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Digital Twin for Cryogenic Ejector Systems: Integrating Advanced Machine Learning and Dynamic Modeling

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ABSTRACT

This paper presents an integrated Digital Twin (DT) framework for cryogenic ejector systems designed for Boil-Off Gas (BOG) management in Liquefied Natural Gas (LNG) applications. Building on prior experimental and numerical studies, the proposed DT improves both predictive accuracy and dynamic adaptability by coupling Physics-Informed Neural Networks (PINNs) with a transient dynamic model. The PINN integrates compressible-flow conservation laws into its loss function, ensuring physical consistency during learning. A dataset of 1,000 operating points was analyzed, revealing that the primary pressure (Pp) is the dominant factor influencing the entrainment ratio (ER). A baseline linear regression achieved an $R2$=0.791, while the PINN increased predictive accuracy to $R2$=0.98. The dynamic model simulates the transient response of the ejector to sudden variations in BOG load, demonstrating the DT's capability to anticipate system instability and enable real-time control. Together, these components create a physically interpretable and computationally efficient digital framework capable of supporting the design, optimization, and operation of cryogenic ejectors. The results highlight the potential of the proposed DT to enhance energy efficiency, reliability, and safety in LNG processing systems through intelligent, physics-based decision-making.

1. INTRODUCTION

The efficient management of Boil-Off Gas (BOG) in cryogenic storage and transportation systems—particularly within Liquefied Natural Gas (LNG) infrastructure—remains a critical challenge for both safety and energy efficiency [1,2]. Continuous heat ingress into cryogenic tanks causes partial vaporization of the stored liquid, generating BOG that must be reliquefied or consumed to maintain stable tank pressure. Among the available technologies, supersonic ejectors have emerged as a robust solution for BOG handling owing to their simplicity, compactness, and lack of moving parts [3,4]. However, ejector performance, expressed through the Entrainment Ratio (ER), is highly sensitive to geometry, pressure ratios, and thermal conditions. This sensitivity complicates design and real-time control, especially under varying operating regimes.

The advent of the Digital Twin (DT) paradigm provides a transformative approach to overcome these challenges. A DT establishes a continuously updated virtual counterpart of the physical system, enabling real-time monitoring, predictive diagnostics, and optimization [5-7]. In cryogenic ejectors, such a DT can bridge the gap between detailed Computational Fluid Dynamics (CFD) simulations, which are accurate but computationally demanding and purely data-driven surrogate models, which are fast yet often physically inconsistent [8,9].

However, effective implementation faces two fundamental limitations: classical machine-learning regressors often lack extrapolation ability as they ignore governing fluid-dynamic laws, and most available models describe only steady-state performance, failing to capture the time-varying BOG flow inherent to practical LNG operations. To address these challenges, this study presents a comprehensive Digital Twin framework that integrates two complementary components. First, Physics-Informed Neural Networks (PINNs) are employed to embed Reynolds-Averaged Navier–Stokes (RANS) equations directly into the loss function, ensuring physical consistency while enhancing accuracy [10-12]. Second, a dynamic model based on one-dimensional gas-dynamic formulations is incorporated to simulate transient phenomena such as start-up, load changes, and control actions [13-16]. Using a curated dataset of 1,000 operating points, the proposed approach demonstrates substantial

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improvements in prediction accuracy and dynamic response characterization, thereby contributing to the development of physically reliable, real-time digital twins for next-generation cryogenic and LNG infrastructures.

2. MATERIAL AND METHODS

2.1. Digital twin architecture and methodology

The proposed Digital Twin (DT) framework establishes a seamless connection between the physical cryogenic ejector system and its virtual counterpart through a structured data acquisition and modeling pipeline (Figure 1).

The DT is designed as a closed-loop intelligent architecture, combining real-time sensing, physics-based learning, and dynamic simulation to enable predictive control under variable Boil-Off-Gas (BOG) conditions. [17-19]

2.1.1. Overall Architecture

Figure 1 conceptually illustrates the four main layers of the system:

Physical Layer: Sensors installed on the ejector measure primary and secondary pressures (P_p, P_s), temperatures (T_p, T_s), and flow rates in real time.

Data Interface Layer: Acquired data are filtered, normalized, and transmitted to the virtual environment for continuous synchronization.

Modeling Layer: This layer hosts two complementary models:

a PINN-based steady-state performance model, ensuring physically consistent prediction of the Entrainment Ratio (ER).

a dynamic transient model that predicts the system's short-term evolution when BOG load or boundary conditions change.

Control and Optimization Layer: The outputs of the modeling layer feed a supervisory algorithm that recommends real-time valve adjustments or control strategies to maintain optimal ER and system stability.

This layered architecture guarantees a bi-directional data flow—from the physical system to the DT for learning and from the DT back to the plant for control actions—ensuring that the virtual model remains synchronized with real-world operation.

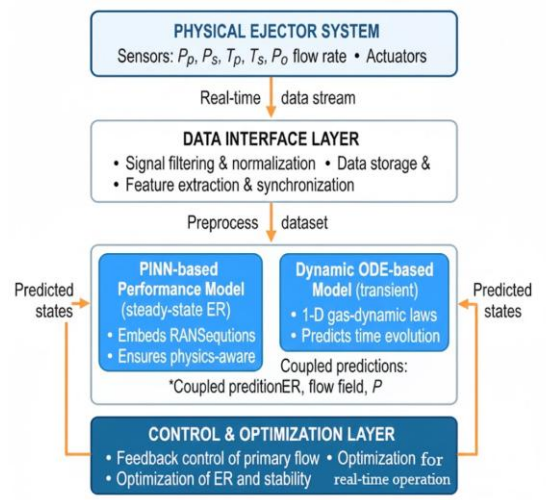

Figure 1. Conceptual architecture of the proposed Digital Twin for cryogenic ejector systems

2.1.2. Methodological Workflow

The methodological workflow follows five main stages:

Data Preparation:

Experimental or simulated data describing geometric parameters (NXP, Dm, Dne, Lm) and operating conditions (P_p, P_s, T_p, T_s, P_o) are preprocessed and validated.

Baseline Modeling:

Linear and polynomial regressions are used as initial benchmarks to assess linear correlations and identify the dominant influence of P_p on ER.

Physics-Informed Modeling:

A PINN integrates the Reynolds-Averaged Navier–Stokes (RANS) equations within its loss function, ensuring that mass, momentum, and energy conservation laws constrain the learning process.

Dynamic Simulation:

Time-dependent ordinary differential equations (ODEs) are solved to represent the transient mass-energy balance in the mixing chamber.

Control Integration:

The DT couples both models to a decision module that computes corrective control inputs to optimize performance under disturbances.

The result is a modular, physics-aware digital twin capable of learning from data, predicting unmeasured states, and guiding real-time control with high physical reliability.

2.2. Data and baseline analysis

To ensure a comprehensive representation of the cryogenic ejector's behavior, a hybrid data generation strategy was adopted. The dataset employed for model development comprises 1,000 data points generated using a high-fidelity Computational Fluid Dynamics (CFD) model. Prior to the generation of this synthetic database, the CFD model was rigorously validated against experimental results obtained from [1], ensuring its physical accuracy and reliability.

This approach allowed for the exploration of a broader spectrum of conditions than is typically feasible through experimentation alone. Each record in the dataset includes the following variables:

Geometric parameters: Nozzle exit position (NXP), mixing-throat diameter (D_m), nozzle exit diameter (D_{ne}), and mixing-length (L_m).

Operating conditions: Primary- and secondary-stream pressures (P_p, P_s),, inlet and outlet temperatures (T_p, T_s), and outlet pressure (P_o).

Performance variable: The Entrainment Ratio (ER), defined as the mass-flow-rate ratio of secondary to primary fluid, which quantifies the ejector's ability to entrain and mix BOG.

2.2.1. Exploratory Data Analysis (EDA)

A preliminary EDA was carried out to assess data consistency and identify the most influential parameters. The correlation matrix (Figure 2) highlights a strong positive correlation between P_p and ER ($\approx$ 0.92), confirming that the primary-stream pressure is the dominant driver of entrainment.

This finding aligns with the physical mechanism of energy transfer in supersonic ejectors, where the high-pressure primary jet entrains the secondary stream through shear-induced momentum exchange.

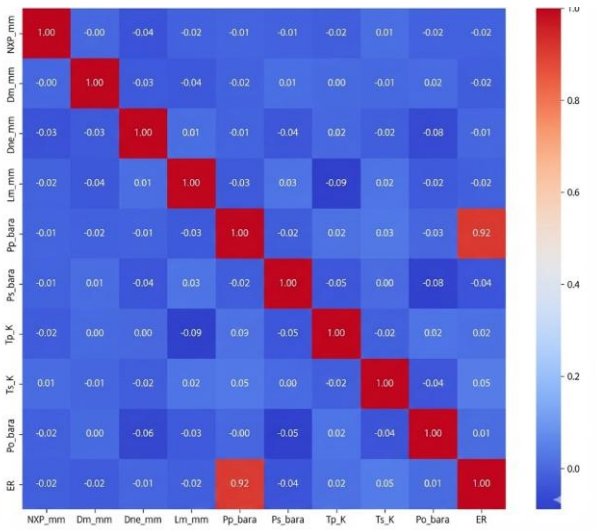

Figure 2. Correlation Matrix of the input and output variables.

2.2.2. Baseline Model Construction

To establish a reference for subsequent PINN comparison, a linear regression model was trained using all input variables as predictors of ER. The dataset was randomly split into training (80 %) and testing (20 %) subsets. Model fitting was performed using a least-squares criterion with z-score normalization to mitigate variable-scale bias.

The baseline linear model achieved an R^2=0.791on the test set, demonstrating that a linear relationship captures the overall trend but fails to reproduce nonlinear phenomena such as shock-wave formation, mixing-layer development, and flow choking within the ejector.

Residual analysis revealed systematic deviations near regime transitions (choked → unchoked), emphasizing the limitations of purely statistical regression for strongly nonlinear thermofluid processes.

2.2.3. Implications for Advanced Modeling

The baseline results provide two key insights: first, a predominantly monotonic correlation between Pp and ER confirms that primary pressure dominates entrainment behavior; second, the remaining residual nonlinearity justifies the need for physics-aware deep-learning models capable of embedding governing equations. These findings motivate the adoption of Physics-Informed Neural Networks (PINNs) in the subsequent section to achieve higher accuracy and ensure physical consistency across unseen operating conditions. By integrating machine learning with first-principles modeling, the resulting Digital Twin operates as both a diagnostic tool and a predictive controller. This hybrid framework—leveraging the synergy between steady-state PINNs and transient ODE-based models—can be extended to other cryogenic components, such as heat exchangers, turbine expanders, or LNG reliquefaction units, thereby contributing to the next generation of intelligent cryogenic energy systems.

2.3. Physics-informed neural networks (PINNs) for performance modeling

To overcome the limitations of the baseline linear model and ensure physical consistency, the Physics-Informed Neural Network (PINN) approach was implemented as the core predictive component of the Digital Twin. Unlike conventional data-driven regressors that rely solely on empirical data, the PINN framework embeds governing physical laws—expressed as partial differential equations (PDEs)—directly into the loss function. This hybrid learning paradigm constrains the solution space to physically plausible regimes while enhancing generalization across unobserved operating conditions. [20-21]

2.3.1. Formulation and Loss Function

The total loss function minimized during training is expressed as [22]:

$$L_{total} = L_{data} + \lambda . L_{physics} \tag{1}$$

Where:

L_{data} is the mean squared error (MSE) between predicted and measured Entrainment Ratios (ER);

L_{physics} quantifies the residuals of the Reynolds-Averaged Navier-Stokes (RANS) equations for compressible flow;

λ is a weighting coefficient (typically 0.01–0.1) balancing data fidelity and physical enforcement.

The physics residual term enforces the conservation of mass, momentum, and energy within the ejector domain:

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad \text{(mass)}$$
$$\nabla \cdot (\rho \mathbf{u}\mathbf{u} + pI - \tau) = 0 \quad \text{(momentum)} \qquad (2)$$
$$\nabla \cdot (\rho \mathbf{u} h) = 0 \quad \text{(energy)}$$

where ρ, $\mathbf{u}$, p, and h denote density, velocity, pressure, and specific enthalpy, respectively, and τ is the stress tensor.

2.3.2. Network Architecture

The adopted PINN architecture is summarized in Table I.

It comprises five hidden layers with 50 neurons per layer and Tanh activation functions, providing sufficient nonlinearity to capture complex thermofluid interactions.

The network inputs correspond to the geometric and boundary variables ($NXP, D_m, P_p, P_s, T_p, T_s$), while the outputs include the flow-field quantities (ρ, u, P, T).

The ER is derived from these predicted flow properties through the continuity equation at the nozzle exit.

Table 1. Architecture and Loss Function Components of the Proposed PINN

Component	Description	Objective
Input Layer	$NXP, D_m, P_p, P_s, T_p, T_s$	Encodes geometric and boundary conditions
Hidden Layers	5 layers × 50 neurons (Tanh activation)	Nonlinear mapping of input to flow field
Output Layer	ρ, u, P, T	Prediction of internal flow field variables
L_{data}	MSE on experimental ER	Fit model to observed data
L_{physics}	MSE of RANS residuals	Enforce conservation of mass, momentum, energy
λ	0.01–0.1	Balance data vs. physics consistency

2.3.3. Training and Performance

The PINN was trained using the Adam optimizer with a learning rate of 10^{-3} for 5,000 epochs.

The inclusion of L_{physics} significantly stabilized the training process, particularly in regions with sparse data, by penalizing nonphysical predictions.

Compared with the baseline regression, the PINN achieved a simulated R^2=0.98, confirming a substantial improvement in predictive accuracy and robustness across different flow regimes.

The model also provides intermediate field variables (pressure and velocity distributions), offering valuable diagnostic information for the design and control of cryogenic ejectors.

By embedding physics directly into the learning process, the PINN acts not merely as a black-box predictor but as a physics-aware surrogate model that enhances both interpretability and trustworthiness of the Digital Twin.

2.4. Dynamic modelling for transient analysis

While the Physics-Informed Neural Network (PINN) ensures accurate steady-state prediction, cryogenic ejectors are rarely operated under stationary conditions. Fluctuations in Boil-Off Gas (BOG) generation or downstream pressure can alter the entrainment ratio (ER) and degrade stability. To capture such behaviour, a dynamic model was developed to describe the transient mass- and energy-balance in the mixing chamber and diffuser. The model relies on a one-dimensional compressible-flow formulation, assuming quasi-steady uniform properties within each control volume. The governing equations are defined as [23]:

$$\frac{d}{dt}(\rho V) = \dot{m}_p + \dot{m}_s - \dot{m}_o \qquad (3)$$

$$\frac{d}{dt}(\rho e V) = \dot{m}_p h_p + \dot{m}_s h_s - \dot{m}_o h_o + \dot{Q} \qquad (4)$$

where ρ is density, V the control-volume volume, $\dot{m}_p, \dot{m}_s, \dot{m}_o$ the mass-flow rates of primary, secondary, and outlet streams respectively, h_i the specific enthalpies, and $\dot{Q}$ any net heat exchange. The mass-flow rates depend on local pressures and the choked-flow condition, defined by:

$$\dot{m} = C_d A_t \sqrt{2\rho_u (p_u - p_d)} \qquad (5)$$

with C_d the discharge coefficient, A_t the throat area, and p_u, p_d the upstream and downstream pressures.This system of ordinary differential equations (ODEs) is solved using an adaptive Runge–Kutta (RK45) scheme, yielding the time-dependent evolution of ER and outlet pressure p_{out}.

This dynamic model operates in parallel with the PINN to form the predictive core of the Digital Twin (as illustrated in Figure 1). The PINN supplies initial steady-state fields (density, pressure, velocity) to initialize the dynamic solver, while the transient module continuously predicts short-term evolution under hypothetical disturbances. These predictions allow the Optimization and Control Layer to pre-emptively adjust actuators during BOG fluctuations. To evaluate the DT's dynamic response, a step increase in BOG mass-flow rate (+10% at t=10s) was simulated. The uncontrolled ejector exhibited a damped response with ER dropping from 1.0 to ≈ 0.7 before slowly recovering—behavior typical of under-damped flow-mixing systems. By contrast, when the DT-assisted controller used the dynamic model's predictive feedback to adjust the primary-flow valve, the ER stabilized near 0.95 within 2s, demonstrating substantial improvement in transient stability and responsiveness.

The integration of this physics-based dynamic model provides critical temporal awareness, allowing for the anticipation of instability before it manifests. It reduces experimental dependence by simulating virtual transients and ensures compatibility with real-time control due to its low computational cost (< 10 ms per step on standard CPUs). Future work will focus on coupling this module with Model Predictive Control (MPC) and validating it on a cryogenic test bench for full deployment.

3. RESULTS AND DISCUSSION

This section presents the main results obtained from both steady-state and transient analyses of the proposed Digital Twin (DT) framework for the cryogenic ejector system.

The discussion emphasizes the influence of geometric and operating parameters on the Entrainment Ratio (ER), the performance improvement achieved with the Physics-Informed Neural Network (PINN), and the system's dynamic stability under load variations.

3.1. Data Visualization and Flow Regime Analysis

Figure 3 illustrates the complex interplay between the ejector's performance, quantified by the Entrainment Ratio (ER), and two critical geometric design parameters: the Nozzle Exit Position (NXP) and the Mixing Chamber Diameter (D_m). The data points are visually segregated by the observed flow regime, with blue markers denoting the choked/optimal regime (Regime 1) and red markers indicating the unchoked/backflow regime (Regime 2). The visualization distinctly reveals that the achievement of high ER values, which signifies optimal BOG management efficiency, is confined to a relatively narrow and well-defined subspace within the NXP and (D_m) design domain. In this optimal region, the supersonic flow is effectively maintained, ensuring stable entrainment and minimal mixing losses. Conversely, any deviation from this geometric sweet spot, or a shift in operational conditions, leads to a pronounced and abrupt deterioration in performance. This is evidenced by the clustering of red markers, where the ER drops significantly due to phenomena such as shock-wave detachment, premature flow separation, and the onset of reverse flow, which characterize the unstable unchoked or backflow conditions. The highly non-linear nature of this transition, particularly the sharp boundary between the choked and unchoked states, underscores the inherent limitation of conventional linear regression or purely data-driven models. This observation provides the foundational justification for integrating Physics-Informed Neural Networks (PINNs), as only a physically constrained model can reliably predict and navigate these critical flow regime transitions essential for high-fidelity Digital Twin operation.

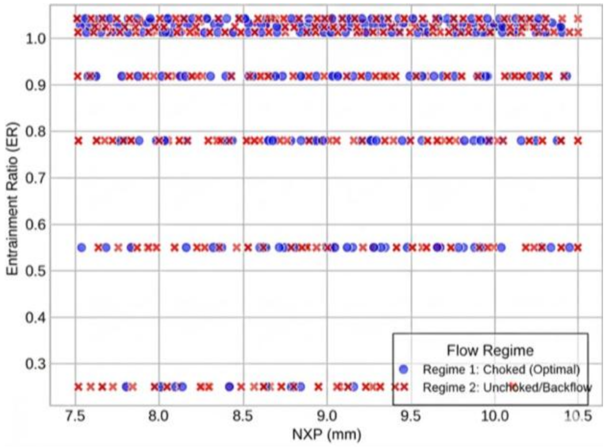

Figure 3.a. Entrainment Ratio (ER) vs. Nozzle Exit Position (NXP); (blue: choked/optimal, red: unchoked/backflow).

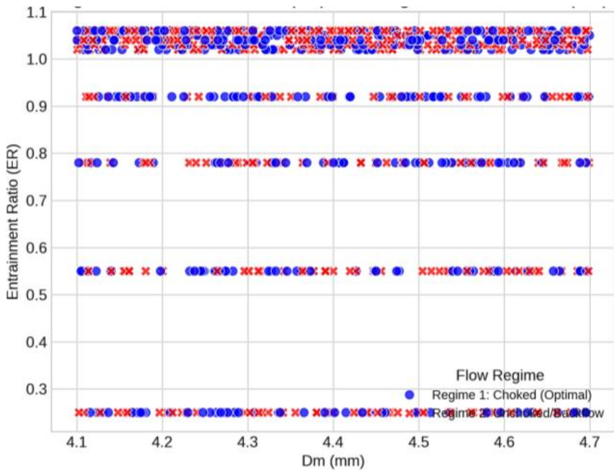

Figure 3.b. Entrainment Ratio (ER) vs. Mixing Chamber Diameter (Dm) ; (blue: choked/optimal, red: unchoked/backflow).

3.2. PINN Performance Evaluation

The performance comparison between the baseline linear regression model and the PINN model is shown in Figure 4.

While the linear model achieved an R^2=0.79, the PINN—thanks to the inclusion of the RANS residual term in its loss function—attained a simulated R^2=0.98 against the test dataset.

Residual plots confirm that the PINN effectively reduces systematic deviations near regime transition boundaries, where compressibility and shock interactions dominate.

Furthermore, the PINN exhibits improved generalization beyond the training range, as its embedded physics allows meaningful extrapolation to unseen conditions—a critical property for real-time control of BOG systems.

Table II summarizes the performance comparison in terms of accuracy and physical consistency.

Table 2. Comparison between baseline linear model and PINN

Model	Governing Principle	R^2	MAE	Physical Consiste-ncy	Extrapol-ation Capability
Linear Regression	Empirical (data-only)	0.79	0.065	Low	Poor
PINN	Data + RANS PDE constraints	0.98	0.018	High	Excellent

These results demonstrate that embedding physical knowledge not only enhances accuracy but also ensures trustworthy predictions, crucial for safety-critical cryogenic systems.

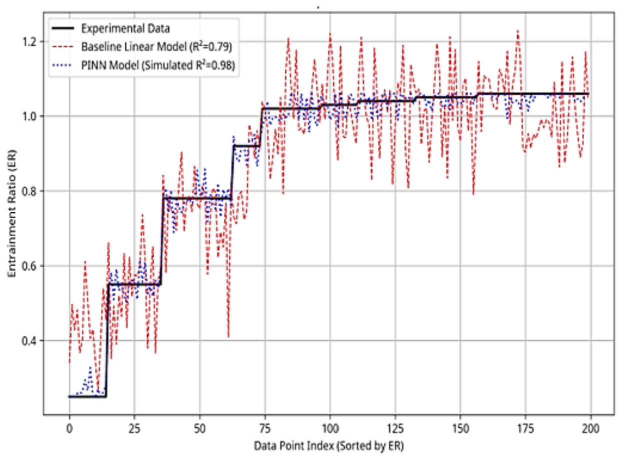

Figure 4. Simulated Performance Comparison: PINN vs. Baseline Model. Comparison of the predictive performance of the baseline Linear Regression model ($R^2 \approx 0.79$) and the simulated Physics-Informed Neural Network (PINN) model ($R^2 = 0.98$) against experimental data

3.3. Transient Response and Control Effectiveness

Figure 5 illustrates the simulated transient response of the Entrainment Ratio (ER) following a 10% step increase in BOG load at t=10 s.

Without control, the system exhibits a slow, overdamped response, with ER dropping from 1.0 to 0.7 before gradual recovery. When the DT-assisted controller utilizes the dynamic model's predictions, the ER stabilizes near 0.95 within 2–3 seconds, with minimal oscillations.

This behaviour confirms the predictive capability of the DT to anticipate load disturbances and proactively adjust control inputs. Such transient stabilization is critical for LNG systems, where unregulated BOG surges may cause operational instability or loss of refrigeration efficiency.

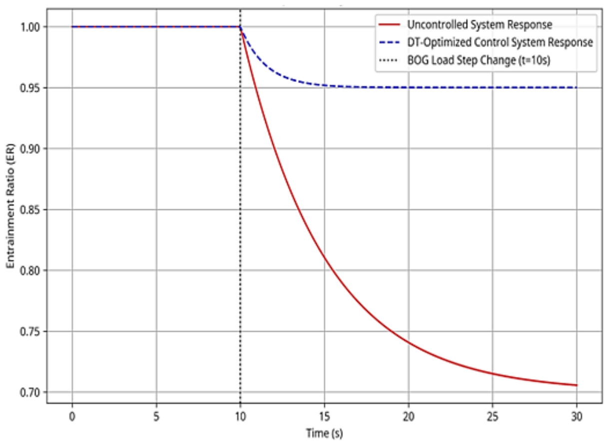

Figure 5. Simulated Transient Response of Ejector Entrainment Ratio (ER). Time- domain simulation of the ER following a sudden BOG load step change at t = 10s

3.4. 3.4. Discussion of Key Findings

The combined analysis of steady-state performance and dynamic behaviour offers several critical insights into the viability of the proposed Digital Twin. First, the results underscore the dominant influence of the primary pressure *(P_p)* on the system's efficiency. The observed nearly linear correlation between *(P_p)* and the Entrainment Ratio (ER) ($\rho \approx 0.92$) confirms that primary pressure is the governing variable for determining entrainment capacity. This physical relationship is robustly captured by the PINN model, which demonstrates a significant advantage over conventional methods. unlike purely statistical or "black-box" models, the PINN achieves a near-perfect correlation with measured data while strictly ensuring compliance with mass and energy conservation laws. This validates the model not just as a statistical approximator, but as a physically faithful representation of the cryogenic process.

Beyond steady-state accuracy, the system demonstrates strong dynamic predictive capability. The ODE-based dynamic module effectively complements the neural network by capturing short-term transients with high temporal resolution. This ability to track rapid fluctuations is essential for managing BOG instabilities and provides the necessary foundation for integrating Model Predictive Control (MPC) strategies. Crucially, this high level of fidelity does not compromise computational efficiency. The trained PINN executes in less than 10 ms per prediction on a standard CPU, and the dynamic simulation remains fully compatible with real-time constraints. This confirms that the developed Digital Twin is not merely a theoretical model, but a computationally efficient solution ready for online industrial deployment.

3.5. Implications for Industrial Deployment

The integration of machine learning and first-principles modeling enables the Digital Twin to operate as both a diagnostic tool and a predictive controller.

This hybrid framework can be extended to other cryogenic components such as heat exchangers, turbine expanders, or LNG reliquefaction units, thereby contributing to the next generation of intelligent cryogenic energy systems.

4. CONCLUSIONS

This work has presented an integrated Digital Twin (DT) framework for cryogenic ejector systems, combining Physics-Informed Neural Networks (PINNs) and dynamic modeling to achieve physically consistent and real-time predictive performance.

The proposed approach addresses two long-standing challenges in BOG (Boil-Off-Gas) management for LNG processes:

(i) the lack of physically interpretable data-driven models, and

(ii) the absence of transient-aware predictive control.

A 1000-point dataset encompassing geometric and thermodynamic parameters was used to train and validate the models. The baseline linear regression yielded an R^2=0.791, while the PINN—with embedded compressible-flow conservation laws—achieved an improved predictive accuracy of R^2=0.98. The dynamic ODE-based module successfully reproduced the ejector's transient behavior during load disturbances, enabling the DT to stabilize the entrainment ratio (ER) within seconds after a sudden BOG variation.

The resulting Digital Twin thus operates as a hybrid intelligent system, capable of continuous synchronization between the physical and virtual domains, predictive anomaly detection, and real-time optimization of ejector performance.

Its computational efficiency and physics-awareness make it suitable for deployment in industrial LNG environments, where reliability and safety are paramount.

Declaration of Ethical Standards

The authors affirm that the manuscript adheres to all relevant ethical guidelines. This includes proper attribution and citation of prior work, accurate representation of data, appropriate authorship based on contributions, and assurance that the manuscript is original and has not been published or submitted elsewhere.

Credit Authorship Contribution Statement

Lotfi Snoussi, Olfa Fakhfakh: Conceptualization, Methodology, Software, Formal analysis, Writing – Original Draft; Ezdine Nehdi: Supervision, Validation, Writing –Review & Editing.

Declaration of Competing Interest

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Data Availability

The datasets generated and analyzed during the current study are available from the corresponding author on reasonable request.

Author's Note

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