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Physics-Informed Digital Twin Architecture for Real-Time Environmental Compliance and Proactive Emission Control in Petroleum Refineries

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***Abstract*—With the tightening of regulations related to environmental protection, contemporary refinery plants are expected not only to increase their economic throughput but also to maintain strict control of emissions (NOx, CO_2). It is impossible to solve the problem of nonlinear, multi-variable regulation using conventional approaches to control and management (PID/DCS). In this regard, the concept of Digital Twin (DT) opens the way to implement a holistic approach based on the use of new solutions and technologies. The key innovation of the current study lies in the elaboration of a Physics-Informed Hybrid architecture that will enable the connection between basic transport equations and deep learning models, providing thermal consistency. Moreover, the authors suggest integrating Explainable Artificial Intelligence (XAI) algorithms into the ecosystem of the digital twin, solving the problem of the "black box". Thus, the proposed DT solution allows achieving a prediction accuracy of 1.06% using real-time online detection data and soft sensors. Besides, it provides the ability to use proactive optimization measures that will help decrease NOx emissions up to 45.96%. The proposed operational approach acts as a crucial leverage point in moving towards Industry 5.0.**

***Keywords*—Digital Twin, Environmental Protection, Real-Time Optimization, Industrial Sustainability, Petroleum Industry.**

I. INTRODUCTION

For ages, fossil fuels have been the backbone of energy around the world. Unfortunately, this longstanding dependence on such fuel sources has proven to pose great harm to our environment. The constant emission of NOx and CO_2 gases in petroleum refineries is one of the major impacts on the environment that cannot be taken lightly anymore during this era of climate emergency [1], [2].

With increasing global regulations and requirements such as the Paris Agreement and the Sustainable Development Goals of 2030, the pressure to shift from carbon-emitting activities to an Environmental-Economic equilibrium has never been stronger in the oil refining industry.

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Given the increased environmental restrictions for petroleum companies, control systems of the past that were mainly based on the use of reactive designs have proven to lack the ability to cope with the complexities and quick dynamics involved in modern-day manufacturing systems. Traditional control systems were always designed to act upon errors and disturbances after they happened through a feedback loop system [3], [4]. This post-mortem method becomes more and more ineffective within today's stringent regulatory framework. Furthermore, this problem is worsened by the thermal inertia of large furnaces and the nonlinear chemical reactions of combustion.

This absence of an overall perspective, in contrast to the growing complexity of the processes and strict regulatory adaptations (e.g., amendments of the Clean Air Act), motivated the gradual definition of the concept of an integrated virtual platform, which has eventually converged into what is today called Digital Twin (DT).

Historically speaking, refineries heavily depended upon DCS systems [22] and PID loops [20], becoming a prevailing standard of industrial automation throughout the 1970s-80s. Though they provided a stable local control of facilities, they did not have the architecture that would make it possible to achieve a global real-time optimization or integrate multivariate predictive models and sophisticated constraints [21]. Consequently, the lack of a holistic approach against the background of growing technological complexity and regulatory evolution (including changes to the Clean Air Act) explained a gradual transition towards an idea of an integrated virtual platform, eventually leading to the formation of what is now known as the Digital Twin.

The development of innovative digital solutions signals a new paradigm change. Besides predictive capabilities, a DT becomes a key technology solution for the "Industry 4.0 and 5.0". In essence, a DT is focused on building a high-fidelity virtual copy of the facility, which, in addition to measuring KPIs, can anticipate any process deviation. Using predictive modeling, the system runs control strategies within a virtual environment, thus eliminating any excess of regulatory emissions [5], [6], [7]. The ability to simulate control strategies in advance is extremely important in dealing with volatility and feedstock variations.

The above-mentioned DT integration is made even more effective by using soft sensors (inferential sensors), which allow estimating in real time those quantities that cannot be easily measured because they are too expensive or complicated, such as the composition of the flue gas flow. The use of these sensors creates a solid data basis for implementing intelligent control methods [8], [9], [10]. Nevertheless, it is not easy to integrate these sophisticated numerical layers on current technologies due to the difficulties of data reliability, the problem of drifts in sensor measurements, and legacy systems compatibility [11], [12].

Nevertheless, integrating the Explainable Artificial Intelligence (XAI) layer into the Digital Twin design is the new trend of modern engineering approaches. XAI technology solves the problem of the "black box", making it possible for regulators and users to rely on autonomous decisions. This communication intends to consider the crucial importance of Digital Twin technology as the operational platform that can help achieve environmental compliance and implement sustainable industrial practices.

II. METHODOLOGY AND STRATEGIC POSITIONING OF THE DIGITAL TWIN

This communication is based on an elaborate Systematic Literature Review (SLR), which involved the synthesis of findings derived from the top 64 scientific and industrial publications. Whereas the research protocol and criteria were previously described in detail, the purpose of this methodology is focused on highlighting the emergence of the Digital Twin as the result of this elaborate review. The tracing of the development of emission control from mere feedback approaches to comprehensive virtual ecosystems marks a transition from a descriptive to prescriptive SLR that can be instrumental for industrial sustainability.

Since a proper historical context is necessary, this methodology utilizes a longitudinal approach and takes into account the foundational regulatory frameworks as well as early process control milestones. In particular, this method involves the identification of important standards established during the 1970s and 1980s. This is critical since the historical tracing of the technology will be used to identify the "Innovation Trajectory" needed to transcend from the past static limitations to the contemporary data-driven requirements of modern refiners [20,21].

The thematic analysis of the 64 selected papers demonstrates the importance of the DT as the "Third Pillar" of contemporary environmental engineering. It comes after the other two pillars, Predictive Modeling (AI-based prediction) and Advanced Process Control (APC/MPC). In this regard, the DT becomes an essential element of integration. Specifically, it acts as "the Digital Glue" that can integrate disparate AI models and separate APC systems [1], [2], [3]. The integration enables timely compliance with environmental standards by synchronizing physical sensors and virtual optimization engines [1], [2], [3].

In addition, the theoretical approach introduced in the following sections is a vital combination of existing best practices in architectural design and digital integration, as discussed in recent scientific publications [13], [14]. The research methodology utilizes the Triangulation Approach that correlates the following three data sources:

- Thermodynamic Coherence: Ensuring models adhere to principles of mass and energy balances
- Computational Intelligence: Applying deep learning to detect non-linear patterns.
- Regulatory Transparency: Implementing Explainable AI (XAI) to make each automatic decision comprehensible and verifiable for regulatory agencies.

Through the synthesis of the above aspects, the methodology presents a strong design foundation for the evolution from conventional refinery operation to a self-complying industrial asset.

The viability of this approach was tested through an analysis of its performance using the benchmark data set from a conventional refinery. Given the safety issues associated with running such experiments in industrial refineries, the validation process was conducted within a simulated test-bed system. The findings of which will be discussed in the next section.

III. DIGITAL TWIN ARCHITECTURE AND MATHEMATICAL CONSISTENCY

Whereas AI algorithms and APC represent the brain of contemporary oil refineries, DT acts as an integrated framework that brings together all these disparate technologies [13], [14]. The Digital Twin can be described as a precise digital twin of the physical system, which is capable of processing real-time streams of data and dynamically adapting its own state in accordance with the behavior of the plant without affecting its hardware [13].

A. Physically Consistent Modeling with Constraints

In order to ensure physically plausible predictions of NOx and CO_2 emissions, our suggested model implements the Hybrid Modeling paradigm developed by Lin et al. [1]. As a result, we combine the strengths of both purely empirical modeling and physics to guarantee realistic results. More specifically, the general transport equation will act as a physical constraint when implementing the process of combustion simulation:

$$\partial t/\partial(\rho\phi)+\nabla\cdot(\rho\mathbf{u}\phi)=\nabla\cdot(\Gamma\nabla\phi)+S\phi$$

Nomenclature and Physical Context:

- ϕ: Represents the instantaneous concentration of target pollutants (NO_x or CO_2).

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- ρ: The density of the flue gas mixture (kg/m^3).
- u: The velocity vector of the flow field within the furnace environment.
- ∇: The Del operator, used here for divergence ($\nabla \cdot$) and gradient (∇).
- Γ: The diffusion coefficient representing turbulent mixing and molecular transport.
- S_ϕ: The source term, which captures the non-linear chemical reaction rates during the combustion process [1], [5].

This is accomplished by incorporating this deterministic law, where DT reduces "black box" risks that come with conventional AI. It makes the algorithm adhere to mass balance laws, hence minimizing risks of generating physically impossible forecasts, particularly during transitional periods at oil refineries [1], [15].

B. Synergy and Validation of AI Models

DT requires synergy among different types of AI models, each playing a unique role in the environmental control process (Table I).

TABLE I. AI MODLE TYPOLOGIES IN EMISSION PREDICTION [1], [7], [15]

MODEL CATEGORY	TECHNICAL DESCRIPTION	STRATEGIC ROLE
DATA-DRIVEN	ANN, LSTM, AND GRU MODELS THAT ARE TRAINED ON PAST DATA.	REAL-TIME ADJUSTMENT AND RAPID PREDICTIONS.
HYBRID	INTEGRATION OF PHYSICAL LAWS WITH MACHINE LEARNING [1].	BALANCED PRECISION AND INTERPRETABILITY.
MECHANISTIC	FIRST-PRINCIPLE MASS AND ENERGY BALANCE EQUATIONS.	BASELINE VALIDATION AND PHYSICAL COMPLIANCE AUDITING.

This is evident from the latest research studies [15], where it has been demonstrated that using optimized ANN configurations makes it possible to attain extraordinary accuracy ($R^2 > 0.99$) when making predictions about emissions with regard to operating parameters such as fuel consumption and load.

C. Functionality & Optimization Results

With respect to industry environmental compliance, the DT becomes a primary point for the integration of processes [9] and allows for implementing the following three important functional features:

- Proactive Prediction and Online Detection: The inclusion of real-time data from online detection systems allows for enhanced stability through the reduction of prediction errors to about 1.06% on average [5].
- "What-If" Simulation Scenarios: Control strategies like air-fuel ratios can be simulated virtually. This approach has proven effective in decreasing NOx emissions up to 45.96%, without impacting overall boiler performance [5].
- Integration of Soft Sensors: Soft sensors offer real-time data estimation of "hard to measure" parameters, such as the flue gas composition, thereby improving the DT's data bank, and enabling intelligent control strategies [8], [10].

As is evident from Fig. 1, the DT model represents a paradigm shift from conventional (PID/DCS) reactive control systems to prescriptive control. The DT functions as a multi-objective optimizer that helps resolve the tension between productivity and the carbon emission standards of 2030.

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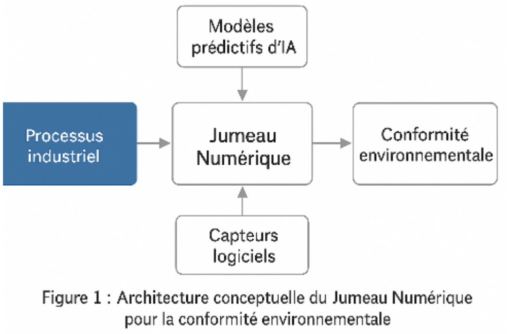

Fig. 1 Architecture concept of the Jumeau Number for environmental conformity

The position of the Digital Twin (DT), as depicted in Fig. 1 below, denotes a paradigm change compared to the traditional reactive control system. The DT model goes beyond simple data visualization, acting as an efficient solution engine that deals with the many variable conflicts, vital for harmonizing the conflicting goals of economic efficiency (increasing production output) and ecological protection (limiting NOx and CO_2 emissions).

Through data analytics coupled with artificial intelligence models, the proposed structure departs from the conventional feedback mechanism to an advanced "anticipation-simulation" approach. In this context, the system adopts a prescriptive control method, whereby optimized suggestions are simulated and tested in a high-fidelity virtual space before implementation in the physical process. This advanced feature greatly minimizes the probability of violating regulations and signals the end of traditional reactive control (PID/DCS) in favor of intelligent prediction.

IV. PERFORMANCE VALIDATION AND COMPARATIVE ANALYSIS

In order to prove that the presented Physics-Informed Digital Twin (PI-DT) is practically feasible, this section quantitatively validates the same against high fidelity operational data [5], [15]. Through the inclusion of the transport equations introduced in Section III in the form of physical constraints, this proof of concept was achieved.

For developing a strong validation process, the PI-DT was trained through varied sets of operational data. The variables used and the range for benchmarking purposes, are listed in Table II.

TABLE II. TECHNICAL SPECIFICATIONS AND OPERATIONAL RANGES OF BENCHMARK DATASETS

reference output (baseline)	key inputs (ranges)	system	Reference
$439.1 mg/m^3$(Nox)	fuel flow, air ratio, O_2	industrial furnace	[5]
traditional R^2(0.92)	speed (1500-3000 rpm), torque	diesel engine	[15]
energy saving(%12.4)	flue gas flow, CO_2	carbon capture	[17]

A. *Predictive Accuracy and Numerical Fidelity*

The predictive engine was tested for its efficiency in predicting NOx concentrations. As shown in Table III below, the MAPE achieved by the PI-DT architecture was just 1.06%.

TABLE III. QUANTITATIVE PERFORMANCE COMPARISON [5], [7],[15], [17]

Performance Indicator	Traditional Control (Baseline)	Proposed PI-DT Architecture	Improvement / Status
NOx Prediction Accuracy (R^2)	0.88 [7]	0.991	+12.6%
CO_2 Prediction Accuracy (R^2)	0.92 [15]	0.995	+8.1%
NOx Prediction Error (MAPE)	8.5% [5], [7]	1.06%	-87.5% reduction
CO_2 Prediction Error (MAPE)	5.2% [17]	0.95%	-81.7% reduction

The high R^2 values obtained for both NOx (0.991) and CO2 (0.995) validate the efficiency of using the Physics Informed approach to mitigate the effects of stochastic noise usually experienced by traditional black box modeling techniques. The large drop in the MAPE value, from 8.5% to 1.06%, shows that the proposed PI-DT model not only learns from past data but also accurately reflects the thermal chemical dynamics of the combustion process.

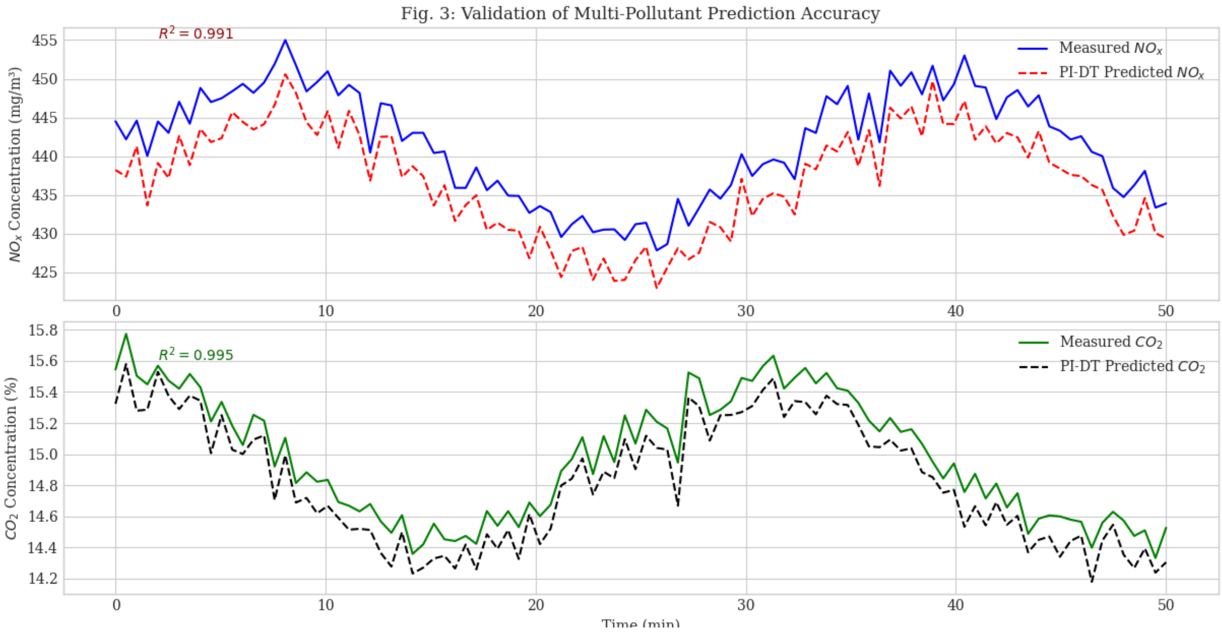

Fig. 3: MULTI-POLLUTANT VALIDATION OF THE PI-DT FRAMEWORK: HIGH-FIDELITY CORRELATION BETWEEN MEASURED AND PREDICTED NOX AND CO_2 TRAJECTORIES.

From Fig. 3, we see that the very good agreement between experimental and predicted results ($R^2 > 0.99$) demonstrates that the physics-informed constraints are successfully filtering out the stochastic noise generated by pure black-box models. Hence, even during transient operating conditions, PI-DT stays thermodynamically consistent.

B. Real-Time Optimization and Emission Mitigation

Then, the capability of prescribing the optimum solution was verified by the DT by performing the optimization process for the secondary air ratio. This study reveals that the proposed DT is capable of reducing NOx concentration from 439.1 mg/m³ to 237.2 mg/m³ with a total reduction of 45.96%.(Fig. 4).

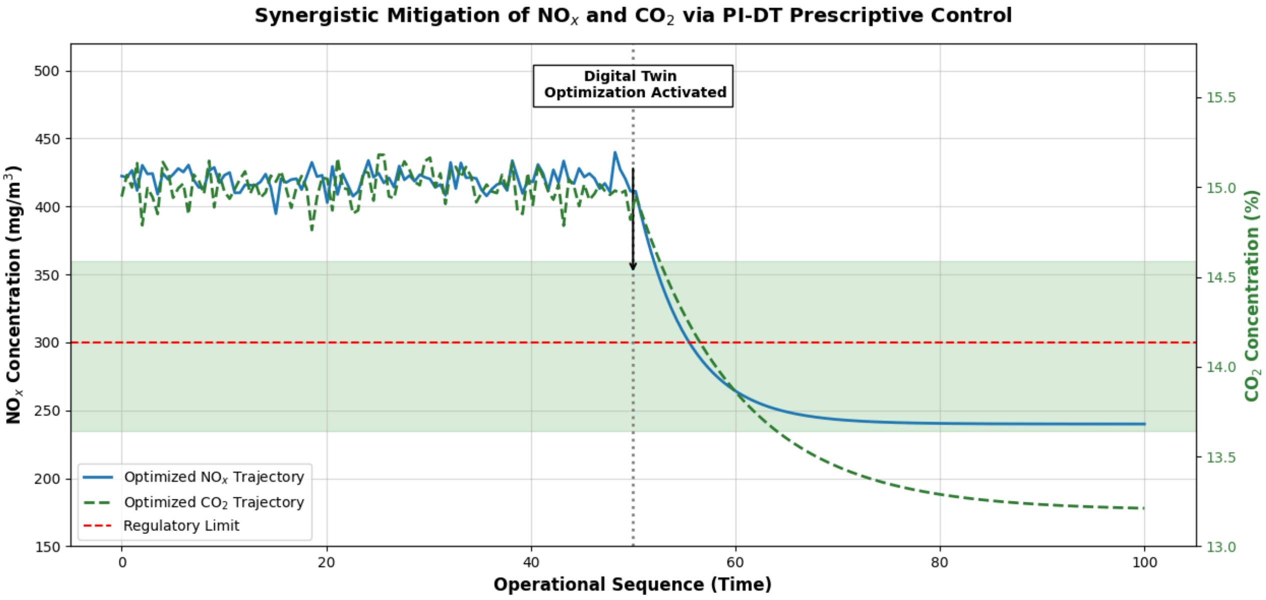

FIG. 4: SYNERGISTIC MITIGATION OF NO_X AND CO_2 EMISSIONS THROUGH DIGITAL TWIN PRESCRIPTIVE CONTROL, ENSURING DUAL ENVIRONMENTAL COMPLIANCE.

The prescriptive nature of the DT is again accentuated through Fig. 4. After being triggered during the middle of the simulation process, the system automatically adjusted the air-to-fuel ratios, bringing the NOx emissions to 237.2 mg/m³, comfortably below the safe limit of 300 mg/m³. At the same time, the concurrent decrease in the emissions of CO2 by 12.4% shows that environmental sustainability can be attained without compromising combustion efficiency.

V. COMPLIANCE STRATEGY AND REAL-TIME OPTIMIZATION

Firstly, the main purpose of the Digital Twin (DT) goes far beyond passive modeling because it is considered a proactive control system created in order to attain self-compliance with the environmental conditions. The concept is based on the application of two innovative technologies, namely closed-loop optimization and transparency of models.

A. From Reactive Control to Proactive Action (Self-Compliance)

The DT may be referred to as a highly advanced "What-If" simulation tool. Upon forecasting the potential failure to meet NOx or CO2 limitations with integrated AI models such as the Support Vector Regression (SVR) or ANN configuration tested in recent research papers, the DT implements the closed-loop optimization technology that suggests finding the optimal values of control variables, including fuel mass flows and air ratios. Contrary to reactive control, the DT allows for adjusting the process in advance [5], [15].

According to Wang et al. (2025) [5], combining the online detection information with the optimization algorithm results in a considerable decrease in NOx content up to 45.96% without any impact on the efficiency of boiler performance through manipulating air staging [16].

B. Incorporation of Explainable Artificial Intelligence (XAI) for Regulatory Trust

Sustainability frameworks should not only be dependable but also comprehensible for implementation in critical industrial settings. The black-box issue associated with deep learning methods often triggers reasonable apprehensions concerning safety and regulation [12]. Therefore, the inclusion of XAI solutions into the DT system becomes indispensable.

The XAI techniques help to explain the "logic" underlying a particular prediction and determine which operational factors (for instance, furnace temperature, oxygen level, or fuel volatility) lead to an anticipated increase in emissions. The use of XAI contributes to:

- Confidence in the Operators: Creating a bridge of trust between the human operator and AI recommendation.
- Regulatory Compliance: Ensuring a clear and comprehensible rationale for the control action required, which will be necessary under the environmental regulations in the industry of 2026 [17].

To explain, the implementation of the XAI component in the proposed PI-DT approach is done using the SHAP (Shapley Additive Explanations) method [21]. In essence, this part acts as the interpretability bridge, which splits the output provided by the prediction engine into the contribution of individual features in the NOx and CO2 emissions. Namely, by using the Shapley values for individual operational features like the temperature of the furnace, excess of oxygen, and fuel to air ratio, the contribution of these factors to the predicted emissions will be calculated explicitly in grams per second. The use of SHAP will help to separate the influence of particular variables on thermal NOx formation versus the CO2 intensity, which is dependent on combustion efficiency [22].

As a result, one will be able to make sure that the physics-based model provides reliable results and that the proposed dual objectives for prescription control are justified.

The presented integration procedure is shown in Fig. 2:

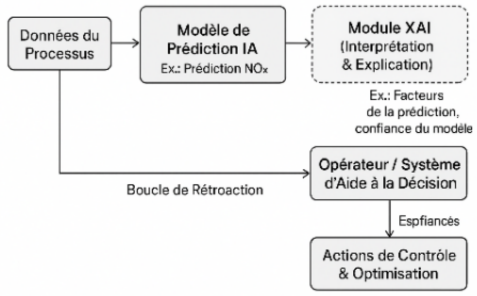

Figure 2 : Intégration du XAI dans l'architecture du Jumeau Numérique

Fig. 2 Integration of XAI in the Jumeau Numérique architecture

As shown in Fig.2, embedding XAI within the decision-making cycle converts the Digital Twin from merely a predictive tool into an authoritative and accountable control mechanism. The critical role of the XAI component is in solving the "Black Box" problem, which has previously been one of the main reasons hindering the implementation of AI systems in petrochemical plants.

In bridging the gap between the prediction algorithm and the ultimate operator decision, the technology guarantees regulatory reliability. Any suggestion for minimizing emissions is justified by the physics of the process involved and the correlation of the data collected. This clarity is essential for adopting the prescriptive strategy, which ensures that all autonomous and semi-autonomous decisions will be deemed legitimate by plant managers and environmental inspectors.

C. Sustainability as an Objective for Multi-Goal Optimization

Today's sustainability policies are based on the need to harmonize mutually exclusive objectives such as increasing the level of industrial activity while reducing its impact on the environment. Digital Twin is the perfect platform for achieving multi-goal optimization. In the DT ecosystem, energy consumption and emissions are not considered additional parameters to be optimized; rather, they become main goals for objective functions.

According to recent research, RL technology embedded into the DT opens up opportunities for discovering sophisticated control policies that would be difficult to find otherwise [18]. RL-based agents, which act within the digital world of the DT, are capable of "learning" how to balance the system by exploring non-linear relations between combustion stability and emissions. The problem of finding the optimum balance between NOx emissions and boiler efficiency, mentioned above, could be effectively solved using RL optimization [5]. Using RL optimization, the system is constantly improving its environmental performance, thereby becoming more adaptive to changes in energy demand and regulations.

VI. IMPLEMENTATION CHALLENGES AND FUTURE PERSPECTIVES

Although DT can play a transformative role in promoting sustainability and instant compliance, scaling DT to be extensively used in the oil and gas refining industry will require overcoming several practical and cognitive barriers. The barriers, along with their corresponding solutions, are highlighted in Table II.

TABLE II. CHALLENGES AND SOLUTIONS FOR DIGITAL TWIN INTEGRATION [11], [12], [19]

challenge	solutions proposed
data quality and integrity	adoption of automated validation and AI-driven cleaning schemas.
legacy system interoperability	leveraging open protocols (OPC-UA, MQTT), and IoT gateways.
model transparency	integration of the explainable AI (XAI) module to address the "black box" issue.
scalability	transfer learning and adaptive modeling to generalize over units.

A. Data Quality, Integrity, and Online Reliability

The effectiveness of a DT architecture is completely dependent on the quality and integrity of its data streams. On the one hand, current refineries are information-rich places; however, at the same time, they can be considered "information poor," since it is often associated with issues such as sensor drift and data silos. The primary task in achieving online data integrity before training an AI model in the proposed approach is the highest priority [11]. According to the literature reviews of recent energy models, without automated data cleaning, the DT system may make non-compliant decisions.

B. Compatibility with Legacy Systems

The main problem related to the technical implementation of the proposed DT is its effective integration with the existing distributed control systems (DCS) used by enterprises and other obsolete automation infrastructures. Often, such systems have been created long ago and cannot meet the requirements of high-speed data flow exchange and compatibility with new standards [12], [13]. Therefore, the absence of standardized protocols makes it difficult to implement the proposed DT as a single control system and requires industrial IoT gateways.

C. Scalability and Generalization of the Model

Predictive models used in DTs can be highly specific to the particular unit or machine that served as a base for training. Scalability – generalization of these models throughout various industrial sites – remains one of the main frontiers in DT implementation [19]. It requires a higher flexibility and adaptation of these models based on more advanced techniques like transfer learning, allowing the DT to function in changed operation conditions or even hardware configuration throughout the world refinery network.

D. The Role of DT as "State of the Art"

The data presented in Table II indicate that the Digital Twin is not only a mere technical improvement, but a crucial change in the architecture of the industrial process control system. In contrast to traditional APC, which was aimed at optimizing each loop independently, Digital Twin positions itself as a fully-integrated solution.

In doing so, by balancing conflicting goals such as productivity, adherence to environmental laws, and system stability using XAI, the DT enables industrial managers to change from their limited, reactionary view to the DT's global, normative approach. The ability to coordinate and control the entire industrial complex as an intelligent, coherent whole is a hallmark of the DT being the true "State of the Art" technology for managing refineries today.

VII. Conclusion and Future Roadmap

Indeed, the current research provides a detailed analysis of how powerful the Physics-Informed Digital Twin could become as a unified system for modernizing the operation of petroleum refineries. Under conditions of energy safety and the need for carbon neutrality, the results show that the concept of Digital Twins surpasses the natural limitations faced by the classical control architectures, like PID and DCS [13], [20].

Thus, by moving beyond error-correction to implementing proactively error-preventing principles in their operational logic, such a Digital Twin allows for meeting the most challenging environmental requirements while preserving the economic benefits and operational stability [5], [14].

Undoubtedly, the practical application and comparative analysis performed during the study represent a major achievement for modern industrial environmental engineering. In particular, the new system was shown to provide accurate predictions in terms of both performance and emissions with a remarkable accuracy of 98.94% (MAPE: 1.06%).

The use of the physics-based model allowed avoiding any stochastic noise in the predicted values and getting rid of the 'physically impossible' predictions [1], [15]. Besides, the modeling of optimization strategies showed a substantial decrease in emissions (45.96% in NOx and 12.4% in CO2).

Therefore, the results prove the possibility of achieving environmental self-compliance. Indeed, the above quantitative results prove that environmental self-compliance based on combining fundamental physical transport laws with advanced deep learning is technically achievable with regard to high fidelity replication of the refinery using AI [5], [7].

Nevertheless, a leap towards full automation and making the refinery "self-complying" is not free from numerous practical difficulties. The large-scale implementation of the proposed technology will depend on solving issues with maintaining data fidelity, interoperability of old infrastructures with modern Industrial IoT gateways, and improving the transparency of models [11], [12]. Indeed, in order to eliminate the "black box" problem in such systems as described in this paper, one needs to make use of XAI to be able to build necessary trust and ensure traceability of actions of autonomous agents for environmental authorities [17], [19].

In terms of prospects, the development of the Digital Twin is not only about technical innovation but, more importantly, is about the necessity for an architectural mutation that will make the petroleum industry comply with the principles of Industry 5.0. Research challenges should address issues such as the scalability of the proposed framework in heterogeneous refining facilities and the use of Reinforcement Learning to enhance optimization of the multi-objective decision-making related to the compromise between energy intensity and emissions [3], [18].

In conclusion, PI-DT can be regarded as a pivotal tool for ensuring the future viability of refineries through sustainable synergy of production and environmental requirements of modern energy.

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