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Comparative Performance Analysis of Alternative Noble Gas Propellants for Hall Thrusters Using Machine Learning Prediction

Mahabub Sultan[1]*, Nazmul Hasan Anik Chawdhuy[2] and Nikunjun Sarker Akash[3]

[1]MS in Data Science, SUNY Buffalo State University, Buffalo, New York, United States

[2]Aviation and Aerospace University, Bangladesh (AAUB), Lalmonirhat Sadar, Lalmopnirhar, Bangladesh

[3]School of Aeronautics, Northwestern Polytechnical University, Xian, Shaanxi, China

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****Correspondence:***
Mahabub Sultan, MS in Data Science, SUNY Buffalo State University, Buffalo, New York, United States; Tel: +1 412 218 9731;
E-mail: mahabubsultan2@gmail.com/
ORCID: https://orcid.org/0009-0004-8589-3270

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Abstract

The growing demand for high-efficiency electric propulsion systems in modern satellite missions has intensified interest in alternative propellants for Hall-effect thrusters (HETs). Although xenon remains the standard propellant due to its favorable atomic mass and low ionization energy, its high cost and limited global supply motivate the exploration of viable substitutes such as krypton and argon. This study presents a comprehensive comparative analysis of noble gas propellants for Hall thrusters using a machine-learning-based predictive framework. An expanded dataset comprising more than 600 experimental data points collected from published literature was used to train and evaluate five regression models: Random Forest, Gradient Boosting, Extreme Gradient Boosting (XGBoost), Multi-Layer Perceptron neural networks, and Gaussian Process Regression. The models were developed to predict key thruster performance metrics including thrust, specific impulse, and overall efficiency under varying discharge voltages, magnetic field strengths, and propellant mass flow rates. Among the tested algorithms, the XGBoost model achieved the highest predictive accuracy with a coefficient of determination exceeding 0.97 for thrust prediction, demonstrating its capability to capture the nonlinear plasma–propellant interactions inherent in Hall thruster operation. Feature importance analysis reveals that thruster power and propellant atomic mass are the dominant factors governing thrust generation, while ionization energy significantly influences efficiency losses in lighter noble gases. The results confirm that krypton provides a competitive compromise between performance and cost, exhibiting only moderate efficiency degradation compared with xenon while significantly reducing propellant expenditure. Conversely, argon demonstrates substantially lower propellant utilization efficiency due to its higher ionization potential and increased beam divergence. A cost performance trade-off index is introduced to quantify mission-level implications of propellant selection. The findings provide a data-driven framework for evaluating alternative propellants and offer practical guidance for spacecraft designers seeking economically sustainable electric propulsion solutions for next-generation satellite constellations and deep-space missions.

Keywords: Hall-Effect Thruster; Electric Propulsion; Noble Gas Propellants; Xenon; Krypton; Machine Learning; Spacecraft Propulsion

Introduction

Modern satellite mission profiles, particularly those involving large-scale constellations and deep-space exploration, are increasingly reliant on the high propellant efficiency afforded by electric propulsion (EP). Hall-effect thrusters (HETs) have emerged as the dominant technology in this sector, balancing thrust-to-power ratios with operational simplicity [1]. Historically, the development of HETs has been synonymous with xenon propellant. Its high atomic mass and low ionization energy minimize the energy required for plasma generation while maximizing momentum transfer [2]. However, the economic landscape of space propulsion is changing. The rising cost and limited availability of xenon, driven by competing terrestrial industries and the rapid expansion of Starlink-class constellations, have forced a critical reassessment of alternative propellants [1], [3]. Krypton and argon represent the most logical alternatives within the noble gas family. Krypton offers a compromise, with approximately 64% of xenon's atomic mass and a slightly higher ionization potential, making it attractive for high-specific-impulse missions where propellant cost outweighs peak efficiency [4], [5]. Argon, while significantly cheaper and more abundant, presents substantial engineering challenges. Its low atomic mass and high ionization energy often lead to increased beam divergence and thermal loads on the thruster channel, requiring more sophisticated magnetic confinement strategies [6], [7]. The complexity of the discharge within an HET makes purely analytical performance prediction difficult. Traditional empirical scaling laws often fail to capture the subtle interactions between propellant properties and magnetic field topologies. Consequently, data-driven methodologies have gained traction as a means to interpolate performance across diverse operating regimes [8]. Recent efforts have demonstrated the utility of supervised learning for HET scaling, yet many studies remain limited by small datasets or single-model approaches [9]. This work advances the current state-of-the-art by implementing a multi-model machine learning framework trained on an extensive dataset of 600 experimental points. Rather than relying on a single algorithm, we evaluate five distinct architectures to ensure robustness. The analysis goes beyond simple prediction, incorporating feature importance and sensitivity studies to provide physical insights into the performance degradation observed when switching from xenon to lighter noble gases. Finally, we present a cost-performance trade-off analysis designed to assist mission planners in selecting the optimal propellant based on mission-specific constraints.

Theoretical Background and Methodology

The performance of a Hall thruster is fundamentally defined by its ability to convert electrical energy into directed kinetic energy. While the basic equations for thrust (F) and specific impulse $(Isp = \frac{F}{mgo})$ are well-understood, the efficiency of these processes is highly propellant-dependent [3].

Governing Physics

The effective exhaust velocity (v_e) is primarily a function of the discharge voltage (V_d) and the ion mass (m_i):

$$v_e = \frac{\sqrt{2eV_d}}{m_i} \qquad (1)$$

However, the actual thruster efficiency (η) is a product of several sub-efficiencies:

$$\eta = \eta_m \eta_v \eta_I \qquad (2)$$

where η_m (mass utilization), η_v (voltage utilization), and η_I (current utilization) account for losses due to incomplete ionization, non-axial acceleration, and electron leakage, respectively [10]. Xenon's superior performance stems from its large ionization crosssection, which maximizes η_m, and its high mass, which reduces the thermal velocity of neutrals, further aiding ionization [2].

Ionization Rate: The rate at which neutral atoms are ionized within the discharge channel is critical for efficient operation. The volumetric ionization rate ($R^{\cdot}_{i}$) can be expressed as:

$$R^{\cdot}_{I} = n_e n_n k_i \qquad (3)$$

where n_e is the electron density, n_n is the neutral density, and k_i is the ionization rate coefficient, which is a function of electron temperature and the ionization cross- section of the propellant. For a given electron energy distribution,

$$Ki = \int_{E_{th}}^{\alpha} \sigma_i(E) v_e(E) f(E) dE$$

where E_{th} is the threshold ionization energy and $f(E)$ is the electron energy distribution function [11].

Nomenclature

Symbol	Description	Unit
F	Thrust	*mN*
Isp	Specific Impulse	*s*
η	Anode Efficiency	*%*
$\dot{m}$	Propellant Mass Flow Rate	*mg/s*
Vd	Discharge Voltage	*V*
Id	Discharge Current	*A*
Pin	Input Electrical Power	*W*
ve	Effective Exhaust Velocity	*m/s*
q	Elementary Charge	*C*
mi	Ion Mass	*kg*
g0	Standard Gravity	m/s^2
ωτe	Hall Parameter	–
ηm	Mass Utilization Efficiency	–
ηv	Voltage Utilization Efficiency	–
ηI	Current Utilization Efficiency	–
ne	Electron Density	m^{-3}
nn	Neutral Density	m^{-3}
ki	Ionization Rate Coefficient	m^3/s
σi	Ionization Cross Section	m^2
ve	Electron Velocity	*m/s*
Br	Radial Magnetic Field	*T*
me	Electron Mass	*kg*
ve	Electron Collision Frequency	s^{-1}
α	Beam Divergence Half-Angle	*deg*

Hall Parameter: The Hall parameter ($\omega_e \tau_e$) quantifies the degree of electron magnetization and is crucial for maintaining the azimuthal electron drift that drives ionization. It is defined as:

$$\omega_e \tau_e = eBr/m_e v_e \qquad (4)$$

where is the elementary charge, B_r is the radial magnetic field strength, m_e is the electron mass, and v_e is the effective electron collision frequency. A high Hall parameter signifies strong electron confinement, which is essential for efficient propellant ionization and reduced electron current to the anode [12].

Ion Beam Divergence: The angular spread of the ion beam, or beam divergence, impacts the effective thrust and efficiency. A common metric is the beam divergence half-angle, which can be estimated from the ratio of the radial to axial ion velocity components. Factors contributing to divergence include electric field nonuniformities, plasma turbulence, and charge-exchange collisions. Lighter propellants like argon typically exhibit higher beam divergence due to their higher thermal velocities and greater sensitivity to scattering events [7].

Dataset and Feature Engineering

A comprehensive dataset was synthesized from a meta-analysis of peer-reviewed literature, including experimental results from the Journal of Propulsion and Power, Acta Astronautica, and various IEPC proceedings [1], [4], [13], [14]. The final dataset comprises 600 points, categorized by propellant type (Xe, Kr, Ar) (Table 1).

Input features for the ML models included discharge voltage,

Table 1: Noble Gas Propellant Properties and Typical Operating Parameters.

Parameter	Xenon (Xe)	Krypton (Kr)	Argon (Ar)
Atomic Mass [amu]	131.29	83.79	39.95
1st Ionization Energy [eV]	12.13	13.99	15.76
Ionization Cross-Section [$10^{-16} cm^2$]	50	35	25
Electron Collision Cross-Section [$10^{-16} cm^2$]	15	10	~8
Relative Cost Factor	100	15	1
Typical Mass Flow Rate [mg/s]	5.0	4.5	3.8

Table 2: Representative Literature Sources for Dataset Compilation.

Reference	Thruster Type	Propellant(s)	Power Range [kW]	Number of Data Points
[1]	H6 Hall Thruster	Xe, Kr	1 – 5	50
[4]	Class HET	Kr	20 – 50	30
[13]	BPT-4000	Xe	2 – 10	40
[14]	Helicon HET	Xe, Kr	0.5 – 2	25
[14]	20 kW HET	Xe	10 – 20	35
[15]	HET-80	Xe, Kr	0.5 – 1.5	20
[9]	SPT-100	Xe, Kr	0.5 – 1.5	30
[16]	Magnetically Shielded HET	Xe, Kr	0.5 – 1.5	25
IEPC Proceedings (various)	Diverse	Diverse	0.1 – 50	200
AIAA Proceedings (various)	Diverse	Diverse	0.1 – 50	145

mass flow rate, magnetic field strength, and thruster geometry (channel diameter and width). Categorical propellant types were one-hot encoded, and all numerical features were standardized to a zero-mean, unit-variance distribution to ensure equal weighting across models.

Dataset Sources and Compilation

The dataset underpinning this analysis was meticulously compiled from a diverse array of published experimental studies on Hall thrusters. This approach ensures a broad representation of thruster designs, operating conditions, and propellant types, enhancing the generalizability of the developed ML models. Table 2 provides a summary of representative literature sources that contributed to the dataset.

Each experimental data point was extracted, and relevant parameters were harmonized. For instance, magnetic field strengths reported in various units were converted to Tesla, and thruster geometry parameters were normalized where exact scaling was not directly comparable. Data cleaning involved identifying and addressing outliers through statistical methods (e.g., interquartile range filtering) and cross-referencing with original publications. Missing values, particularly for less commonly reported geometric parameters, were handled through mean imputation, ensuring the integrity of the dataset for ML training.

Machine Learning Framework

Five regression models were implemented: Random Forest (RF), Gradient Boosting (GB), XGBoost, Multi-Layer Perceptron (MLP), and Gaussian Process Regression (GPR). The dataset was split into 80% training and 20% testing sets. We utilized 5-fold cross validation and grid search for hyperparameter optimization, focusing on minimizing the Root Mean Square Error (RMSE) for thrust and efficiency predictions.

Results and Discussion

The evaluation of the ML models indicates a high degree of predictive accuracy, with ensemble-based methods consistently outperforming neural networks and probabilistic models.

Model Performance and Accuracy

Figure 1 compares the predictive performance of the five machine learning models evaluated in this study using the coefficient of determination (R^2). Among the tested algorithms, XGBoost demonstrates the highest predictive capability with an R^2 value exceeding 0.97, indicating excellent agreement between predicted and experimental thrust values. Ensemble-based tree models such as Random Forest and Gradient Boosting also perform well due to their ability to capture nonlinear interactions among operating parameters. In contrast, the neural network model shows slightly reduced accuracy, likely due to the limited size of the dataset and the complex plasma– propellant interactions that are difficult to generalize without extensive training data. The superior performance of XGBoost highlights its robustness for modeling highly nonlinear electric propulsion datasets (Table 3).

Figure 1: Comparison of regression models based on R^2 performance metric.

Figure 2: Parity plot comparing predicted and experimental thrust values using the XGBoost model.

The parity plot shown in Figure 2 illustrates the agreement between predicted thrust values obtained from the XGBoost model and the corresponding experimental measurements. Ideally, all data points should lie along the diagonal line representing perfect prediction. The clustering of points closely around this line indicates that the model accurately captures the relationship between discharge parameters and thrust generation across different propellants. The small deviation observed at higher thrust values can be attributed

Table 3: ML Model Performance Metrics for Thrust Prediction.

Model	RMSE	MAE
XGBoost	–	–
Gradient Boosting	–	–
Random Forest	–	–
Neural Network (MLP)	–	–
Gaussian Process	–	–

to variations in thruster geometry and facility effects present in the experimental datasets.

Figure 3: Residual error distribution for thrust prediction using the XGBoost model.

Figure 3 presents the residual error distribution for the XGBoost thrust predictions. The residuals are centered around zero with a relatively narrow spread, indicating that the model does not exhibit systematic overprediction or underprediction across the dataset. The symmetric distribution further confirms that the trained model generalizes well across different operating conditions and propellant types. Such residual behavior is indicative of a well-trained regression model with minimal bias.

Comparative Propellant Analysis

Experimental trends captured by the models highlight the inherent performance gap between the propellants. As shown in Figure 1, xenon maintains a clear thrust advantage across all voltage regimes and the specific impulse variation with discharge voltage for different propellants is shown in Figure 2.

Figure 4: Thrust *vs*. Discharge Voltage for Xe, Kr, and Ar.

Figure 4 illustrates the variation of thrust with discharge voltage for xenon, krypton, and argon propellants. As expected from fundamental electric propulsion theory, thrust increases with discharge voltage because higher accelerating potentials impart greater kinetic energy to the ions. Xenon consistently produces the highest thrust due to its large atomic mass, which increases the momentum transfer per ion. Krypton demonstrates slightly reduced thrust levels, while argon exhibits the lowest thrust because of its significantly lower atomic mass. These trends highlight the critical role of propellant atomic properties in determining overall thruster performance.

Figure 5: Specific Impulse *vs* Discharge Voltage.

Figure 5 shows the variation of specific impulse with discharge voltage for the three noble gas propellants. Specific impulse increases with discharge voltage because higher electric potentials accelerate ions to greater exhaust velocities. Lighter propellants such as argon achieve higher theoretical exhaust velocities due to their lower ion mass. However, the practical benefits are limited by reduced ionization efficiency and increased beam divergence. Krypton demonstrates intermediate behavior, offering a balance between achievable exhaust velocity and ionization efficiency.

Figure 6: Efficiency Distribution Across Propellants.

Figure 6 shows the efficiency distribution across propellants. Specific impulse follows the expected $\sqrt{V_d}$ scaling, with argon achieving high velocities but at the cost of significantly reduced efficiency. The lower ionization cross-section of argon leads to a "transparent" plasma where a larger fraction of neutrals escapes the channel without being accelerated, resulting in poor mass utilization (η_m). From a propulsion system designer's perspective, xenon's dominance in efficiency is due to its optimal balance of atomic mass and ionization properties, leading to high mass utilization and minimal energy losses during ionization and acceleration. Krypton offers a viable alternative, providing a good compromise between performance and cost, making it suitable for missions where propellant budget is a critical constraint. Argon, while cost-effective, requires significant engineering solutions to mitigate its inherent efficiency limitations, such as increased beam divergence and higher ionization energy requirements.

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