, the sector is likely to benefit more from domain-grounded assistants trained on procedures, alarm logs, maintenance reports, and engineering standards but tied to verified plant contexts. A fourth direction is stronger twin governance, including model-risk management, traceable retraining, and cyber-resilient architectures.

Research should also pay greater attention to techno-organizational deployment in the Gulf region. Many published studies are technology-forward but light on regional industrial realities such as localization targets, workforce transition, data sovereignty, and integration with existing process simulation and enterprise platforms. Saudi Vision 2030 makes these dimensions particularly important because industrial digitalization is expected to generate both economic and institutional value. Future studies should therefore examine measured performance outcomes from petrochemical pilots in the Kingdom, compare hybrid modelling strategies across plant types, and evaluate how twin-enabled decisions affect operator trust, maintenance productivity, emissions intensity, and business responsiveness over time.

The review has several limitations that also define a future research agenda. First, much of the published evidence still comes from pilots, simulations, or cross-industry analogies rather than large bodies of openly reported petrochemical deployment data. Second, performance indicators are not standardized; some studies prioritize prediction accuracy, others economic gain, and others sustainability proxies, making direct

comparison difficult. Third, there is still limited empirical reporting from Gulf-based operating environments, despite the region’s strategic importance to global petrochemicals. Future work should therefore adopt more transparent benchmarking across use cases, compare hybrid-model architectures under shared datasets, and document the organizational conditions that determine adoption success. It would also be valuable to assess how twin-enabled optimization affects operator cognition, turnaround planning, process safety management, and carbon-accounting quality over multiple years. Such longitudinal evidence would strengthen the business case for Saudi deployments and move the field from promising prototypes toward reproducible industrial practice.

Finally, the review highlights the importance of architecture choices. Edge analytics, cloud integration, and enterprise interoperability should be selected according to latency, sovereignty, and reliability requirements rather than technology fashion. Safety-critical recommendations may need on-premise execution with strict validation, while broader planning and benchmarking workloads can benefit from cloud elasticity. Likewise, integration with SAP, maintenance systems, and sustainability reporting platforms should be governed through open data models and disciplined master-data management. These choices determine whether the twin becomes an enterprise capability or remains an isolated pilot. For Saudi petrochemical operators, architecture discipline is especially important because future industrial competitiveness will depend on the ability to scale digital intelligence across multiple assets, sites, and value-chain interfaces without losing trust, security, or operational continuity. It also supports stronger localization by embedding reusable engineering knowledge within governed industrial operating models.

IX. CONCLUSION

This review has argued that digital twins and AI are most valuable in petrochemical operations when implemented as an integrated optimization framework rather than as separate digital initiatives. The literature from 2020 to 2025 shows clear momentum toward hybrid twins that fuse process knowledge, industrial data, AI analytics, and enterprise workflows. Across process monitoring, abnormal situation management, predictive maintenance, energy optimization, planning, and operator support, the combined approach can deliver faster decisions, better asset reliability, improved energy performance, and stronger sustainability outcomes. At the same time, the review finds that technical potential alone is insufficient. Data quality, semantic structure, model explainability, cybersecurity, and organizational readiness remain decisive factors in real-world performance.

For Saudi Arabia, these findings align strongly with Vision 2030. Smart petrochemical operations supported by digital twins and AI can contribute to industrial competitiveness, localization, environmental performance, and capability development. The proposed six-layer framework offers a practical path for adoption, starting with secure data connectivity and contextualization, then progressing through hybrid models, AI analytics, prescriptive optimization, and governed human integration. The central implication is straightforward: petrochemical digitalization should be designed as operational intelligence architecture. When that architecture is aligned to process realities and human decision structures, digital twins and AI become not just technologies of observation, but technologies of sustained industrial transformation.

Table 1. Enabling Layers, AI Functions, and Petrochemical Value Creation

Framework Layer	Typical Petrochemical Function	AI/Analytics Role	Expected Value
Sensing & connectivity	Collect process, asset, lab, and enterprise data	Stream ingestion, signal validation, event capture	Trusted live operational picture

Contextualization	Map tags to units, assets, maintenance objects, and business rules	Semantic linking and data harmonization	Decision-ready industrial context
Hybrid modelling	Represent process physics, asset behavior, and operating constraints	First-principles + ML fusion	Reliable prediction beyond historical data
AI analytics	Forecast failures, estimate hidden states, detect anomalies	Soft sensing, diagnosis, prediction, classification	Faster and more accurate operational awareness
Prescriptive optimization	Recommend setpoints, cleaning schedules, and production plans	Multi-objective optimization under constraints	Higher yield, lower energy use, reduced downtime
Human & governance	Support engineers, operators, and managers	Explainability, approval logic, KPI monitoring	Adoption, auditability, and safer deployment

Figure 1. Layered digital twin and AI optimization framework for smart petrochemical operations

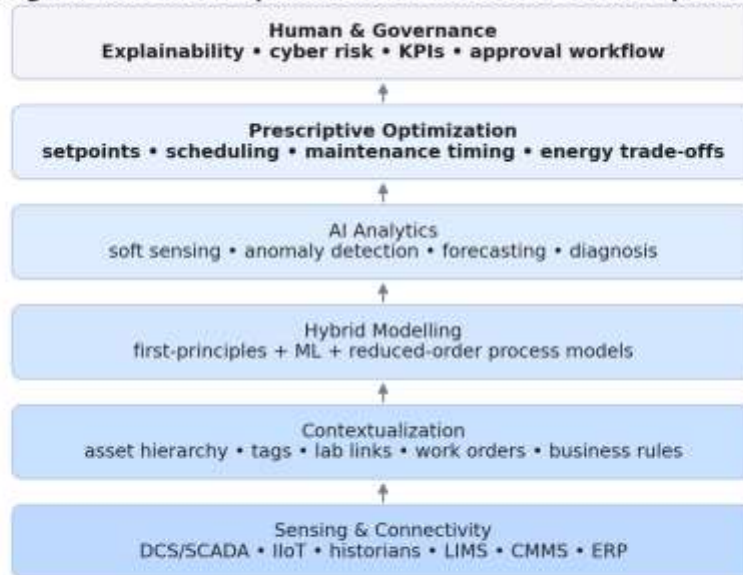


Figure 1. Layered digital twin and AI optimization framework for smart petrochemical operations.

Table 2. Common Deployment Barriers and Recommended Mitigation Actions

Barrier	Operational Manifestation	Primary Risk	Recommended Mitigation
Poor data quality	Noisy tags, missing values, weak synchronization	Model drift and false recommendations	Tag governance, validation rules, historian cleanup, contextual data stewardship

Semantic fragmentation	Disconnected process, maintenance, and lab systems	Fragmented decisions and poor traceability	Unified asset hierarchy and interoperable data models
Cybersecurity exposure	Expanded attack surface across OT and IT layers	Operational disruption and data compromise	Zero-trust access, network segmentation, model and API governance
Low explainability	Operators cannot justify model outputs	Resistance to adoption and unsafe automation	Explainable AI, confidence scoring, human approval thresholds
Weak change management	Pilot remains disconnected from workflows	Limited business value realization	Cross-functional ownership and staged deployment
Insufficient reskilling	Teams lack digital and analytical capability	Underuse of tools and dependence on vendors	Role-based training and localized capability programs

Figure 2. Phased Implementation Roadmap for Saudi Petrochemical Digital Twin Deployment

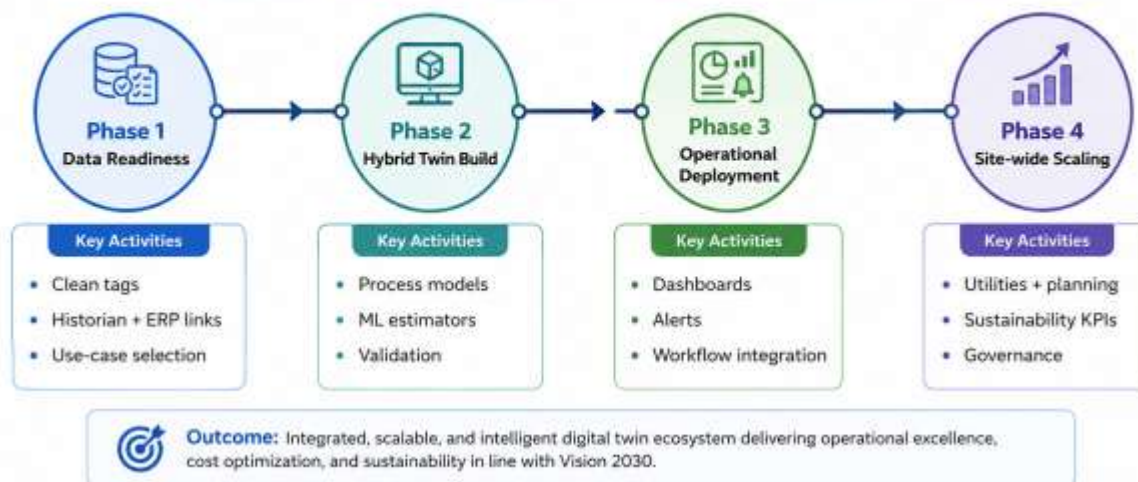


Figure 2. Phased implementation roadmap for Saudi petrochemical digital twin deployment.

REFERENCES

[1] Ali, M., Mahmood, T., & Khan, F. (2025). Review of artificial intelligence applications in sustainable chemical engineering. *Discover Sustainability*, 6, 1-32.

[2] Ansari, T., Taqvi, S. A. A., & Almansoori, A. (2024). Artificial intelligence for chemical process safety and sustainable operations: A review. *Process Safety and Environmental Protection*, 181, 1250-1268.

- [3] Aramco Careers. (2025). Process simulation twin and optimization engineer: Refinery operations and online process digital twins. Saudi Aramco Careers.
- [4] Bortz, M., Tinsley, A., & Reklaitis, G. (2024). Artificial intelligence in process industries: Current practice, limitations, and industrial opportunities. *Computers & Chemical Engineering*, 186, 108613.
- [5] Das, A., Date, A., & Alami, A. H. (2023). AI-powered approaches for water desalination and process sustainability: A review. *Desalination*, 563, 116793.
- [6] Elgarahy, A. M., Elwakeel, K. Z., & Elgarahy, A. M. (2024). Circular valorization of biowaste using AI-assisted optimization frameworks. *Journal of Environmental Management*, 362, 121004.
- [7] Goel, P., & Singh, S. P. (2024). Enterprise data integration and real-time process analytics for intelligent operations. *International Journal of Information Technology*, 16(3), 1451-1464.
- [8] Hydrocarbon Processing. (2024). Deliver sustainable benefits through site-wide process digital twins. *Hydrocarbon Processing*, 103(9), 41-47.
- [9] Jafari, M., Ghaffari, A., & Khorasani, M. (2024). Artificial intelligence for membrane separation and fouling control: State of the art and future opportunities. *Separation and Purification Technology*, 340, 127948.
- [10] Jampani, S., Cheruku, S. R., Thakur, D., Prasad, M. S. R., Kaushik, S., & Goel, P. (2023). Leveraging AI in SAP for real-time data processing. *International Journal of Progressive Research in Engineering Management and Science*, 3(11), 428-448.
- [11] Jiao, Y., Zhang, H., & Liu, X. (2021). Digital twin-driven optimization and control for intelligent industrial systems. *Journal of Manufacturing Systems*, 61, 229-243.
- [12] Karkaria, V., Skoogh, A., & Johansson, B. (2025). An optimization-centric review on integrating artificial intelligence and digital twins in manufacturing. *International Journal of Production Research*, 63(4), 1021-1048.
- [13] Kim, J., Lee, H., & Park, S. (2024). AI-assisted sustainability optimization in petrochemical process systems. *Chemical Engineering Research and Design*, 204, 357-371.
- [14] Li, X., Zhao, Y., & Chen, Q. (2024). Multiscale modelling and optimization for sustainable process operations using digital twins. *Industrial & Engineering Chemistry Research*, 63(18), 7614-7629.
- [15] Mahamod, I., Shayea, I., & Ergen, M. (2023). Intelligent optimization strategies for future industrial cyber-physical systems. *IEEE Access*, 11, 77412-77439.
- [16] Marquez, F. P. G., Schmitt, R. H., & Wang, Z. (2024). Digital twins for predictive maintenance and resource efficiency in process and manufacturing industries. *Machines*, 12(4), 221.
- [17] Meng, J., Suo, H., & Gao, L. (2023). Development and analysis of a petrochemical smart factory utilizing digital twin technology. *ESCAPE Proceedings*, 34, 1-6.
- [18] Mousavi, S. H., Mirjalili, S., & Ahmadianfar, I. (2025). Generative AI and digital intelligence for optimizing renewable and industrial energy systems. *Energy AI*, 12, 100261.
- [19] Narayanan, P., Nair, A., & Rajan, K. (2024). AI techniques for intelligent wastewater and utility management in process industries. *Journal of Cleaner Production*, 452, 142157.
- [20] Pascoschi, G., Cimini, C., & Cavalieri, S. (2024). AI-assisted energy optimization in manufacturing systems: Evidence from injection moulding and process plants. *Journal of Manufacturing Technology Management*, 35(7), 1061-1083.
- [21] Pham, T., Nguyen, M., & Tran, H. (2024). Machine learning and digital twins for circular petrochemical operations and polymer recycling. *Resources, Conservation and Recycling*, 207, 107609.
- [22] Rangel-Martinez, D., Martinez, N., & Ponce, P. (2024). Artificial intelligence in sustainable energy systems and catalysis: A review. *Energy Reports*, 10, 5168-5190.

- [23] Redchuk, A., Kliueva, I., & Boichenko, S. (2025). Industry 5.0 and digital twins in the chemical industry. *ChemEngineering*, 9(4), 78.
- [24] Rivera, J., Gomez, M., & Serrano, D. (2024). Computer-aided sustainability improvement in bioethanol and process industries. *Sustainable Production and Consumption*, 46, 437-451.
- [25] Sun, H., Diao, C., & Zhao, M. (2024). Data-centric optimization for smart chemical operations under Industry 5.0. *AIChE Journal*, 70(11), e18482.
- [26] Usman, M., Khan, M. U., & Imran, M. (2024). Artificial intelligence for sustainable treatment and separation operations in industrial wastewater systems. *Journal of Water Process Engineering*, 61, 105063.
- [27] Wang, S., Zhang, Y., & Liu, Z. (2022). Process digital twin and its application in petrochemical industry. *Journal of Service Science and Management*, 15(4), 308-321.
- [28] Xuan, Y., Li, P., & Zhao, J. (2025). Intelligent membrane and process monitoring with AI-enhanced digital twins. *Membranes*, 15(2), 131.
- [29] Zhang, H., Li, Y., & Xu, J. (2025). Artificial intelligence-enhanced digital twin systems for intelligent industry: Concepts, architecture, and optimization. *International Journal of Advanced Manufacturing Technology*, 136, 1123-1145.
- [30] Zhou, Y., Zhu, K., & Du, Z. (2024). Intelligent process digital twins for real-time optimization, diagnostics, and decision support. *Computers in Industry*, 159, 104058.