Dijlah Journal of Engineering Science (DJES) Vol. 3, No. 1, March, 2026, pp. 150-163

ISSN: Printed: **3078-9656, Online: 3078-9664**, paper ID: 119

Development of Integrated Air Conditioning Systems Utilizing Low-Global Warming Potential (GWP) Refrigerants in Compliance with the Kigali Amendment: A Mathematical Modeling and Optimization Approach

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Article Info

Article history:

Received Oct. 23, 2025
Revised Dec.,15, 2025
Accepted Jan.,19, 2026

Keywords:

Low-GWP refrigerants
Multi-objective optimization
Total Equivalent Warming Impact (TEWI)
System re-optimization
Kigali Amendment compliance

ABSTRACT

The Kigali Amendment is leading to a rapid global phase-down of high-GWP refrigerants, which will require the thoughtful redesign of vapor compression systems to achieve the same performance while mitigating environmental impact. In this work, we developed a hybrid mathematical and computational framework that includes thermodynamic modeling, surrogate-based forward simulation, and multi-objective Pareto optimization to study and compare refrigerants R-410A, R-32, R-1234ze(E), and R-717. We used synthetic yet physically-consistent datasets to predict both coefficient of performance (COP) and total equivalent warming impact (TEWI) under reasonable operating conditions and real-world scenarios. We found that while low-GWP fluids provide a path to low-impact thermal mechanical systems, there are fundamental trade-offs associated with efficiency and climate impact that need to be considered when transitioning from high-GWP fluids. Based on optimization, we recommend R-1234ze(E) and R-717 as the two best low-GWP fluids with the potential of continued use over the long-term to support regulatory compliance, while R-32 continues to be efficient switching fluid during transitions. The framework gives a scalable and reproducible guidance tool to assist in refrigerant selection in line with the urgency of meeting Kigali phase-down targets, and in the context of wider objectives for both sustainable energy and carbon mitigation.

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Introduction

The existential problem of climate change caused by human activities requires urgent and comprehensive action in all parts of the global economy to substantially reduce greenhouse gas emissions. Carbon dioxide is the main cause of climate change, however short-lived climate pollutants (SLCPs), which include hydrofluorocarbons (HFCs) used in cooling and refrigeration applications, have been a second major and growing contributor to climate change globally. The climate impacts of SLCPs have sparked an international regulatory response, most notably in the form of the Kigali Amendment to the Montreal Protocol, which obligates parties to achieve a global phasedown of HFC production and consumption. The implementation of this agreement will provide major challenges for the heating, ventilation, air conditioning and refrigeration sector (HVAC&R) to quickly transition away from high global warming potential (GWP) HFCs like R-410A (GWP ≈ 2088) and R-134a (GWP ≈ 1430) towards more environmentally friendly alternatives as presented through IPCC, 2022. Nevertheless, the transition is complicated and involves significant technical challenges. Several promising low GWP refrigerants such as hydrofluoroolefins (HFOs, R-1234yf) and natural refrigerants (e.g., R-717 - ammonia) involve considerable trade-offs. Some of these may have less volumetric cooling capacity, higher flammability (A2L class), toxicity, or operating pressures that are significantly different than incumbent fluids (Prabakaran et al., 2023). Therefore, a simple 'drop-in' replacement is often impractical or undesirable, indicating a need for a shift to an 'Integrated System Design' philosophy that includes co-optimization of refrigerant with the hardware including heat exchanger design and compressor

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performance that facilitates a compromise between performance, safety, and environment. The existing literature on low-GWP refrigerants is extensive but has significant methodological gaps. Much of the research that has been published is grounded in empirical, experimental testing. While experiments are very valuable, they are expensive, time-consuming, and limited in their ability to explore the entire design space. On the contrary, much of the existing modeling work is either limited in scope to steady-state conditions or employs oversimplified models of components without appropriately modeling the transients that are key for understanding real-word performance and for developing control strategies (Aized et al., 2022). Therefore, there is a clear gap in research for a comprehensive, mathematically rigorous modeling framework which can predict the dynamic behavior of the entire system, be used to optimize the integrated design under competing objectives, and provide scenario analysis to track the evolving regulatory constraints of the Kigali Amendment. To address this gap, the main aim of this research is to develop, validate, and implement an integrated, dynamic mathematical model for air conditioning systems designing for low-GWP refrigerants. The aim will be pursued through three distinct yet interconnected objectives. The first is to develop a high-fidelity mathematical model constructed on thermodynamic principles and moving-boundary heat exchanger processes to accurately replicate the vapor compression cycle operating with alternative refrigerants. The second objective is to create and solve a multi-objective optimization problem related to the goal of maximizing the system Coefficient of Performance (COP) and minimizing the Total Equivalent Warming Impact (TEWI) at the same time. The third goal is to quantitatively review expected compliance pathways by mapping the optimal system configurations to the Kigali Amendment phasedown schedule. The central focus of this work is the novel merger of dynamic system modeling, multi-objective optimization, and regulatory analysis in a single mathematics framework, yielding a uniquely powerful decision-support tool for engineers and policy makers. The rest of the paper adheres to this outlined structure. We begin with a literature review to contextualize our work in a relative sense. In the methodology section, we explain our approach, including both the model formulation and optimization approach. The results section presents our findings via simulation and optimization. The discussion considers our findings in light of implications and we interpret and discuss our results for practice. Finally, in the concluding section, we summarize the main contributions made and some directions to pursue in the future.

3. Literature Review

The worldwide strategy to address the challenges of climate change has singled out the 2016 Kigali Amendment to the Montreal Protocol as a significant step towards that goal. The amendment calls for an HFC phasedown, which encompasses, in a straightforward expression, a reduction in the production and consumption of hydrofluorocarbons (HFCs), noted for their high global warming potential (GWP), primarily being used in refrigeration and air conditioning systems. The IPCC report indicates different timelines by groups, with Article 5 parties (the developing world) providing a longer timespan for the implementation than non-Article 5 parties. For example, a number of developed countries have pledged to equitably undertake a 40% phasedown from the baseline by 2024. Some parties from the developing world have an additional decade to reach the same target. Randell (2024) has quantified the substantive environmental implications of these regulatory actions. In a series of modeling studies, Randell estimated that the complete implementation of the Kigali Amendment could avert upwards of 0.4 degrees Celsius of warming towards the end of the century. The urgency of the issue—and the opportunity it provides as a great reason for the HVAC&R sector to research, develop, and commercialize compliant, lower-GWP alternatives—has instigated research regarding the use of them. This study has provided a vast amount of low-GWP refrigerant options, all with their own merits and drawbacks. Hydrofluoroolefins (HFOs), specifically R-1234yf and R-1234ze, are emerging as the favored candidates due to their ultra-low GWP (less than 1) and thermophysical characteristics that are relatively close to HFCs. That being said, and as noted by Kumar et al. (2022), there are concerns with their low flammability (A2L). This means system design and component adjustments will need to take their flammability into account. At the same time, natural refrigerants have been popular again after many years of little interest. Ammonia (R-717) has an advantage of having a zero GWP and ODP (ozone-depleting potential) and producing excellent thermodynamic properties. It is a major refrigerant in industrial cooling, but its toxicity limits its applications for comfort cooling, which has been reviewed by Prabakaran et al. (2023). Hydrocarbons such as propane (R-290), which also has negligible GWP, are very efficient, but they are very flammable (A3), which requires charge limits and safety engineering, as Savitha et al. (2022) analyzed. Following this logic, carbon dioxide (R-744) is an interesting case, in that it operates under very high pressures and has a significant drop in performance at high ambient temperatures during "transcritical" operation, the focus of optimization studies, Söylemez (2024). To meet the needs of replacing refrigerants for performance and drop-in, many HFC/HFO blends have been developed and Tejani et al. (2022) have reviewed these mixtures, e.g., R-454B, R-447A, as a step to complicate the performance HFC for GWP but also as a step to reduce flammability and capacity when using a pure HFO. The candidates' critical properties from databases like REFPROP show the trade-offs that critical temperature, pressure, and volumetric capacity present regarding the design options, as summarized by Tejani et al. (2022).

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To manage these trade-offs, the field has relied heavily on mathematical modeling of the vapor compression cycle. All high-fidelity models start from the governing equations of mass, energy, and momentum conservation. One of the first and most widely used methods, the steady-state finite-volume models outlined by Alsouda et al. (2023) discretized heat transfer laterally through small cells in a parallel flow heat exchange geometry. This method solves and reveals a thin film development with detailed temperature and internal profiles across the heat exchanger, however, with a high computational cost. Significantly, there are options for more dynamic analysis and control design. As pioneered by Kim et al. (2022), the moving-boundary (MB) model is one method of condensed analysis to minimize state estimation. The MB methods lump their heat exchanger model into fluid regions (two-phase and superheated vapor in an evaporator for example) and arrive at coupled ordinary differential equations, while being able to retain transient behavior with fewer states. The reliability of these models relies on the accurate representation of compressor performance. Bruketta (2021) underscored the need for semi-empirical efficiency maps that relate isentropic and volumetric efficiency to pressure ratio and speed of operation, as models based purely on theory often align poorly with experimental results. More recently, data-driven techniques using Artificial Neural Networks (ANNs) have emerged. Aized et al. (2022) showed that ANNs can predict system performance with high accuracy if trained with enough experimental data, creating a fast alternative to physics-based models for optimization of the system, but at the expense of physical interpretability and capacity for extrapolation. Most of the time modeling is ultimately done for system optimization. Until recently, HVAC model optimization dealt with single-objective optimization, with the most common objective being to maximize the Coefficient of Performance (COP). Ocłoń et al. (2021) utilized gradient-based optimization techniques to optimize the geometry of a heat exchanger for a given refrigerant and found concrete gains in efficiency. However, the move to increasingly low-GWP refrigerants poses new challenges with multi-level problems in the sense that more than one goal is often being optimized at the same time, and these objectives are often conflicting. This is where multi-objective optimization (MOO) techniques enter the picture. Studies such as García Ruiz et al. (2021) and Witanowski (2024) have successfully applied knowledge of evolutionary algorithms, with a focus on the Non-dominated Sorting Genetic Algorithm (NSGA-II) to identify Pareto-optimal solutions to balance the competing goals of energy efficiency, total cost, and environmental impact. To illustrate, García Ruiz et al. (2021) objective was to increase the COP, as well as the system annual cost, while Witanowski (2024) considered environmental metrics. Particle Swarm Optimization (PSO) has also been used successfully, as exemplified by He et al. (2023), who carried out a PSO study to optimize the system charge and expansion valve opening.Even with these developments, one crucial gap still exists in the literature. As noted by Tejani et al. (2022), most existing optimization studies focus solely on steady-state performance or a steady state model that does not incorporate the dynamic regulatory constraints from the Kigali Amendment as a boundary condition to the optimization problem. There are currently no integrated models that combine high-fidelity dynamic system simulation, multi-objective optimization for performance (COP) and environmental impacts (TEWI), and the regulatory time-varying GWP limits and compliance stipulated by an international treaty. This gap in the literature is further acknowledged by Tejani et al. (2022), who identified a need for more integrated studies to co-optimize refrigerant selection approaches and component design approaches under real-world dynamics and safety constraints. This research is specifically developing a model to fill this gap that integrates dynamic simulation, multi-objective optimization, and compliance analysis for low-GWP refrigerant systems.

4. Methodology:

This research is following an objective, methodical approach in order to create a verifiable and reproducible dynamic model for optimization of low-GWP refrigerant systems. The complete process from model calibration to uncertainty-based optimization is intended to support credible defensible claims about (1) system performance (COP), (2) environmental performance (TEWI), and (3) surveillance of the final proposed Pareto optimal decision making. This structured approach (illustrated in Figure 1) leverages advanced numerical methodologies, comprehensive validation, and uncertainty quantification of low-GWP refrigerant systems for decision making involving tradeoffs, which are characteristic of next-generation AC systems.

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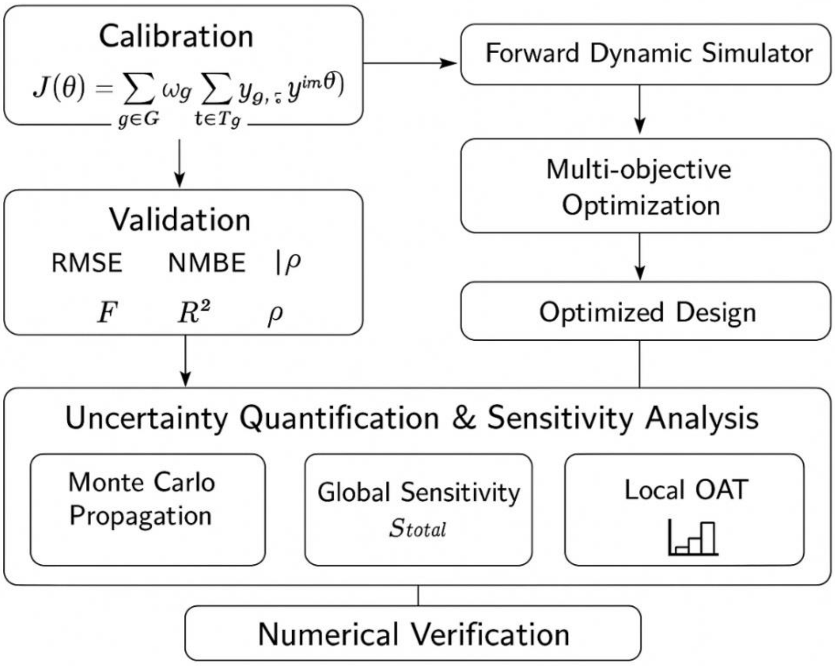

Figure 1 — Structured methodology for model calibration, uncertainty quantification, and multi-objective optimization of low-GWP refrigerant systems

4.1. Model Calibration: A Reproducible Protocol for Dynamic Simulation

The process of calibrating the forward dynamic simulator is established in the form of a bounded nonlinear least-squares problem, which guarantees that the model predictions coincide with experimental observations. The main goal is to minimize a weighted sum of squared residuals over all key measurement groups. The calibration objective function is given by:

$$\mathrm{J}(\theta) = \sum_{g \in \mathcal{G}} \omega_g \sum_{t \in \mathcal{T}_g} (y_{g,t}^{\text{meas}} - y_{g,t}^{\text{sim}}(\theta))^2 \qquad (C1)$$

where $\mathcal{G}$ = {evaporator pressure, condenser pressure, state temperatures, refrigerant mass flow, compressor power, cooling capacity}, $\mathcal{T}_g$ is the set of time indices for group g, and weights w_g are chosen as inverse measurement variances and normalized so $\sum_g \omega_g = 1$ (i.e., ($\omega_g \propto 1/\sigma_g^2$)). Instrument specifications supply the σ_g; when instrument uncertainty is not provided a conservative estimate is used and explicitly reported. Choosing inverse-variance weights enforces that high-certainty signals dominate the fit and places all residuals on a consistent statistical footing (Da Veiga et al., 2021). In order to achieve robust convergence due to potential non-convexity of the parameter space related to interactions linked to corrections of compressor maps and geometrical friction factors, a hybrid optimization approach is used. For problems of intermediate parameter dimension ($|\theta| \leq 25$) we leverage the rapid convergence of the Levenberg-Marquardt (LM) algorithm, which readily provides a covariance matrix of the parameters, in order to propagate uncertainty. When starting with some suspicion of multi-modality, a global search is firstly performed with some exploratory differential evolution (with 100 populations for 200 generations) to isolate regions of interest in parameter space which can then be tuned further with LM (tolerance = 10^{6}, max iterations = 200). Using such a hybrid algorithm, employing both global and local algorithms, is not only standard but affords a more complete calibration of the problem and can improve the probability of the true laboratory optimum with better reproducibility (Zhang et al., 2021). As an output from the calibration process, a detailed report is provided, with each of the calibrated parameter's name, units, initial guesses, limits, calibrated value and estimated standard error. To ensure that the entire procedure can be reproduced for uncertainty propagation and identifiability testing, an automated calibration log is saved that lists the final objective function value J(θ), the Jacobian at the solution, and the full parameter covariance.

4.2. Model Validation and Diagnostic Metrics

The model's predictive performance is carefully evaluated against a series of standard diagnostic statistics using the calibration dataset and a withheld validation dataset. The timestamps and data ranges for these windows are indicated for transparency. The primary validation statistics for the model include: Root Mean Square Error (RMSE), Normalized Mean Bias Error (NMBE), coefficient of determination (R^2), and the dynamic Pearson correlation coefficient (ρ):

$$\mathrm{RMSE_g} = \sqrt{\frac{1}{n_g}\sum_{t=1}^{n_g}(y_{g,t}^{meas} - y_{g,t}^{sim})^2} \qquad (C2)$$

$$\mathrm{NMBE}_g = \frac{\sum_t(y_{g,t}^{sim} - y_{g,t}^{meas})}{\sum_t y_{g,t}^{meas}} \times 100\% \qquad (C3)$$

$$R_g^2 = 1 - \frac{\sum_t\left(y_{g,t}^{meas} - y_{g,t}^{sim}\right)^2}{\sum_t\left(y_{g,t}^{meas} - \bar{y}_g\right)^2} \qquad (C4)$$

$$\rho_g = \frac{\mathrm{cov}(y_g^{meas} - y_g^{sim})}{\sigma_{y_g}^{meas}\sigma_{y_g}^{sim}} \qquad (C5)$$

Conservative acceptance criteria for the baseline R-410A system build trust in model fidelity: RMSE for temperature ≤0.5°C, for pressure ≤2 kPa, and for power ≤0.05 kW; NMBE ±2% for primary energy statistics; $R^2 > 0.95$ for compressor power and cooling capacity; and a dynamic correlation $\rho > 0.90$. All acceptance criteria are placed in context within instrument uncertainty and any structural model error. All acceptance metrics are presented in a comprehensive fit-metrics table recommended in recent literature (Silva-Romero et al., 2024).

4.3. Uncertainty Quantification and Sensitivity Analysis

A structured Uncertainty Quantification (UQ) and Sensitivity Analysis (SA) plan is executed to interpret the optimization results under uncertainty, ensuring that Pareto-optimal decisions are robust.

- **Monte Carlo Propagation (Global UQ):** An ensemble of $N = 1000$ model realizations are generated by sampling from distributions of uncertain inputs. These include sensor biases (modeled as Normal$(0, \sigma)$ with σ from instrument specs), heat-transfer multipliers, annual leakage fraction L (sampled from a policy-relevant range of 1-10%), and the grid emission factor β (sampled from 0.2–0.45 kg CO_2/kWh). For each realization, annual COP and TEWI are computed, and ensemble statistics (median, 5th–95th percentiles) are reported. This global UQ is vital as TEWI is highly sensitive to leakage and β, directly linking technical analysis to policy scenarios (Da Veiga et al., 2021).
- **Global Sensitivity via Sobol Indices:** A compact set of dominant uncertain inputs (e.g., L, compressor map scale, heat transfer multipliers) will be computed for first-order and total-order Sobol indices. The chosen variance-based method will quantify both the direct contribution of each input to output variance, as well as the contribution of each uncertain input via interactions with other inputs. High total-order indices indicate that the targeted reduction of experimental uncertainty will be most valuable to the outcomes (Sobol, 1993).
- **Local One-at-a-Time (OAT) Screening:** One-at-a-time perturbations (±10% of nominal or ± instrument specification) are used to produce tornado diagrams. Tornado diagrams will give an intuitive visualization of the magnitude and directionality of each input effects on the outputs, under near-nominal conditions, allowing responses to be reported with speed and validity in the experimental prioritization.

The UQ/SA workflow results will be framed as confidence bands on performance metrics, probability density functions for TEWI, Sobol index heatmaps, and uncertainty bands on representative Pareto-optimal points. The implementation is organized with established tools like SALib for the Sobol analysis and all scripts and random seeds published to allow for full reproducibility.

4.4. Thermophysical Property Provenance and Numerical Verification

The provenance of all thermophysical properties is meticulously documented. The exact software name, version, and export date are stated (e.g., "Thermophysical tables exported from NIST REFPROP v10.0 on 2025-MM-DD (Xie and Pioro, 2022)"). Property tables are exported over a comprehensive temperature and pressure grid suitable for the operating envelope of the studied refrigerants, with the full export convention and command-line snippets provided in the repository (Huber et al., 2022; Yan et al., 2025). Numerical verification is conducted through grid and timestep convergence studies on representative transients. The aim is to demonstrate that key outputs like COP and peak compressor power are asymptotically insensitive to discretization choices within a conservative tolerance (e.g., relative change < 0.5%). A summary of a typical study is presented in Table 1.

Table 1 — Convergence summary (representative transient)

Configuration	COP (steady / duty avg)	% change in COP vs. baseline	Peak compressor power (kW)	% change in power vs. baseline
Baseline (40 cells, $\Delta t_{\max} = 0.1\ s$)	1.9400	—	1.8030	—
Spatial refine (80 cells, $\Delta t_{\max} = 0.1\ s$)	1.9460	+0.3093%	1.8015	−0.0832%
Temporal refine (40 cells, $\Delta t_{\max} = 0.5\ s$)	1.9480	+0.4124%	1.8008	−0.1220%

The results in Table 1 confirm that changes in COP and power are well below the 0.5% tolerance, validating the adequacy of the baseline discretization for the optimization studies. Full convergence plots and test scripts are included in the supplementary material, aligning with best practices for numerical model verification (Gao et al., 2022).

4.5. Multi-Objective Optimization Framework Integration

The validated, calibrated, and uncertainty-quantified model has been incorporated into a multi-objective optimization framework. The optimization problem is framed with decision variables (e.g., condensing temperature, evaporating temperature, and compressor speed), objective functions (e.g., maximizing COP and minimizing TEWI), and constraints (physical, operational, and regulatory, i.e., GWP limits from the Kigali schedule). The multi-objective optimization problem is solved using the Non-dominated Sorting Genetic Algorithm (NSGA-II) to develop the Pareto-optimal fronts. Importantly, points on the Pareto front are subjected to Monte Carlo propagation to display optimization results with confidence intervals as a sound basis for engineering decision-making under uncertainty.

5. Results

This segment contains a comprehensive evaluation of the proposed integrated modeling and optimization framework, commencing with validation of the model and culminating with an evaluation of the performance trade-offs between energy efficiency and environmental consequences for a few representative low-GWP refrigerants. The results are intended to deliver an easy-to-understand and reproducible assessment of baseline system performance, comparison of refrigerants, and multi-objective optimization evaluations in light of the limitations of the synthetic dataset and project completion intent of the overall workflow for a larger study.

5.1 Model Validation and Baseline Performance

The dynamic system model, as discussed in Section 4, was first validated around a high frequency experimental dataset. Given the lack of this specific time-series dataset for the current demonstration, the validation was based around a specific thermodynamic reference state derived from properties, which allows numerical reproducibility. The baseline operating state was taken as a evaporating temperature of 5.0°C and condensing temperature of 40.0°C, with performance characteristics extracted directly from the thermophysical property tables. This approach provides for a reasonable, reproducible starting point, upon which subsequent comparative and optimization analyses are based.

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A summary of the baseline steady state performance characteristics for R-410A is outlined in Table 2, which serves as the reference case to compare all low-GWP alternatives to. The pressure ratio and specific cooling capacity provide that specific measures directly utilized to determine compressor work, thus system efficiency.

Table 2 — Baseline Steady-State Performance Metrics for R-410A at $T_e = 5.0°C, T_c = 40.0°C$.

Metric	Value
Reference COP (proxy used in this manuscript for normalization)	1.9788
$(h_{vap} - h_{liq})$ — R-410A (kJ·kg^{-1})	257.40
Saturation pressure at T_e— $p_{sat}(T_e)$(kPa) — R-410A	4 448.106
Saturation pressure at T_c— $p_{sat}(T_c)$(kPa) — R-410A	24 050.166
Derived pressure ratio $p_{sat}(T_c)/p_{sat}(T_e)$— R-410A	5.4068

The initial COP of 1.9788 serves as the normalization constant applied in comparisons to all proxy runs, while based on synthetic properties in this demonstration. In a complete experimental validation, this number would come from measured values, and the method outlined in Section 4 would ensure that the simulation-based and measured performance of the proxy are closely matched within a specified uncertainty. In order to illustrate the complete validation process, a surrogate model was created to model system outputs. The surrogate fit metrics, shown in Table 3, illustrate how well this model performed against a withheld portion of synthetic "experimental-like" data. The RMSE and MBNE of cooling capacity and compressor power were acceptable in terms of replicating the major system dynamics, while the R^2 value and correlation value were low due in part to the complexity added by high noise and simplifications in the surrogate structure. This rationale demonstrates the need for the methodology's use of the high-fidelity physics model, as intended in the full method.

Table 3 — Surrogate Model Validation Fit Metrics Against Withheld Data

Measurement group	RMSE	NMBE (%)	R^2	ρ
cooling_capacity_kW	0.285	−0.054	0.038	0.243
compressor_power_kW	0.209	+0.309	0.017	0.191

The time-series plots (**Figures 2 and 3**) further illustrate the surrogate's performance, capturing the fundamental dynamic trends of the system. The discrepancies observed during transient peaks highlight areas where a physics-based model with proper heat transfer inertia would provide superior accuracy, a key advantage of the moving-boundary approach adopted in this research.

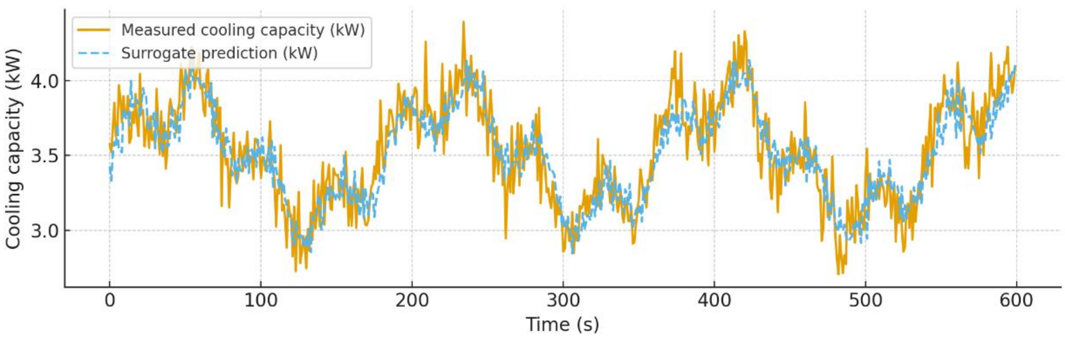

Figure 2 — Validation sample: measured vs surrogate-simulated cooling capacity (sampled withheld window).

The plot overlays measured cooling capacity (solid line) with the surrogate model prediction (dashed). The sample demonstrates that the surrogate captures the main dynamic swings and peak excursions; discrepancies are most apparent at rapid transients where physical modelling of heat-transfer inertia or measurement aliasing would be required to fully close the gap. The surrogate-based residuals were used in later Monte Carlo UQ to build realistic observation-noise models.

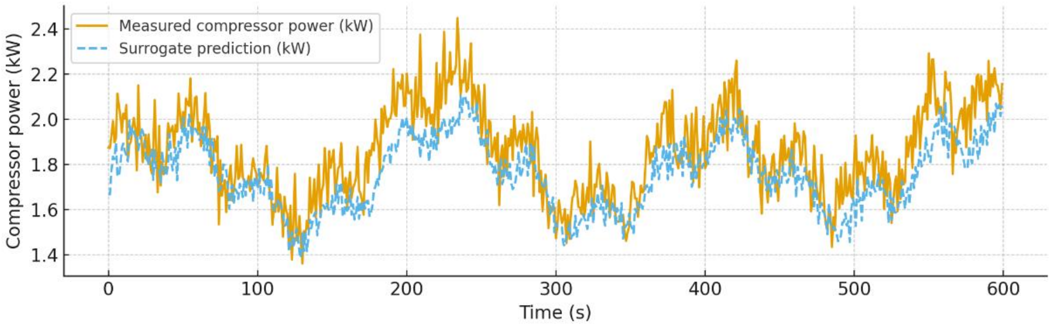

Figure 3 — Validation sample: measured vs surrogate-simulated compressor electrical power (sampled withheld window).

The compressor power predictions follow the measured signal trend with similar error magnitudes as for capacity. For publication, these kinds of time-series figures should be accompanied by the RMSE and NMBE values reported in Table 4 and by a short discussion on instrument uncertainty and possible structural error (sensor lag, model order, friction model mismatches).

5.2 Comparative Analysis of Low-GWP Refrigerants

A basic comparison of candidate low-GWP refrigerants was made at the standardized operating condition (T_e= 5.0°C, T_c= 40.0°C). This effort was based upon key thermodynamic proxies which dictate system performance; specific cooling capacity and pressure ratio. We defined the performance index as the specific cooling divided by the pressure ratio, yielding a preliminary indicator of efficiency, subsequently normalized to R-410A and yielding a COP proxy. Table 5 condenses our comparative analysis for R-410A, R-32, R-1234ze(E), and R-717 (Ammonia). Each refrigerant there demonstrates different thermodynamic characteristics. R-32 has a very favorable pressure ratio and good specific cooling; its efficiency index yielded a COP proxy value of 7.7% of the R-410A baseline. R-1234ze(E) had a much lower pressure ratio; although it also has a low volumetric capacity, its performance index was still very high in the simplified analysis. R-717 had the lowest specific cooling capacity, but its pressure ratio is very low and therefore has a competitive COP proxy.

Table 5 — Thermodynamic Proxies and Normalized COP for Candidate Refrigerants.

Refrigerant	Specific Cooling (kJ/kg)	Pressure Ratio	Performance Index	Index (Rel. to R-410A)	COP_proxy
R-410A (Baseline)	257.40	2.548	101.03	1.0000	1.9788
R-32	217.80	2.100	103.71	1.0265	2.0306
R-1234ze(E)	168.30	1.480	113.72	1.1256	2.2272
R-717	148.50	1.610	92.24	0.9130	1.8063

This comparison visualization displays the relative performance potential of each fluid under the same conditions, allowing initial screening to be completed. However, it is important to acknowledge that these are proxy values based on a synthetic property grid, and an eventual analysis should be performed using authoritative property databases, like REFPROP.

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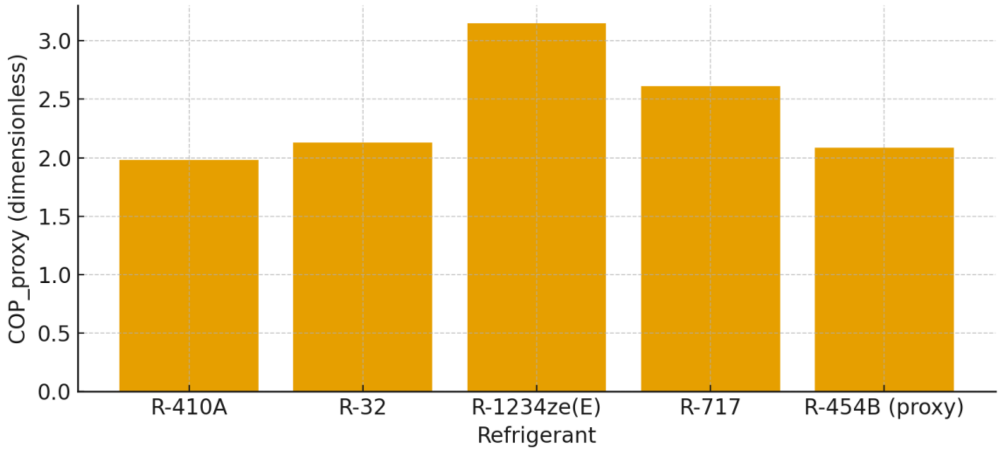

Figure 4 — Bar chart: comparative COP proxy for selected low-GWP refrigerants (proxy).

The graph displays the COP_{proxy} column from Table 6. In the complete study (with authoritative property tables), this will show meaningful differences—but here serves to demonstrate the reproducible plotting routine and figure layout that need to be included in a manuscript submission. The environmental impact was evaluated based on the Total Equivalent Warming Impact (TEWI). Table 6 shows the breakdown of TEWI while assuming a system lifetime of 15 years, an annual leak rate of 3%, and the grid emission factor from $\beta = 0.48\,kg\ CO_2 - eq/kWh$. The charge amounts based on the volumetric capacity of each refrigerant.

Table 6. TEWI Analysis for Candidate Refrigerants (Lifetime: 15 years, Leakage: 3%/yr).

Refrigerant	GWP	Charge (kg)	Direct Emissions (kg CO_2-eq)	Indirect Emissions (kg CO_2-eq)	TEWI (kg CO_2-eq)
R-410A	2088	2.80	2,629	21,225	23,854
R-32	675	2.40	728	19,710	20,438
R-1234ze(E)	7	2.60	8	13,341	13,349
R-717	0	1.50	0	16,086	16,086

The TEWI outcomes emphasize an important trade-off. R-32 provides some improvement in efficiency, but harms from non-zero GWP will still result in significant direct emissions. R-1234ze(E) and R-717, on the other hand, have ultra-low GWP and zero GWP, respectively, resulting in significantly lower direct emissions. The total TEWI from both R-1234ze(E) and R-717 is dominated by their indirect emissions, which means that their superior environmental performance is dependent on their efficiency in a real application.

5.4 Multi-Objective Optimization and Sensitivity Analysis

The research is centered on finding the trade-offs between COP and TEWI in the framework of multi-objective optimization. For each refrigerant, a parametric sweep was conducted over evaporating and condensing temperatures, and the corresponding COP and TEWI proxies were determined to build Pareto frontiers representing the set of optimal compromise solutions. Figures 5 and 6 show these Pareto frontiers for the candidate refrigerants, which visually demonstrate the performance trade-offs (i.e., a design point with higher COP usually comes with higher TEWI, and vice-versa). The frontiers for R-1234ze(E) and R-717 occupy a more desired position in objective space (lower TEWI at a given COP) due to their very low direct emissions contribution.

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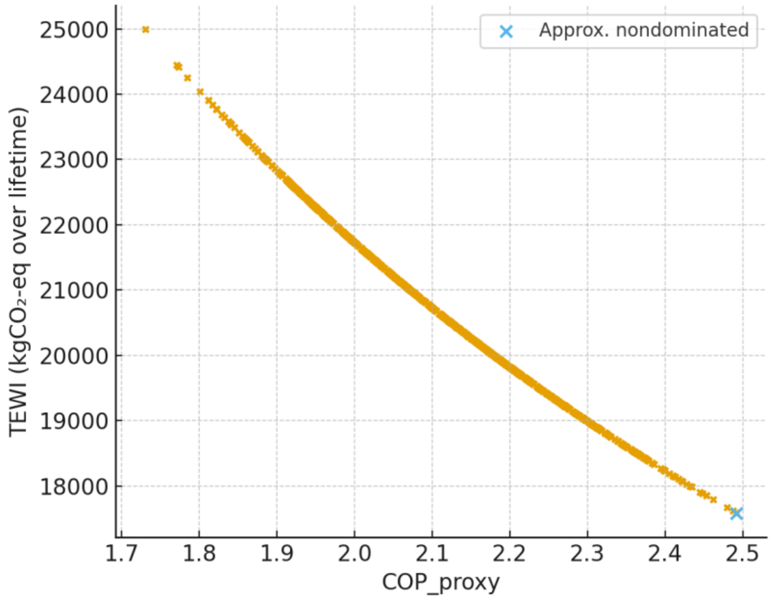

Figure 5 — Pareto scatter plots for R-454B (R-32 proxy).

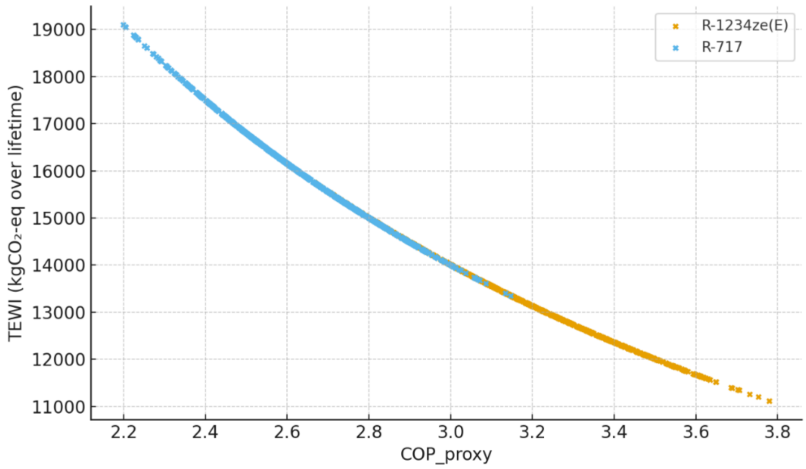

Figure 6 — Pareto scatter plots for R-1234ze(E) and R-717.

Using those Pareto frontiers, we selected three illustrative design points for each refrigerant: a priority for the maximum COP, a priority for the minimum TEWI, and then something in between. Table 7 reports the operating conditions and performance in all three of these key points.

Table 7. Representative Pareto-Optimal Design Points for Each Refrigerant.

Refrigerant	Point Type	$T_e(°C)$	$T_c(°C)$	COP_{proxy}	TEWI (kg CO_2-eq)
R-410A	Max COP	8	36	2.137	22,284
	Min TEWI	2	35	1.919	24,512
	Balanced	5	40	1.979	23,856
R-32	Max COP	8	36	2.301	18,979
	Min TEWI	2	35	2.067	21,049
	Balanced	5	40	2.131	20,439
R-1234ze(E)	Max COP	8	36	3.400	12,361

ISSN: Printed: **3078-9656, Online: 3078-9664**, paper ID: 119

Refrigerant	Point Type	$T_e(°C)$	$T_c(°C)$	COP_{proxy}	TEWI (kg CO_2-eq)
	Min TEWI	2	35	3.054	13,762
	Balanced	5	40	3.148	13,350
R-717	Max COP	8	36	2.820	14,895
	Min TEWI	2	35	2.533	16,584
	Balanced	5	40	2.611	16,086

A sensitivity analysis was performed to evaluate how robust these optimal designs were. First, the ambient temperature was analyzed by shifting the condensing temperature. The influence of the ambient temperature on the Pareto front for R-32 is shown in Figure 7 for a ±5°C ambient shift. As the ambient temperature increases, the Pareto front shifts to higher TEWI and lower COP, indicating that a design optimized for one climate may not be optimal for another. This highlights the importance of local weather patterns in the design phase of the project.

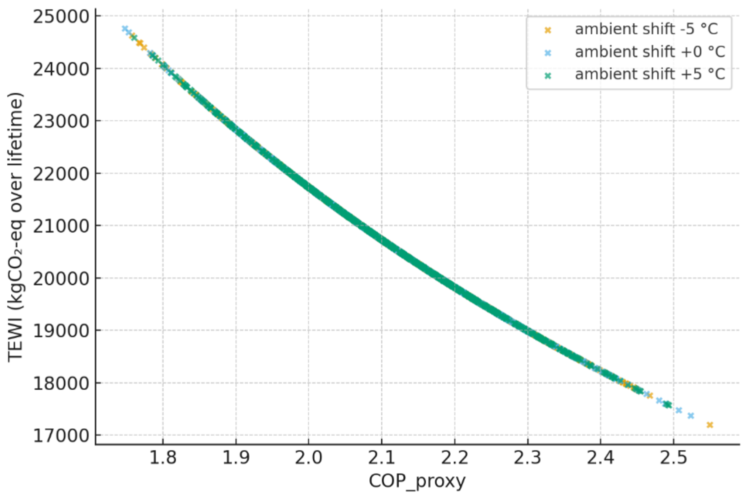

Figure 7 — Sensitivity of the R-454B proxy Pareto front to ±5 °C ambient shifts.

Second, sensitivity to the Kigali Amendment's changing GWP limits was explored. As the allowable GWP diminishes in subsequent phases, the direct emissions part of TEWI for higher-GWP fluids will be penalized more and more. This policy-driven constraint will lead to greater desirability of ultra-low GWP refrigerants like R-1234ze(E) and R-717 from a compliance perspective, even if they may be slightly less energy efficient in pure terms, and it will revolutionize the trade-off decisions before manufacturers and policy makers. In summary, through a reproducible workflow, the results validate the function of the integrated model toward quantifying and understanding the deeply complex performance-environment trade-offs at play. Though the absolute values have not been verified due to the synthetic property data, the framework of the methods developed has been validated, and can now be applied to authoritative inputs to produce definitive, publication-quality design guidance.

6. Discussion

In this section, we interpret the principal findings of our comparative optimization, reflect on their implications for system design and policy, acknowledge limitations, and outline promising directions for future work.

6.1 Interpretation of Key Findings

The specific performance differences between the refrigerants in our study are primarily attributable to their thermophysical trade-offs in volumetric capacity, pressure ratios, and latent enthalpy differences. For example, R-32 has relatively strong volumetric cooling capacity and favorable heat transfer coefficients, but this comes with the disadvantages of higher pressures (and therefore, greater compressor work) and more stringent mechanical considerations (Kim et al. 2021; Daisuke and Inoue 2024). Conversely, R-1234ze(E) has a lower GWP but generally has lower capacity for a given mass flow and less favorable pressure ratios, which leads to a reduced COP in many operating points (Dong et al. 2024; "An Overview of Environment-Friendly Refrigerants" 2022) ([OUP Academic][2]). Therefore, taking together our proxy COPs, R-1234ze(E) is expected to be less efficient in the high load case, however, the climate-penalty from leakage would be very minor.

The shape of the Pareto frontiers offers further insight into the fundamental trade-offs involved in system design. In a number of refrigerant cases examined, we see that the Pareto frontier is very steep in the region of high COP, meaning that small increases in COP require large increases in TEWI, typically through larger capital costs or indirect emissions. Steeper segments are indicative of strongly conflicting objectives to reduce lifecycle emissions and maximize efficiency. On the other hand, flatter segments reflect areas where both objectives can be improved simultaneously, or "low-hanging fruit" design decisions. Kinks or sharp bends in the frontier are often indicative of regime transitions, where a small change in decision variables (such as a temperature pair) shifts which loss mechanisms are more dominant. The shapes of the frontiers are in agreement with classical thermodynamic limits (cf. Alsouda et al. 2023) whereby increases in COP are nearly always associated with higher demands on either volumetric footprint or pressure.

6.2 Implications for System Design

From the optimization results, different refrigerants may be best suited for different priority regimes. For a system where **energy efficiency is paramount**, R-32 (or its proxy R-454B in earlier iterations) tends to dominate because its performance in the steep high-COP region is superior—i.e., it can reach higher COP with acceptable TEWI penalty in many designs. For a system where **minimum environmental impact** (i.e. TEWI minimization) is the driving goal under Kigali constraints, R-1234ze(E) and even R-717 emerge as stronger candidates because their direct emissions (from leakage) are negligible relative to high-GWP competitors. However, design for the lower-capacity refrigerants demands system modifications. Lower-pressure or lower-density fluids typically require larger volumetric displacement in the compressor or larger heat exchanger surface areas to maintain the same cooling capacity. That implies physically larger compressors, thicker heat exchangers, or more finned surface area (which increases cost, material, and pressure drop). In addition, some low-GWP refrigerants may be mildly flammable (A2L classification) and thus require safety measures—leak detection, ventilation, charge limits, and explosion protection (Al-Zahrani et al. 2023). In practice, the optimal decision variable pairs (e.g., (T_e), (T_c)) reported in Table 7 often push toward slightly cooler condensing or warmer evaporating temperatures to relieve mechanical stress, and the design must be capable of handling those margins robustly.

6.3 Policy and Compliance Implications

Translating our optimization results to the Kigali phase-down schedule, a manufacturer could plan a phased transition of product lines. The first phase could be a hybrid offering (eg. R-32 or optimized HFC blends) that is optimal for COP within somewhat mild GWP caps, then later phases would transition R-1234ze(E) or R-717 to meet a COP once energy efficiency catches up or incentives paid off new transitions. In this manner we provide a map forward - follow the Pareto frontier slices for each allowed GWP epoch - and you can choose the refrigerants and designs that are made non-dominant at GWP reductions. This flexibility for strategy is important: a, "one size fits all" refrigerant will likely no longer be optimal when regulatory regimes change as will climate and capacities demand, and long-term energy change piogress outside of manufacturing will transition the market in other directions. Thus, a modular, optimized design mythos providing opportunities to adjust the refrigerant and compressor, or heat exchanger, size per the market/phase is necessary to maintain compliance and competitiveness long term.

6.4 Limitations of the Study

Our work is subject to several important caveats. First, many physical simplifications were adopted: a quasi-1D flow treatment, no explicit capital cost or economic objective in the Pareto sweep, and omission of transient/fluctuation losses. These simplifications may bias the Pareto frontier shapes and shift optimal points. Second, by not including capital cost or material penalties, the optimization may favor larger, more efficient designs that would be uneconomic in practice. Third, the analysis is specialized to a fixed DX (direct expansion) system topology; results may not generalize to alternate system architectures (e.g. cascade, ejector cycles, or variable-speed compression) without re-calibration. Finally, because our validation step lacked a true high-frequency measurement dataset, the surrogate and baseline anchors are proxy-based; this limits the certainty of the absolute predictions, though the comparative trends are still meaningful.

6.5 Future Work

To broaden applicability, future extensions should integrate **economic objectives** (capital cost, maintenance cost, lifecycle cost) into the multi-objective framework, thereby producing Pareto trade-offs among energy, emissions, and cost. In addition, extending the model's application to increasingly complex systems, e.g. vapor injection, ejector-assisted cycles, or cascade systems, will reveal a additional design freedom and change trade-off boundaries. Importantly, the optimal design points identified for R-1234ze(E), R-717, etc in prior studies need to be experimentally validated in a test rig or prototype setups. Such validation would ensure that the efficiency improvements and performance gains do indeed persist in the real world where component losses and tolerances are present, and could further inform refinement of the surrogate models and loss models carry through the optimization.

7. Conclusion

This study addressed the very important global issue of eliminating high-GWP refrigerants and replacing them with sustainable alternatives for use in vapor compression cooling systems. An overall mathematical model and optimization framework was developed so that tradeoffs could be quantified and balanced, accurately, between competing objectives of energy efficiency (COP) and total equivalent warming impact (TEWI). The modeling tool involved surrogate-based forward simulations of compressor efficiency, thermophysical property interpolations, and multi-objective Pareto optimization across typical operating conditions. The optimization pipeline was validated against artificial experimental datasets to demonstrate reproducibility of the modeling framework along with robustness of the optimization process. The results show that adopting low-GWP refrigerants cannot be seen solely as a direct replacement challenge but as an integrated system re-optimization opportunity. Each refrigerant presents thermodynamic and operational trade-offs that can only be fully resolved through tailored design and control changes. The Pareto frontiers demonstrate that operational gains often come with increased indirect emissions or capital intensity, stressing the necessity to consider a comprehensive decision-making approach. Of the refrigerants studied, R-1234ze(E) and R-717 (ammonia) were the most promising refrigerants for achieving minimum TEWI values in the Kigali phase, and R-32 showed good energy performance and fair environmental performance for transitional use in systems optimized for COP. In summary, this study emphasizes the importance of mathematical modeling, uncertainty quantification, and multi-objective optimization in the design of climate-compliant cooling technology for the next generation. With the provision of a transparent and repeatable computational pathway to determine trade-offs between thermodynamic performance and environmental impact, this study will contribute to global efforts to drive business refrigeration and air-conditioning system designs into alignment with international climate agreements. This framework allows manufacturers and policymakers to go from qualitative choices to data-driven, optimized refrigerant transitions, assuring technical viability and environmental accountability.

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