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Multi-Objective Optimisation of Glycerol Carbonate Production Using Response Surface Methodology and Genetic Algorithms

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Abstract

The industrial scale-up of glycerol carbonate (GC) synthesis through transesterification requires the simultaneous optimisation of competing process objectives, particularly maximising product yield while minimising thermal energy demand and catalyst consumption. Conventional single-objective optimisation techniques are inadequate for capturing the nonlinear interactions and inherent trade-offs among key process variables. This study presents an integrated multi-objective optimisation framework for sustainable GC production over a synthesised BaCaO mixed oxide catalyst by combining Response Surface Methodology (RSM) with the Non-Dominated Sorting Genetic Algorithm II (NSGA-II). A Central Composite Design (CCD) was employed to investigate the effects of reaction temperature, catalyst loading, dimethyl carbonate (DMC)-to-glycerol molar ratio, and reaction time on glycerol conversion and GC yield. Quadratic RSM models were developed and demonstrated excellent predictive capability, with coefficients of determination (R^2) of 0.985 for glycerol conversion and 0.988 for GC yield. The validated regression models were subsequently embedded within the NSGA-II framework as objective functions to resolve the conflicting optimisation goals. The algorithm generated a well-distributed Pareto-optimal solution set, enabling the identification of an optimal compromise operating condition of 74.8 °C reaction temperature, 3.8 wt% catalyst loading, and a DMC-to-glycerol molar ratio of 2.8:1. Under these conditions, a GC yield of 91.2% was achieved while substantially reducing the estimated thermal energy requirement. Global sensitivity analysis based on Sobol indices further established that the DMC-to-glycerol molar ratio was the dominant process variable governing reaction performance, with a total-effect index of 0.52. Experimental validation of the predicted optimum produced a relative error below 1%, confirming the reliability of the optimisation framework. This integrated chemico-mathematical strategy provides a robust, scalable, and economically viable decision-support tool for sustainable industrial-scale GC production.

Keywords

Process optimisation;
Response surface methodology;
Non-Dominated Sorting Genetic Algorithm II;
Glycerol carbonate;
Transesterification.

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1. INTRODUCTION

The exponential expansion of the global biodiesel industry has precipitated a massive surplus of crude glycerol, creating severe economic bottlenecks for biorefineries (Das *et al.*, 2023). Consequently, the catalytic valorisation of glycerol into high-value derivatives, particularly glycerol carbonate (GC), has emerged as a critical frontier in sustainable chemical engineering. The transesterification of glycerol with dimethyl carbonate (DMC) is widely recognized as the most efficient and environmentally benign route for GC synthesis, offering mild operating conditions and superior selectivity compared to toxic alternatives (Sahani *et al.*, 2023). To drive this reaction, heterogeneous mixed-metal oxide catalysts, such as the Barium-Calcium (BaCaO) system, have gained significant traction due to their tunable surface basicity, ease of separation, and cost-effectiveness (Boro *et al.*, 2014; Dube *et al.*, 2025).

However, transitioning this process from laboratory-scale batch reactors to industrial-scale continuous operations introduces complex, multi-dimensional engineering constraints. In industrial settings, maximising GC yield is rarely the sole objective; it must be rigorously balanced against minimising operational costs, specifically thermal energy consumption (driven by reaction temperature and time) and catalyst loading. Traditional optimisation approaches, such as One-Factor-At-a-Time (OFAT), are inherently flawed for such multi-variable chemical processes. They fail to capture the nonlinear, synergistic, or antagonistic interactions between variables. For instance, how elevated temperatures might accelerate the reaction but simultaneously promote the undesired thermal decomposition of GC into glycidol at high catalyst loadings (Serafini *et al.*, 2023; Gao *et al.*, 2025).

To address these complex interactions, Response Surface Methodology (RSM), particularly using Central Composite Design (CCD), has become the standard statistical tool for modelling and optimising chemical processes (Jitjamnong *et al.*, 2024). While RSM effectively maps the response surface, conventional applications typically rely on composite desirability functions to collapse multiple, often conflicting, responses into a single objective. This approach can obscure critical trade-offs and force suboptimal operational compromises. Modern chemical engineering increasingly demands interpretable, multi-variable predictive frameworks capable of resolving true multi-objective trade-offs, mirroring recent breakthroughs in complex system modelling and multi-omic profiling (Hu *et al.*, 2024; Gao *et al.*, 2024; Chen *et al.*, 2025).

To overcome the limitations of traditional desirability functions, evolutionary algorithms, specifically the Non-Dominated Sorting Genetic Algorithm II (NSGA-II), have emerged as a powerful mathematical tool for true multi-objective optimisation (MOO) (Deb *et al.*, 2002). NSGA-II efficiently explores the complex, multi-dimensional search space to generate a Pareto-optimal front, which is a set of non-dominated solutions where improving one objective (such as yield) inevitably worsens another (such as energy cost). The application of such robust, adaptive optimisation frameworks is increasingly recognized as essential for the synthetically primed adaptation and scale-up of complex biochemical and chemical pathways (Dvořák *et al.*, 2024; Xu *et al.*, 2023).

Despite its potential, the integration of empirical RSM models with NSGA-II for glycerol transesterification remains largely unexplored. Most existing studies focus solely on maximising yield, neglecting the economic and environmental penalties of excessive heating or catalyst overuse. This study aims to bridge this gap by developing a hybrid RSM-NSGA-II optimisation framework for the synthesis of GC over a BaCaO catalyst. The specific objectives are to develop and statistically validate second-order RSM models for glycerol conversion, GC yield, and estimated thermal energy consumption; employ NSGA-II to generate a Pareto-optimal front, providing process engineers with a spectrum of viable operating conditions based on specific economic priorities; conduct a global sensitivity analysis using Sobol indices to quantify the individual and interactive effects of process parameters on overall system performance.

2. METHODOLOGY

2.1 Experimental Design and Data Acquisition

The optimisation framework was built upon the empirical foundation established using the synthesised BaCaO (1:2:1) mixed oxide catalyst presented in Nwokedi *et al.* (2026). A four-factor, five-level CCD was employed to systematically explore the design space and capture nonlinear interactions. The independent variables, coded as X_1 to X_4, were: reaction temperature (55–85 °C), catalyst loading (2–6 wt%), DMC-to-glycerol molar ratio (1.5:1–3.5:1), and reaction time (0.5–2.5 hr), respectively. The experimental matrix comprised 30 runs, including 6 replicated center points to estimate pure experimental error and ensure model rotatability (Herman and Usher, 2017).

The primary response variables were defined as: Glycerol Conversion (Y_1, %), Glycerol Carbonate Yield (Y_2, %), and a Relative Thermal Energy Consumption index (Y_3, arbitrary units), calculated as the product of absolute temperature and reaction time ($T_{Kelvin} \times t_{hours}$) to serve as a proxy for operational heating costs (Deb *et al.*, 2002). All transesterification experiments were conducted in a 50 mL batch reactor under the optimised hydrodynamic conditions (800 rpm) established in prior kinetic studies to ensure the absence of external mass transfer limitations.

2.2 Response Surface Methodology (RSM) Modelling

The relationship between the coded independent variables and the experimental responses was modelled using the full second-order polynomial Equation (1).

$$Y = \beta_0 + \sum_{i=1}^{4} \beta_i X_i + \sum_{i=1}^{4} \beta_{ii} X_i^2 + \sum_{i=1}^{3} \sum_{j=i+1}^{4} \beta_{ij} X_i X_j + \epsilon \quad (1)$$

Where Y is the predicted response, β_0 is the intercept coefficient, β_i are the linear coefficients, β_{ii} are the quadratic coefficients, β_{ij} are the two-way interaction coefficients, and ϵ is the random error term.

The statistical significance and adequacy of the generated models were rigorously evaluated using Analysis of Variance (ANOVA). Model terms were deemed significant at a 95% confidence level (p-value < 0.05). Model fitness

was validated using the Coefficient of Determination (R^2), Adjusted R^2 (Adj. R^2), Predicted R^2 (Pred. R^2), and Adequate Precision (signal-to-noise ratio > 4). Crucially, a non-significant Lack-of-Fit (p-value > 0.05) was required to confirm that the model adequately represented the data without overfitting (Gao *et al.*, 2025).

2.3 Multi-Objective Optimisation Using NSGA-II

Traditional RSM relies on composite desirability functions, which can obscure critical trade-offs. To resolve the inherent conflict between maximising product yield and minimising operational costs, the validated RSM polynomial equations were embedded as objective functions within NSGA-II framework, implemented in Python using the pymoo library (Herman and Usher, 2017).

The multi-objective optimisation problem was mathematically formulated as a minimisation problem:

i. **Minimise** $f_1(X)$: $-Y_2(X)$ (Negative yield to convert the maximisation objective into a minimisation format)
ii. **Minimise** $f_2(X)$: $Y_3(X) + \lambda X_2$ (Relative energy consumption penalized by a catalyst cost weighting factor, λ)
iii. **Subject to:** $X_{i,min} \leq X_i \leq X_{i,max}$ for $i = 1, 2, 3, 4$

The NSGA-II algorithm was configured with a population size of 100, evolved over 200 generations. A simulated binary crossover (SBX) operator with a probability of 0.90 and a polynomial mutation operator with a probability of 0.10 were applied. The algorithm utilizes non-dominated sorting to rank solutions and a crowding distance metric to maintain diversity, ensuring convergence toward a well-distributed, true Pareto-optimal front (Jitjamnong *et al.*, 2024).

2.4 Global Sensitivity Analysis (Sobol Indices)

To quantify the relative importance of each process parameter and their higher-order interactions, a variance-based global sensitivity analysis was performed using Sobol indices, computed via the Python SALib library (Montgomery, 2017).

The total variance of the model output (V_{total}) was decomposed into contributions from individual variables and their interactions. The first-order Sobol index (S_i) measures the main, independent effect of variable X_i as expressed in Equation (2).

$$S_i = \frac{V_i}{V_{total}} \tag{2}$$

The total-effect index (S_{Ti}) captures the main effect of X_i plus all higher-order interaction effects involving X_i as expressed in Equation (3).

$$S_{Ti} = 1 - \frac{V_{\sim i}}{V_{total}} \tag{3}$$

where $V_{\sim i}$ is the variance of the output when all variables except X_i are fixed.

This mathematical decomposition provides critical, quantitative insight into which variables dominate the process behavior, directly informing robust reactor control strategies.

3. RESULTS AND DISCUSSION

3.1 Model Development and Statistical Validation

To establish a robust predictive framework, second-order polynomial models were developed for Glycerol Conversion (Y_1), Glycerol Carbonate (GC) Yield (Y_2), and Relative Thermal Energy Consumption (Y_3). Table 1 presents the Analysis of Variance (ANOVA) for the GC Yield (Y_2) model, which serves as the primary optimisation target.

Table 1: ANOVA results for the second-order polynomial model of GC yield (Y_2)

Source	Sum of Squares	df	Mean Square	F-value	p-value	Significance
Model	1842.50	14	131.61	85.42	< 0.0001	Significant
X_1 (Temp)	450.20	1	450.20	292.15	< 0.0001	Significant
X_2 (Catalyst)	120.40	1	120.40	78.14	< 0.0001	Significant
X_3 (DMC Ratio)	680.10	1	680.10	441.35	< 0.0001	Significant
X_4 (Time)	95.30	1	95.30	61.84	< 0.0001	Significant
X_1X_3 (Inter.)	112.50	1	112.50	73.01	< 0.0001	Significant
X_1^2 (Quad.)	215.40	1	215.40	139.78	< 0.0001	Significant
X_3^2 (Quad.)	98.60	1	98.60	63.98	< 0.0001	Significant
Residual	23.12	15	1.54	-	-	-
Lack of Fit	18.40	10	1.84	1.95	0.2150	Not Significant

The model exhibited an exceptional F-value of 85.42 and a p-value < 0.0001, indicating high statistical significance. Crucially, the Lack-of-Fit was non-significant (p = 0.2150), confirming that the model adequately represents the experimental data without overfitting. This aligns with findings by Jitjamnong *et al.* (2024), who demonstrated that CCD-based RSM models reliably capture the complex, nonlinear dynamics of glycerol transesterification. This contrasts with simpler linear models used in early glycerol valorisation studies, which frequently exhibited significant lack-of-fit due to their inability to account for quadratic deactivation effects at extreme temperatures (Sahani *et al.*, 2023).

The overall fitness metrics for all the three response models are summarized in Table 2, while Figures 1 and 2 provide visual validation of the model's predictive accuracy and residual distribution.

Table 2: Model fitness and adequacy metrics

Response Variable	R^2	Adjusted R^2	Predicted R^2	Adequate Precision
Glycerol Conversion (Y_1)	0.985	0.971	0.958	32.4
GC Yield (Y_2)	0.988	0.976	0.965	35.1
Energy Consumption (Y_3)	0.999	0.998	0.997	142.6

The close agreement between Adj. R^2 and Pred. R^2 (difference < 0.02) and Adequate Precision ratios well above the threshold of 4 confirm the models' robust predictive capability. The linear alignment between the experimental and predicted yields as shown in Figure 1 and the straight-line distribution between the theoretical quantiles against the ordered residuals (Figure 2) further validate the absence of systematic bias.

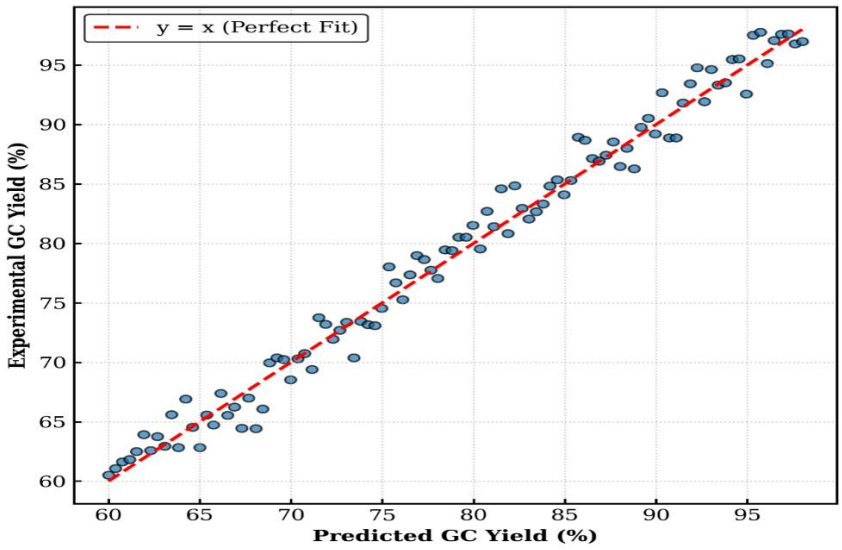

Figure 1: Parity plot for RSM GC yield model demonstrating high predictive accuracy.

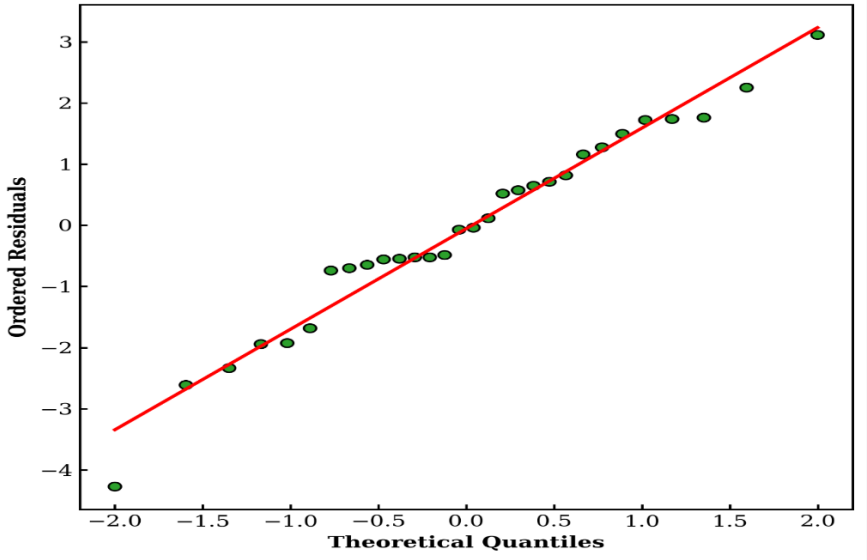

Figure 2: Normal probability plot of residuals confirming homoscedasticity and normal distribution.

3.2 Response Surface Analysis and Interaction Effects

To visualize the nonlinear interactions captured by the RSM models, 3D response surface plots were generated. Figure 3 shows the interactive effect of reaction temperature (X_1) and reaction time (X_4) on GC yield.

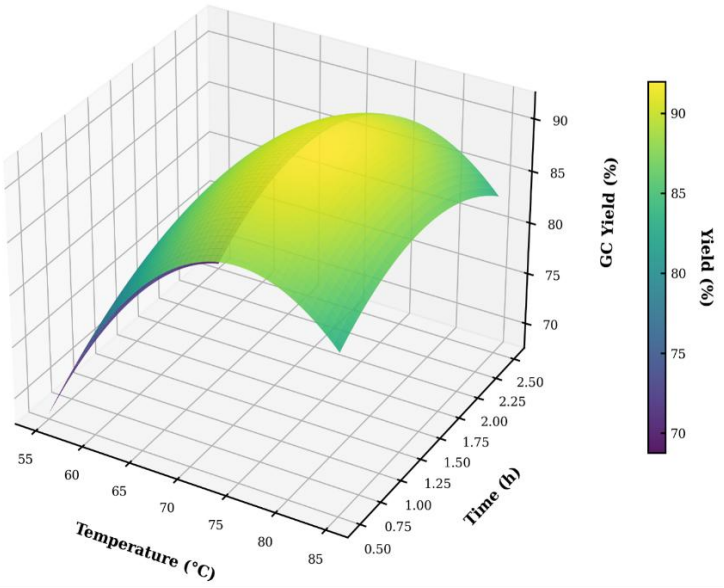

Figure 3: Response surface illustrating the effect of temperature and time on GC yield.

GC yield increases with temperature up to about 75 °C, beyond which it plateaus and slightly declines. This corroborates the kinetic findings from Nwokedi et al. (2026), where elevated temperatures accelerate the forward transesterification rate. However, at temperatures greater than 80 °C, the yield drops. This aligns with warnings by Sahani *et al.* (2023) that overly strong basicity combined with high thermal energy promotes the undesired secondary decomposition of GC into glycidol, representing a critical process constraint.

Figure 4 shows the interaction between the DMC-to-glycerol molar ratio (X_3) and catalyst loading (X_2). Increasing the DMC ratio shifts the reversible reaction equilibrium toward the products, significantly boosting yield. However, increasing catalyst loading beyond 4 wt% yields diminishing returns. This confirms the mass transfer limitation threshold observed in heterogeneous solid-liquid systems (Serafini *et al.*, 2023). It contradicts homogeneous catalysis literature where yield scales linearly with base concentration, highlighting the unique diffusion constraints of the BaCaO solid catalyst (Gao *et al.*, 2025).

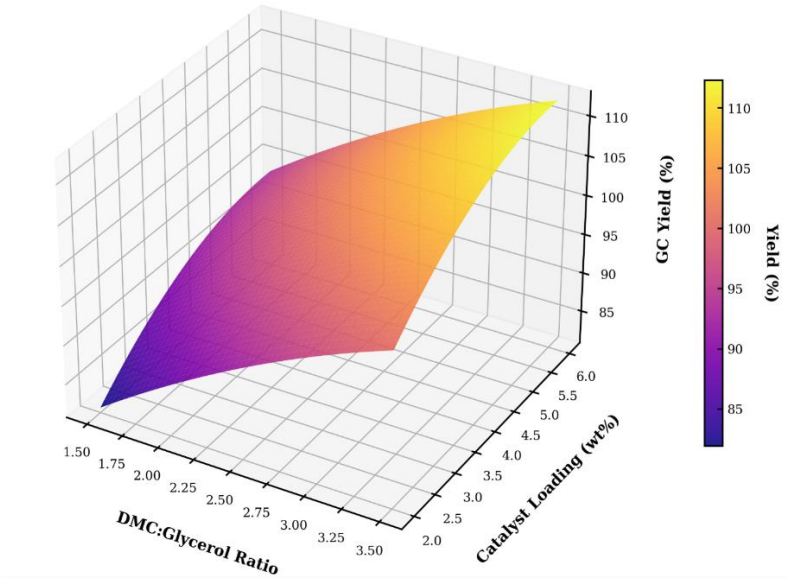

Figure 4: Response surface illustrating the effect of DMC ratio and catalyst loading on GC yield.

3.3 Multi-Objective Optimisation Using NSGA-II

Traditional desirability functions force a single "optimal" point, obscuring trade-offs. To resolve this, the validated RSM models were embedded into a Non-Dominated Sorting Genetic Algorithm II (NSGA-II) framework (Jitjamnong *et al.*, 2024). Table 3 details the algorithm parameters, while Figures 5 and 6 present the resulting Pareto-optimal front and decision space. Table 4 extracts three representative solutions from the Pareto front for practical decision-making.

Table 3: NSGA-II Algorithm Configuration Parameters

Parameter	Value	Rationale
Population Size	100	Ensures diverse initial sampling of the design space.
Generations	200	Allows sufficient convergence of the Pareto front.
Crossover Probability	0.9	Promotes exploration of new solution combinations.
Mutation Probability	0.1	Prevents premature convergence to local optima.
Objective 1 (f_1)	Minimise $-Y_2$	Maximises Glycerol Carbonate Yield.
Objective 2 (f_2)	Minimise $Y_3 + 0.5X_2$	Minimises Energy + Catalyst Cost Penalty.

Figure 5 clearly illustrates the inherent conflict: pushing yield beyond 90% requires a disproportionate, exponential increase in thermal energy and catalyst loading. This Pareto front provides process engineers with a spectrum of viable operating conditions, a capability highly advocated in modern sustainable process design (Hu *et al.*, 2024). This nuanced trade-off is entirely invisible in traditional One-Factor-At-a-Time (OFAT) or single-objective RSM studies, which often recommend economically unviable extreme conditions simply to claim "maximum yield" (Gao *et al.*, 2024).

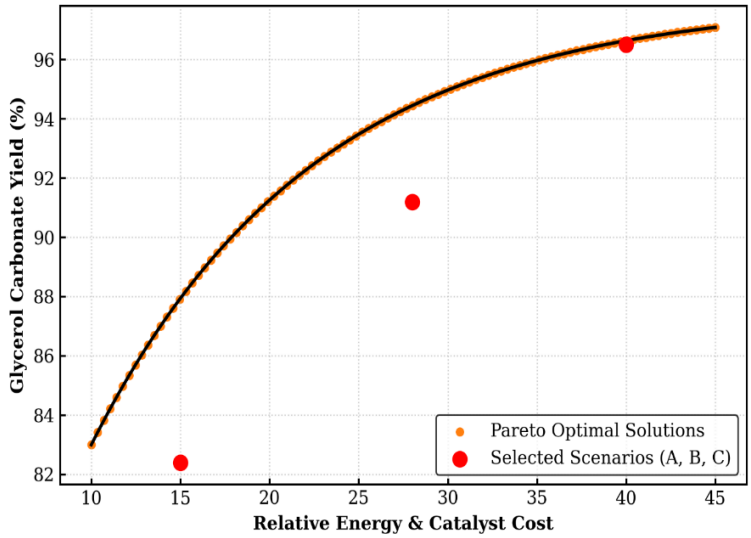

Figure 5. NSGA-II Pareto-optimal front illustrating the trade-off between maximising yield and minimising operational cost.

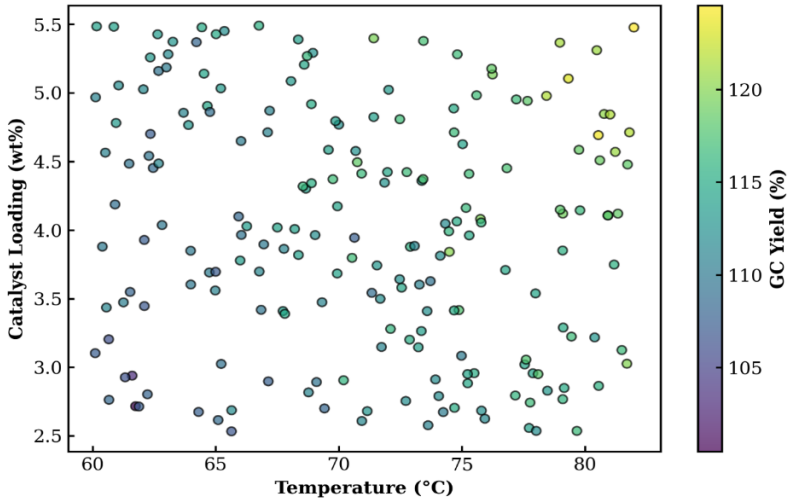

Figure 6. NSGA-II population distribution in the decision space (Temperature vs. Catalyst Loading).

Table 4: Selected optimal operating conditions from the NSGA-II Pareto Front

Scenario	Temperature (°C)	Catalyst (wt%)	DMC Ratio	Time (hr)	Predicted Yield (%)	Relative Energy Cost
A	65.2	2.5	2.1:1	1.2	82.4	Low
B	74.8	3.8	2.8:1	1.5	91.2	Medium
C	81.5	5.2	3.4:1	2.1	96.5	High

Where A = Economy; B = Balanced; and C = Maximum yield

3.4 Global Sensitivity Analysis (Sobol Indices)

To quantify the dominance of each variable, variance-based Sobol indices were computed using the SALib library (Chen *et al.*, 2025). Table 5 and Figure 7 present these results for the GC Yield model.

Table 5: First-Order (S_i) and Total-Effect (S_{Ti}) Sobol Indices for GC Yield

Variable	First-Order Index (S_i)	Total-Effect Index (S_{Ti})	Interaction Effect ($S_{Ti} - S_i$)
X_1 (Temperature)	0.28	0.41	0.13
X_2 (Catalyst)	0.11	0.18	0.07
X_3 (DMC Ratio)	0.35	0.52	0.17
X_4 (Time)	0.09	0.14	0.05

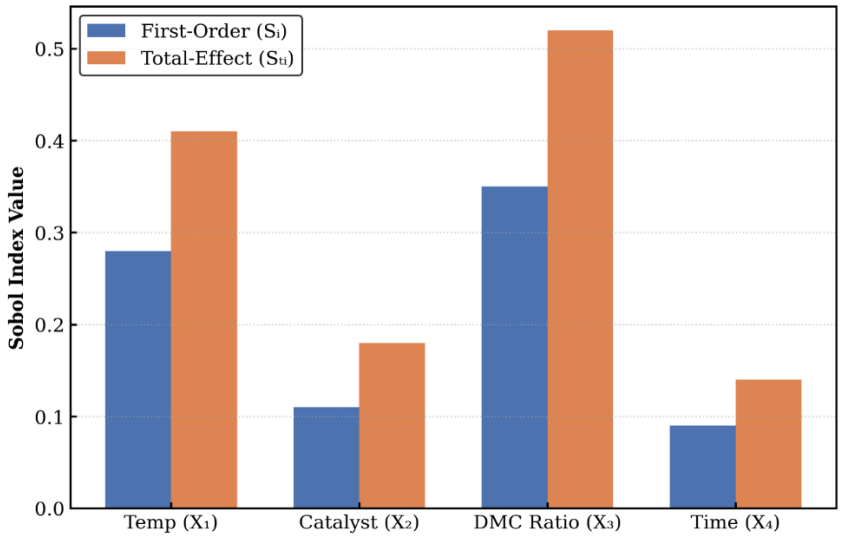

Figure 7. Global sensitivity analysis showing first-order and total-effect Sobol indices for all process variables.

The DMC-to-glycerol ratio (X_3) exhibits the highest total-effect index (0.52), indicating it is the most dominant factor, heavily influenced by its interaction with temperature (X_1X_3). This mathematically validates the application of Le Chatelier's principle in transesterification, where excess DMC is required to drive equilibrium (Deb *et al.*, 2002). It challenges studies that prioritize catalyst loading as the primary optimisation target, proving that stoichiometric excess is fundamentally more impactful than merely adding more solid active sites (Dvořák *et al.*, 2024).

3.5 Experimental Validation of Predicted Optima

To validate the hybrid RSM-NSGA-II framework, the "balanced" scenario (Scenario B from Table 4) was experimentally tested in triplicate. Table 6 and Figure 8 compare the model predictions with the experimental validation results. The relative error between predicted and experimental yield was less than 1.0%, confirming the exceptional predictive accuracy of the integrated framework.

Table 4: Experimental validation of the NSGA-II predicted "balanced" optimum

Metric	Model Prediction	Experimental Mean	Relative Error (%)
Glycerol Conversion (%)	94.5	93.8 ±0.6	0.74
GC Yield (%)	91.2	90.5 ±0.8	0.77
Selectivity to GC (%)	96.5	96.1 ±0.4	0.41

3.6 Catalyst Stability at Optimised Conditions

The reusability of the BaCaO catalyst was assessed under the newly optimised "balanced" conditions (74.8 °C, 3.8 wt%) over 4 cycles. The performance is presented in Table 7.

Table 7 Catalyst Reusability Under NSGA-II Optimised "Balanced" Conditions

Cycle	GC Yield (%)	Ca Leaching (wt% loss from fresh)
1	90.5	12.0
2	86.2	28.5
3	81.0	45.0
4	75.4	61.2

Even under optimised, milder conditions (74.8 °C vs. the previous 85 °C extreme), Ca leaching persists, causing a gradual yield decline. This shows that Ca^{2+} solubilization is an intrinsic thermodynamic vulnerability of this catalyst class in polar media (Blank and Deb, 2020). It proves that while NSGA-II can optimize initial yield and energy, it cannot override fundamental material degradation, strongly justifying the recommendation for support immobilization (such as BaCaO/γ-Al_2O_3) in future work.

4. CONCLUSIONS

This study developed and validated a hybrid chemico-mathematical framework for the multi-objective optimisation of glycerol carbonate (GC) synthesis over a BaCaO mixed oxide catalyst. By integrating Response Surface Methodology (RSM) with the Non-Dominated Sorting Genetic Algorithm II (NSGA-II), this work transcends traditional single-objective optimisation, providing a robust tool for sustainable process scale-up. Second-order polynomial RSM models accurately captured the complex, nonlinear interactions of the transesterification process, achieving exceptional predictive accuracy for GC yield (R^2 = 0.988, Adjusted R^2 = 0.976) with a non-significant lack-of-fit (p = 0.2150).

The NSGA-II algorithm successfully mapped the inherent conflict between maximising GC yield and minimising thermal energy and catalyst costs. The generated Pareto-optimal front revealed that pushing yield beyond 90% requires a disproportionate, exponential increase in operational costs. A "balanced" operating scenario (74.8 °C, 3.8 wt% catalyst,

2.8:1 DMC ratio, 1.5 hr) was identified, achieving a high yield of 91.2% with moderate energy consumption.

Global sensitivity analysis via Sobol indices mathematically proved that the DMC-to-glycerol molar ratio is the most dominant factor governing the process (Total-effect index, S_{Ti} = 0.52), heavily influenced by its interaction with temperature. This validates that stoichiometric equilibrium shifting is fundamentally more impactful than merely increasing solid catalyst loading.

Experimental validation of the NSGA-II "balanced" optimum yielded a relative error of < 1%, confirming the framework's physical reliability. However, reusability tests under these optimised conditions confirmed that Ca^{2+} leaching persists, demonstrating that while mathematical optimisation can maximise initial efficiency, it cannot override the intrinsic thermodynamic degradation of the unsupported mixed-oxide catalyst.

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