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Research Articles

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Sensitivity Analysis of CubeSat Orbital Parameters for Enhancing Revisit Time and Regional Coverage: A Case Study of the Najran–Yemen Desert Border

Ghadi Mahdi Al Amer and Asia Saeed Kajo Habila
(Aerospace engineering)

1
- 

Software-Driven Imaging Mission Planning and Attitude Control for Super-Agile Satellite

Fatimah Alzedany and Atif Mahmood
(Aerospace Engineering)

9
- 

Adapting Urban Digital Twins for Greenfield Vertical Urbanism: A Deployment Strategy for NEOM's The Line

Yousif Turki AlGurain and Mustafa Faisal Ahmed
(Architecture Engineering and Design)

20
- 

Development of a Microwave Metamaterial Sensor for Noninvasive Glucose Detection

Dhay Al-Harathi and Ibraheem Al-Naib
(Bioengineering)

27
- 

Computational Investigation of Continuum-Like Behavior in Segmented Beam Structures with Frictional Interfaces

Mohannad F. Al Sindhi and Ahmed S. Dalaq
(Bioengineering)

34
- 

XGBoost-Based Prediction of pKa Values from Molecular Descriptors

Fahad Ali Atwi and Mohammed Al-Khater
(Chemical Engineering)

41
- 

Building and Evaluating an Arabic Social-Media Dataset for Deepfake Text Detection

Budoor Alshehri, Amal Sunba, and Tarek Helmy
(Computer Science)

48
- 

Collection and Generation of Arabic E-Commerce Text Data: A Study on Deepfake Detection and Dataset Development

Funoon Albalawi, Amal Sunba, and Tarek Helmy
(Computer Science)

56
- 

Evaluation of Azure Pronunciation Assessment Tool for Arabic-Speaking Learners

Jalal Zainaddin and Mohammad Amro
(Computer Engineering)

65
- 

Simulation-Based Modeling and PID control optimization for quadcopter UAV using genetic algorithm

Sajjad Al Mahmud and Ahmed Eltayeb
(Control and Instrumentation Engineering)

74
- 

Enhancing 2-DOF Helicopter MIMO System Control using ZOA-Tuned Single Neuron PID Algorithm

Abdullah Aljuaid and Fadi Alyoussef
(Control and Instrumentation Engineering)

91

-  **Experimental Modeling and Control of a DC Servo Motor Based on System Identification: A Comparative PID with Policy Iteration** 99
Hassan K. Misbah and Nezar M. Alyazidi
(Control and Instrumentation Engineering)
-  **Techno-Economic Optimization of a Grid-Tied Photovoltaic System for Schools in Saudi Arabia** 110
Jarah Alqasim, Fahad Alhamli, Khaled Kunnah, Osama Alghunaim, and Nagmeldeen A. M. Hassanain
(Electrical Engineering)
-  **Monitoring Carbonate Levels in Saline Water Using Electrical Resistivity in Carbonate Formations** 119
Abdullah Deya Al-Qisoom and Ahmed Al-Yaseri
(Geosciences)
-  **Video Based Sperm Motility Grading and YOLOv8 Detection: A Tracking-Free Approach to Automated Semen Analysis** 130
Abdulrahman Alshaikh and Anis Elgabli
(Industrial Engineering)
-  **Investigating the Fouling Tendency of Polyelectrolyte Complex Membranes** 138
Mousa Ibrahim Bokhamseen and Muhammad Irshad Baig
(Material Science and Engineering)
-  **Enhanced CO₂ Adsorption Performance of Amine-Functionalized MCM-41 Mesoporous Silica** 143
Mohammed Alali and Ahmed Alsmail
(Material Science and Engineering)
-  **Enhanced Photocatalytic Performance of Ball-Milled Graphitic Carbon Nitride for Methylene Blue Degradation** 150
Layan Mohammed Alhomidan and Muhammad Ihsan-Ul-Haq
(Material Science and Engineering)
-  **Sputtered TiO₂/Al₂O₃ Multilayer Coatings as Transparent Anti-Soiling Solutions for Solar Photovoltaics in Humid-Arid Regions** 158
Ghadah Khalid Mobaireek and Amir Al-Ahmed
(Material Science and Engineering)
-  **Impact of Cation Dissolution on Kinetics of CO₂ Mineralization in Carbonate Rocks** 164
Turki Aljuaid and Dhafer Al Shehri
(Petroleum Engineering)
-  **Methanol Slug Sizing as a Mobility Control Strategy for Viscous Fingering Supersession in Miscible scCO₂ EOR: A CMG-GEM Simulation Study** 172
Wafa Alahmed and Sidqi Abu-Khamsin
(Petroleum Engineering)

Sensitivity Analysis of CubeSat Orbital Parameters for Enhancing Revisit Time and Regional Coverage: A Case Study of the Najran–Yemen Desert Border

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ABSTRACT

Frequent satellite observations play an important role in enhancing the security of border regions. However, maintaining adequate coverage by using a single CubeSat remains challenging. This study investigates the feasibility of employing a single CubeSat to monitor the Najran–Yemen desert border by optimizing orbital parameters to minimize revisit time while preserving effective regional coverage. This study aimed to determine the orbital configuration, specifically the optimal values of inclination and right ascension of the ascending node (RAAN) to maximize temporal access to the targeted area. A one-year simulation was conducted using Systems Tool Kit (STK) software, in which a nadir-pointing CMOS sensor with fixed imaging parameters was attached to the CubeSat. Two main orbital scenarios were analyzed: a Sun-synchronous orbit (SSO) and a user-defined orbit with varying inclinations and RAAN values. Coverage and Figure-of-Merit (FoM) tools in STK were used to generate coverage metrics, including the overall coverage percentage. The results reveal that the SSO configuration exhibits very long revisit intervals and limited temporal visibility across the border. In contrast, the optimized orbit reduces the average revisit time by more than one order of magnitude and increases access opportunities by over threefold compared to the SSO baseline, with optimal performance achieved at an inclination of 20° and $RAAN = 120^\circ$. These findings confirm that careful orbital tuning improves temporal monitoring capability, providing a practical approach for efficient single-satellite border surveillance.

Keywords: CubeSat, earth observation, satellite coverage analysis, revisit time, figure of merit, STK simulation

1. INTRODUCTION

Satellite technology has become a critical component in various fields, including communications, environmental monitoring, and border surveillance¹. Traditional satellites, however, often entail high costs and face challenges during launch, which limit their deployment. However, recent years have seen a remarkable increase in the utilization and exploration of cube satellites (CubeSats)^{2,3}, a popular type of nanosatellite. Each CubeSat comprises one or more units, with each unit measuring $10 \times 10 \times 10$ cm and possessing a mass of approximately 1 kg⁴. Owing to their comparatively low manufacturing, launch, and maintenance costs, they have emerged as a promising platform for various applications, including Earth observation and remote sensing⁵. This shift toward miniaturized satellite platforms has motivated researchers to investigate their feasibility for security-sensitive applications.

Using CubeSats to monitor sensitive and dynamic regions such as the desert borders between Saudi Arabia and Yemen presents significant challenges in terms of image quality and revisit time (Figure 1). This region is a critical conduit for the illicit trafficking of weaponry, narcotics, and qat into Saudi Arabia⁶. However, due to the small CubeSat form factor, it is

challenging to equip them with cameras capable of achieving both high spatial resolution and wide-swath coverage simultaneously. Moreover, the use of a single CubeSat may also affect access and revisit times. This inherent tradeoff between revisit time and maintaining good imaging quality limits the effectiveness of CubeSats for border monitoring, making it crucial to investigate and evaluate the sensitivity of orbital parameters to balance both objectives.

Research by Selva and Krejci⁷ explored various applications of satellite technology in communication systems, disaster monitoring, border surveillance, and military intelligence. Satellites provide reliable, near-real-time, high-resolution data that support both civilian and defense-related activities. For example, communication satellites can transmit information rapidly and securely worldwide. Similarly, large remote-sensing satellites, such as ASTER and Sentinel-2, have been successful in environmental change detection and disaster response. These studies highlight the strategic importance of space-based assets in surveillance operations; however, they primarily focus on large, high-performance satellite platforms.

The high camera specifications, large apertures, and high altitudes of Sentinel 2 and other large satellites provide excellent

coverage for various remote-sensing applications. In contrast, CubeSats, with lower-specification imagery systems, orbit at lower altitudes, achieving lower spatial resolution and smaller coverage. These limitations motivated the present study, in which the role of satellites in enhancing regional security and resilience was investigated.

Although a single CubeSat has a significant advantage owing to its reduced system complexity and cost, its ability to provide frequent observations is limited due to longer revisit times. One of the possible ways to overcome such limitations, already pursued in previous works, is the deployment of a multisatellite CubeSat architecture optimized to minimize revisit time. Santilli et al.⁸ investigated the potential of CubeSat constellations for disaster management by designing an optimal architecture aimed at minimizing revisit time over remote regions of Brazil. It was demonstrated that deploying multiple CubeSats across appropriately selected orbital planes can reduce revisit intervals. However, constellation-based approaches increase mission complexity, cost, and operational requirements. Furthermore, existing CubeSat coverage studies have largely focused on either constellation design or general Earth observation missions, rather than examining how a single CubeSat can be geometrically optimized for a specific regional security application.

Despite the growing interest in CubeSat-based Earth observation, existing research has not adequately examined how a single CubeSat can be optimally configured for effective border surveillance in desert environments, nor has it addressed context-specific applications within the Kingdom of Saudi Arabia.

To address these challenges, the effective implementation of CubeSats was investigated for continuous security monitoring of the Najran–Yemen desert border by determining the optimal orbital parameters that maximize the revisit frequency over the target area and relying on orbital parameter optimization rather than additional spacecraft. Unlike previous studies that prioritized increasing satellite numbers or enhancing payload capabilities, orbital inclination and right ascension of the ascending node (RAAN) were isolated as controllable design variables in this study; their direct impact on revisit performance was evaluated for a defined border region. The ultimate contribution of this study lies in providing an optimized framework for

single-satellite mission design and offering practical insights for enhancing border surveillance using CubeSat systems.

2. METHODS

2.1. CubeSat Platform and Orbital Parameters. A CubeSat with six units, equipped with a fixed solar panel within its body and keeping the nadir face free of panels for camera mounting, was considered in this study. The CubeSat was modeled at an orbital altitude of 500 km above Earth's surface. The key orbital parameters considered as primary variables in the analysis are listed in Table 1. Each parameter was selected based on a typical configuration utilized for Earth observation in low-Earth orbit. A schematic illustration of the fundamental orbital elements is presented in Figure 2 to clarify their geometric meanings within the orbital plane. The two main planes that define most of the parameters are Earth's equatorial plane and the orbital plane defined by the inclination and RAAN.

The inclination range was based on the latitude of the region of interest (ROI), which is near 18° N. Because a satellite can access latitudes only up to its orbital inclination, moderate inclinations slightly higher than the target latitude were expected to concentrate ground track intersections over the region while avoiding unnecessary coverage at higher latitudes. Consequently, low-to-moderate inclinations were evaluated to assess their impact on revisit performance for localized monitoring.

Similarly, RAAN was varied across a broad interval to assess the effect of the orbital plane orientation on the longitudinal ground track alignment. Because RAAN determines the spatial relationship between the orbital plane and Earth's rotation, sweeping this parameter enables the identification of configurations that produce more favorable temporal clustering of accesses over the target area. This approach represents a structured geometric sensitivity analysis based on orbital mechanics principles.

2.2. Sensor and Imaging Model. The simulated CubeSat was assumed to carry a CMOS-based optical sensor, consistent with the CubeSat's constraints, such as low power consumption and high-resolution images during rapid orbital motion¹⁰. The imaging system pixel resolution was 4096 × 3072 with a 5-μm



Figure 1. Map of the desert border region between Najran, Saudi Arabia, and Yemen⁶

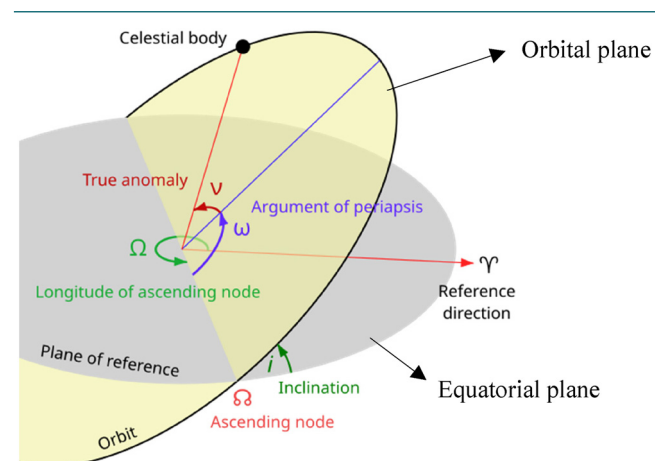


Figure 2. Schematic diagram of orbital elements (adapted from Wikipedia, 2025)

Table 1. Description of Key Orbital Parameters Used in the Study

Parameter	Symbol / Unit	Typical Range Tested	Purpose / Effect in simulation
Altitude	h (km)	500	Controls the satellite's height above Earth; affects image resolution, coverage area, and revisit time. Lower altitude means higher resolution but smaller coverage area.
Inclination	i (°)	20–98	Determines the latitude range the satellite can cover. Higher inclinations allow more frequent passes over mid-latitude regions such as the border region targeted in this study.
Right ascension of ascending node (RAAN)	Ω (°)	30–180	Defines the orbit's orientation relative to the Sun and epoch; affects the local time of day when the satellite passes over the target area
Eccentricity	e	0 (circular orbit)	Fixed in this simulation, to simplify the analysis; ensures uniform altitude throughout each orbit.
Argument of perigee	ω (°)	0 (fixed)	Not significant for circular orbits; kept constant in all simulations.

Table 2. Summary of Scenario 1 (FoM Results)

Number of Access	Access Duration (s)	Average revisit Time (days)	Average Coverage Percentage (%)
127	9.346	251.73	0.0750

pixel size and a 100-mm focal length, resulting in a rectangular field of view defined by half-angles of 5° (cross-track) and 4° (along-track), corresponding to full angular extents of 10°×8°. The sensor was mounted in a nadir-pointing configuration to maximize scene stability and simplify the geometric projection of the footprint onto the Earth's surface. At an altitude of 500 km, this configuration yields an approximate ground swath of 87.5 km (cross-track) and 70.0 km (along-track), computed using $W = 2h/\tan(\Theta)$. The GSD, which represents the ground resolution of the image, was estimated by

$$GSD = \frac{H \times P}{f}$$

where H is the satellite altitude, P is the pixel size, and f is the focal length.

Lower GSD values indicate finer image details, whereas higher orbital altitudes result in coarser resolutions. However, both scenarios (described in the next section) simulated in this study were implemented at the same altitude using an identical camera and nadir-pointing configuration; therefore, the GSD values remained constant at approximately 25 m/pixel (at 500 km altitude).

2.3. Overview of STK Simulation and Coverage Analysis. The simulation was conducted using Systems Tool Kit (STK) version 12.9, which is typically used in the aerospace field for spacecraft mission design, analysis, and visualization¹¹. Specifically, it is used for modeling, analyzing, and visualizing different space missions, including orbit propagation, sensor geometry, and coverage assessment¹². In the context of this research, STK was used to model the CubeSat orbit, onboard sensor, and

interaction between the satellite and the defined region of interest (ROI) over the simulation period.

In this paper, coverage refers to the number of grid points within the ROI that were observed at least once during the simulation. It is also described using different parameters, such as

- Access duration: Time period during which the grid point is visible to the sensor during a single pass.
- Number of accesses: Total number of distinct access intervals between the sensor and target/grid points.
- Revisit time: Time interval between consecutive access events to the same grid point.
- Coverage percentage: Percentage of grid points that achieved at least one access point during the simulation.

These metrics were obtained using the STK Coverage and Figure of Merit (FoM) tools, which are commonly applied in satellite coverage and revisit analysis studies¹³.

Table 3. Summary of Scenario 2 FoM results

Inclination	Number of access	Access duration (s)	Average revisit time (days)	Average coverage percentage (%)
20°	335	6.020	9.355	0.1632
25°	267	10.374	12.383	0.2603
30°	203	5.206	8.489	0.0694
40°	168	4.805	11.17	0.0483
98°	122	4.967	18.8	0.0290

Note: The "Number of access" represents the total number of access events recorded by the STK Coverage Definition over the entire ROI during the simulation period. This value corresponds to the cumulative access count across all grid points. In contrast, the "Average revisit time" represents the mean revisit interval computed per grid point using the STK Revisit Time FoM and then averaged over all grid points within the ROI. Because these metrics were computed at different aggregation levels, their numerical values were not directly reciprocal.

2.3.1. Simulation scenario setup and region of interest.

The simulation epoch was set to November 17, 2025, 09:00:00 UTCG, and the analysis duration was one year. The initial orbital state was defined using classical orbital elements: inclination = 97° , RAAN = 0° , semi-major axis of approximately 6878 km, corresponding to an orbital altitude of 500 km, argument of perigee = 0° , and initial mean anomaly = 5.01143×10^{-17} . For simplicity, the orbit was assumed to be circular with an eccentricity equal to zero, neglecting the effects of atmospheric drag and perturbations. In STK, this region was defined as a rectangular area target with latitude and longitude bounds that were approximately between 16.8°N – 17.8°N and 44°E – 47.1°E . The ROI was modeled as a rectangular target area in STK for consistency in the grid-based coverage evaluation. This simplification may include non-border terrain; therefore, the reported metrics represent coverage within the defined ROI window rather than a strictly border-aligned strip. A narrower corridor aligned with the

border can modify the absolute coverage values and is identified as a potential refinement.

Reproducibility summary: All simulations were performed using STK v12.9 with a two-body propagator over a one-year scenario duration. The epoch, coordinate frame, orbital parameters, and sensor configuration were defined as described previously. The coverage analysis employed a grid-based area target with a specified mesh resolution and default STK access constraints under nadir-pointing assumptions.

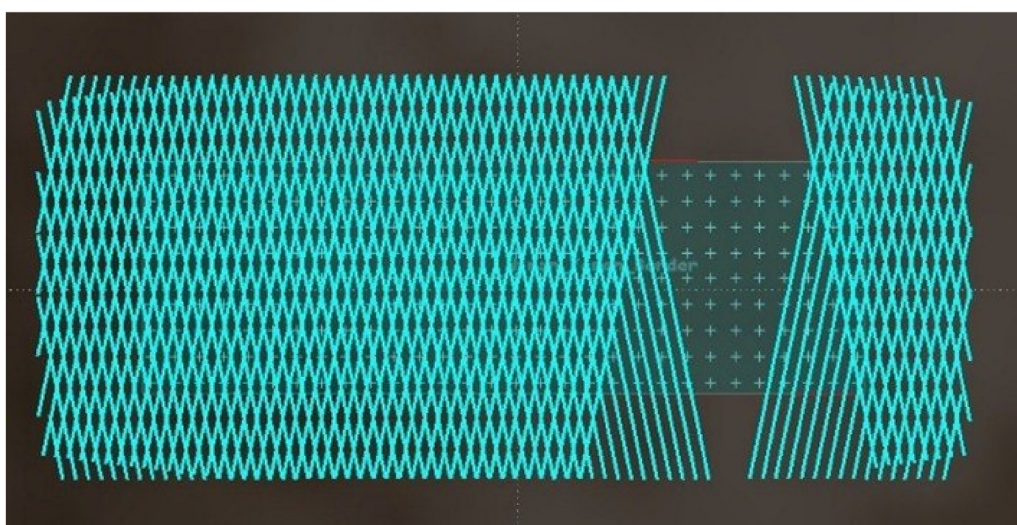
For the simulation, two scenarios were assumed: the sun-synchronous orbit (SSO) scenario and a customized optimal orbital parameter scenario, where the inclination and RAAN values were changed to achieve satisfactory coverage quality and revisit time.

2.3.2. First scenario: baseline sun-synchronous orbit

. The baseline SSO scenario utilized the orbital parameters



(a)



(b)

Figure 3. Satellite coverage footprint over the Najran–Yemen border: (a) 2D coverage projection, illustrating the sensor swath over the target region; (b) 3D representation of the CubeSat's nadir-viewing footprint projected onto the Earth's surface

described in Section 2.1, where the CubeSat was in the SSO at an altitude of 500 km. The sensor was modeled as a rectangular sensor with vertical and horizontal half-angles of 5° and 4°, respectively. The coverage definition object was used to conduct coverage analysis, in which the mesh was set to 0.1° to enable accurate coverage assessment. The coverage definition, together with the STK FoM module, was used to calculate the access periods between the CubeSat and the border area, defined as time intervals during which the satellite maintains a direct line of sight visibility of the target area. From these data, the key performance metrics were derived to evaluate the effectiveness of each scenario. These included the access duration, number of accesses, maximum revisit time, and coverage percentage. The analysis was repeated for multiple orbital configurations by varying inclination and RAAN, enabling direct comparison of how different orbital designs affect the frequency and duration of satellite passes over the targeted area. The optimal configuration was subsequently selected based on these comparative results, as discussed in Section 3.

2.3.3. Second scenario: customized optimal orbital parameters. In this scenario, the orbital inclination and RAAN were changed across a range appropriate for the latitude and longitude of the ROI. This test was conducted to determine the values that provided the best coverage performance. The satellite orbit was propagated using the STK J2 perturbation propagator, which accounts for the Earth's oblateness effects and the associated nodal regression. The atmospheric drag and higher-order perturbations were neglected. The second scenario provides a meaningful comparison to evaluate how different orbital parameters affect the number of accesses, coverage percentage, and revisit time.

3. RESULTS AND DISCUSSION

3.1. Coverage Metrics (Figure of Merit Results).

Figure 3 shows the satellite footprint coverage of the ROI as 2D and 3D maps that align with the results of the four main performance parameters listed in Table 2. The parameters describe how well the satellite observed the Najran–Yemen border during the one-year simulation period. The first is the number of accesses, which represents how many times the satellite observed the target

Table 4. Effect of RAAN on coverage performance (inclination fixed at 20°)

RAAN	Number of accesses	Access duration (s)	Average revisit time (days)	Average coverage percentage (%)
30°	340	6.250	4.363	0.1642
60°	341	6.261	4.318	0.1662
90°	344	6.267	9.087	0.1679
120°	434	6.261	4.322	0.1660
180°	338	6.235	9.627	0.1636

area. The second parameter is the average access duration, which indicates how long the satellite could continuously see the region during each successful pass. The third parameter is the revisit time, which indicates the time gap between passes over the target area, and fourth, the average percentage of coverage, indicates the part of the target area that could be seen successfully. The results for the four parameters demonstrate that the baseline SSO provided weak, infrequent coverage and could not support continuous monitoring of the target region. This finding is attributed to the fact that the SSO has an inclination range from 97° to 98°, which leads to a low access number (127 passes per year) in the low-ground track of the altitude of the ROI. Although the access duration and average revisit time were marginally acceptable, the coverage percentage was quite low because the orbit was nearly polar, providing SSO coverage of a limited portion of the ROI.

3.2. Second Scenario: Customized Optimal Orbital Parameters.

3.2.1. Inclination study – results and interpretation.

Table 3 shows the effect of varying the orbital inclination on the coverage performance of the CubeSat over the Najran–Yemen border region. All reported statistics represent the mean values averaged over all grid points within the ROI generated using the STK Coverage Definition and FoM tools. Revisit time values were exported from STK in seconds and converted to days by dividing by 86,400. The coverage percentage corresponds to the STK Percent Time Covered (Percent Satisfied) metric.

The results show the relationship between the inclination angle and access opportunities. For lower angles, such as those

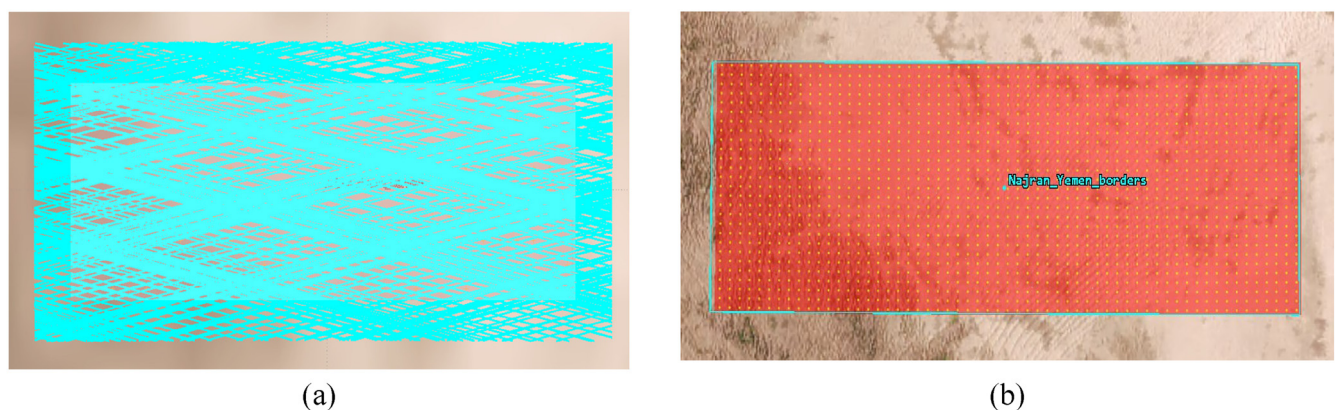


Figure 4. Satellite coverage footprint over the Najran–Yemen Border: (a) 2D coverage projection, illustrating the sensor swath over the target region; (b) 3D representation of the CubeSat's nadir-viewing footprint projected onto the Earth's surface

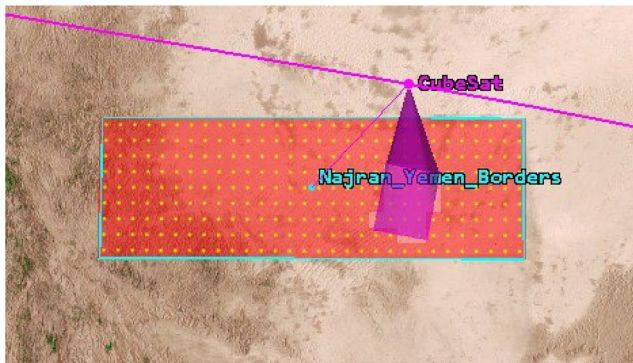


Figure 5. Sensor boresight alignment with the Najran–Yemen border during an access event

between 20° and 30° , the 20° angle provided better visibility. It had the highest number of access points at 335, with a short revisit time per grid point of 9.355 days. The 25° angle provided a slightly lower number of accesses, but achieved the longest access duration and the highest average coverage percentage at 0.2603%. This result suggests more continuous observation during each pass. As the angles increased beyond 30° , there was a significant decrease in both the number of accesses and coverage percentage. This result shows that these orbits do not work well in the latitude of the target area (17° N). Therefore, the best angles for monitoring the Najran–Yemen border region are 20° and 25° . The 25° angle is better for coverage duration and continuity, whereas a 20° angle is preferred for access frequency.

3.2.2. RAAN study – results and interpretation. Table 4 shows the effect of RAAN variation (30° – 180°) while keeping the inclination fixed at 20° . The results show that the RAAN

influences the coverage quality. RAAN values of 30° , 60° , and 120° exhibited comparable performance, whereas $RAAN = 90^\circ$ showed significantly higher revisit time and degraded temporal performance, with access between 334 and 344 and coverage percentages ranging from 0.1642% to 0.1660%. This behavior can be explained by the role of the RAAN in defining the longitudinal alignment of the orbital plane relative to Earth's rotation. Changing the RAAN effectively shifts the ground track pattern longitudinally, thereby modifying the temporal alignment between the satellite passes and the ROI. For certain RAAN values, the orbital plane intersects the target region more favorably, leading to shorter temporal gaps and improved revisit characteristics, as reported in orbital coverage design studies¹⁴. The highest accessibility (434) was achieved at $RAAN = 120^\circ$, which also provided a considerable coverage percentage (0.1660%) versus radius and a relatively short average revisit time (4.322 days), the lowest in extent, resulting in the orbital plane with this value of RAAN optimally timing the satellite crossover with respect to the target area. On average, the best RAAN range was approximately 60° to 120° , and $RAAN = 120^\circ$ provided the maximum performance for various simulated values.

3.2.3. Sensor footprint and coverage visualization. To validate the results for the best orbital parameters, a satellite with the same values was simulated. The best-performing configuration identified in this sensitivity analysis was 20° inclination and $RAAN = 120^\circ$, which provided a clear visual confirmation of the numerical results. Figure 4(a) shows the footprint coverage distribution, where the dense and repeated swaths across the Najran–Yemen border confirmed the frequent access opportunities reported in the inclination and RAAN tables. Figure 4(b) shows the coverage grid, in which the uniformly populated grid points demonstrate that the sensor repeatedly intersected

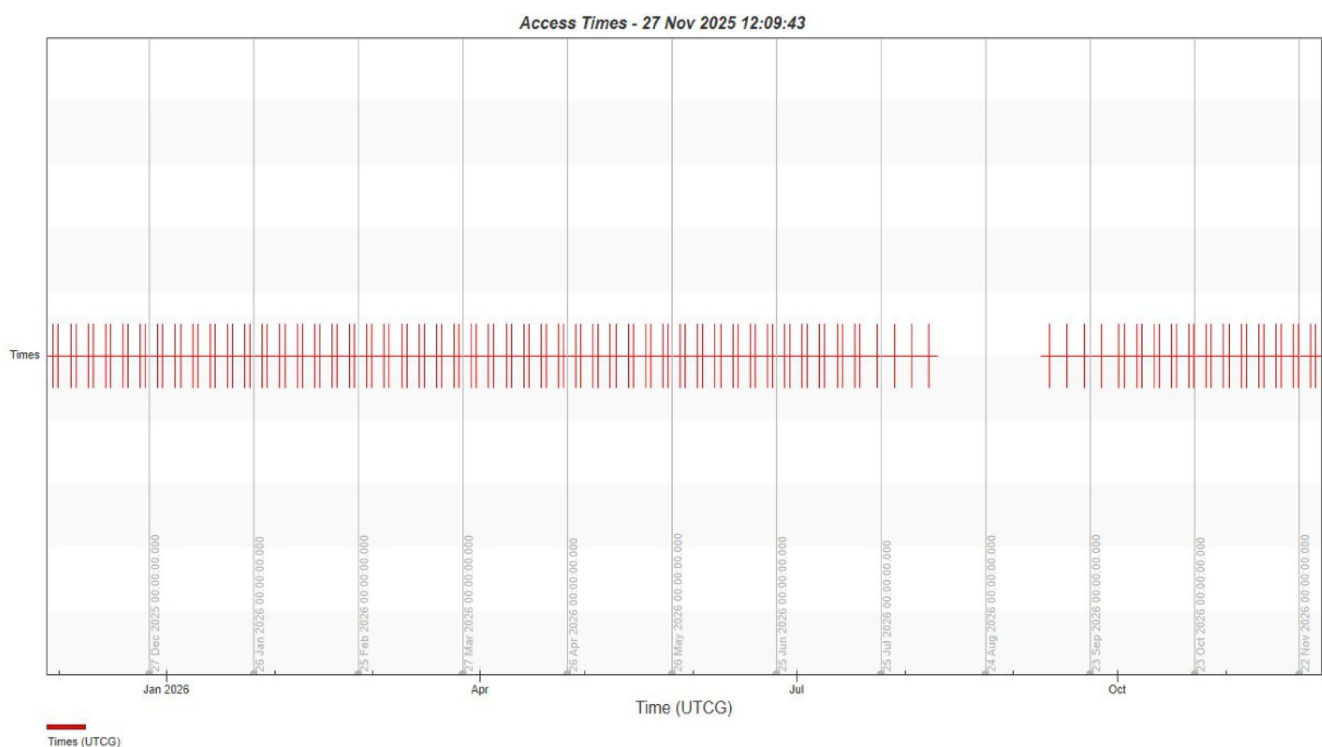


Figure 6. Access timeline for Scenario 1 (SSO)

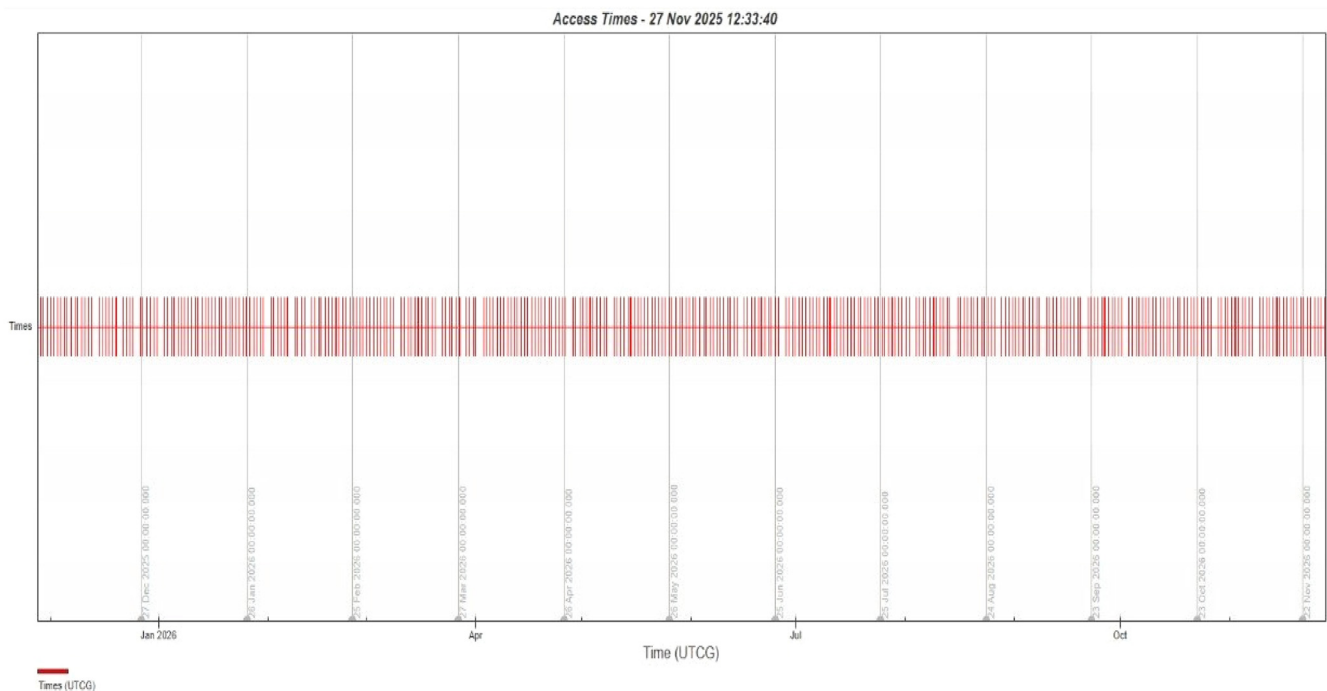


Figure 7. Access timeline for Scenario 2 (20° inclination, $RAAN = 120^\circ$)

the entire region, supporting the improved coverage percentage observed in the results.

Finally, Figure 5 shows the sensor boresight directly aligned with the target area during an actual access event, confirming that each computed access corresponds to true line-of-sight visibility. Together, these three figures validate that the optimized orbit achieves strong geometric alignment with the region, thereby supporting the quantitative findings.

Figures 6 and 7 compare the temporal distribution of access events for Scenarios 1 and 2, respectively. Scenario 1 (SSO) exhibited long gaps between successive accesses, particularly visible during the mid-year, when access opportunities became sparse and irregular. This pattern reflects the misalignment between the Sun-synchronous repeat cycle and the elongated east-west orientation of the Najran–Yemen border region. In contrast, Scenario 2 (20° inclination, $RAAN = 120^\circ$) demonstrated a much denser and more continuous access timeline, with events distributed consistently throughout the year. This behavior confirms that aligning the orbital plane with the region's latitude significantly increases the revisit frequency and reduces long coverage gaps. Therefore, Scenario 2 provides substantially superior temporal coverage and more operationally reliable monitoring performance than the baseline SSO configuration.

4. MODELING ASSUMPTIONS AND PRACTICAL CONSIDERATIONS

The results of this study should be interpreted within the scope of the adopted modeling assumptions. The simulated CubeSat was equipped with a nadir-pointing optical sensor that provided an approximate GSD of 25 m at 500-km altitude. At this spatial resolution, the system is more suitable for wide-area contextual monitoring than for the direct identification of small objects such

as individual vehicles or persons. Therefore, the results primarily reflect improvements in temporal access and regional observation opportunities rather than high-resolution tactical surveillance capability.

The reported coverage percentages and revisit metrics were calculated using geometric line-of-sight analysis with STK Coverage and FoM tools. The simulations assumed ideal imaging conditions and did not incorporate atmospheric attenuation, cloud cover, sensor noise, or operational task constraints. In addition, the analysis focused on geometric access without explicitly enforcing daylight or illumination constraints. Consequently, the comparison between the SSO and non-SSO configurations represents relative geometric performance rather than illumination-optimized imaging feasibility.

5. CONCLUSIONS

In this study, the effect of orbital parameters on CubeSat performance was investigated in monitoring the border region of Najran in Saudi Arabia and Yemen. The results show that the SSO, which was used as the basic model, has limited temporal coverage and long gaps between revisits. In contrast, the second scenario demonstrates that an inclination from 20° to 25° and $RAAN$ of approximately 120° significantly increase the number of accesses and reduce revisit time. Overall, the optimized orbit represents a significant improvement in coverage performance. This finding demonstrates the potential of a single CubeSat to improve temporal access opportunities for regional border observations. These results show that orbital parameter optimization could be an effective and feasible approach to enhance regional monitoring capabilities without increasing system complexity or using multiple satellites. However, these findings are based on an idealized geometric analysis and should be interpreted within

the scope of the modeling assumptions. It is worth noting that the simulations in the current study assumed geometric coverage conditions with a constant altitude and nadir-pointing arrangement and did not consider atmospheric conditions, daylight constraints, or adaptive pointing models.

These limitations indicate that the reported improvements reflect geometric access potential rather than operational performance. Future studies could include the assessment of off-nadir imaging, the incorporation of daylight constraints, and the consideration of propulsion-enabled orbit maintenance and agile pointing strategies, which have become increasingly feasible in modern nanosatellite platforms¹⁵. Such extensions would provide a more comprehensive evaluation of CubeSat performance under realistic mission conditions and support the practical implementation of optimized orbital configurations.

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Software-Driven Imaging Mission Planning and Attitude Control for Super-Agile Satellite

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ABSTRACT

This study evaluates multitarget imaging within a single orbital pass using a software-driven 6U CubeSat simulation. Advances in software-defined operations have enabled small Earth observation satellites to perform imaging tasks beyond their hardware limitations. Leveraging this capability, a simulation was developed using the Systems Tool Kit (STK) to assess agile imaging performance. Six observation sites in the Eastern Province of Saudi Arabia were selected to evaluate the effectiveness of dynamic, software-driven attitude planning. By integrating access analysis with a multi-segment mission plan, the satellite executes rapid attitude maneuvers to sequentially align the onboard sensor with each target. The results demonstrate that the proposed strategy successfully acquires six spatially distributed targets within a single orbital pass, achieving a six-fold increase in coverage compared with conventional nadir-pointing operation. The required maneuvers remain within the operational limits of typical commercial 6U CubeSat attitude determination and control systems (ADCS), with peak slew rates below $8^\circ/\text{s}$. This study validates the feasibility of software-driven agile imaging through high fidelity simulation and highlights the potential of software-defined mission planning to enhance Earth observation performance without hardware modification.

Keywords: agile imaging, 6u cubesat, earth observation, multi-target acquisition, attitude control, systems tool kit

1. INTRODUCTION

Earth observation (EO) is an essential component of modern scientific, environmental, and strategic decision-making. Nations increasingly rely on timely satellite imagery to support applications ranging from climate and environmental monitoring to infrastructure planning, disaster response, and national security operations. As global urbanization accelerates and climate-driven risks intensify, the demand for high-frequency multiregion imaging has increased dramatically¹. Although improvements in sensor resolution and onboard processing have advanced the field of EO, the key challenge now lies in achieving rapid revisits, expanded area coverage, and flexible imaging using cost-efficient satellite systems.

Historically, EO systems have been dominated by large satellites² equipped with wide-swath imaging payloads and multi-satellite constellations designed to deliver consistent temporal coverage. Sentinel-2, for instance, achieves a five-day revisit at medium spatial resolution using a twin-spacecraft architecture³. Commercial operators such as Planet Scope perform daily global imaging by deploying dozens of small satellites arranged in coordinated constellations^{4,5}. While these systems offer excellent operational performances, their high manufacturing costs, complex deployment requirements, and large-scale ground infrastructure render them inaccessible to many institutions, particularly emerging space programs or region-specific missions.

The abovementioned limitations have encouraged a shift toward smaller platforms, particularly CubeSats, owing to their low cost, rapid development cycles, and adaptability. However, small satellites face fundamental constraints such as a limited optical aperture, narrow native swath, reduced signal-to-noise ratio, and restricted power availability for continuous imaging⁶. A single 6U CubeSat equipped with a typical narrow-swath payload can only revisit a mid-latitude region every 15–30 days when operated in a purely nadir-pointing mode⁷. Such revisit intervals are insufficient for regions with fast-changing surface conditions or high monitoring needs, such as the Kingdom of Saudi Arabia, where rapid urban development, coastal expansion, and Vision 2030 environmental initiatives demand more frequent imaging of targeted areas⁸.

To overcome these limitations, without increasing the number of satellites or modifying the payload hardware, recent research introduced the concept of agile imaging, which exploits the attitude control capabilities of a satellite to dynamically repoint its line of sight during a single orbital pass. Critical studies have demonstrated that off-nadir slewing enables multi-strip imaging, thereby virtually expanding the effective swath width beyond the physical limits of the onboard imager⁹. Controlled attitude maneuvers allow a CubeSat to image adjacent or spatially separated regions in a rapid sequence and can increase the number of targets imaged per pass, as demonstrated in this study^{8,10}. However, agile maneuvers also introduce engineering challenges, such

as increased geometric distortions, a higher risk of motion blur, increased attitude settling times, and non-uniform ground sampling¹¹. A proper mission design must balance agility, viewing geometry, sensor limitations, and image stability.

The Ansys Systems Tool Kit (STK), developed by Ansys, Inc. (Pennsylvania, USA) has emerged as one of the most capable platforms for modeling high-fidelity EO missions. STK enables precise access window analysis, sensor geometry modeling, and multisegment attitude scheduling¹². In addition, it allows analysts to validate the feasibility of rapid re-targeting sequences by simulating realistic slew rates, stabilization times, and imaging durations for small-satellite attitude determination and control systems (ADCSs).

Building on these advancements, this study investigates a software-driven agile imaging mission for a 6U CubeSat operating over the Eastern Province of Saudi Arabia. A set of geographically distributed targets was selected to represent practical, multi-interest observation points within a densely populated urban corridor. This study aims to evaluate whether a single 6U satellite can acquire all six targets within a single orbital pass through appropriately sequenced attitude commands. The results confirm the system-level feasibility of software-driven, time-tagged agile imaging by a single 6U CubeSat by integrating access analysis, attitude maneuver planning, and execution timeline verification to enable multi-target acquisition within a single orbital pass.

The satellite mission planning workflow consists of three integrated phases: (1) time-window analysis, (2) multi-segment attitude scheduling, and (3) simulation and feasibility verification.

(1) Window Analysis

STK is used to compute the visibility intervals between the CubeSat sensor and each target, identifying when each target becomes observable and establishing the temporal foundation for constructing the imaging sequence.

(2) Multi-Segment Attitude Scheduling

A time-tagged mission plan is created, in which the satellite transitions between targets using rapid but feasible

slews. Each segment specifies the target name, start time, pointing command, and dwell duration. This mirrors real operational behavior, where precise time-stamped commands are uplinked to the onboard computer for execution.

(3) Simulation and Feasibility Verification

The full mission was executed in the high-fidelity 3D environment of STK to verify pointing performance, ensure target alignment, and assess whether attitude transitions satisfy realistic ADCS limits for a 6U CubeSat platform.

Through this workflow, this study demonstrates that software-defined imaging strategies can substantially expand the effective coverage of a single 6U satellite. By leveraging agile attitude maneuvers and optimized scheduling, a satellite can image multiple spatially separated targets in a single pass, achieving performance previously associated with larger satellites or multi-satellite constellations. This provides a compelling pathway for regional EO missions in Saudi Arabia, where flexible and frequent observations are essential for environmental, developmental, and strategic decision making.

2. BACKGROUND, MOTIVATION, AND OBJECTIVES

2.1. Background and Motivation. A 6U CubeSat with a narrow-swath optical payload is often unable to observe multiple geographically-separated targets during a single orbital pass. In this study, the region of interest consisted of six distributed urban locations in the Eastern Province of Saudi Arabia, which spans a large geographical area of approximately 529,000 km², extending significantly in both the east–west and north–south directions.

Under conventional nadir-pointing operations, these targets would typically require multiple passes to be observed, reducing the temporal responsiveness of applications that require timely regional monitoring. Because the platform is constrained by volume, mass, power, and thermal limitations, increasing coverage through larger optics or additional payload hardware is not practical. Therefore, this study adopts a software-driven approach in which the spacecraft attitude is actively repointed to sequentially

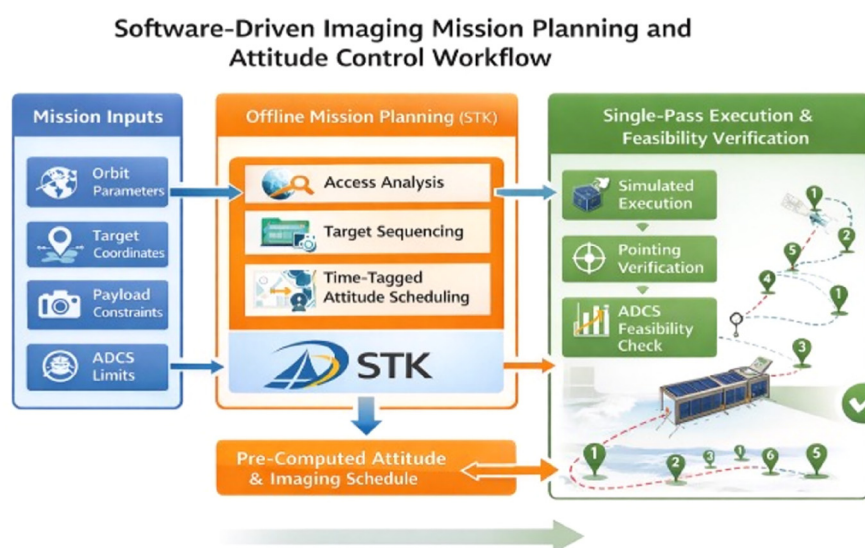


Figure 1. Software-driven agile imaging mission planning workflow showing mission inputs, STK-based access analysis and time-tagged attitude scheduling, and single-pass execution feasibility verification

image multiple targets during one pass. The objective is not to change the payload itself but to improve the mission performance through time-tagged attitude planning.

Moreover, this study validated whether such a multitarget imaging sequence could be executed within realistic 6U CubeSat operational limits. Using STK, the access windows, target visibility, maneuver timing, and attitude transitions were analyzed to verify whether all selected targets could be observed in a single pass while maintaining a feasible slew rate and pointing requirements. Unlike studies that primarily focus on optimization algorithms for target scheduling, this study emphasizes system-level feasibility. Consequently, this study confirms that software-driven agile imaging can be implemented as a practical mission concept for a 6U CubeSat using realistic timing, geometry, and ADCS constraints.

2.2. 6U CubeSat Mission Objectives. The core mission objective is to minimize the effective revisit time over an elongated region of interest (ROI) by expanding the coverage through agile multi-directional imaging and forward motion compensation (FMC). Instead of waiting for multiple orbital cycles, the attitude system is leveraged to command time-tagged pointing maneuvers that allow a spacecraft to image multiple strips or discrete targets during a single orbital pass.

Formally, the objective can be expressed as:

$$\text{Minimize } T_{(\text{revisit})} = \frac{A_t}{W_{\text{eff}} * V_g} \quad (1)$$

where A_t is the total area of the region of interest, W_{eff} is the effective swath width after multistrip imaging, and V_g is the ground track velocity. This equation captures the relationship between imaging coverage and revisit performance by modeling how an increased effective swath width reduces the time required to observe the ROI.

Note that Eq. 1 represents a first-order approximation. A rigorous revisit time analysis requires the modeling of orbital repeat cycles, Earth rotation, access geometry, and multipass coverage accumulation. However, the objective of this study is not to derive a precise orbital revisit model, but to demonstrate how software-driven attitude agility increases W_{eff} , thereby reducing the revisit time at the system level. Thus, this simplified equation was used to support the mission design concept and provide intuitive insights into the performance improvement achieved through agile imaging. For a single-pass agile imaging scenario, an effective revisit reduction can also be interpreted as an increase in instantaneous coverage, rather than a change in orbital periodicity.

Accordingly, because the native swath width ($W = 20.3$ km) was insufficient, the mission sought to increase W_{eff} using agile pointing. Therefore, the mission optimizes (1) spacecraft attitude transitions, (2) exposure timing, (3) pointing stability, and (4) FMC stabilization while respecting all constraints to ensure safe and reliable operations.

3. SATELLITE MISSION WORKFLOW AND PAYLOAD SPECIFICATIONS

3.1. Mission Workflow. The workflow adopted in this study is illustrated in Figure 1. It is important to note that the

Table 1. Mission Execution Pattern

Orbital Parameter	Value
Semimajor axis	6903 km
Altitude	525 km
Inclination	96.77°
Eccentricity	0
RAAN	85
Argument of Perigee	0

imaging sequence in this study was constructed directly from the access windows obtained through STK analysis rather than through an automated optimization algorithm. The ordering of the targets follows their temporal visibility while ensuring feasible attitude transitions between consecutive imaging events. This approach reflects realistic operational practices, in which mission planners generate time-tagged command sequences based on geometric access constraints and system limitations. This study validates the feasibility of such a sequence under practical conditions rather than optimizing the scheduling performance.

The satellite mission inputs, including the orbital parameters, target coordinates, payload characteristics, and ADCS constraints, are first processed through offline mission planning in STK to perform access analysis, target sequencing, and time-tagged attitude scheduling. The resulting precomputed mission timeline was then executed in the simulation to verify the single-pass feasibility and compliance with the spacecraft pointing and slew-rate limits.

3.2. Orbit and Imaging Specifications. The satellite operates in a near-circular low-earth orbit (LEO) with characteristics summarized in Table 1. This orbit is typical of Sun-synchronous regimes, enabling consistent lighting conditions and repeatable ground-track geometry. A visualization of the satellite's orbital pass is shown in Figure 2.

The imaging sensor used in this study was based on a representative commercial CubeSat-class Earth-observation payload with specifications consistent with those of the HyperScape100 hyperspectral imager (Simera Sense, South Africa)^{14,15}. The assumed sensor characteristics are summarized as follows:

Linear push-broom imaging sensors rely on precise knowledge of the satellite ephemeris and attitude to achieve an accurate ground projection. The sensitivity of push broom imaging geometry to attitude and orbit uncertainties has been extensively analyzed in earlier high-resolution missions, demonstrating

Table 2. Representative CubeSat Imaging Payload Specifications

Parameter	Value
Optical configuration	Push broom
Focal length	580 mm
Aperture	95 mm
Field of view	2.22°
Detector	CMOS, 4096 pixels
Pixel size	5.5 μm
Radiometric depth	12-bit

the importance of accurate physical sensor modeling for image quality and geolocation accuracy⁴. This payload configuration is representative of modern CubeSat-compatible EO cameras and was used to approximate the imaging footprint, resolution, and attitude maneuver requirements during the simulation.

3.3. Payload Description. The optical payload features are summarized below:

- GSD: 4.75 m, suitable for regional mapping
- Native swath: 20 km
- Optics: 95 mm aperture, 580 mm focal length
- Detector: 4096-pixel CMOS line array, 5.5 μm pixel pitch
- Dynamic range: 12-bit
- Spectral bands: 32 VNIR bands + optional panchromatic
- Mass: 1.1–1.3 kg
- Power usage: 5–8 W
- Internal storage: 128 GB

Although highly performing for its class, the payload's swath limitations motivate the adoption of agile pointing to cover wider scenes. A representative photo of the CubeSat optical payload is shown in Figure 3.

4. SATELLITE MISSION PLANNING

4.1. Problem Formulation.

4.1.1. Expanded optimization statement. The CubeSat mission's optimization task involves maximizing effective imaging coverage under operational constraints.

4.1.2. Goal. The objective of the mission was to minimize the effective revisit time ($T_{revisit}$) by increasing the effective imaging swath achievable within a single orbital pass.

4.2. Mission Constraints. The mission constraints are summarized below:

1. ADCS Power Constraint

$$P_{ADCS}(t) \leq P_{max}$$

2. Slew Rate Constraint

$$\omega_{sat}(t) \leq \omega_{limit}$$

3. Image Quality Constraint (MTF Preservation)

$$MTF_{actual} \geq MTF_{min}$$

4. Pointing Stability Constraint

$$\sigma_{pointing} \leq \sigma_{allowed}$$

5. Exposure Timing Constraint

$$t_{exp} \leq t_{FMC-corrected}$$

6. Thermal and Power Budget Constraints

Because attitude slews require demand significant ADCS effort, the duty cycle is constrained by the available energy per orbit.

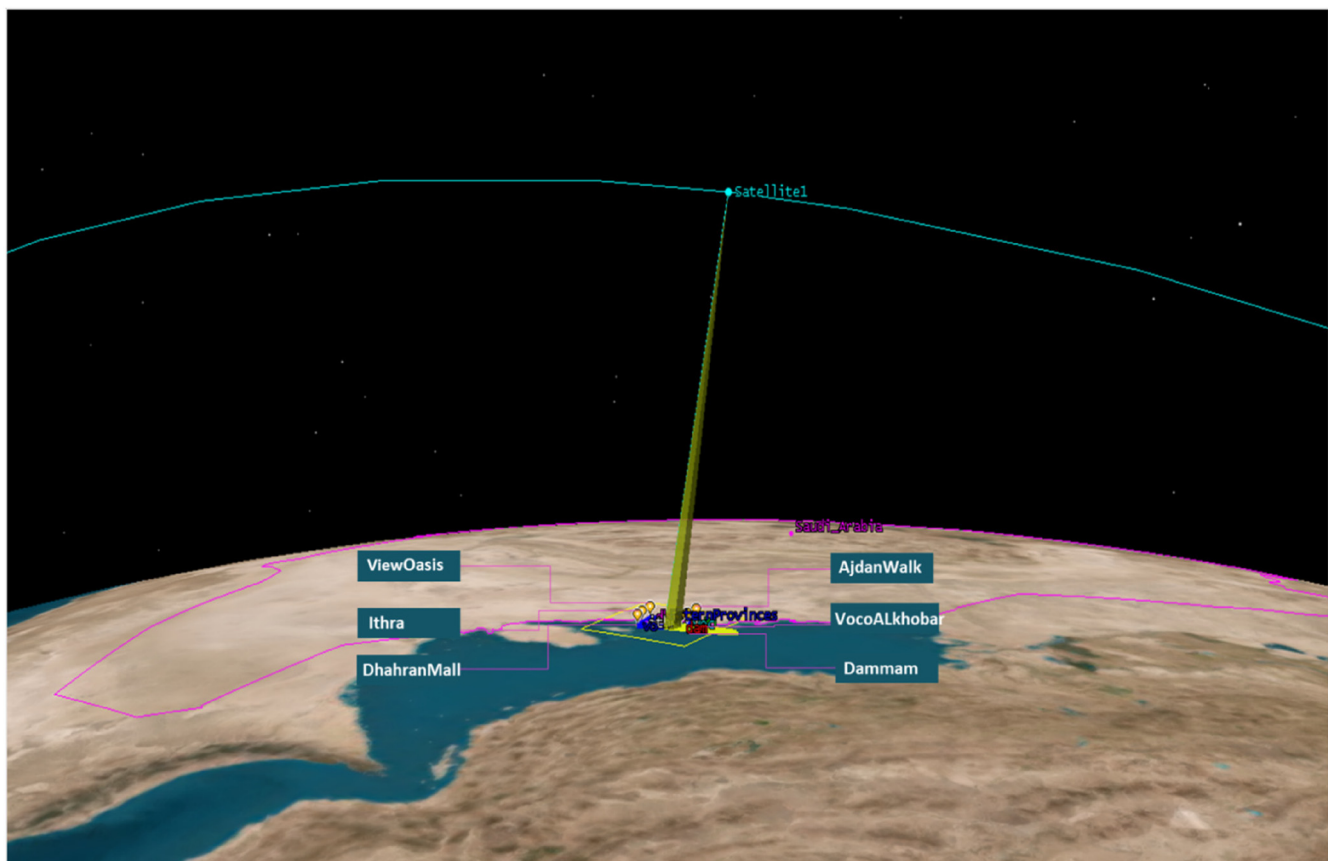


Figure 2. 3D visualization of the satellite's orbital pass over the Eastern Province showing the sensor line-of-sight and the six ground targets

4.3. Decision Variables. The decision variables include the following: (1) slew angles (pitch, yaw, roll), (2) slew rate profiles, (3) segment durations, (4) imaging window placement, and (5) FMC adjustment magnitude.

4.4. Outputs. The desired outputs are the following: (1) achieved effective swath, (2) number of strips imaged per pass, (3) effective revisit time, (4) total imaging duration, and (5) attitude maneuver feasibility.

4.5. Expanded Assumptions. The mission implements the following expanded assumptions:

1. *Sufficient Power Margin:* The power subsystem provides enough margin for aggressive ADCS maneuvers during one pass.
2. *FMC Availability:* The payload electronics allow FMC techniques to increase exposure time and prevent motion blur.
3. *ADCS Capability:* Satellite reaction wheels support multi-degree-per-second slewing at 5–6°/s with rapid stabilization.
4. *ROI Observability:* All strips of interest fall within observable latitude limits.
5. *Environmental Consistency:* The illumination conditions remain appropriate for VNIR imaging at 525 km.
6. *Operational Temperature Stability:* Slewing does not introduce thermal instabilities affecting optics.
7. *Perfect Timing Execution:* The onboard computer executes time-stamped commands with negligible delay.

4.6. Agile Attitude Scheduling. Agile attitude scheduling was implemented to enable sequential imaging of multiple spatially distributed targets within a single orbital pass. Based on the access windows identified in the previous section, time-tagged attitude commands were generated to coordinate the sensor pointing, imaging activation, and slew transitions between targets. The mission execution timeline summarized in Table 4 is structured into distinct operational modes, including pre-imaging preparation, target-track mode, active imaging windows, and post-imaging stabilization.



Figure 3. Representative CubeSat-class push broom optical payload used to illustrate typical Earth observation imaging configurations and mission simulation assumptions, based on the HyperScape100 hyperspectral imager¹⁶

Table 3. Geographic coordinates of selected ground targets

Target Location	Latitude	Longitude
Ajdan Walk	26.4137 deg	50.0688 deg
Dammam	26.4398 deg	50.1058 deg
Dhahran Mall	26.2698 deg	50.1775 deg
Ithra Center	26.28 deg	50.2 deg
View Oasis	26.3054 deg	50.2237 deg
Voco Al Khobar	26.4248 deg	50.0855 deg

In target-track mode, the attitude control system executes commanded slews to align the sensor line-of-sight with each target, followed by short imaging windows and inter-target transitions. The imaging windows and slew intervals were scheduled in a tightly coordinated sequence to ensure that all targets were imaged within their respective access intervals while respecting the spacecraft operational constraints. The resulting timeline demonstrates the feasibility of executing agile multitarget imaging within a single orbital pass. Similar agile imaging strategies have been demonstrated for push-broom EO satellites, where attitude maneuvers are exploited to increase imaging flexibility and multitarget acquisition within a single orbital pass¹⁴.

5. MISSION EXECUTION PLAN

5.1. Mission Definition and Inputs. An agile imaging mission is defined as the execution of a sequence of EO tasks over six selected ground targets within a single orbital pass. The mission inputs include the predefined target locations, satellite orbital configuration, and assumed payload and attitude control system characteristics. These inputs define the initial conditions for mission planning and establish the operational constraints within which the access analysis and mission execution are performed.

In this study, the imaging sequence was constructed directly from the access windows obtained in STK rather than through an automated optimization algorithm. The ordering of targets follows the temporal availability of visibility intervals while ensuring feasible attitude transitions between consecutive imaging events.

5.2. Access Window-Based Mission Execution Plan.

Access analysis was conducted using STK to determine the geometric visibility between the satellite sensor and six selected ground targets within the Eastern Province of Saudi Arabia. Table 3 lists the geographical coordinates of the selected targets used in the access analysis. Figure 4 shows the imaging sequence over the targets located in the Eastern Province of Saudi Arabia.

The analysis focused on identifying feasible access windows during a single orbital pass, accounting for orbital geometry, Earth's rotation, and sensor line-of-sight constraints. The results indicated that all six selected targets were within the observable latitude limits and were accessible during the same orbital pass. These access intervals define the temporal bounds within which imaging operations can be scheduled and form the basis for the subsequent agile attitude planning.

The extracted access windows provide the required timing information for sequencing imaging operations while respecting operational constraints, including the attitude maneuvering capability and sensor exposure requirements.

5.3. Mission Operating Modes and Execution Timeline.

5.3.1. Mission operating modes . In the initial phase, the satellite prepares both its payload and attitude control systems prior to the first imaging event. This phase involves: (i) powering and initializing the imaging payload through the onboard computer (OBC); (ii) synchronizing internal timing with the mission schedule; (iii) stabilizing the satellite in nadir-hold or inertial-hold mode; and (iv) verifying that power and thermal conditions support agile operations. This mode ends when the satellite is ready to initiate the first attitude maneuver toward the initial target, as shown in Figure 5.

5.3.2. Target-track mode. In this phase, the satellite's ADCS begins executing preplanned slews to aim for the payload's line-of-sight at the upcoming ground targets. During this period, the satellite may (1) be actively slewing between targets as demonstrated in the Figure 6 or (2) holding a precise inertial attitude until the optimal imaging instant. All maneuvers were precomputed based on the STK access analysis and executed according to the exact time tags.

5.3.3. Imaging sequence mode. This mode represents the period of active data acquisition. During each imaging window the imaging sequence is as follows:

1. The payload captures imagery in its operational mode.
2. The OBC enforces the start and stop times.
3. Image data are buffered into onboard storage.
4. The ADCS maintains stable pointing to avoid motion blur.

The imaging sequence consists of multiple consecutive windows targeting six selected ground locations in the Eastern Province, executed in the order defined by the mission plan.

5.3.4. Nadir-hold mode. After the final imaging window, the satellite transitioned back to a nadir-pointing attitude. During this phase the sequence of operations is as follows:

1. The payload is powered down or placed into standby.
2. The ADCS stabilizes the satellite for routine Earth-pointing operations.
3. The OBC finalizes data logging and prepares the collected imagery for future downlink.

This mode concludes the single-pass agile imaging mission.

5.4. Imaging Timeline. The total imaging duration is 6 s, yielding a total mission execution time of 16 s, as shown in Table 4.

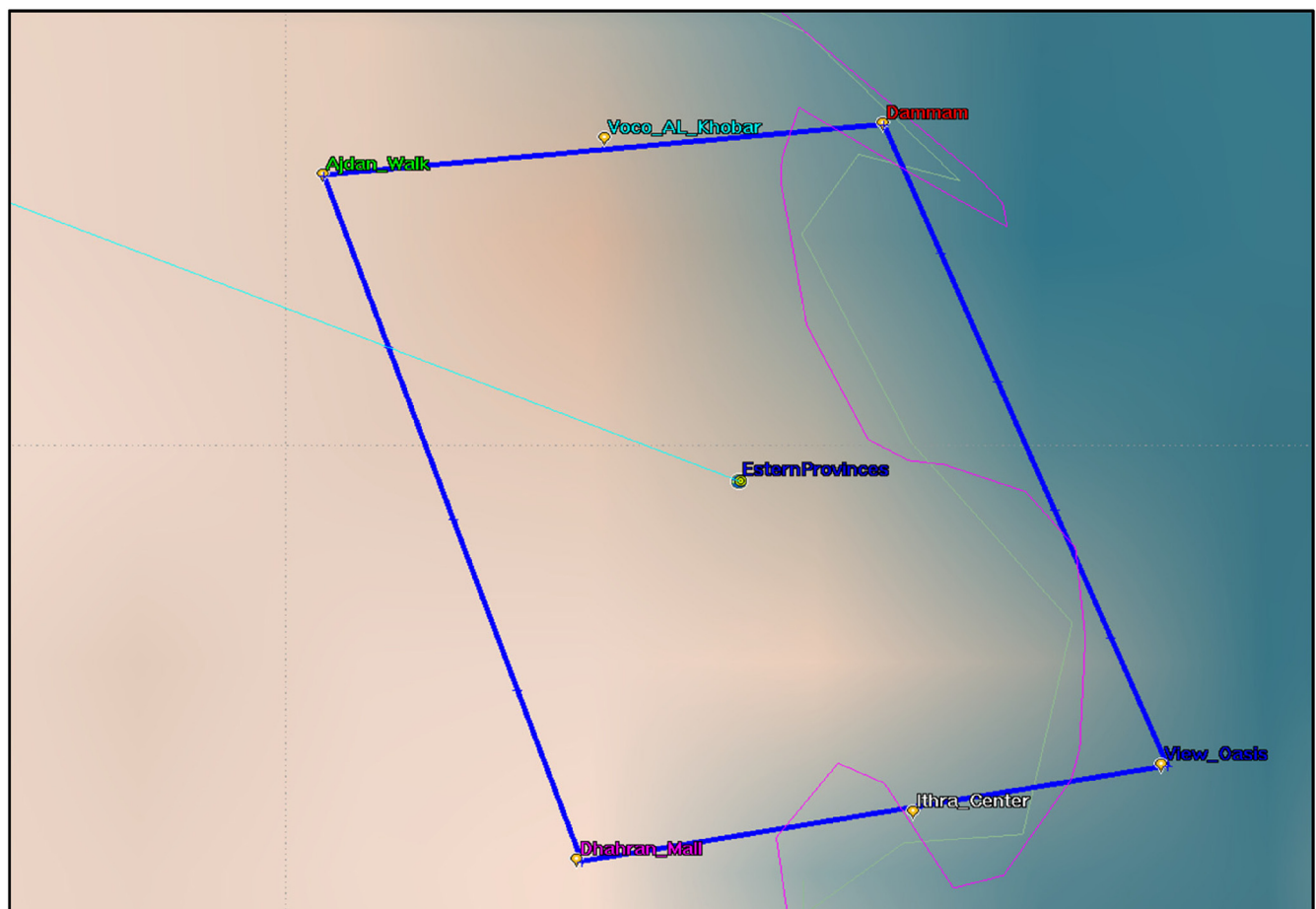


Figure 4. Agile imaging sequence over the Eastern Province of Saudi Arabia showing the satellite ground track and the spatial distribution of the six selected targets imaged sequentially within a single orbital pass

Table 4. Imaging timeline for multi-target mission execution

Targets	Pre-imaging preparation	Slew transition
Place/Dammam	4 Dec 2025 09:40:27.472	4 Dec 2025 09:40:27.472
	4 Dec 2025 09:40:27.472	4 Dec 2025 09:40:29.472
Place/View Oasis	4 Dec 2025 09:40:29.472	4 Dec 2025 09:40:30.472
	4 Dec 2025 09:40:30.472	4 Dec 2025 09:40:32.472
Place/Ithra Center	4 Dec 2025 09:40:32.472	4 Dec 2025 09:40:33.472
	4 Dec 2025 09:40:33.472	4 Dec 2025 09:40:35.472
Place/Voco	4 Dec 2025 09:40:35.472	4 Dec 2025 09:40:36.472
	4 Dec 2025 09:40:36.472	4 Dec 2025 09:40:38.472
Place/Ajdan Walk	4 Dec 2025 09:40:38.472	4 Dec 2025 09:40:39.472
	4 Dec 2025 09:40:39.472	4 Dec 2025 09:40:41.472
Place/Dhahran Mall	4 Dec 2025 09:40:41.472	4 Dec 2025 09:40:43.472
	4 Dec 2025 09:40:43.472	4 Dec 2025 09:40:45.472

5.5. Slew Segments. The maneuver parameters listed in Table 5 provide quantitative validation of the ADCS feasibility for the proposed agile imaging mission. The largest retargeting maneuver requires a yaw change of approximately 15° . The maximum average yaw rate observed during the simulation was approximately $7.5^\circ/\text{s}$, while the peak slew rate was approximately $7.9^\circ/\text{s}$. These values remain within the typical operational capabilities of the commercial CubeSat ADCS, which commonly supports multi-degree-per-second slewing. Furthermore, the roll rates remain below $3^\circ/\text{s}$, and the maneuver durations are approxi-

mately 2 s, indicating that the required control authority and slew performance can be achieved using existing commercial-off-the-shelf (COTS) ADCS solutions.

Typical commercial CubeSat ADCS systems support slew rates in the range of $8\text{--}10^\circ/\text{s}$ with pointing accuracies in the order of tens of arcseconds¹⁶, indicating that the maneuver rates observed for the proposed agile imaging sequence remain well within the achievable operational limits for CubeSat class ADCS systems.

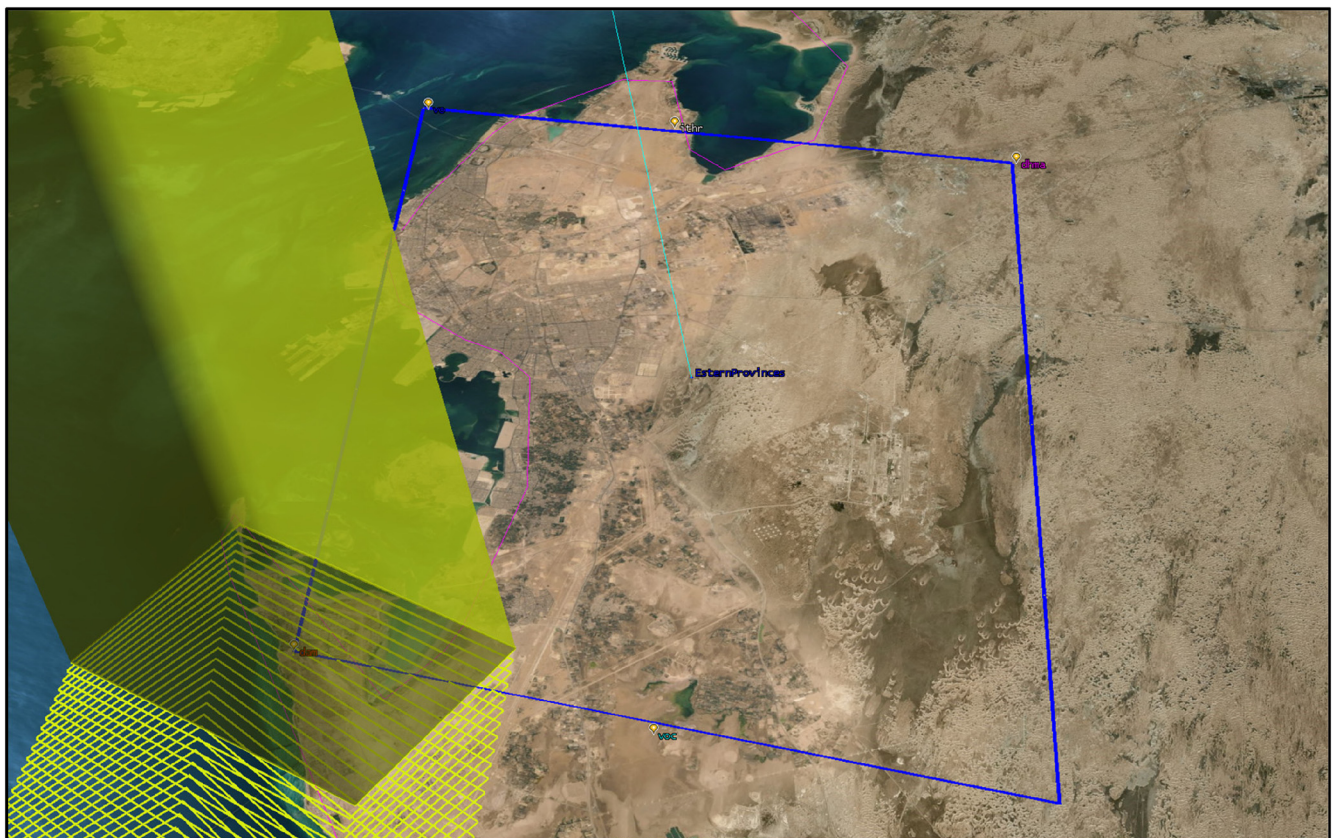


Figure 5. Satellite pointing toward the first target point to start mission execution

Table 5. Attitude maneuver parameters for inter-target slew segments

Segment	Duration(s)	Δ Yaw (°)	Δ Pitch (°)	Δ Roll (°)	AvgYawRate (°/s)	Avg Roll Rate (°/s)	Slew Rate ω (°/s)
Place/vo→Place/dammam	2	10	0.3	3.3	5.0	1.7	5.4
Place/dam→Place/voco	2	8	0.3	2.7	4.0	1.3	4.2
Place/voc→Place/ithra	2	12	0.7	4.0	6.0	2.0	6.3
Place/ithr→Place/dhmall	2	10	0.4	3.3	5.0	1.7	5.4
Place/dhma→Place/ajdan	2	15	0.4	5.0	7.5	2.5	7.9

5.6. ADCS Slew-Rate Capability Requirement. The required average slew rate, ω_{req} , is given by:

$$\omega_{req} = \frac{\Delta\theta}{(t_{gap} - t_{settle})} \quad (2)$$

where $\Delta\theta$ is the required angular displacement between consecutive targets, t_{gap} is the available time interval between imaging events, and t_{settle} is the required attitude stabilization time after each maneuver.

The acceleration-limited minimum slew time, t_{min} , is calculated as:

$$t_{min} \approx 2\sqrt{\frac{\Delta\theta}{\alpha_{max}}} \quad (3)$$

where α_{max} is the maximum angular acceleration provided by the spacecraft attitude control system.

The feasibility condition is $t_{min} \leq t_{gap} - t_{settle}$. The feasibility can be evaluated using the mission-specific parameters.

5.7. ADCS Capability Requirements. The agile imaging mission requires an ADCS capable of providing the following:

- (1) Sufficiently high maximum body rates.
- (2) Angular acceleration adequate for the largest planned retargeting maneuver.
- (3) Fine pointing stability during imaging.
- (4) Absolute pointing accuracy within mission tolerance.
- (5) Settling times of 1–1.5 s between slews.

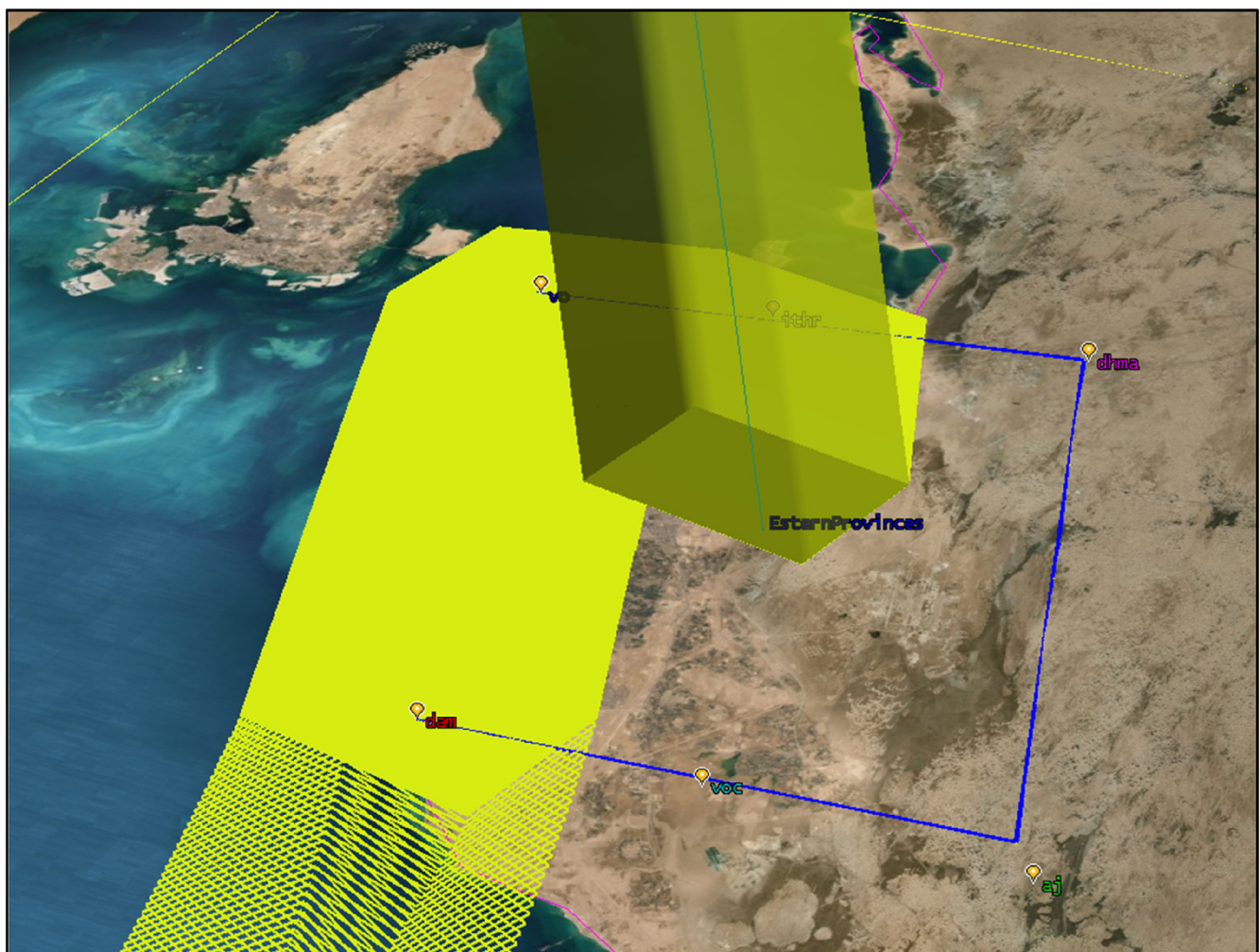


Figure 6. Satellite payload heading towards target 4 from 3 during the second strip imaging

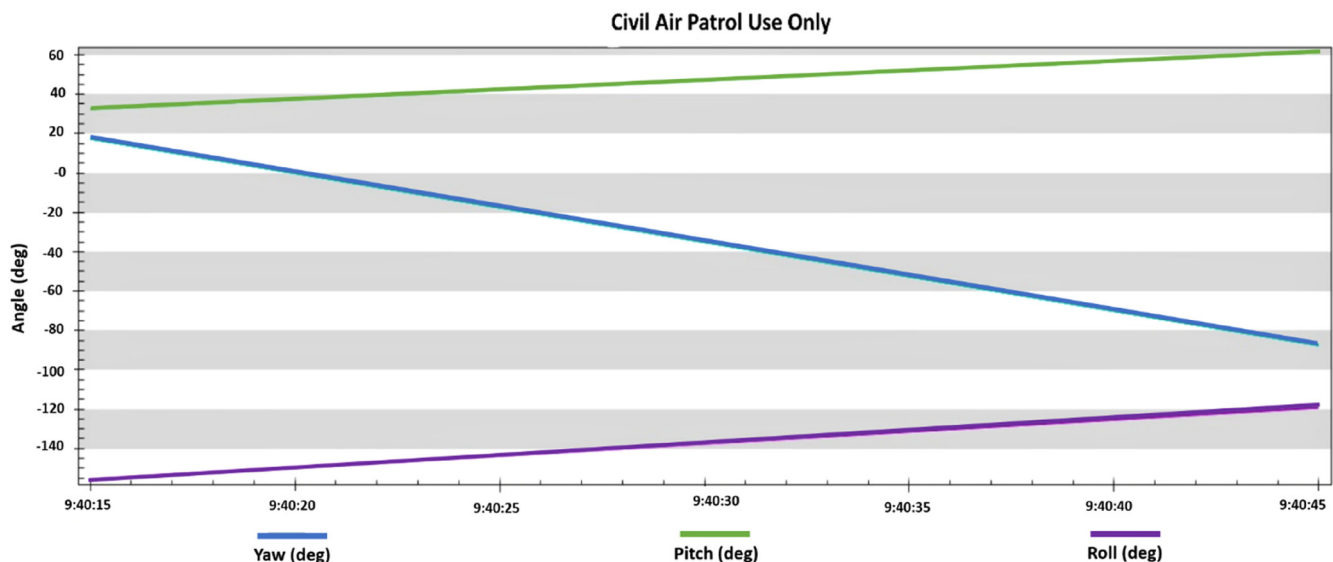


Figure 7. Satellite yaw, pitch, and roll angles versus time during the agile imaging maneuver sequence

- (6) Smooth jerk-limited S-curve profiles to preserve image quality.
- (7) Maximum yaw maneuver = 15°
- (8) Required average slew rates = $4\text{--}8^\circ/\text{s}$
- (9) Average roll rates = $1\text{--}3^\circ/\text{s}$

These requirements fall within the operational range of current commercial 6U ADCS systems.

5.8. COTS ADCS Feasibility. Modern commercial ADCS solutions for 6U satellites, such as the cube space ADCS Gen-2 and GomSpace ADCS modules, support multi-degree-per-second slewing and provide sufficient pointing accuracy for agile imaging. They incorporate reaction wheels, advanced control loops, and optional star trackers, which make them suitable for the maneuvering profile required by the mission.

A quantitative analysis of the maneuver parameters confirmed that the proposed agile imaging sequence remained within the operational capabilities of typical commercial CubeSat ADCS systems. The maximum observed slew rate of approximately $7.9^\circ/\text{s}$ and average rates in the range of $4\text{--}8^\circ/\text{s}$ are consistent with the performance specifications of widely available 6U-class ADCS solutions. Additionally, maneuver durations of approximately 2 s and moderate roll rates below $3^\circ/\text{s}$ indicate that the required control authority and stabilization performance can be achieved using existing COTS hardware. This provides strong evidence that the proposed mission concept is theoretically and practically viable.

6. RESULTS AND DISCUSSION

An agile imaging scenario was executed in STK for a single orbital pass over the Eastern Province of Saudi Arabia. Six distinct ground targets were incorporated into the mission timeline. Access analysis demonstrated the visibility windows for each target, which were subsequently used to construct a multi-segment imaging sequence.

To provide a baseline comparison, a nadir-only imaging scenario was simulated using the same orbital configuration and

target set, with the satellite maintaining a fixed nadir-pointing attitude and no agile slewing maneuvers.

To further quantify the performance improvement, a comparative analysis of the nadir-only and agile imaging modes was conducted. Under the nadir-pointing operation, only one target can be effectively imaged within a single orbital pass owing to the limited swath coverage and restricted access geometry. In contrast, the agile imaging strategy enabled all six targets to be acquired within the same pass, representing a six-fold increase in target coverage. The total imaging duration was approximately 6 s, with an overall mission execution time of 16 s, including the intertarget slews and stabilization intervals. These results highlight the substantial performance enhancement achieved through agile attitude control without the need to increase the system complexity or payload capability.

The extracted imaging windows from STK confirmed that each target was successfully observed within its corresponding access interval. The satellite completed all six imaging tasks in a single pass with an aggregate imaging duration of 6 s distributed across six individual target imaging time windows. The slewing and attitude settling phases between imaging windows required an additional 10 s, resulting in a total operational execution time of 16 s.

A series of inter-target slews were simulated to assess the maneuvering workload imposed on the ADCS. The yaw, pitch, and roll adjustments for each re-targeting maneuver summarized in Table 5 are plotted in Figure 7. The largest retarget required a yaw change of approximately 15° and roll change of 5° , which are consistent with the geometry of the target distribution. The average yaw rate remained within $5.5^\circ/\text{s}$, which is well below the maximum allowable rate for 6U-class ADCS.

Timeline analysis demonstrated that the satellite maintained a stable pointing during all imaging windows, with attitude variations remaining within acceptable bounds for EOs. No imaging interval violated the alignment or exposure constraints.

The maximum required attitude rates observed in the simulation are within the assumed ADCS capabilities. Specifically, the highest average yaw rate required was approximately

5.5°/s, which is consistent with the multi-degree-per-second slewing performance reported for commercial 6U-class ADCS. No maneuver exceeded the assumed control authority, confirming the internal consistency between the attitude assumptions and simulated maneuver profile.

Although the primary focus of this study was on mission feasibility and attitude maneuvering, detailed optical image quality modeling, including modulation transfer function degradation and motion smear effects, is beyond the scope of this study. Nevertheless, the maneuvering characteristics observed in the agile imaging sequence suggest that the image quality should remain within acceptable operational bounds. The simulated attitude transitions maintained moderate slew rates, with maximum values below approximately 8°/s, and maneuver durations of approximately 2 s between the targets, allowing sufficient stabilization before each imaging event.

In addition, the off-nadir pointing angles remained moderate relative to the satellite ground track, thus limiting geometric distortion and maintaining adequate ground-sampling consistency. These factors indicate that the image degradation remains limited for the push broom imaging configuration considered in this study.

7. CONCLUSIONS AND FUTURE WORK

This study demonstrated the feasibility and effectiveness of a software-driven agile imaging mission for a 6U EO satellite using STK. These findings reinforce the growing importance of software-driven mission planning for next-generation small satellite systems. By leveraging agile attitude control and time-tagged command execution, it is possible to significantly enhance imaging coverage and revisit performance without increasing the hardware complexity. This reflects a paradigm shift in EO mission design, where software-driven operational strategies complement physical system capabilities to achieve performance levels that are traditionally associated with larger or multi-satellite systems.

The simulated maneuver profiles remained within the capability envelope of representative 6U-class ADCS, confirming both operational feasibility and engineering consistency. These results highlight the practical value of optimizing attitude agility and mission timing to enhance coverage and responsiveness in small-satellite EO missions. While this study demonstrates the feasibility of agile multitarget imaging using STK-based mission planning, several aspects warrant further investigation. These include explicit modeling of ADCS actuator dynamics and jitter effects, detailed analysis of image blur and exposure-time during slewing, automated target scheduling under competing access constraints, and the incorporation of spacecraft power availability and duty cycle limitations to further enhance operational realism.

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Adapting Urban Digital Twins for Greenfield Vertical Urbanism: A Deployment Strategy for NEOM's The Line

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ABSTRACT

Accelerating global urbanization underscores the limits of reactive urban planning systems. The Smart City paradigm has facilitated a transition to predictive control; however, traditional development places an increasing strain on infrastructure, contributing to resource depletion and environmental pollution. Urban digital twins (UDTs) have been deployed to retrofit brownfield infrastructure; however, they have not been strategically deployed in greenfield vertical urban projects. This study investigates the adaptation of UDT architecture in NEOM's The Line, a prototype for vertical urbanism. Strategic documentation was synthesized to evaluate UDT adaptation in greenfield zero-gravity environments. The analysis identified a structural shift from 2D geospatial grids to 3D volumetric stacks, enabled by synchronization using a high-density fiber backbone. The findings indicated that this strategy employs artificial intelligence for predictive operations, dynamic load balancing, and vehicle-to-everything communication. Numerical sensitivity analysis established functional stability bounds, validating the resilience of the orchestration engine, independent of planning intent. However, governance barriers specifically sector siloing persist. Although the technical architecture is sound, the absence of a unified regulatory framework remains a critical single point of failure. This study provides a strategic blueprint for hyper-connected vertical cities.

Keywords: urban digital twin, NEOM The Line, vertical urbanism, greenfield urbanism, smart city, data governance, AI-driven infrastructure optimization

1. INTRODUCTION

Global urbanization necessitates a foundational shift from reactive planning to predictive control, a transition facilitated by the Smart City paradigm^{1,2}. Traditional development of smart cities places an increasing strain on infrastructure, contributing to resource depletion and environmental pollution³. Urban digital twins (UDTs), real-time virtual replica of urban systems, enable planners to optimize complex infrastructure through the seamless integration of physical objects, digital models, and continuous data streams^{4,5}. Although current research demonstrate their effectiveness in retrofitting brownfield infrastructure, limited work addresses deployment strategies in greenfield vertical urban systems with radical unorthodox constraints^{3,6}.

Therefore, to investigate the adaptation of UDT to address the distinctive constraints of vertical urbanism, the role of artificial intelligence (AI)-driven predictive models in optimizing vital infrastructure systems, and the fundamental technical and governance challenges impeding optimal greenfield deployment, this study examines the digital twin deployment strategy for NEOM's The Line, a case study in which vertical urbanism and a car-free environment demand a customized UDT framework designed for predictive orchestration rather than mere monitoring^{2,7,8}. Examining this strategy provides a vital frame of reference

for future urban planning globally⁹. Utilizing an exploratory case study¹⁰, this research investigates the adaptation of traditional frameworks by the strategy to overcome the distinctive constraints of vertical urbanism; optimization of vital infrastructure systems using AI-driven predictive models; and the fundamental technical and governance challenges inherent in this greenfield deployment. Although mathematical logic is grounded in existing sector specifications^{8,11,12}, this analysis evaluates the theoretical feasibility of the proposed orchestration architecture rather than the live system performance. Furthermore, this study empirically validates the global cost function using a stochastic Monte Carlo simulation ($n = 1,000$), thereby providing a quantitative baseline for assessing the resilience of the orchestration engine under greenfield operational volatility.

2. LITERATURE REVIEW

This section synthesizes the existing academic literature to establish a theoretical framework for analyzing the deployment strategy of NEOM. It examines the evolution of UDT models from static representations to dynamic, multilayered systems. This review is structured around three critical dimensions required for greenfield implementation: the foundational architecture of

the digital ecosystem, the role of AI in driving predictive infrastructure optimization, and the governance challenges inherent in city-wide deployment of these systems.

2.1. Urban Digital Twin Architecture. Although traditional frameworks often rely on static representations, a functional UDT requires a continuous, bidirectional flow of data between physical and digital entities. A common architectural discrepancy exists between the theoretical component models and operational layered stacks. The model utilized in this study synthesizes a six-component framework comprising physical entities, data, virtual entities, services, users, and connection⁹ into a five-layer operational structure. As illustrated in Figure 1, the architecture integrates cross-industry standards¹³ to progress from the physical and data acquisition layers to the digital modeling, simulation, and service layers. This synthesis maps virtual entities and service components from the literature into modeling and simulation layers to better reflect the predictive orchestration required for greenfield, high-density environments. This structure enables the “what-if” scenario modeling necessary for managing radical vertical urban compositions.

2.2. AI-Driven Infrastructure Optimization. The integration of AI into the UDT system transforms it from a passive mirror to an active optimization instrument^{5,14}. Machine-learning algorithms utilize digital threads to analyze historical and real-time data and predict demand spikes in infrastructure. In the energy sector, this enables dynamic load balancing and optimization of renewable energy reserves based on consumption forecasts¹⁵. In the mobility sector, the framework integrates vehicle-to-everything (V2X) communication and edge computing to enable autonomous transit scheduling and predictive congestion management^{15,16}. Table 1 summarizes this shift, comparing the specific functional differences between traditional frameworks and AI-driven UDT optimization strategies required for data-driven urban environments^{15,16}.

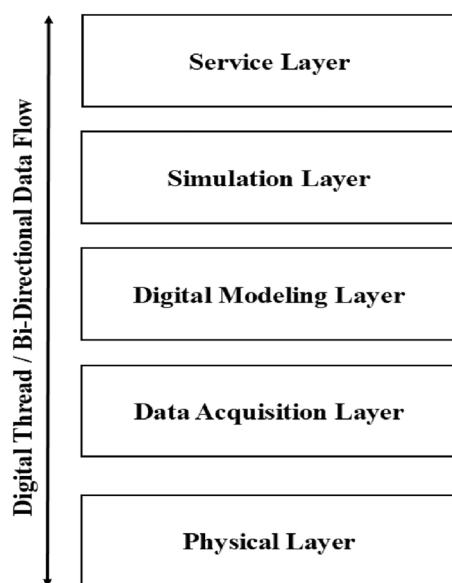


Figure 1. Synthesis of the proposed five-layer UDT architecture for vertical urban orchestration^{5,9}

2.3. Governance and Implementation Challenges.

Despite their technological potential, the deployment of UDTs in greenfield environments faces notable sociotechnical barriers, with institutional friction hampering digital integration. The primary challenges identified in the literature extend beyond technical compatibility, encompassing organizational interoperability between disparate city departments, legal entanglements of cybersecurity¹⁴, and the lack of standardized data stewardship frameworks. A major obstacle is the “silo effect,” where administrative fragmentation causes data from energy, water, and transport sectors to remain isolated, hindering the multi-functional analysis essential for city-wide optimization⁴. Establishing a resilient deployment strategy requires resolving these governance hurdles by moving toward unified ecosystems supported by application programming interface (API) gateways to facilitate a digital foundation that is as interoperable and resilient as a physical entity, as verified through high-concurrency stress testing. Current research emphasize that although technological capabilities have advanced, the strategic frameworks for governance and data integration in the region remain underdeveloped and require customized solutions⁶.

3. METHODOLOGY

This section outlines the research design and analytical framework used to evaluate UDT deployment strategies in the NEOM context. Given the development stage of the project, this study utilizes a qualitative exploratory approach to synthesize strategic intent using theoretical frameworks. This methodology was designed to bridge the gap between established UDT architectures and the peculiar emergent requirements of vertical urbanism by analyzing planning documents rather than post-implementation metrics.

3.1. Research Design. A systematic extraction protocol was applied to the primary technical documentation of the project to ensure the reliability of the parameters used in the orchestration model. This process involved a three-stage target-to-variable mapping to convert strategic mandates into a functional computational framework:

- **Technical Source Filtering:** Data were exclusively extracted from the technical white papers of ENOWA (NEOM’s energy, water, and hydrogen subsidiary) and NEOM, as shown in Table 2. This filtering process prioritizes high-fidelity engineering specifications^{8,11} over general visionary statements, ensuring that the baseline variables used in the function represent established technical targets rather than promotional projections.
- **Axiomatic Parameter Coding:** Each strategic mandate was translated into a corresponding mathematical constraint. For instance, mobility synchronization and commute mandates⁸ were formalized as transit latency variables (L_i), with the mean calibrated at 4.5 minutes to reflect the project’s modular urban design. Similarly, renewable energy mix and grid parity requirements¹¹ were used to define the energy supply baseline (S_e).
- **Greenfield Variance Calibration:** In instances where specific standard deviations were not explicitly defined in the literature,

Table 1. Comparative analysis of operational paradigms: Traditional smart city frameworks versus AI-driven UDT optimization strategies^{15,16}

Operational Domain	Traditional Smart City (Reactive Paradigm)	AI-Driven UDT (Predictive Paradigm)	Enabling Technologies
System Function	Status Monitoring: Sensors report state; alerts triggered <i>after</i> faults occur.	Predictive Orchestration: Algorithms forecast state changes; interventions occur <i>pre-event</i> .	Machine Learning, Edge Computing
Energy Grid	Demand Response: Reactive load shedding during peak stress.	Dynamic Load Balancing: Proactive distribution based on predicted consumption.	Smart Grids, AI-IoT, Digital Twin Simulation
Urban Mobility	Traffic Management: Signal timing based on current counters.	Autonomous Optimization: Predictive route adjustment for autonomous fleets.	V2X Communication, Deep Learning, 6G
Governance	Siloed Stewardship: Data locked within specific departments.	Federated Ecosystem: Cross-domain interoperability and exchange.	Cloud-Native Platforms, API Gateways

values were derived from automated closed-loop infrastructure benchmarks (e.g., high-speed autonomous rail headways). The synchronization variance (x) was calibrated based on data stewardship and the M3LD framework logic¹⁷, representing the projected data parity of a digital-first urban environment.

3.2. Case Selection. NEOM's The Line was utilized as an extreme case study to reveal architectural patterns often obscured in traditional municipal environments¹⁰. It provides a controlled greenfield environment to investigate UDT orchestration in a context where the absence of legacy infrastructure enables the testing of theoretical stability bounds (J_{total}) without the interference of brownfield variables.

4. RESULTS AND DISCUSSION

This section presents findings from a systematic review of NEOM's strategic planning documents, technical white papers, and architectural specifications. The analysis was structured to answer the core research questions, moving from physical architectural constraints to digital optimization strategies, and finally to the governance frameworks required for implementation. By synthesizing these strategic documents with the theoretical models established in the literature review, this section evaluates how the deployment strategy addresses the unique challenges of vertical urbanism. The results presented in this section constitute a conceptual validation of the UDT architecture by mapping the strategic targets identified in the document analysis to the formal mathematical constraints of the proposed framework.

4.1. Architectural Adaptation for Vertical Urbanism.

A review of the architectural specifications of The Line establishes a foundational deviation from traditional horizontal UDT

layers. The city is organized as a standard vertical stack extending up to 500 m above sea level rather than as a geospatial grid⁷. This physical constraint forces the UDT deployment strategy to adopt a volumetric data model capable of simulating the microclimate and asset performance at multiple altitudes⁷. Figure 2 illustrates this radical composition, showing three distinct functional layers (pedestrian, service, and spine) that the digital twin must simultaneously simulate. Moreover, the technical design replaces urban sensor networks with a high-density fiber backbone integrated directly into the structural spine of the modules, ensuring ultralow deterministic latency in data transmission across the vertical axis⁵. These findings indicate that traditional Geographic Information Systems are insufficient for this environment, necessitating bespoke city-scale Building Information Modeling integration to support synchronization between digital and physical entities^{3,13}.

4.2. AI-Driven Optimization of Critical Infrastructure.

The operational metrics listed in Table 3 provide a quantitative baseline for assessing the orchestration engine. These metrics serve as input parameters for the simulation layer, where AI optimizes the infrastructure response based on real-time demand fluctuations. To balance the competing demands between energy efficiency and mobility latency, the system utilizes a global cost function designed to minimize the system-wide variance.

The orchestration engine applies a cost function (J_{total}) across three primary domains: energy (S_e), water (W_d), and mobility (L_i). As detailed in Tables 1 and 3, the transition from reactive to predictive management enables 100% renewable grid balancing, zero-liquid discharge recycling, and autonomous transit scheduling^{8,11,12,15,16}. This predictive optimization ensures system-wide

Table 2. Mapping of Strategic Documents to Operational Variables

Strategic Document Analyzed	Year	Operational Variable / Target Supported
ENOWA: 100% Renewable System	2023	Smart grid technical parity ($S_{e(t)}$) and renewable energy mix requirements.
ENOWA: Water Environmental, Social, and Governance Report	2023	Water distribution efficiency and desalination operational targets ($W_{d(t)}$).
NEOM: The Line Whitepaper	2024	20-minute commute mandate and mobility synchronization latency (L_i).
NEOM Personal Data Management	2022	M3LD framework logic and user-centric data stewardship protocols.

Table 3. Projected operational metrics of NEOM's The Line vs. traditional urban benchmarks^{8,11,12,17}

Metric	Traditional Smart Cities (Global Average)	NEOM (The Line) Target	Deployment Strategy Enabler
Energy Mix	~10–30% Renewable	100% Renewable (Solar/Wind/H2)	ENOWA Smart Grid & Storage Balancing
Water Efficiency	30–60% Network Loss	<3% Network Loss (zero-liquid discharge)	IoW & Digital Twin
Commute Time	>60 minutes (average urban)	<20 minutes (end-to-end)	The Spine (High-Speed Rail) & AI-Scheduling
Land Footprint	Sprawling (>1000 km ²)	34 km ² (physical footprint)	Vertical Density (500-meter Height)
Data Usage	<5% of urban data utilized	>90% of data utilized	M3LD Platform & Data-Driven OS

parity within the synchronization tolerance (ϵ) limits, addressing the technical risks of desynchronization and latency inherent in high-density vertical environments^{15,16}. To synthesize these diverse requirements into a unified response, the orchestration engine applies a global cost function designed to minimize the system-wide variance:

$$J_{total} = \min_{u(t)} \int_{t=1}^T (w_e |D_e(t) - S_e(t)| + w_m \sum_{i=1}^N (L_i(t)) dt \quad (1)$$

where J_{total} is the global cost function of urban resource orchestration. w_e and w_m are weighted factors for the energy and mobility variance, $D_e(t)$ and $S_e(t)$ denote the time-dependent energy demand and supply, respectively, and $L_i(t)$ represents the latency of the i -th mobility node within the network of nodes.

The optimization framework is further governed by a set of hard constraints to ensure system stability and operational safety. These boundary conditions define the feasible region for the orchestration engine, preventing divergence during high-concurrency events.

Subject to

$$S_{e(t)} \geq D_{crit} \text{ and } L_i \leq 20 \text{ and } |X_{phys} - X_{dig}| < \epsilon \quad (2)$$

where D_{crit} is the critical energy threshold required to sustain life-support and emergency infrastructure, $L_i \leq 20$ is the latency ceiling (in minutes) to maintain travel duration standards, and

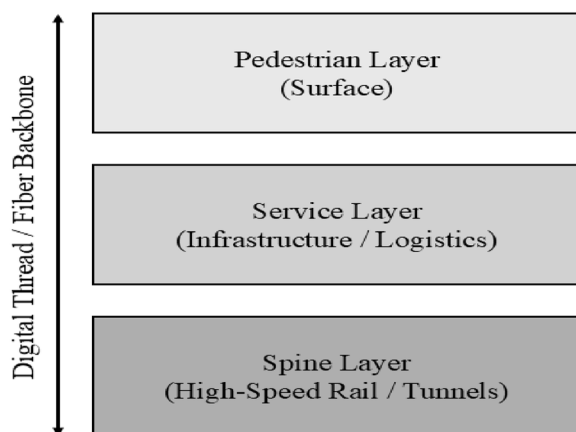


Figure 2. Schematic of the three-tier vertical stratification (pedestrian, service, and spine layers) demonstrating the volumetric data requirements²

ϵ denotes the maximum allowable desynchronization between physical infrastructure (X_{phys}) and its digital twin (X_{dig}).

The critical energy floor (D_{crit}) maintains supply side integrity by prioritizing essential services, whereas the latency ceiling (20) stabilizes the mobility network against runaway transit delays. Finally, the synchronization tolerance (ϵ) manages desynchronization risk, ensuring the digital twin remains a high-fidelity mirror of physical infrastructure, thereby mitigating the risk of divergent logic errors common in unconstrained autonomous frameworks.

4.2.1. Sensitivity Analysis and Stability Bounds. To evaluate the computational stability of the proposed cost function, numerical sensitivity analysis was conducted to simulate the operational stress in a UDT environment. By varying the synchronization variance (x) between the digital and physical twins, the model demonstrates a non-linear escalation in the global cost function (J_{total}) as it approaches the axiomatic stability threshold ($\epsilon = 10$).

As shown in Figure 3, the cost-to-risk ratio remains relatively linear during low-variance states ($x < 6$), which provides an independent stress test for the proposed operational targets. Divergence observed for $x = 8$. serves as an objective validation of the system's functional bounds (D_{crit}), verifying the resilience of the orchestration engine independent of the strategic intent described in the planning artifacts^{11,12}.

This rapid divergence validates the necessity of a deterministic fail-safe override and the human-in-the-loop (HITL) architecture defined in Section 4.3. By enforcing a manual intervention protocol before the system reaches the $\epsilon = 10$ limit, the deployment strategy effectively mitigates the risk of opaque algorithmic decision-making and ensures the interpretability of the orchestration engine⁵.

4.3. Control Architecture and Strategic Governance Barriers. The control architecture utilized in this study operates on an HITL framework to manage the operational risks inherent to high-frequency autonomous systems. Although the simulation layer provides autonomous optimization for routine infrastructure adjustments, a tiered override protocol ensures that human agency remains central to the city's governance⁶. Under this protocol, the orchestration engine is restricted to an advisory role for any decision impacting the critical energy floor ($S_{e(t)} \geq D_{crit}$) or safety-critical mobility shifts.

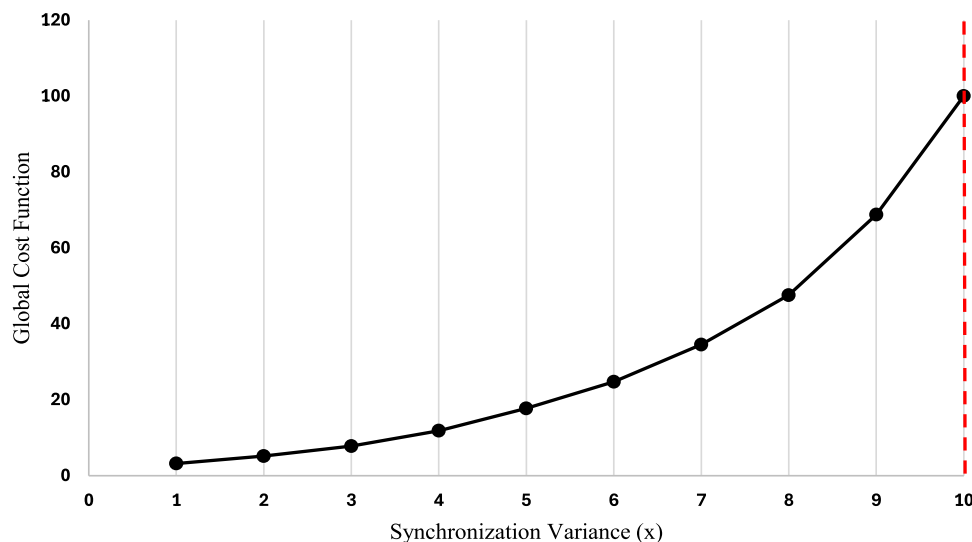


Figure 3. Sensitivity analysis of the UDT orchestration engine

In the event of a desynchronization error where the digital-physical variance exceeds the established synchronization tolerance ($|X_{phys} - X_{dig}| \geq \epsilon$), the system triggers an automatic fail-safe override. This override reverts control to manual operators until digital-physical parity is restored, mitigating algorithmic opacity and the risk of untraceable autonomous decision-making⁶ common in unconstrained autonomous frameworks. However, the high-frequency nature of this orchestration introduces the risks of cognitive overload and operator fatigue⁵. By integrating these mathematical safety rails with human oversight, the architecture ensures that algorithmic efficiency never supersedes human-verified safety parameters.

However, the practical implementation of this integrated control architecture is contingent on overcoming the systemic governance barriers inherent in cross-sector urban management. The technical sophistication of UDT contrasts with the significant governance barriers identified in the documentation. The analysis indicated a high risk of data silos, where cross-sector integration between energy, water, and mobility is hindered⁴. Solutions for technical interoperability and data privacy must be differentiated. The strategic response is M3LD, a platform designed to operationalize data stewardship by incentivizing user consent¹⁷. M3LD functions as a decentralized data exchange layer⁵, utilizing federated identity protocols to ensure that data remain interoperable across utility sectors without compromising resident privacy. System performance is maintained by the framework's ability to ensure parity within the synchronization tolerance (ϵ) limit defined in Section 4.2, where any breach triggers the fail-safe override. However, the effectiveness of this technical architecture is fundamentally predicated on NEOM's unique

institutional power dynamics⁶. Unlike traditional municipal governance, NEOM's 'sector-owner' model utilizes a centralized administrative authority to bypass multi-jurisdictional friction, enabling the top-down enforcement of data-sharing mandates². By transforming cross-sector data from contested political assets into a unified operational utility, this governance structure provides the institutional authority required to prevent fragmentation⁴. This integrated workflow, shown in Figure 4, restores data sovereignty to the user while maintaining system-wide orchestration, although it ultimately renders definitive legislative enforcement a prerequisite for long-term scalability. Notably, the effectiveness of an AI-powered orchestration engine is strictly contingent upon the fidelity and velocity of the underlying data streams within a vertical urban environment. Physical sensor reliability and network latency represent significant operational risks that could compromise the accuracy of the predictive outputs of the twin and, consequently, the stability of the global cost function¹⁴.

4.4. Comparative Analysis and Transferability. To establish a comparative baseline, the proposed framework was evaluated against the implementation hurdles of prior smart city archetypes such as Masdar City¹⁸ and Songdo IBD¹⁹. Unlike Masdar City which relies on specialized, high-cost physical infrastructure that limits its commercial scalability¹⁸, the proposed framework utilizes a software-defined orchestration engine⁵. By prioritizing the global cost function (J_{total}) over rigid architectural constraints, this approach provides greater resilience than "static" models. The framework, by decoupling orchestration logic from physical infrastructure, remains analytically transferable to brownfield cities, regardless of governance structures.

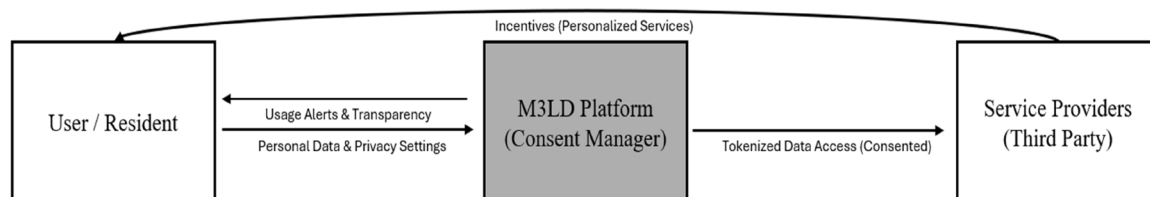


Figure 4. Conceptual model of the M3LD consent management platform, illustrating the user-centric data stewardship framework. Adapted from¹⁷

Table 4. Stochastic stability and performance metrics

Performance Metrics	Operational Definition	Simulation Result
System Success Rate	$J_{total} < 10$ (Axiomatic Threshold)	90.6%
Mean Global Cost	Average cumulative system variance	7.33
Operational Warning Rate	$10 \leq J_{total} \leq 15$ (Sub-optimal)	9.2%
Fail-Safe Trigger Rate	$J_{total} > 15$ (Critical Divergence)	0.2%

This shift from physical-centric to software-defined logic directly addresses the transferability of UDT development principles to urban environments lacking NEOM's specific financial and centralized resources⁴. Because the stability constraints in Equation 2 are modular, they do not require a "totalizing" greenfield environment to be effective. Instead, these principles can be exported as sector-specific API gateways for cities operating under decentralized governance or constrained budgets, enabling high-fidelity energy and water optimization without requiring an all-encompassing, top-down infrastructure overhaul. NEOM, as an outlier case study owing to its greenfield nature and centralized sector-owner governance model, bypasses the legacy infrastructure and jurisdictional fragmentation typical of brownfield cities^{4,18}. Consequently, although the specific institutional power dynamics are site-specific, the mathematical orchestration logic, specifically the synchronization tolerance (ϵ) and fail-safe override protocols remain generalizable^{5,6}. These elements provide a transferable framework for any high-frequency UDT environment that seeks to maintain digital-physical parity, regardless of the underlying political structure.

4.5. Synthetic Performance Validation. To evaluate the operational resilience of the proposed orchestration engine, a stochastic Monte Carlo simulation ($n = 1,000$) was conducted. As shown in Table 4, the analysis tested the global cost function (J_{total}) against the inherent volatility of a greenfield cognitive city by utilizing operational bounds derived from the project's technical mandates^{8,11}. The simulation utilized high-precision operational bounds derived from NEOM's technical mandates to simulate a high-efficiency greenfield environment. The transit latency ($\mu = 4.5, \sigma = 1.2$) was aligned with the five-minute walkability mandate, and energy demand ($\sigma = 2.5$) and data synchronization ($\sigma = 0.5$) reflect the integration of ENOWA's cognitive grid and ultra-low latency 6G connectivity standards^{8,17}.

The results demonstrate that the orchestration logic maintained urban equilibrium within the established stability threshold ($\epsilon = 10$) in 90.6% of scenarios. The negligible fail-safe trigger rate (0.2%) indicates that although extreme stochastic "shocks" are possible, the system's baseline configuration, grounded in the M3LD framework logic is robust enough to prevent catastrophic divergence without frequent human intervention¹⁷. It should be noted that the results presented here constitute a pre-operational baseline. In the absence of live-sensor data from a currently under-constructed greenfield site, this synthetic validation establishes the necessary stability bounds for the orchestration engine. This provides a benchmark against which future real-world operational data can be calibrated.

4.6. Discussion. These findings reveal a paradigm shift from the traditional Smart City model of reactive monitoring

to a model of predictive orchestration^{2,8}. Although previous frameworks focused on retrofitting digital layers onto horizontal assets⁴, "The Line" establishes that vertical urbanism requires the digital twin to be a foundational design parameter rather than a post-construction add-on. This reliance on AI for infrastructure balancing verifies that the UDT serves as the city's operating system, ensuring viability within radical physical constraints. However, as seen in previous greenfield projects^{18,19}, technical optimization remains contingent on a governance structure that can manage the tension between system efficiency and resident data privacy^{17,19}. Ultimately, the mathematical logic presented here serves as a generalizable framework for the next generation of high-density urban development.

5. CONCLUSIONS

This study investigated the deployment strategy of UDTs within the unprecedented context of NEOM's The Line, addressing the critical lack of frameworks for vertical urban environments. The study identified a foundational shift from passive, monitoring-based twins of brownfield environments to an active, orchestration-based AI-powered digital twin. However, although it provides a robust logical foundation for UDT deployment, it only represents the conceptual design phase. The empirical findings of the synthetic performance validation confirm the technical viability of this orchestration logic. With a recorded 90.6% system success rate and a negligible 0.2% fail-safe trigger rate, the simulation demonstrates that the framework maintains urban equilibrium even under high-variance stochastic shocks.

Subsequent empirical validation is required as The Line's physical infrastructure and live data streams become operational. More importantly, a distinction must be maintained between mathematical orchestration logic, which serves as a generalizable framework for UDT research, and the centralized governance model of The Line, which serves as a critical testbed for these technologies.

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Development of a Microwave Metamaterial Sensor for Noninvasive Glucose Detection

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ABSTRACT

Diabetes is a chronic disease requiring frequent monitoring. However, traditional methods are invasive and can cause discomfort. Although prior studies have focused on various microwave and metamaterial geometries in noninvasive sensor applications, they exhibit multiple limitations, including the need for large sample volumes and complex fabrication processes. In this study, a non-invasive microwave sensor was designed, fabricated, and evaluated for fingertip glucose detection. The proposed sensor comprises a single-metal-layer coplanar waveguide with four nested split-ring resonators on an FR4 substrate to enhance electric field confinement and maximize the interaction with biological samples. Experimental validation was performed using a Vector Network Analyzer with various concentrations of glucose samples ranging from 100 to 400 mg/dL. The sensor exhibited a general structural resonance near 4.18 GHz, whereas distilled water measurements exhibited a resonance at 3.584 GHz, which shifted with increasing glucose concentration, yielding a sensitivity of approximately 36.4 kHz/(mg · dL⁻¹). These findings highlight the potential of the compact microwave metamaterial sensor as a foundation for real-time glucose-monitoring systems.

Keywords: microwave biosensor, glucose monitoring, split-ring resonator, noninvasive sensing

1. INTRODUCTION

Diabetes is a chronic disease that occurs when the body either cannot produce insulin or use it effectively. Over time, this limitation causes severe damage to the heart, kidneys, eyes, and other vital organs. According to the World Health Organization, diabetes affects approximately 830 million people worldwide, with the majority living in low- and middle-income countries¹. Traditional glucose measurement methods, such as finger-prick blood glucose tests, are invasive and may cause pain, discomfort, and an increased risk of infection. Moreover, they do not support continuous monitoring, which is critical for managing chronic conditions such as diabetes². Consequently, the demand for non-invasive, continuous, and reliable glucose-monitoring techniques is increasing. Researchers are increasingly exploring promising alternatives such as microwave biosensors. The various types of glucose-monitoring techniques are illustrated in Figure 1.

Microwaves (1–300 GHz) are electromagnetic waves that are widely used in healthcare and biosensing. They propagate without a medium, are reflected by metals, and are partially transmitted through nonmetallic materials such as biological tissue, offering both good penetration depth and sensitivity to variations in glucose concentration. Moreover, recent studies have shown that metamaterials can significantly enhance the sensitivity of microwave sensors owing to their engineered electromagnetic properties, which are not observed in natural materials. These structures can concentrate and shape electromagnetic fields,

enabling stronger interactions with biomolecules and facilitating noncontact, noninvasive detection, which are key advantages for biomedical applications³.

Recently, several studies have advanced the field of microwave-based biosensing for noninvasive glucose monitoring. Baghelani et al. developed a chipless printable split-ring resonator (SRR) sensor that enabled real-time glucose detection without complex circuitry, demonstrating the feasibility of low-cost monitoring⁴. Chien designed a 1.8 GHz near-field dielectric plethysmography sensor for heart-rate detection, validating the capability of microwave sensing to monitor physiological changes⁵. Hassan et al. proposed a minimally invasive implantable passive resonator for wireless continuous glucose monitoring, offering reliable operation with reduced discomfort⁶. Omer et al. used whispering gallery mode resonators at millimeter-wave frequencies to characterize aqueous glucose solutions, achieving high sensitivity with the strong confinement of the electromagnetic field⁷.

Souza et al. employed double-circular SRRs to evaluate artificial blood plasma solutions, and achieved good sensitivity and reproducibility⁸. Omer et al. proposed a hexagonal complementary SRR (CSRR) sensor on an FR4 substrate that operates near 2.45 GHz and validated it through both Vector Network Analyzer (VNA) measurements and in vivo fingertip tests⁹. In vitro tests of this sensor over the 40–500 mg · dL⁻¹ range demonstrated a sensitivity of 0.94 MHz/mg · dL⁻¹. Harnsoongnoen et al. reported a planar microwave sensor fabricated on Rogers

RT/duroid 6002 for fingertip glucose detection with a nonlinear signal response, demonstrating a sensitivity of $0.282 \text{ dB}/(\text{mg} \cdot \text{dL}^{-1})$ ¹⁰. Hosseinzadeh and Pakvarjouy developed a single-port microwave sensor integrating interdigital and CSRR structures on FR4 that detected glucose in distilled water and saline solutions with limits of detection of 3 and 5 mM, respectively¹¹. Srisai et al.¹² demonstrated a noncontact microwave sensor coupled with an artificial neural network for enhanced prediction accuracy, whereas Marzouk et al.¹³ introduced a rectangular dielectric resonator system capable of comprehensive, noninvasive glucose monitoring. Other studies have similarly demonstrated high sensitivity to subtle changes in glucose levels using metamaterial-based microwave sensors.

However, limited studies have optimized sensor geometry specifically focusing on fingertip compatibility. Despite prior work employing various microwave and metamaterial geometries, further improvement is needed in two key areas: (i) optimizing the electric field (EF) distribution to enhance sensitivity and (ii) matching the physical dimensions of the sensor to the fingertip anatomy for better electromagnetic coupling. Moreover, reducing the fabrication complexity, such as implementing the sensor in a single-metallic-layer design, can support manufacturability and integration into practical systems¹⁴. To address these limitations, this study proposes a metamaterial-based microwave sensor that offers several advantages, including a compact design, low sample requirements, and a fingertip-compatible geometry. The integration of this sensor into wearable or noninvasive glucose-monitoring platforms will provide significant advantages in terms of portability, real-time monitoring, and user convenience.

2. METHODOLOGY

2.1. Sensor Design and Optimization. The primary design objective of this study was to develop a compact sensor structure with dimensions compatible with fingertip-scale applications, enabling its potential use in noninvasive glucose detection systems. The proposed microwave metamaterial glucose sensor was designed and evaluated using the CST Microwave Studio simulation software to numerically analyze its electromagnetic response and EF distribution within the sensing region. The sensor structure, shown in Figure 2 (a), comprises a coplanar waveguide (CPW) integrated with symmetrically arranged nested square SRRs. The CPW configuration enables the resonators to be implemented within a single metallic layer, simplifying the fabrication compared to that of the multilayer structures reported in the literature. Design adjustments were performed iteratively, and the geometry was modified and evaluated in the simulation until satisfactory resonance characteristics and strong field localization in the sensing region were achieved.

The substrate material plays a critical role in the electromagnetic performance of microwave sensors. An appropriate substrate should ensure low dielectric loss, a moderate dielectric constant, and good mechanical stability. FR4 was selected as the substrate for this study owing to its affordability, availability, and acceptable microwave performance. The thickness and dielectric constant (ϵ_r) of the substrate were 1.56 mm and ~ 4.7 , respectively. The conductive layer comprised a $35 \mu\text{m}$ thick copper film.

2.1.1. Geometrical design. The overall sensor dimensions were 31.51 mm in width and 29.25 mm in height. The side length,

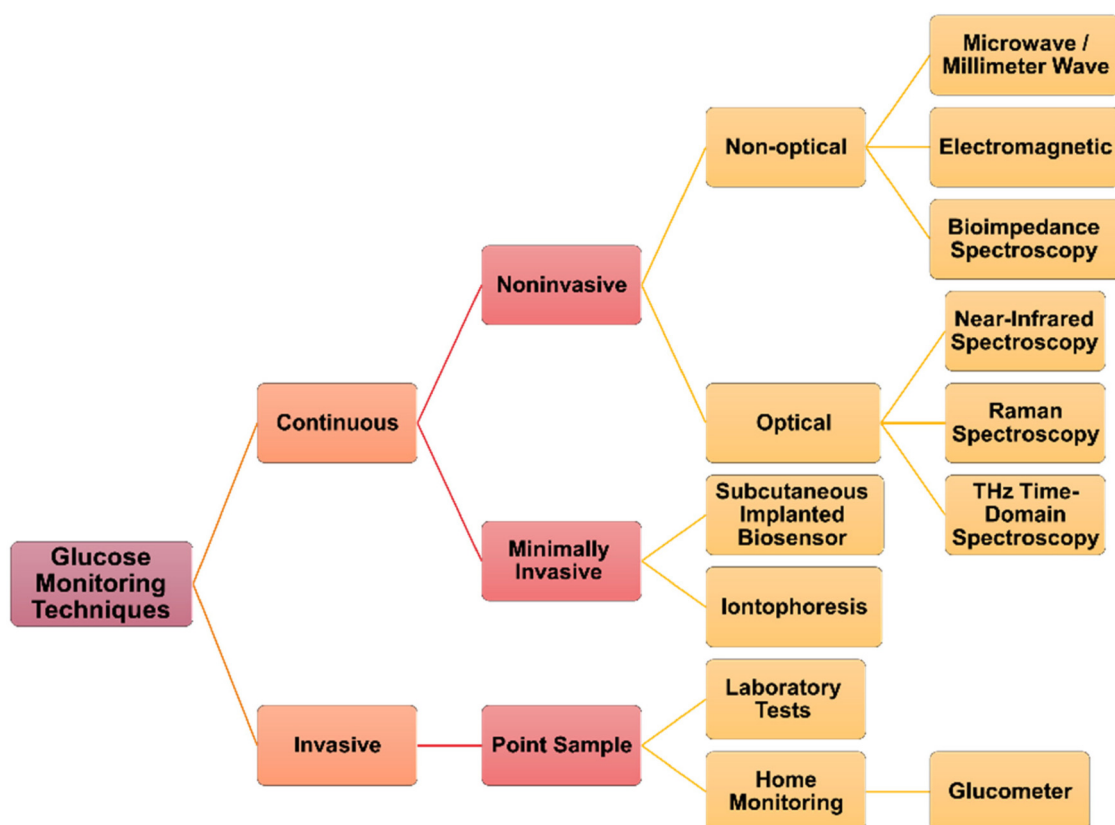


Figure 1. Different techniques for blood glucose monitoring

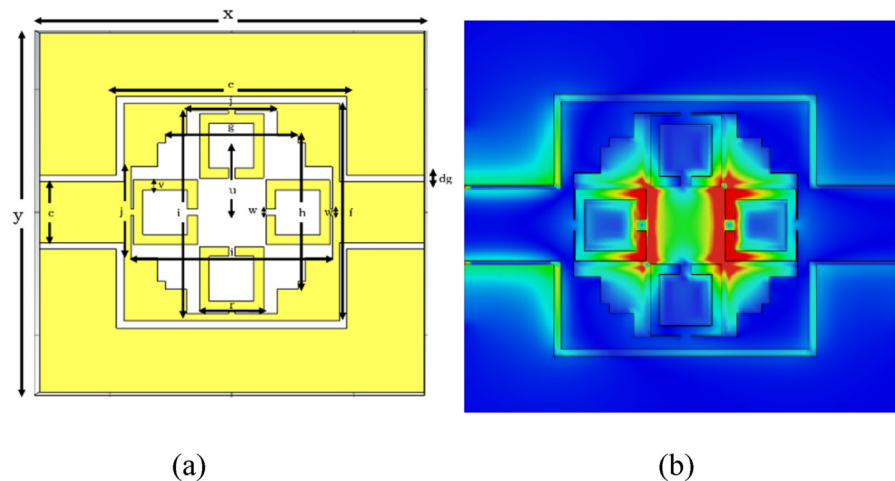


Figure 2. (a) Geometry of proposed metamaterial microwave glucose sensor indicating the key parameters on an FR4 substrate; (b) Electric field distribution of the sensor at the resonance frequency, showing strong field localization

conductor width, and resonator gaps of each SRR were 5.25, 0.4, and 0.77 mm, respectively. The horizontal and vertical lengths of the resonator frame were 18.88 and 17.68 mm, respectively. The main dimensions of the sensor were selected to match the size of a human fingertip, whereas the other parameters were optimized to achieve a deep and sharp transmission response. The geometry was iteratively refined in the simulation software by modifying the resonator and CPW dimensions until the desired resonance behavior and field localization were obtained.

To ensure appropriate impedance matching, the CPW dimensions were adjusted to obtain a characteristic impedance of approximately 50Ω . When the gap between the ground planes was 0.5 mm and the signal line width was 5 mm, the resulting impedance closely matched the standard 50Ω , thereby minimizing the signal reflection and enabling efficient power transfer when connected to a VNA. As shown in Figure 2 (b), the symmetrical SRR arrangement produced a strongly localized EF at the center of the structure, where the sensing sample, such as a glucose solution or fingertip, interacts with the resonant field. This confined EF region significantly enhanced the sensitivity of the sensor to changes in the dielectric properties due to varying glucose concentrations.

The sensor was simulated using the time-domain solver of the CST Microwave Studio Suite. Waveguide ports were placed at both ends of the CPW feed to excite the structure and extract the scattering (S)-parameters (S_{11} and S_{21}) over a frequency

range of 2–6 GHz. The simulated response exhibited a resonant frequency of approximately 4.27 GHz.

3. EXPERIMENTAL WORK

3.1. Fabrication. After fabrication, the geometrical parameters of the sensor, including the resonator gaps, CPW line width, and substrate thickness, were measured using a calibrated digital caliper with a resolution of 0.1 mm to verify fabrication accuracy. Each dimension was measured multiple times, and the average value was recorded. Minor deviations were observed compared to the design values obtained from the simulation, which can be attributed to the manufacturing tolerances and etching variations associated with the standard printed circuit board fabrication. For example, the FR4 substrate thickness increased from the intended value of 1.56 mm to approximately 1.7 mm, whereas the inner gap of the resonators increased from 0.77 mm to approximately 0.8 mm. These deviations were within acceptable fabrication limits and did not significantly affect the electromagnetic response of the sensor.

Figure 3 illustrates the fabricated sensor and highlights the observed dimensional variations. The fabricated sensor exhibited a measurable shift in the resonant frequency relative to the simulation results, as listed in Table 1. In the CST Microwave Studio simulations, the design featured a resonance at 4.27 GHz; however, during the VNA measurements, the resonance frequency was 4.18 GHz, exhibiting a discrepancy of only 0.09 GHz. This

Table 1. Comparison Between Designed and Fabricated Parameters

Parameter	Simulation	Fabricated	Parameter	Simulation	Fabricated
Width (x)	31.51	31.6	h	12.44	12.5
Length (y)	29.25	29.3	i	16.48	16.2
Thickness (z)	1.56	1.7	j	7.44	7.45
Signal line width is 5 (c)	5	5.1	SRR side length (r)	5.25	5.1
Resonator frame horizontal length (e)	18.88	18.85	Conductor width (v)	0.4	0.7
Resonator frame vertical length (f)	17.68	17.8	Resonator gaps (w)	0.77	0.8
g	10.89	10.2	CPW line width (dg)	0.3	0.3

shift may have resulted from dimensional deviations during fabrication or tolerances in the dielectric constant (ϵ_r) of the FR4 substrate. Despite this variation, the measured resonance closely aligned with the simulated result, confirming the validity of the sensor design.

3.2. Test Setup. All measurements were performed using a Keysight N9914B VNA. Before data collection, a calibration procedure was conducted to eliminate the effects of cable loss and connector imperfections, as illustrated in Figure 3 (a). Following calibration, the VNA was used to record the reflection (S_{11}) and transmission (S_{21}) coefficients under various test conditions, including distilled water and glucose solutions. Figure 3 (b) shows a comparison of the simulated S_{21} response with its measured counterpart.

3.3. Experimental Samples. Glucose solutions with concentrations of 100, 200, 300, and 400 mg/dL were prepared in distilled water using the mass–volume method. Glucose powder was weighed using a calibrated analytical balance, dissolved in distilled water, and transferred to volumetric containers to ensure accurate dilution. To ensure homogeneity, the solutions were stirred continuously until complete dissolution was achieved. The concentration of each solution was calculated using the following formula.

$$C \left(\frac{\text{mg}}{\text{dL}} \right) = \frac{\text{mass of glucose (mg)}}{\text{volume of solution (dL)}}$$

A fixed volume of 150 μL was dispensed using a calibrated micropipette into a 3D-printed sensing cell (10 mm $\times$ 10 mm $\times$ 2

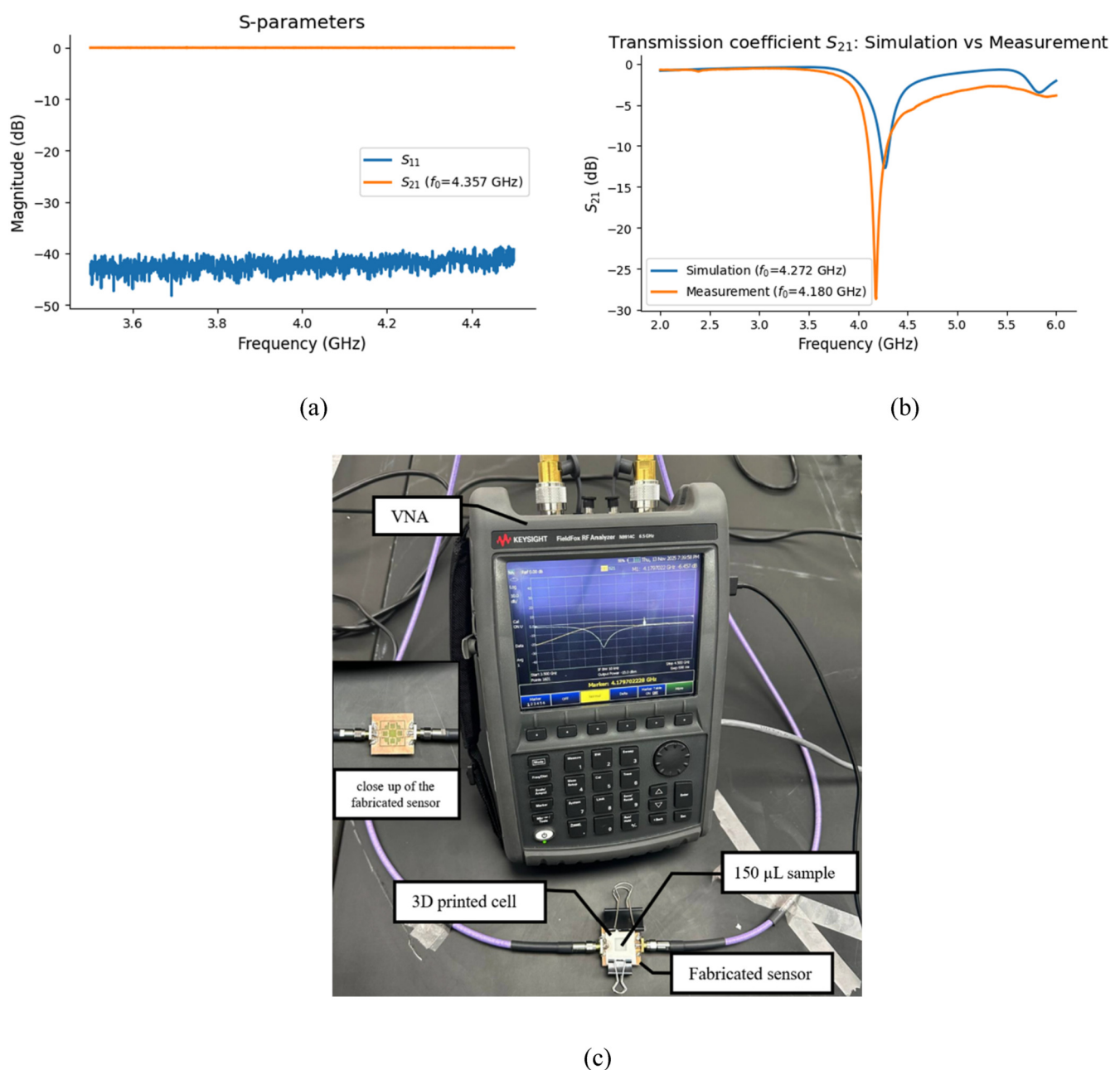


Figure 3. (a) S-parameters after performing the calibration; (b) Simulated and measured S_{21} values across the 2–6 GHz frequency range; (c) Experimental setup with the resonator and 3D printed cell

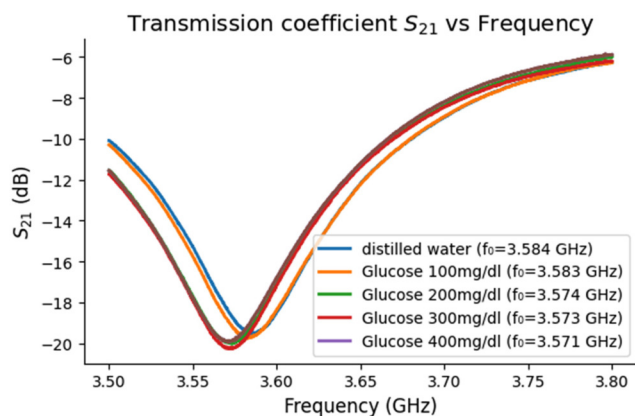


Figure 4. Measured S_{21} response of the fabricated sensor for distilled water and glucose solutions (100–400 mg/dL)

mm) fabricated from polylactic acid-based material, as shown in Figure 3 (c). Each sample was carefully placed over the sensing region to maintain consistent electromagnetic interaction. All measurements were conducted at room temperature (approximately 25 °C).

3.4. Experimental Measurements. For each prepared glucose concentration, the sensor was connected to a calibrated VNA, and S_{21} was measured across the operating frequency range. The resonant frequency for each sample was determined by identifying the minimum magnitude of the S_{21} response. A reference measurement was obtained using distilled water, and the frequency shifts for all glucose concentrations were calculated relative to this baseline. The data-collection process involved detecting the resonance dip and extracting the corresponding resonant frequency for each sample. These values were compiled to evaluate the sensor response to various glucose concentrations.

All data processing steps, including resonance dip identification, frequency extraction, visualization, and regression analysis, were performed using Python to ensure reproducibility and automation. A calibration curve was constructed by plotting the extracted resonant frequencies against the corresponding glucose concentrations. Linear regression was applied to model the relationship between glucose level and frequency shift, with the slope

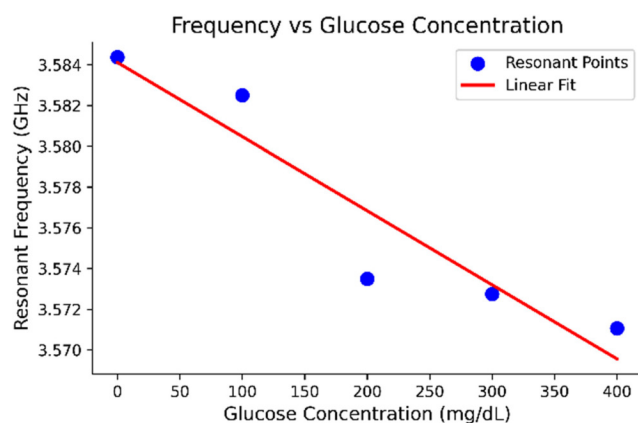


Figure 5. Calibration curve showing resonant frequency as a function of glucose concentration with fitting

of the resulting line representing the sensitivity of the sensor, which is expressed in $\text{kHz}/(\text{mg} \cdot \text{dL}^{-1})$.

4. RESULTS AND DISCUSSION

4.1. S_{21} Frequency Response for Glucose Concentrations. Figure 4 shows the measured S_{21} response of the fabricated sensor for distilled water and glucose solutions with concentrations ranging from 100 to 400 mg/dL. A distinct resonance dip was observed in all measurements, accompanied by amplitude variations. As the glucose concentration increased, the resonance curve progressively shifted toward lower frequencies. Distilled water exhibited the highest resonant frequency at 3.584 GHz, whereas the lowest value (~ 3.571 GHz) was recorded for the 400 mg/dL sample. This trend indicates that increasing the glucose concentration modified the dielectric properties of the test sample, which directly influenced the electromagnetic response of the sensor.

4.2. Sensitivity. The calibration curve illustrated in Figure 5 shows a clear inverse relationship between the glucose concentration and resonant frequency. Linear regression analysis revealed a sensitivity of approximately $36.4 \text{ kHz}/(\text{mg} \cdot \text{dL}^{-1})$, indicating that for every 1 mg/dL increase in glucose concentration, the sensor exhibits a frequency shift of approximately 36.4 kHz. Although this sensitivity is moderate, the value is highly promising given the simplicity of the sensor and minimal sample volume requirement. Deviations from ideal linearity may result from experimental limitations such as marginal temperature variations, inhomogeneous sample distribution, or mechanical disturbances. Future improvements could involve the implementation of a temperature-controlled measurement setup and a microfluidic channel to stabilize the sample and improve repeatability.

A comparative overview of recent microwave glucose sensors is presented in Table 2. Notably, previous designs predominantly required large sample volumes (up to 3000 μL), limiting their practicality for point-of-care use. Conversely, the proposed sensor achieves a full clinical glucose concentration range (0–400 mg/dL) using only 150 μL of solution. Operating at 4.18 GHz, it balances compact form factor, fabrication simplicity, and low-volume usage. These advantages make the proposed sensor a compelling candidate for integration into wearable or noninvasive glucose-monitoring platforms. In the future, the sensor can be fabricated on lower-loss substrates with significantly smaller loss tangents. Moreover, the sample cell can be manufactured from materials with a lower dielectric loss than that of polylactic acid. These enhancements should reduce the dissipative losses and improve the sensor sensitivity.

Although the sensitivity of the proposed sensor is moderate compared to that of certain high-performance designs, important tradeoffs must be considered, including sample volume, structural simplicity, and fabrication practicality. Compact design, low sample requirements, and fingertip-compatible geometry provide significant advantages for noninvasive sensing applications, where user comfort and integration into portable systems are essential. Overall, the sensor demonstrates a well-balanced solution, and future optimization efforts may further enhance its sensitivity.

Table 2. Comparison Table

Reference	Sample type	Sample volume (μL)	Concentration range (mg/dL)	Material	Dimension (mm^2)	Operating frequency (GHz)	Sensing parameter	Advantages	Drawbacks
[9]	Aqueous glucose	600	70,90,110,1000	FR4	66 $\times$ 1.5	2.45	S_{21}	-High sensitivity -Compact and low cost -Enhanced field interaction -Application of machine learning	-Large sample volume -High loss tangent
[10]	Aqueous glucose	200	0-200	Rogers RO6002	60 $\times$ 26	1-1.6	S_{11}	-Use of tube chamber -Integration of machine learning	-Sensitivity variation -Nonlinear response
[12]	Aqueous glucose	3000	0-200	DiClad 880	706.5 (sensor area, based on 30 mm diameter)	2-3	S_{F7}	-Compact single-port design -Simple setup -Good sensitivity	-Large sample volume -Sensitivity variation -Limited to liquid samples
[15]	Finger phantoms	-	0-500	FR4	35 $\times$ 13.5	2.45	S_{11}	-Use of a solid phantom model -Good sensitivity -Compact size	-Sensitivity variation -Nonlinear response
This work	Aqueous glucose	150	0-400	FR4	31.51 $\times$ 29.25	4.18	S_{21}	-Compact, simple fabrication -Smallest sample volume	-High loss tangent

5. CONCLUSIONS

This study investigated a compact metamaterial-based microwave sensor designed for potential noninvasive glucose detection using a fingertip-compatible geometry. The sensor comprised SRRs integrated into a single metallic layer of a CPW structure, demonstrating a simple fabrication as compared to the complex processes associated with the double-layer printed circuit boards that are commonly reported in the literature. The resonance characteristics and sensitivity of the sensor to varying glucose concentrations were evaluated through numerical simulations and experimental validation. The fabricated sensor exhibited a measurable resonance shift with increasing glucose concentration, confirming its ability to detect dielectric variations in aqueous glucose solutions. The calibration curve demonstrated a negative linear relationship between glucose concentration and resonant frequency, with a measured sensitivity of approximately $36.4 \text{ kHz}/(\text{mg} \cdot \text{dL}^{-1})$. Factors such as temperature variation, sample homogeneity, and fabrication tolerance may influence performance. Nevertheless, these results support the feasibility of using metamaterial resonators for glucose monitoring. Overall, the findings highlight the potential of the proposed sensor as a foundation for future noninvasive real-time glucose measurement systems. Future work may include temperature-controlled testing, improved sample handling, integration with portable wireless electronics, and evaluation of human samples to advance practical applications.

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Computational Investigation of Continuum-Like Behavior in Segmented Beam Structures with Frictional Interfaces

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ABSTRACT

The prevalence and consistency of segmented materials in nature have resulted in increased research attention aiming to use them to produce tough materials from brittle and fragile basic constituents. Therefore, studies have been conducted to determine the underlying mechanics of segmented materials. Some investigators argue that segmented configurations are better described as engineered structures rather than materials because their properties arise from geometry and assembly rather than intrinsic composition. In this study, a computational model was developed to predict the kinematics and kinetics of an array of linear elastic blocks that form a beam under a transverse load, in which the blocks interact via contact and dry friction. The model was experimentally validated and used to explore the design space characterized by the number of blocks and friction coefficient between them. The results showed that the mechanical response increased with increasing friction akin to block fusion, and with an increasing number of blocks analogous to the separation of the scale argument of periodic materials. The increase in friction coefficient from 0.2 to 1.0 improved strength by up to $6 \times$ at low N ($N = 3$), without changing the deformation modes. Although increasing f and N induced a transition in the deformation mode to “hinging,” with strength increasing by up to $3 \times$ (e.g., at $N = 7, f = 1.0$), competition with the increased compliance associated with higher N remains. These findings show that increasing friction or block number promotes the transition of segmented structures toward continuum-like behavior, offering insight into the design of architected materials with tunable properties.

Keywords: segmented beam structures, topologically interlocked materials, continuum-like behavior, frictional contact mechanics, finite element modeling, structural mechanics

1. INTRODUCTION

In biology, segmentation, also known as metamerism, refers to repeated structural units along a body axis. Multicellular animals and plants commonly exhibit such repetition, for example, in limbs¹. Segmentation spans multiple length scales and includes the fundamental structural system of animals, the skeleton.

Natural structural materials, such as bone, teeth, and mollusk shells, consist of stiff building blocks of defined sizes and shapes arranged in periodic patterns. Their mechanical performance arises from the interplay between their building block properties, geometry, and arrangement⁴. Notable examples are the tesserae in sharks (*Lamna nasus*)² (Fig. 1a, b) and intervertebral columns (Fig. 1a, c), which form a segmented series of robust blocks optimized for flexibility and load bearing. In species such as sharks and aquatic mammals, this design enables the spine to act as either a spring or a brake, depending on swimming requirements^{5–8}.

Biological examples have inspired engineered segmented materials, in which patterned elastic (relatively rigid) blocks are set to interlock, slide, or rotate to produce tuneable mechanical responses⁶. Segmented structures form the basis of topologically

interlocked materials (TIMs), which are assemblies in which blocks are secured to one another (i.e., maintain static stability) through geometry and edge abutments. The load is transmitted through friction and contact, resulting in ductility and tunable strength^{4,6–8}. Topological interlocking combines the damage tolerance of fragmented assemblies with the overall structural integrity of a continuous structure^{9–14}.

Segmentation or fragmentation improves strength by allowing arrest at interfaces and maintaining stability, even when some blocks fail^{15,16}. By tailoring the geometry and interfaces, TIMs can achieve combinations of properties rarely found in monolithic materials, including simultaneous strength and toughness and high resistance to impact^{9,15,17,18}. Their mechanical responses are governed by block interactions, which are often studied using load-line analysis, finite element methods, or discrete element methods. Distributed deformation and delayed strain localization increase toughness and resistance to damage^{15,19–23}. Although TIMs can initially be less stiff because the blocks can move relative to one another, they are much tougher than brittle solids. Some TIMs also exhibit mechanical chirality²⁶, and hollow blocks do not compromise their performance^{21,25}.

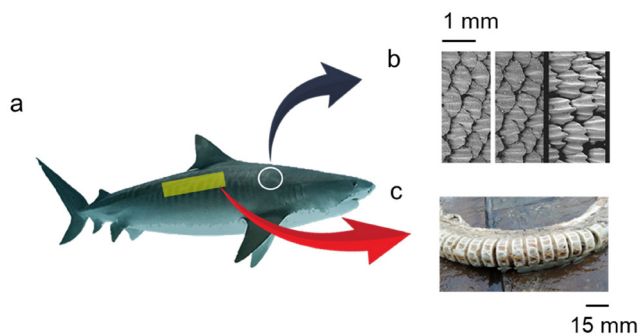


Figure 1. Segmentation in nature. (a) Shark (*Lamna nasus*), (b) tesserae in shark skin (*Lamna nasus*), adapted from², and (c) part of the shark's intervertebral column, which forms a cartilaginous segmented column, adapted from³

Despite extensive research on TIMs and, segmented or fragmented beams and panels, the connection between fragmentation and TIMs remains unclear. TIMs are designed to behave as tough materials; however, fragmentation often gives rise to structures rather than materials. Studies typically consider these systems separately; therefore, it is difficult to establish a unified understanding of how segmented or fragmented structures, such as masonry, relate to fragmented materials. However, the relationship between segmented structures and topologically interlocked materials remains insufficiently understood, particularly in terms of when a segmented assembly begins to exhibit continuum-like behavior. Existing studies typically treat these systems independently, and a clear framework linking discrete structural response to material-like behavior is lacking. This gap limits the ability to rationally design segmented systems with predictable and tunable mechanical properties. Understanding whether increasing the number of blocks in a segmented structure causes it to behave as a material is crucial. To address this, we progressively increased the block count and friction between blocks to determine when a segmented assembly begins to exhibit material-like behavior. We used a simple quasi-static finite element model with dry contact mechanics enforced at the interfaces between different elastic domains. These elastic domains represent the blocks that interact within a fragmented beam. The finite element model was first validated against experimental results from the literature and then used to identify the point at which a segmented structure transitions into a continuum (i.e., a material). In this work, we focused on a fragmented beam, which provides a tractable base model for investigating the distinction between segmentation and fragmentation and for identifying the thresholds at which a structure transitions into a material.

2. METHODOLOGY

2.1. Computational Model. The segmented beam comprised N linearly elastic blocks in an array configuration. Each block forms a standalone elastic domain governed by the equilibrium equation²⁶

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0, \quad \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0. \quad (1)$$

Where σ_{xx} , σ_{xy} , and σ_{yy} are the stress tensor components in the 2D domain. We assume a plane-strain case with the following constitutive law (Fig. 2)²⁶:

$$\begin{aligned} \sigma_{xx} &= (\lambda + 2\mu) \varepsilon_{xx} + \lambda \varepsilon_{yy} \\ \sigma_{yy} &= \lambda \varepsilon_{xx} + (\lambda + 2\mu) \varepsilon_{yy} \\ \sigma_{xy} &= 2\mu \varepsilon_{xy}. \end{aligned} \quad (2)$$

Where the strains are:

$$\varepsilon_{xx} = \frac{\partial u}{\partial x}, \quad \varepsilon_{yy} = \frac{\partial v}{\partial y}, \quad \varepsilon_{xy} = \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right). \quad (3)$$

where u and v are the components of the displacement vector along the x and y directions, respectively.

The contact interfaces were defined at the boundaries between all elastic blocks (see the red interfaces in Fig. 2). Contact was enforced using an augmented Lagrangian algorithm²⁷. Coulombic friction was considered for the frictional interaction between the blocks⁵. Other boundary conditions included a fixed displacement in the vertical direction along the vertical sides of the segmented beam (see blue domain Ω), which can be expressed as follows (Fig. 2):

$$v(\mathbf{x}) = 0 \text{ for} \quad (4)$$

$$u(\mathbf{x}) = \pm \Delta \text{ for } \mathbf{x} \in \Omega \quad (5)$$

where $\mathbf{x}$ denotes the position vector. The horizontal abutment support on which the segmented beam rests provides vertical support (black domain in Fig. 2).

$$v(\mathbf{x}) = 0 \text{ for} \quad (6)$$

The central block located at $(x = NL/2, y = L/2)$ is subjected to transverse displacement (red arrow in Fig. 2).

$$v(x = NL/2, y = L/2) = -L \quad (7)$$

This boundary value problem was solved using COMSOL Multiphysics²⁸ with pseudo-increments until the model stopped converging owing to the loss of stability or high nonlinearity arising from the contact interaction. Quadratic quadrilateral elements were also used.

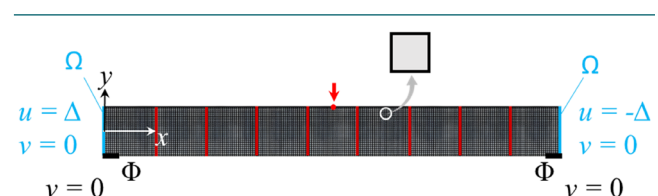


Figure 2. Meshed elastic domain and numerical problem setup, showing the applied boundary conditions. The gray regions represent the elastic blocks forming the segmented beam, with red vertical lines indicating contact interfaces between adjacent blocks. Blue symbols (Ω) denote the constrained boundary regions at both ends, while Φ symbols indicate horizontal abutment supports. Prescribed displacements include $u = \pm \Delta$ and $v = 0$. The white and red arrows indicate the directions of axial loading and applied transverse displacement, respectively, while the curved gray arrow illustrates the resulting rotation of the central block. A sample element is enlarged for demonstration.

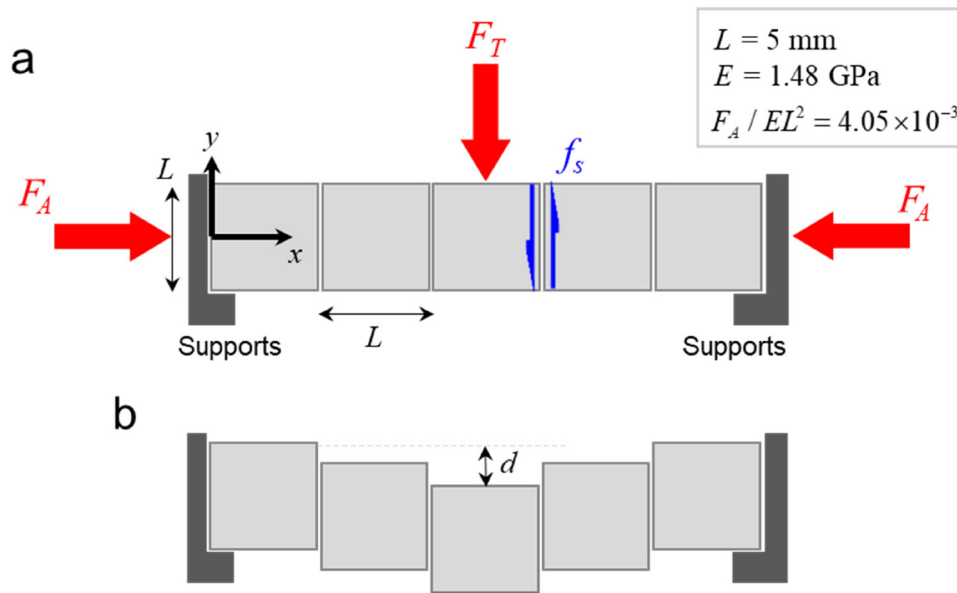


Figure 3. (a) Schematic of the segmented beam subjected to an axial load F_A and a transverse load F_T . (b) Deformed configuration of the segmented beam showing a transverse deflection d .

3. RESULTS AND DISCUSSION

3.1. Segmented Beam Structure. In this section, we introduce the concept of a segmented beam. In this study, we focused on presenting a segmented beam because beam mechanics are well established, and any distinctions that emerge from segmentation would reveal interesting underlying behaviors inherent to the segmented architecture⁵.

An array of N identical elastic blocks was considered, each made from an ABS-like material with a Young's modulus $E = 1.48$ GPa and Poisson's ratio $\nu = 0.3$ (Fig. 3a). This study considered only an odd number of blocks. Each block has a length of $L = 5$ mm. To ensure mechanical interaction and static equilibrium among the blocks, we subjected their lateral faces to an axial pre-stress of $F_A/EL^2 = 4.05 \times 10^{-3}$. The blocks rested on the rigid abutments of height $0.1L$.

When a transverse load F_T is applied to the central block located at $x = NL/2$, the block undergoes a vertical downward displacement. The model accounts for dry contact interactions between adjacent blocks through frictional contact (governed by the friction coefficient f) and normal contact enforcement, implemented via an augmented Lagrangian algorithm. We assume here

that the dynamic friction is equivalent to static friction, i.e., $f_s = f_d = f$. Two intersecting surfaces with concomitant stresses are subjected to localized shear stress, τ , and only when τ exceeds the local normal interfacial strength, $\tau \geq f\sigma$, where σ is the localized compressive stress, does slip initiate. At that instant, crack-like behavior ensued and localized slip occurred, which tended to depend on the static friction coefficient. Upon movement of the blocks relative to each other, the localized strength decreased slightly, and the dynamic friction coefficient was used. Assuming that equal static and dynamic friction coefficients are associated with a less catastrophic onset of sliding, the interfaces were not too brittle.

Consequently, the displaced block interacts with its neighbors and may drag adjacent blocks either via sliding or hinging⁵. As such, the blocks are deflected by d (Fig. 3b). The overall motion of the array, that is, block translations, local deformations, and rotations, is governed by the parameters F_A/EL^2 , N , f , and L . In this study, E and L were fixed, as described above. The objective of this work was to understand the effect of the parameters N and f on the global kinematics of the segmented beam and on the resulting force–deflection response F_T-d .

The elastic domain, which comprises the square block domain, is governed by equilibrium equations. Numerically, we imposed a displacement-driven problem, in which displacements are applied at the central block ($x = NL/2$, $y = L/2$). The contact was enforced using an augmented Lagrangian method. To solve this contact-based boundary value problem under static conditions with no inertial terms, we used COMSOL Multiphysics²⁸. The axial force F_A was applied at $x = 0$ and $x = NL$ and was maintained constant using pseudo increments of the solver. The reaction forces were summed at the location where the transverse displacement was applied (i.e., $x = NL/2$, $y = L/2$). See Methods for further details.

3.2. Transverse Response. Figure 4 shows the transverse responses of the three blocks. The force–deflection curve exhibits

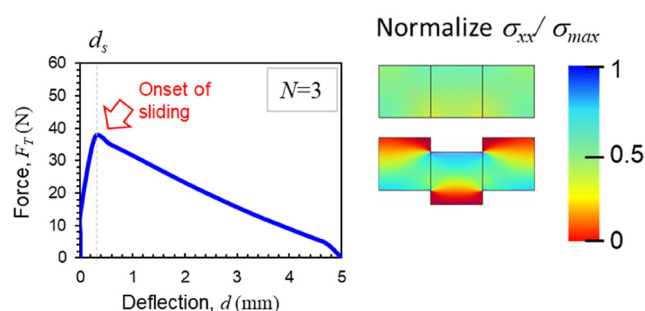


Figure 4. $F_T - d$ response for the case $N = 3$. The corresponding block deformation owing to sliding and the normalized axial stress distribution are shown adjacent to the plot at $d = 1.5$ mm.

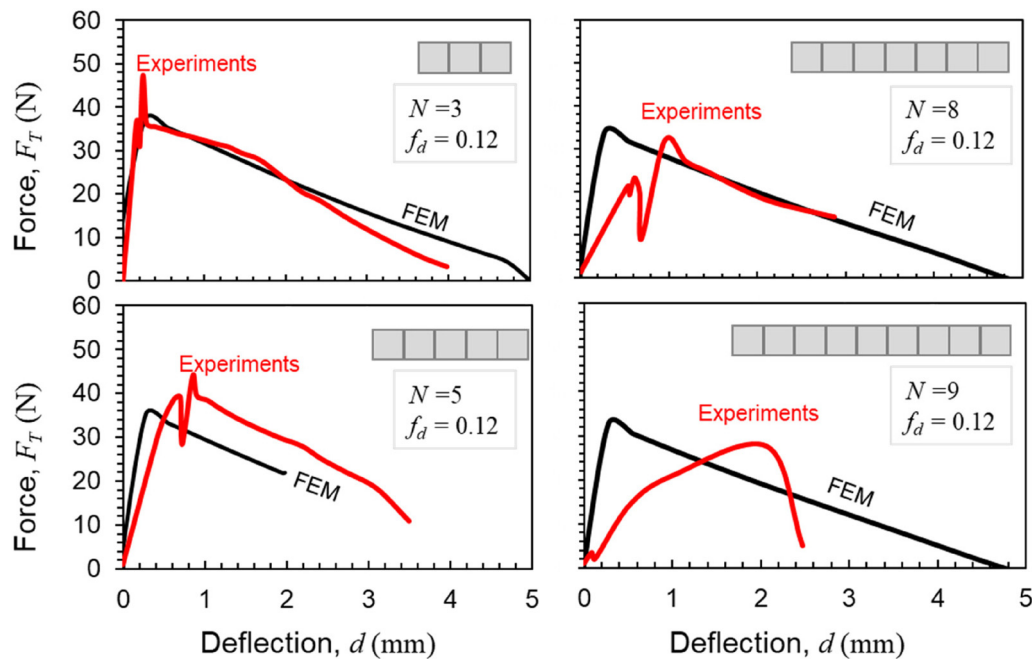


Figure 5. $F_T - d$ responses from experiments (red) compared with FEM simulations (black) for $N = 3, 5, 7$, and 9 .

a sharp linear increase until the onset of sliding $F_T^{(s)}$. Beyond this point, the blocks began to slide, causing the compressed elastic volume to decrease^{5,29}. Consequently, the sliding force F_T decreased almost linearly until the displaced block lost contact with its neighboring blocks. At this stage, the axial compression vanishes, and the static equilibrium was lost. The deformation prior to sliding followed the simple analytical expression derived in Ref.⁵:

$$\frac{F_T^{(s)}}{F_A} = \frac{16f}{3(4 + f^2(N - 2)^2)} \quad 0 < d < d_s \quad (8)$$

where the subscript s denotes the onset of sliding. First, for $N = 3$ and $f = 0.18$, the onset of sliding predicted from Eq. (1), $F_T^{(s)} = 35.7$ agrees with the numerical simulation results within 4% (Fig. 4). Thus far, Eq. (1), and the simulations verified each other. In the post-sliding regime, the sliding force for $d > d_s$ can be expressed using Ref.⁵:

$$\frac{F_T}{F_A} = 2f \left(1 - \frac{d}{L} \right) \quad d_s < d < L \quad (9)$$

This explains the observed linear decline. Equation (1) describes the reduction in the onset of sliding as the number of blocks N increases.

Figure 4 shows the axial stress σ_{xx} normalized by the maximum axial stress. The highest stress occurred at the leading edge of the sliding interface, where the edge was sharpest.

Segmentation at low block numbers breaks the beam into discrete interfaces, causing the system to behave more like a granular assembly than a homogeneous continuum. Importantly, for a brittle counterpart, such as a glass beam, the segmented configuration makes the system predictable, as demonstrated by both simulations (Figure 4) and simple Euler-based expressions (Eqs. (1)–(2)). Significantly, segmentation endows an otherwise brittle system with ductility; the resulting beam can deform smoothly

and dissipate energy through friction³⁰ instead of failing suddenly through a catastrophic fracture, in which the stored energy is released as fracture noise and the dynamic spread of glass fragments.

3.3. Experimental Verification of the Model. Once we developed a basic understanding of the transverse loading response of the segmented beams, the FEM model introduced above was validated experimentally. Existing literature contains several measurements of segmented beam deformation and their corresponding force–deflection curves⁵. We extracted the raw experimental data for the same segmented beam setup shown in Figure 6 and the same friction coefficient values from Ref.⁵. The experimental data are represented by a red curve. Using the same parameters reported in these experiments: $f = 0.18$, $N = 3-9$, $F_A = 150$ N, and $E = 1.48$ GPa, we ran simulations and compared the results with the experimental data shown in Fig. 5.

For $N = 3$, the FEM prediction (black curve) closely follows the experimental response (red curve). For $N = 5$, the FEM also captured the experimental trend but with slightly larger deviations. For $N = 7$ and $N = 9$, the FEM predicted a graceful sliding deformation, whereas the experiments showed the same deformation mode, but with a noticeably smaller response. In the experiments, the initial linear rise (elastic region) was lower than that in the simulations, and the subsequent behavior exhibited a parabolic-like decline, indicating significant softening as the stiffness decreased.

This softening suggests that the segmented beam entered an elastic deformation regime dominated by the geometric jamming of the blocks, causing the system to behave like a standing truss, where the increased transverse load stores more elastic energy. Overall, the FEM model captured the essential physics of the segmented beam accurately, although the deviation increased as the number of blocks N became larger.

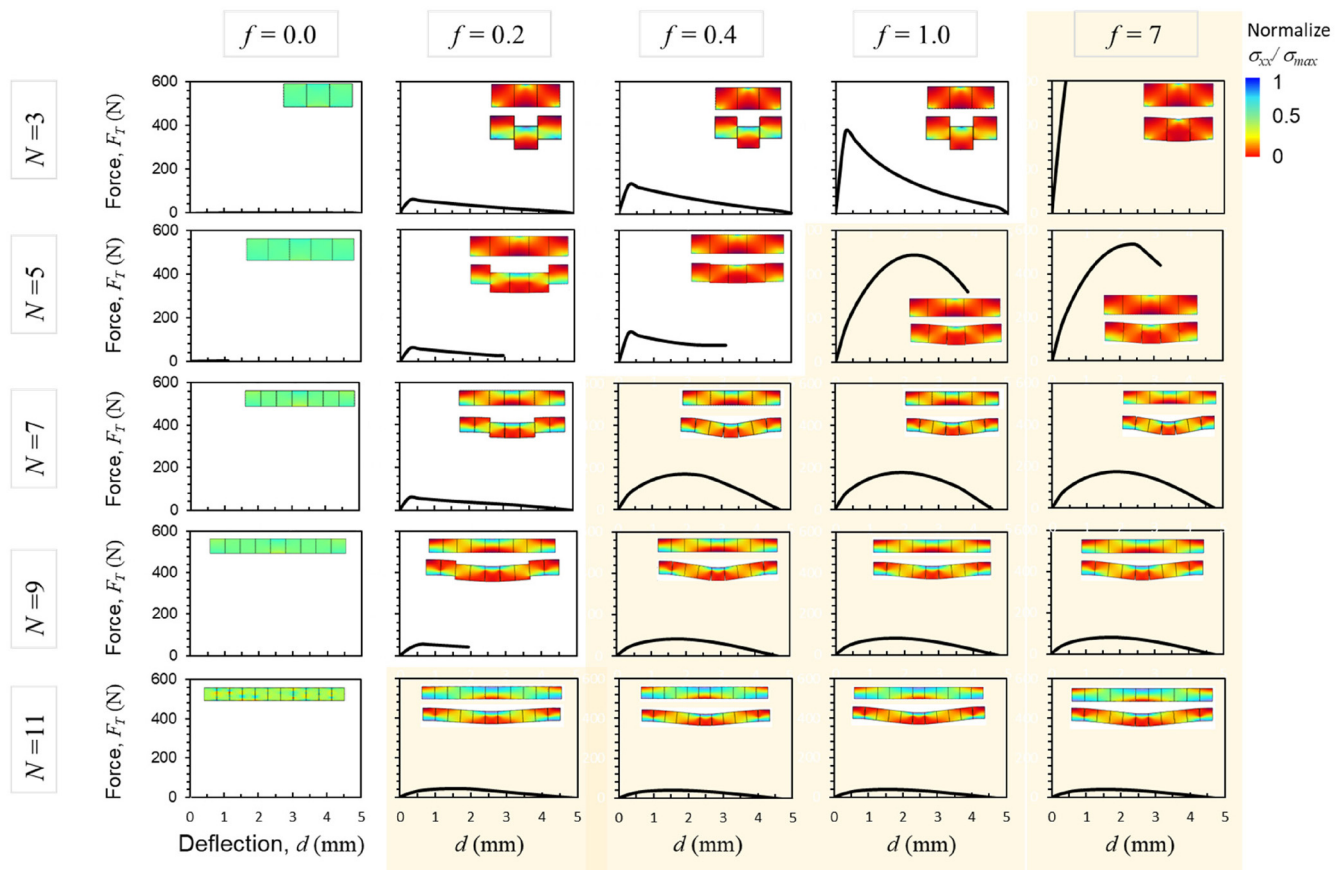


Figure 6. $F_T - d$ responses based on the FEM; $N = 3, 5, 7, 9$ and 11 and friction coefficients; and $f = 0, 0.2, 0.4, 1.0$, and 7.0 .

3.4. Beam Structure as a Material. Once the FEM model was verified and validated experimentally, we proceeded with a computational sweep over the parameter design space (N, f). We ran the FEM for $f = 0, 0.2, 1.0$, and 7 , from low friction to extreme levels, and for $N = 3, 5, 7, 9$, and 11 blocks, using the same elastic and axial force parameters as before. Figure 6 shows all the force-deflection plots ($F_T - d$) for the above-mentioned parametric sweep. For the frictionless cases ($f = 0$), as shown in the first column, the solver registered extremely low forces near the machine zero $\sim 10^{-13}$ N, and thus, the system was unstable and the solver could not proceed except for a few pseudo increments. Therefore, without friction, the segmented beam could not maintain its stability and had no load-bearing capacity (Fig. 6). In Fig. 6, the insets of each plot show the undeformed and deformed beams.

With increased friction, i.e., the second column for $f = 0.2$, the segmented array exhibited a linear increase and onset of sliding, followed by sliding until loss of bearing capacity (as in Fig. 4) only for the case of 3–9 blocks. With an increased number of blocks ($N > 9$), the array transitioned into another mode of deformation where the blocks bent like a continuous beam, characterized by the tendency of the interfaces to open due to block rotation, which we called “hinging” as per Ref. ⁵. This mode was also characterized by a gradual softening in stiffness during deformation (the slope of the force-deflection curve), showing a parabolic trend. One major difference is that the area under the curve (AUC), which visualizes the absorbed energy, is predominantly due to the elastic energy built into the structure. The structure

acted more like a continuous beam but with enhanced deformation (more compliant). Thus, the structure lost its energy-dissipation mechanism. The regions characterized by the hinging mode are highlighted with an orange background in the grid in Fig. 6.

With a further increase in the number of blocks ($N = 9$ and 11), the tendency of the interfaces to open diminished, and the segmented beam began to exhibit the behavior of a continuous beam. In other words, the segmented beam structure began to behave as a homogeneous continuum for $N > 11$ at $f = 0.2$. At $f = 0.4$, the sliding persisted up to $N = 5$. For larger numbers of blocks, $N > 5$, parabolic hinging-mode deformation emerged, and the tendency of the interfaces to open ceased around $N \geq 9$. By increasing the friction to extreme levels, such as $f = 1.0$ and 7 , sliding was only observed at $N = 3$ for $f = 1.0$, and the structure exhibited only hinging for $f = 7$. For $f = 1.0$, the tendency of interface opening ceased for $N \geq 7$, and for $f = 7$ it ceased already at $N \geq 3$. Thus, it is reasonable to suggest that for $f > 7$, the material interfaces act as fused blocks, and the system behaves more like a continuous beam (i.e., approaching a continuum) without the homogenization of its apparent properties. In this regime, the segmented beam transitions from discrete granules (i.e., individual blocks) to continuum-like behavior, where the interfaces remain intact and the stiffness modulation is preserved across scales. Maintaining the advantage of interfaces is important for ensuring crack resistance because cracks are forced to deflect along these interfaces^{4,17}.

In summary, segmented structures can be transitioned, at least for the beam case presented herein, via increased friction or an increased number of blocks. Both are analogous to interatomic bonding and increase the number of units (i.e., separation of scale) in lattice materials and composites¹⁶. Increased friction also caused the maximum traverse force to increase. Therefore, both the strength and stiffness of the beam increased with friction. An increase in N softens the beam and decreases its strength. Increasing both N and f promotes hinging over sliding and makes the beam structure behave more like a continuous beam.

4. CONCLUSION

This study introduced the mechanics of segmented beams and established their basic transverse responses, including the linear regime, sliding onset, and post-sliding behavior. The FEM model was further validated against existing experiments and captured the main deformation modes, with deviations increasing only for larger values of N . With the model verified, a parametric study of (N and f) showed that friction stabilized the segmented beam and increased its strength and stiffness, whereas an increase in N softened the beam and decreased its strength. High friction or N suppressed sliding and promoted hinging, causing the segmented beam to behave more like a continuous beam, effectively transitioning from a structure to a continuum. This behavior is analogous to increased bonding or scale separation in lattice materials and composites. Despite these findings, this study has several limitations that should be acknowledged. The model is developed under quasi-static conditions, meaning that dynamic and rate-dependent effects are not considered; therefore, the results are most applicable to slow loading scenarios. Friction between blocks is represented using a simplified Coulomb model with equal static and dynamic coefficients, which does not capture more complex behaviors such as stick-slip transitions or surface wear. In addition, the analysis focuses on a segmented beam configuration, selected as a simple and well-understood system to isolate the key mechanics; consequently, extending these findings to more complex geometries or fully three-dimensional architected materials should be done with caution. Finally, the conclusions are based on a specific parameter space defined by block number and friction coefficient; while they provide useful mechanistic insight, they are not intended to be universally applicable to all segmented systems.

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DATA AVAILABILITY

Data will be made available upon request

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XGBoost-Based Prediction of pKa Values from Molecular Descriptors

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ABSTRACT

The acid dissociation constant (pKa) is a fundamental physicochemical property that governs molecular ionization, solubility, and bioavailability, rendering its accurate prediction essential in drug design and environmental toxicology. This study entailed a systematic comparison of molecular descriptor representations for pKa prediction using eXtreme Gradient Boosting (XGBoost) regression. Four descriptor categories were evaluated: Morgan circular fingerprints, known as extended-connectivity fingerprints (ECFP), with varying radii (one to four) and bit lengths (12–16,384), Molecular ACCess System (MACCS) structural keys, physicochemical descriptors (molecular weight, logP, rotatable bond count, and fragment counts), and combined representations. A comprehensive grid search optimized the XGBoost hyperparameters across all configurations using five-fold cross-validation on a curated dataset of 7,912 compounds with experimental pKa values obtained from DataWarrior. Morgan fingerprints with radius two and 16,384 bits achieved the highest standalone performance (test $R^2 = 0.795$, root mean squared error, RMSE = 1.539), whereas combining Morgan fingerprints (radius one, 2,048 bits) with MACCS keys and physicochemical descriptors yielded the optimal overall result (test $R^2 = 0.817$; RMSE = 1.455). An extended analysis employing 1,135 Mordred and RDKit cheminformatic descriptors with XGBoost feature selection further improved the prediction accuracy (test $R^2 = 0.829$; RMSE = 1.404). Moreover, feature importance analysis identified the number of acidic groups, spectral descriptors, and aromatic amine fragments as the most influential predictors. These results demonstrate that multisource descriptor fusion consistently outperforms individual representations and that XGBoost provides a computationally efficient and interpretable framework for pKa modeling.

Keywords: pKa prediction, XGBoost, molecular fingerprints, Morgan fingerprints, MACCS keys, QSAR, molecular descriptors

1. INTRODUCTION

The acid dissociation constant (pKa) quantifies the tendency of a molecule to donate a proton in an aqueous solution and is one of the most critical physicochemical properties in medicinal chemistry, environmental science, and chemical engineering¹. Because pKa governs the molecular charge state at physiological pH, it directly influences drug absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiles. Therefore, accurate pKa values are indispensable for lead optimization in pharmaceutical development and for predicting the environmental fate of organic pollutants.

The experimental determination of pKa via potentiometric titration or spectrophotometric methods, although reliable, is time-consuming and resource-intensive, particularly for the screening of large compound libraries. Consequently, computational approaches to pKa prediction have attracted sustained research interest over the past few decades. Empirical methods based on linear free-energy relationships represent some of the earliest pKa-prediction strategies; however, their applicability is often restricted to structurally similar compound series². Alternatively, quantum-mechanical approaches, including density functional theory (DFT) combined with continuum

solvation models, offer higher accuracy; however, they remain computationally prohibitive for large-scale virtual screening^{3,4}.

More recently, machine learning (ML) methods have emerged as attractive compromises between accuracy and computational cost. For instance, quantitative structure–activity relationship (QSAR) models trained on molecular descriptors or fingerprints can rapidly predict pKa values of thousands of compounds following the establishment of a robust training set^{1,5}. Among available ML algorithms, gradient boosting methods, particularly eXtreme Gradient Boosting (XGBoost), have demonstrated competitive performance across diverse molecular property prediction tasks^{6,7}. XGBoost employs regularized gradient boosting of decision trees, incorporating L1 and L2 regularization terms, which mitigate overfitting while maintaining predictive power, thereby making the method particularly well-suited for high-dimensional descriptor spaces common in cheminformatics⁶.

Previous studies have reported that the choice of molecular representation profoundly affects QSAR model performance. For instance, binary fingerprints, such as Morgan (extended-connectivity) fingerprints⁸ and Molecular ACCess System (MACCS) structural keys⁹, encode substructural information as fixed-length bit vectors and have been widely employed in

similarity searching and property prediction. Additionally, continuous physicochemical descriptors computed from molecular graphs (e.g., molecular weight, polar surface area, and partition coefficients) capture complementary global properties. More recently, comprehensive descriptor calculators such as Mordred¹⁰ and PaDEL have enabled the generation of thousands of descriptors per molecule, raising questions regarding optimal feature-selection strategies. Nevertheless, despite the wide range of descriptor options, systematic comparisons of representation types for pKa prediction using modern gradient-boosting frameworks remain limited.

As one example, Mansouri et al.¹ established an important benchmark by developing open-source pKa prediction models using support vector machines, XGBoost, and deep neural networks on a curated dataset of 7,912 compounds from DataWarrior¹¹. These models achieved root mean squared error (RMSE) values of approximately 1.5 pKa units on external test sets, comparable to those of commercial software packages. Additionally, Yang et al.¹² applied XGBoost with structural and physical-organic parameter-based (SPOC) descriptors for pKa prediction across 39 solvents, achieving a mean absolute error (MAE) of 0.87 pKa units. Furthermore, graph-based neural network approaches, such as MolGpKa¹³ have also shown promise for pKa prediction. However, the relative contributions of different descriptor types (fingerprints versus continuous descriptors, as well as their combinations) to the XGBoost-based pKa models have not yet been comprehensively evaluated.

The present study addresses this gap by systematically comparing four molecular descriptor categories for pKa prediction using XGBoost regression: (i) Morgan circular fingerprints with varying radii and bit lengths, (ii) MACCS structural keys, (iii) a set of physicochemical descriptors and fragment counts, and (iv) combined multisource descriptor vectors. A grid search of the XGBoost hyperparameters with five-fold cross-validation was performed for each configuration. Furthermore, an extended analysis employing 1,135 Mordred and RDKit descriptors was conducted to assess the potential of a high-dimensional descriptor space. The key objectives of this work are to determine the descriptor representation that yields the most accurate pKa prediction, quantify the benefit of descriptor fusion, and identify the most informative molecular features using XGBoost feature-importance analysis.

2. METHODOLOGY

2.1. Dataset. The experimental pKa values for 7,912 organic compounds were obtained from the DataWarrior software package¹¹, which aggregates data from multiple public repositories. This dataset, originally curated by Mansouri et al.¹, includes the strongest acidic pKa for each compound measured in aqueous solution at 25 °C. The chemical structures were represented as Simplified Molecular Input Line Entry System (SMILES) strings. Prior to descriptor computation, salt forms were removed using a custom salt-removal protocol based on the RDKit SaltRemover module¹⁴ with a curated salt definition file. Molecules that could not be parsed by RDKit or that yielded invalid molecular objects after salt removal were excluded, yielding the final working dataset. For the fingerprint

comparison experiments (Sections 2.2–2.5), this dataset was split into 75% training and 25% test sets using a random partition (random_state = 11) to ensure reproducibility.

2.2. Morgan Circular Fingerprints. Morgan fingerprints, also known as ECFPs⁸, were generated using the RDKit library¹⁴. Each fingerprint encodes a substructural environment around every atom up to a specified radius and is hashed into a fixed-length bit vector. To evaluate the effect of the fingerprint parameters on predictive performance, a comprehensive grid was constructed over four radii (one, two, three, and four) and ten bit lengths (12, 64, 128, 256, 512, 1,024, 2,048, 4,096, 8,192, and 16,384), yielding 40 distinct fingerprint configurations.

2.3. MACCS Structural Keys. MACCS keys⁹ are a set of 166 predefined binary structural keys that indicate the presence or absence of specific substructural patterns (e.g., aromatic rings, functional groups, and ring sizes). Unlike Morgan fingerprints, MACCS keys do not require parameter tuning as the key definitions are fixed. MACCS fingerprints were generated for all valid molecules using the RDKit MACCSKey module¹⁴.

2.4. Physicochemical Descriptors. A set of five continuous molecular descriptors and fragment counts was computed for each molecule using RDKit¹⁴: molecular weight (MolWt), calculated octanol–water partition coefficient (MolLogP), number of rotatable bonds (NumRotatableBonds), number of aliphatic hydroxyl groups (fr_Al_OH), and number of aromatic nitrogen atoms (fr_Ar_N). These descriptors were selected to capture fundamental size, lipophilicity, flexibility, and functional group properties relevant to acid–base equilibria.

2.5. Combined Descriptor Vectors. For each of the 40 Morgan fingerprint configurations, a combined feature vector was constructed by concatenating the Morgan fingerprint with a 166-bit MACCS key vector and five continuous descriptors, resulting in a total dimensionality of (Morgan size + 171). This experimental design allowed the assessment of whether multisource descriptor fusion improved pKa prediction relative to individual descriptor types.

2.6. Extended Descriptor Analysis. In a separate analysis, a comprehensive set of molecular descriptors was computed for an independent subset of the data (Opt2 acidic partition:

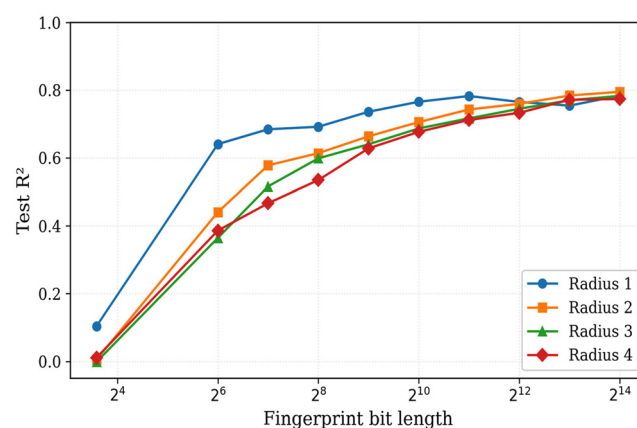


Figure 1. Effect of Morgan fingerprint bit length on the test R^2 value for radii 1–4

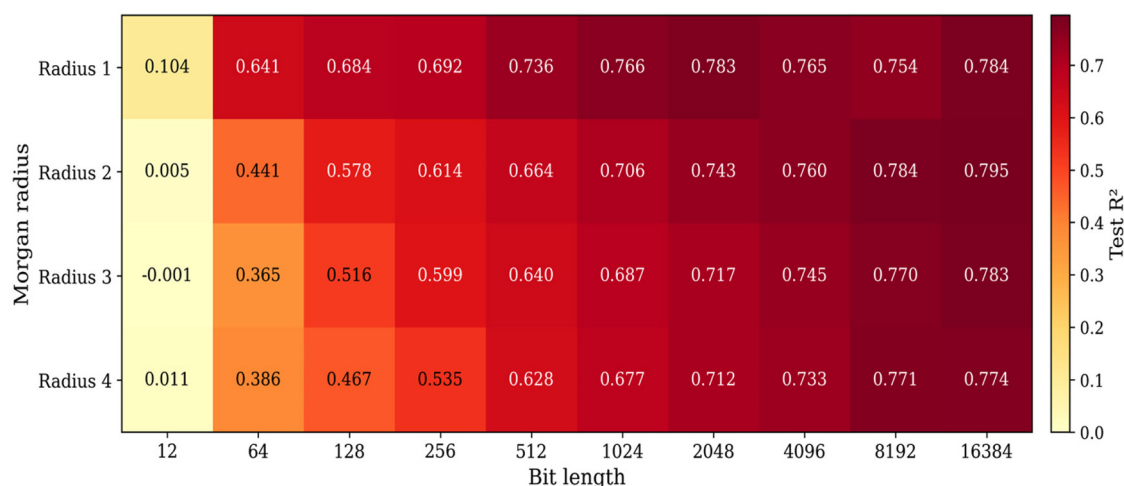


Figure 2. Heatmap of the Morgan fingerprint test R^2 values across all radius and bit-length combinations. Darker shading reflects superior performance

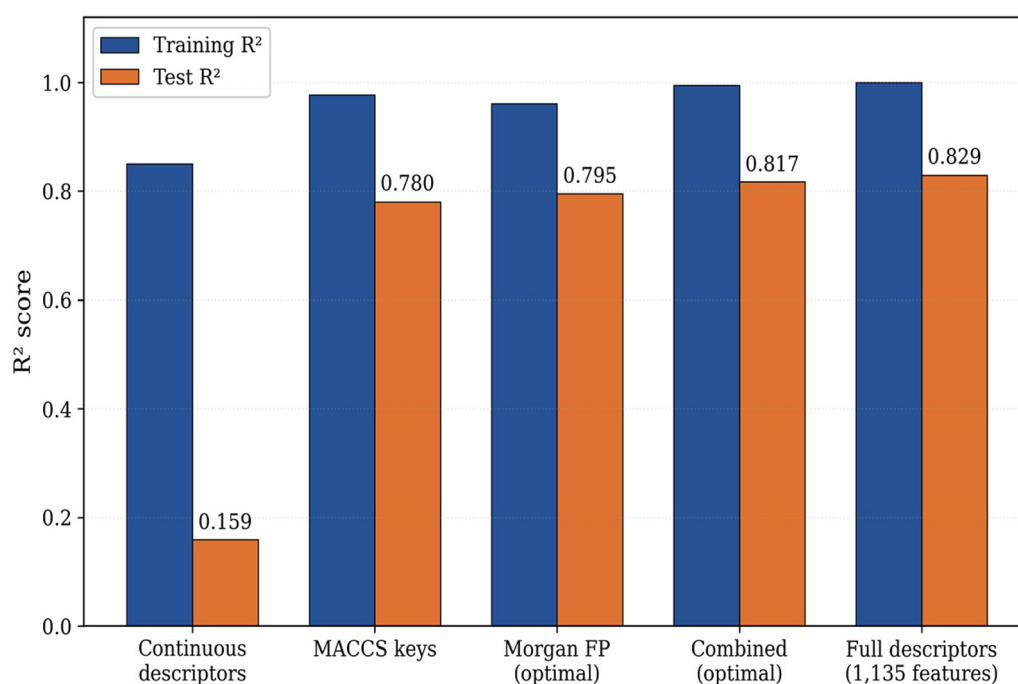


Figure 3. Comparison of the training and test R^2 values across descriptor categories

2,293 training compounds and 765 test compounds with predefined splits from DataWarrior). Three descriptor families were calculated: (i) all 210 RDKit two-dimensional (2D) descriptors¹⁴, (ii) 85 RDKit fragment counts (fr_* functions), and (iii) approximately 1,800 Mordred of 2D descriptors¹⁰. After removal

of zero-variance columns, conversion of all values to numeric format, and removal of rows with missing values, the final descriptor matrix contained 1,135 features. This high-dimensional representation was used to train an XGBoost model with the same hyperparameters described in Section 2.7, and to extract feature importance for chemical interpretation.

Table 1. Performance comparison of XGBoost models across descriptor categories

Descriptor type	Features	Training R^2	Test R^2	MAE	RMSE
Continuous descriptors	5	0.850	0.159	2.385	3.117
MACCS keys	166	0.977	0.780	1.056	1.596
Morgan FP (optimal)	16384	0.961	0.795	1.040	1.539
Combined (optimal)	2219	0.995	0.817	0.913	1.454
Full descriptors	1,135	0.9998	0.829	0.887	1.404

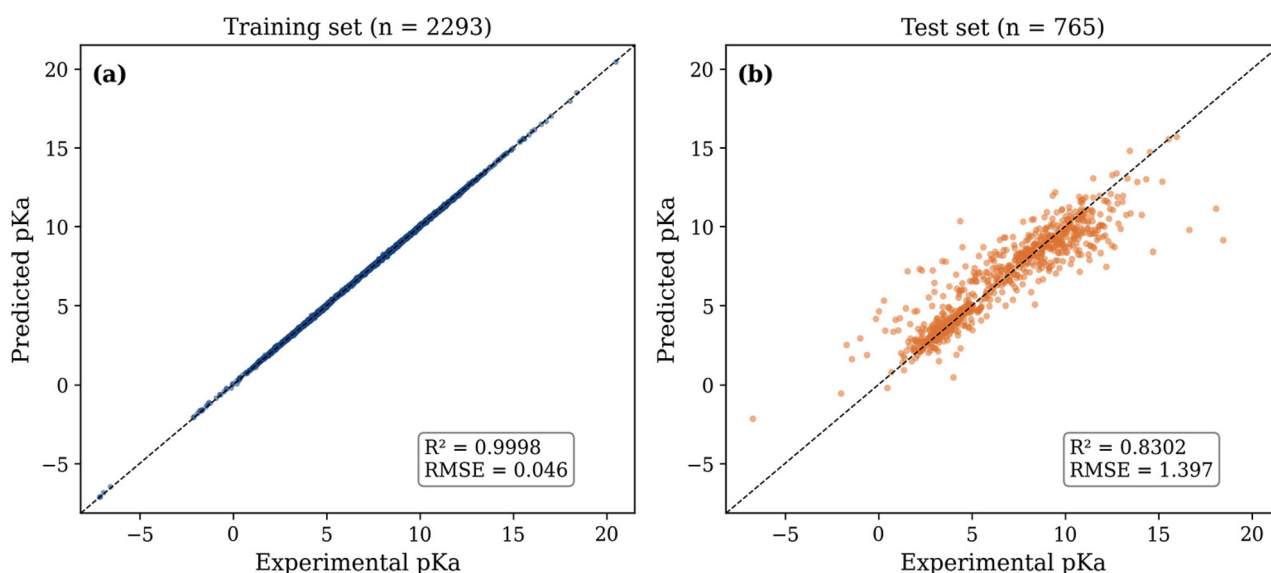


Figure 4. Predicted versus experimental pKa values for the full-descriptor XGBoost model. (a) Training set ($n = 2293$). (b) Test set ($n = 765$). The dashed line represents perfect prediction

2.7. XGBoost Model Training and Evaluation. All models were trained using XGBoost⁶ with a squared-error regression objective (squarederror). For fingerprint comparison experiments, hyperparameter optimization was performed via an exhaustive grid search with five-fold cross-validation using GridSearchCV¹⁵. The search space included $n_estimators = \{300\}$, $max_depth = \{3, 6\}$, $learning_rate = \{0.1, 0.2\}$, $subsample = \{0.8\}$, $colsample_bytree = \{0.8, 1.0\}$, and $reg_lambda = \{1, 5\}$. The optimal model determined by cross-validation was evaluated using the held-out test set. For the extended descriptor analysis, fixed hyperparameters were employed ($n_estimators = 300$, $max_depth = 6$, $learning_rate = 0.1$, $subsample = 0.8$, $colsample_bytree = 0.8$, and $reg_lambda = 1$), following published guidelines for gradient boosting in QSAR⁷. Model performance was assessed using the coefficient of determination (R^2), RMSE, and MAE for both the training and test sets. Feature importance was extracted from the trained XGBoost model using a gain-based importance metric.

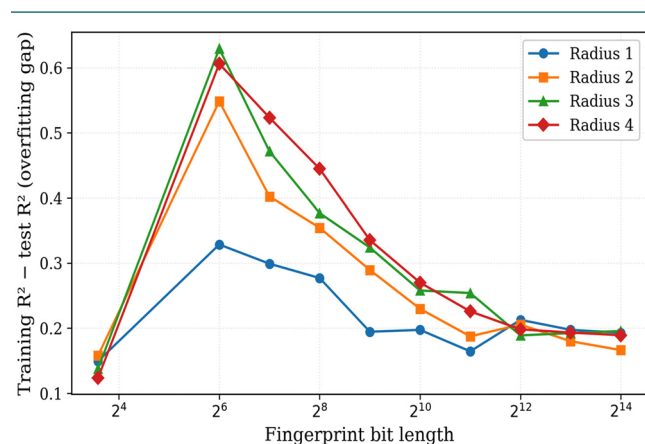


Figure 5. Overfitting gap (training R^2 – test R^2) for Morgan fingerprint models as a function of bit length and radius

3. RESULTS AND DISCUSSION

3.1. Effect of Morgan Fingerprint Parameters. The predictive performance of the Morgan fingerprints varied substantially with both radius and bit length. Figure 1 illustrates the relationship between the fingerprint bit length and R^2 for each radius. At the smallest bit length tested (12 bits), all radii yielded poor model performance (test $R^2 < 0.20$), reflecting severe information loss due to hash collisions. Performance increased monotonically with bit length up to approximately 2,048–4,096 bits, beyond which the gain plateaued. Radius 2 consistently outperformed the other radii at higher bit lengths, achieving superior individual Morgan fingerprint results: test $R^2 = 0.795$ and RMSE = 1.539 at 16,384 bits. This finding is consistent with the observation that ECFP4 (radius 2) captures a balance between local atomic environments and broader substructural context⁸.

Figure 2 presents a heatmap of the test R^2 values across the full-radius-bit-length grid. A clear pattern emerged: radii 1 and 2 generally outperformed radii 3 and 4 at equivalent bit lengths. This can be attributed to the fact that larger radii encode increasingly specific substructural environments, which may introduce noise and reduce generalizability when the training set does not contain sufficient structural diversity. Additionally, extremely small bit lengths (12–64 bits) were found to be consistently inadequate, regardless of radius, confirming that fingerprint dimensionality represents a critical design parameter.

3.2. Comparison Across Descriptor Types. Table 1 summarizes the best-performing models for each descriptor category. Use of the five continuous physicochemical descriptors alone yielded a low R^2 value of 0.159 (RMSE = 3.117), indicating that this minimal feature set was insufficient for pKa prediction across a structurally diverse compound library. This result underscores the importance of substructural information for capturing the electronic and steric factors that govern the acid–base equilibria. MACCS keys (166 bits) produced a significantly superior R^2 of 0.780 (RMSE = 1.596), demonstrating the utility of predefined structural keys despite their modest dimensionality. The

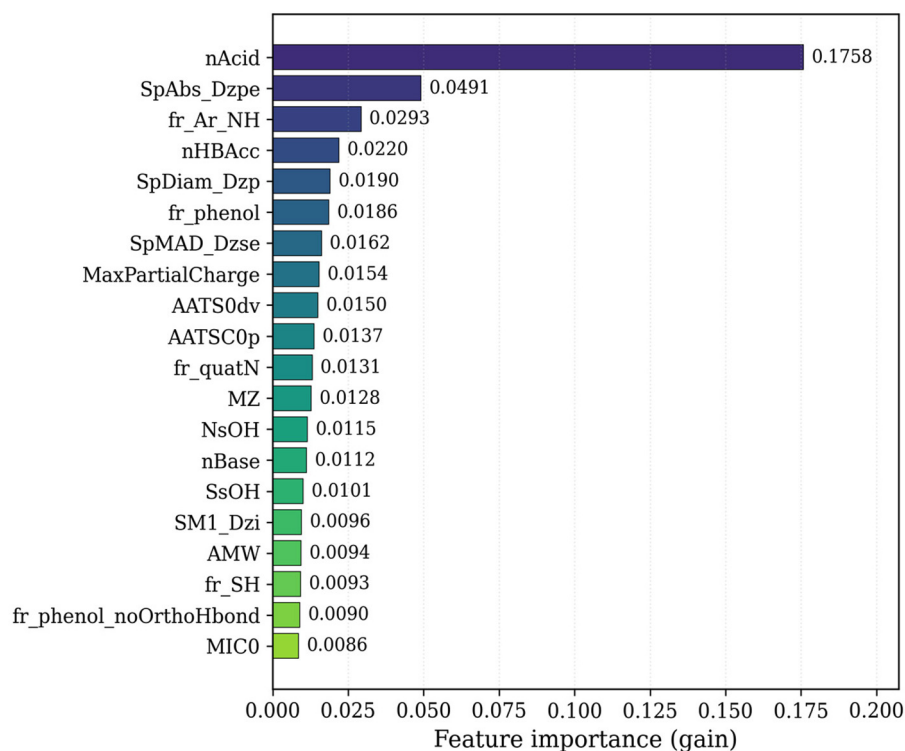


Figure 6. Top 20 features ranked by importance (gain metric) identified by the full-descriptor XGBoost model

optimal Morgan fingerprint configuration (radius two, 16,384 bits) slightly outperformed MACCS, with a test R^2 of 0.795, which can be attributed to its data-driven encoding of circular substructures rather than the fixed key set^{8,9}.

As detailed in the table, the combined descriptor vectors consistently outperformed the individual components. The optimal combined configuration (Morgan radius 1, 2,048 bits + MACCS + continuous descriptors) achieved a test R^2 of 0.817 (RMSE = 1.454), representing a 2.8% improvement over the optimal individual Morgan fingerprints. This result corroborates previous findings that heterogeneous descriptor fusion can capture complementary structural information^{5,7}. Figure 3 presents a visual comparison of the training and test R^2 values across all five model categories.

3.3. Predicted Versus Experimental pKa. Figure 4 presents scatter plots of the predicted versus experimental pKa values obtained using the full-descriptor XGBoost model for both the training and test sets. The training set ($n = 2293$) exhibited a near-perfect fit ($R^2 = 0.9998$, RMSE = 0.047), whereas the test set ($n = 765$) showed good generalization ($R^2 = 0.829$, RMSE = 1.404). The scatter around the diagonal identity line remained relatively uniform across the pKa range of -3 to 14 , suggesting that the model does not exhibit systematic bias toward any particular pKa region.

3.4. Overfitting Analysis. The gap between the training and test R^2 values was used as an indicator of overfitting. Figure 5 plots this gap for the Morgan fingerprint models across all radii and bit lengths. Models with $\text{max_depth} = 6$ exhibited larger train-test gaps (up to $0.20 R^2$ units) than those with $\text{max_depth} = 3$, consistent with the known tendency of deeper trees to memorize training data⁶. Nevertheless, the regularization

provided by XGBoost (L2 penalty via reg_lambda) prevented catastrophic overfitting, even at high dimensionalities. The full-descriptor model showed the largest absolute training-test gap (training $R^2 = 0.9998$ vs. test $R^2 = 0.829$), suggesting that some degree of overfitting was inevitable with 1,135 features and 2,293 training samples. Future studies should therefore explore additional regularization strategies (e.g., feature selection or ensemble averaging) to narrow this gap.

3.5. Feature Importance Analysis. The feature importance extracted from the full-descriptor XGBoost model provided chemical insights into the structural drivers of pKa variation (Figure 6). The most important feature was nAcid (importance = 0.176), which is a Mordred descriptor that counts the number of acidic functional groups in the molecule. This is chemically intuitive because the presence and number of acidic groups directly determine the pKa landscape. The second-ranked feature, SpAbs_Dzpe (importance = 0.049), is a spectral descriptor related to Barysz-weighted electronegativity that captures electronic distribution patterns. The third most important feature, fr_Ar_NH (importance = 0.029), reflects the influence of aromatic amine groups, which are well-known weak acids.

Other highly ranked features included nHBAcc (hydrogen-bond acceptor count, importance = 0.022), fr_phenol (phenolic hydroxyl groups, importance = 0.019), and MaxPartialCharge (importance = 0.015). This feature-importance profile is consistent with chemical theory: molecular acidity is primarily governed by the presence of ionizable functional groups, the electronic environment around those groups (i.e., partial charges and electronegativity), and intramolecular hydrogen bonding². The top ten features identified in this work are listed in Table 2.

Table 2. Top ten molecular descriptors ranked by XGBoost feature importance (gain metric)

Rank	Descriptor	Importance	Description
1	nAcid	0.176	Number of acidic groups
2	SpAbs_Dzpe	0.049	Spectral Barysz electronegativity
3	fr_Ar_NH	0.029	Aromatic amine count
4	nHBAcc	0.022	H-bond acceptor count
5	SpDiam_Dzp	0.019	Spectral Barysz polarizability
6	fr_phenol	0.019	Phenol group count
7	SpMAD_Dzse	0.016	Spectral distance descriptor
8	MaxPartialCharge	0.015	Maximum partial charge
9	AATS0dv	0.015	Moreau–Broto autocorrelation
10	AATSC0p	0.014	Centered Moreau–Broto polarizability

3.6. Residual Analysis. Figure 7 shows the residual distribution and the residual-versus-predicted plot for the full-descriptor model on the test set. The residual histogram is approximately symmetric about zero, with a slight positive skew. The majority of predictions (>80%) fall within ± 2 pKa units of the experimental value. Additionally, the residual-versus-predicted plot shows no pronounced systematic pattern, although larger absolute residuals were observed at extreme pKa values (i.e., below -1 and above 12), where the training-data density is lower. These observations indicate that the prediction errors of the model are predominantly random rather than systematic and suggest that the performance could be improved by augmenting the training set in these extreme pKa ranges.

3.7. Comparison with the Literature. The results of this study are consistent with the findings of Mansouri et al.¹, who reported RMSE values of approximately 1.5 pKa units for XGBoost models trained on the same DataWarrior dataset. The present combined fingerprint model (RMSE = 1.454) and full-descriptor model (RMSE = 1.404) both fall within this range. Although Yang et al.¹² achieved a lower MAE of 0.87 pKa units using solvent-specific SPOC descriptors, their study was restricted to a smaller, more homogeneous dataset. Additionally,

Sanchez et al.⁴ achieved high prediction accuracy by combining DFT-computed features with molecular fragmentation descriptors, albeit at a substantially higher computational cost than the purely descriptor-based approach presented herein. These results demonstrate that purely 2D descriptor-based XGBoost models provide a favorable balance between accuracy, interpretability, and computational efficiency for large-scale pKa predictions.

4. CONCLUSIONS

This study systematically evaluated the performance of four molecular descriptor categories for pKa prediction using XGBoost regression on a curated dataset of 7,912 compounds.

It was revealed that Morgan circular fingerprints at radius 2 with 16,384 bits achieved the optimal standalone fingerprint performance (test $R^2 = 0.795$, RMSE = 1.539), whereas bit lengths below 128 were insufficient for accurate prediction, regardless of radius. The MACCS structural keys (166 bits) provided competitive performance (test $R^2 = 0.780$) relative to their low dimensionality. However, the use of continuous physicochemical descriptors alone resulted in poor predictability ($R^2 = 0.159$), confirming the requirement for substructural

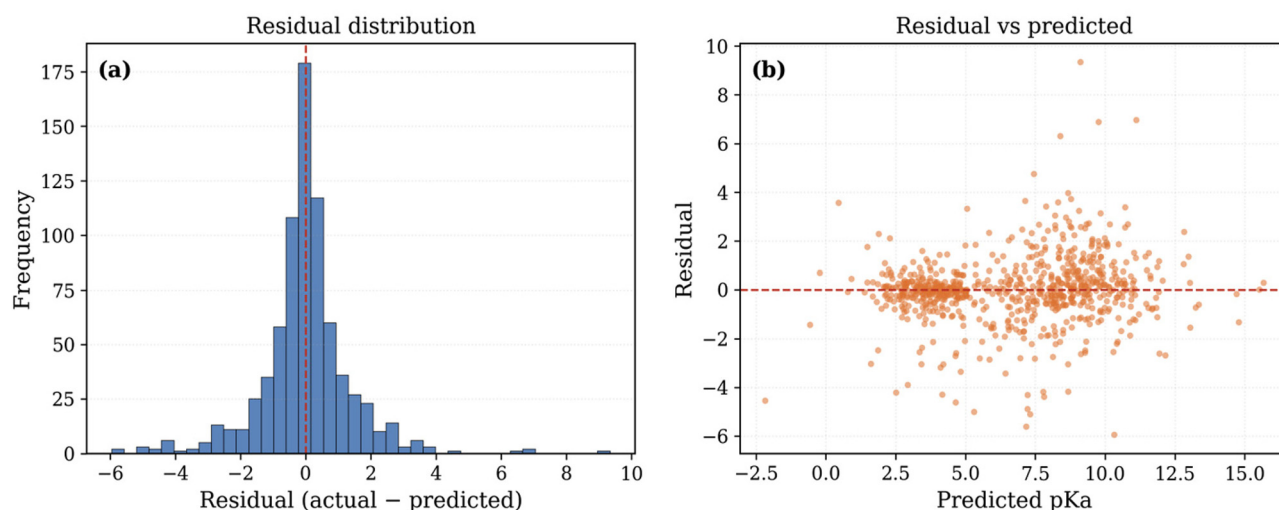


Figure 7. Residual analysis of the full-descriptor XGBoost model on the test set. (a) Residual histogram. (b) Residuals versus predicted pKa values

information. Notably, a combination of Morgan fingerprints, MACCS keys, and physicochemical descriptors consistently outperformed the individual representations, with the optimal combined model achieving $R^2 = 0.817$ (RMSE = 1.454). An extended analysis with 1,135 Mordred and RDKit descriptors further improved the prediction accuracy to $R^2 = 0.829$ (RMSE = 1.404). Furthermore, feature importance analysis revealed that the acidic group count, spectral electronegativity descriptors, and aromatic amine fragments were the most influential predictors, consistent with established chemical theory of acid–base equilibria.

These findings demonstrate that descriptor fusion is a simple yet effective strategy for improving pKa prediction accuracy and that XGBoost offers a computationally efficient and interpretable framework suitable for large-scale virtual screening. Future studies should explore the application of these models to external validation sets, the integration of three-dimensional molecular descriptors, and comparisons with graph neural network approaches to further advance the field.

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Building and Evaluating an Arabic Social-Media Dataset for Deepfake Text Detection

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ABSTRACT

Rapid advances in large language models have enabled the creation of sophisticated deepfake text, which poses a significant threat to social media information integrity. Arabic deepfake text detection is underexplored owing to the morphological complexity of the language and its diverse regional dialects. Studies in this domain often rely on narrow datasets or focus exclusively on Modern Standard Arabic and fail to capture the informal linguistic nuances prevalent on platforms like X. This study addresses these gaps by compiling a high-quality Arabic dataset spanning six major dialects and seven distinct domains, providing a representative benchmark for real-world environments. Real Arabic texts were collected from X, deepfake texts were generated via a prompt-based approach using GPT-4o-mini across multiple deception styles, and a pretrained BERT-base-uncased model was fine-tuned for binary classification using the Hugging Face Transformers framework. Experimental results validated the high quality of the proposed dataset. The model achieved training, validation, and test accuracies of 93.7%, 93.2%, and 92.5%, respectively, with an F1 score of 92.5%. A significant finding of this study was the variation in performance across different data sources. The highest accuracy was observed in entertainment content from YouTube, suggesting that the model effectively identifies the stylistic and expressive markers inherent in synthetic conversational Arabic. Our contributions include the curation of an authentic multi-dialectal corpus and validation of transformer-based architectures tailored for identifying AI-manipulated text. This study provides a benchmark for the Arabic natural language processing community.

Keywords: deepfake detection, Arabic text, machine learning, social media

1. INTRODUCTION

The rapid evolution of large language models (LLMs) has ushered in an era of synthetic text being increasingly indistinguishable from that written by humans. Although these advances offer transformative benefits in natural language processing (NLP), they also facilitate the creation of highly realistic deepfake texts, which are frequently used to spread misinformation, conduct large-scale phishing, and manipulate public discourse, especially across social-media platforms^{1,11}. Recent findings indicate that although LLMs excel at generating coherent text, they introduce significant ethical risks by enabling the production of deceptive content, which can deceive even human experts^{11,12}. Despite the global prevalence of this threat, existing detection frameworks are overwhelmingly optimized for English and Indo-European languages, often overlooking the linguistic complexity and vulnerability of Arabic¹².

This study is motivated by several fundamental challenges in the detection of deceptive Arabic content. The primary obstacle is the inherent morphological complexity of the language—Arabic is characterized by a root-and-pattern system where a single semantic root can generate numerous forms with distinct

meanings, making it one of the most intricate languages. Therefore, there is a persistent shortage of standardized and inclusive datasets that capture the linguistic diversity of Arabic, including the variability between Arabic dialects commonly used on social media¹².

The complexity of Arabic is mirrored in other morphologically rich and right-to-left languages such as Urdu, where standard, unsupervised models often struggle without specialized feature extraction and syntactic rules¹³. Just as document clustering in Urdu requires specific handling of complex syntax—where the absence of Latin-script features such as capitalization complicates standard NLP approaches—Arabic detection requires models that consider its unique agglutinative nature and intricate orthography^{12,13}.

The absence of comprehensive, multi-dialectal Arabic datasets and the lack of detection models tailored to Arabic's morphological complexity represent critical gaps in the literature. This study addresses these gaps through three steps: collecting diverse data from social media, generating synthetic counterparts using LLM, and implementing rigorous quality control to address the morphological framework.



Figure 1. Workflow of the proposed approach

2. RELATED WORK

Although detecting machine-generated text in Arabic is critical, it is an emerging research field. Current literature can be mainly categorized into three main directions: rumor and fake news detection, deep learning approaches for synthetic text, and development of large-scale Arabic corpora.

Early research focused on rumors rather than AI-generated text. Alzanin and Azmi⁴ used semi-supervised and unsupervised expectation maximization to detect rumors in Arabic on Twitter. Although pioneering, this approach targeted misinformation patterns rather than LLM linguistic markers. Similarly, Awajan¹ explored shallow learning techniques for fake news detection, emphasizing the importance of platform-specific features on X. Qasem et al.⁷ expanded this into ensemble learning specifically for COVID-19 rumors, demonstrating that domain-specific models achieve high accuracy but often fail to generalize to broader contexts.

Recent studies have shifted toward identifying deepfake or machine-generated text. Sadiq et al.² leveraged FastText embeddings combined with deep learning to identify synthetic tweets, providing a baseline for how machine-generated Arabic differs from human prose. For data-collection methodology, Fagni et al.³ established the TweepFake dataset; although focused on English, it provided a blueprint for using application programming interfaces (APIs) and heuristic searches to build deepfake-specific corpora, which were subsequently adapted by Arabic researchers.

The introduction of AraBERT by Antoun et al.⁸ revolutionized the field by providing a robust transformer-based encoder

for Arabic. Building on this, Alshammari et al.¹¹ recently proposed a dedicated detector for AI-generated Arabic text using an encoder-based transformer architecture, specifically designed to distinguish between human-written text and LLM output. To evaluate these complex models, Swaminathan and Tantri¹⁰ recently emphasized the use of advanced metrics based on confusion matrices to ensure that performance is not skewed by imbalanced datasets.

Despite these technical leaps, the progress in this field is hindered by lack diverse data. Nofal⁵ and Seddik⁶ provided large-scale datasets through web scraping and APIs; however, these are largely restricted to Modern Standard Arabic (MSA) and Egyptian dialects. As noted by Alayba¹² in a 2025 comprehensive review, the primary challenge remains "Diglossia"—the vast difference between MSA and regional dialects. Most datasets focus on news and political content, leaving a notable gap in social and creative domains, where machine-generated text and deepfakes are increasingly prevalent. These limitations—narrow dialect coverage, domain imbalance, and models inadequate to Arabic's morphological complexity—collectively motivate the present study. This study aims to address these challenges by constructing a benchmark dataset spanning six Arabic dialects and seven domains, and by evaluating a transformer-based model for deepfake text detection. The key contributions of this work include the curation of an authentic multi-dialectal corpus collected from X, the generation of deepfake texts using multiple deception styles, and the fine-tuning of a BERT-based classifier.

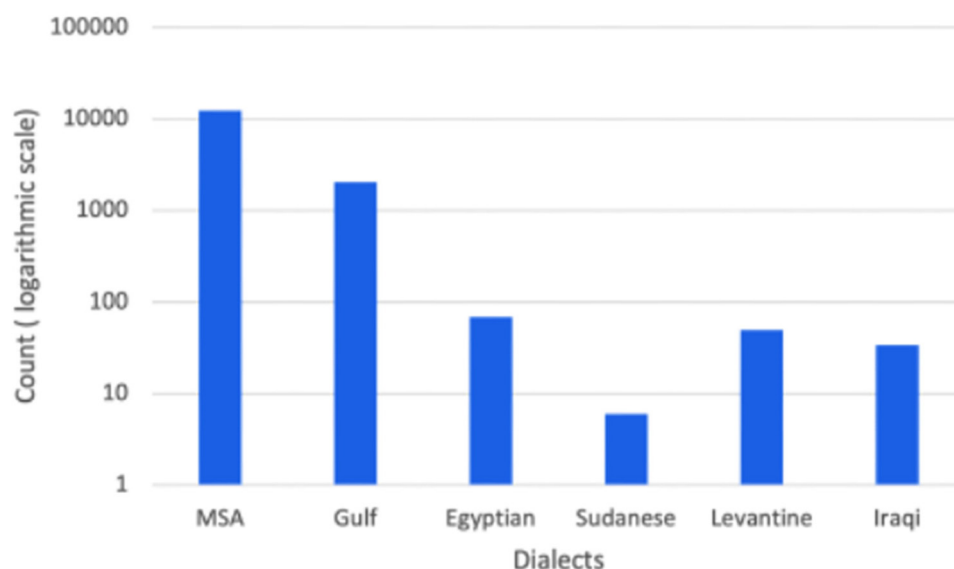


Figure 2. Distribution of the dataset across dialects

Table 1. *Attributes of the dataset*

Attribute	Description
Text	Target text
Type	Tweet, Reply
Platform Type	Social media
Source	X (formerly Twitter)
Dialect	MSA, Gulf, Egyptian, Levantine, Iraqi, and Sudanese
Domain	Health, Politics, Education, Ads, Sports, Religion, and Economy
Class	Real or Deepfake

3. METHODOLOGY

This section explains the methodology followed in this study to construct and validate an Arabic deepfake-detection dataset, as shown in Figure 1.

3.1. Real Data Collection. We gathered real Arabic text from X and compiled a representative dataset using a wide range of linguistic and thematic variations across Arabic dialects. Public posts and replies were searched and collected using a combination of hashtag queries, keyword searches, automated scraping, and manual reviews. The search targeted diverse domains, including news, opinions, e-commerce, and general discussions. The text was collection between June 2022 and November 2022, focusing on posts shared before the public release of ChatGPT to minimize the likelihood of AI-generated content. No private or personal identifiable information was collected; all data were obtained from publicly accessible sources according to data usage and content access policies of X. The resulting dataset reflects natural Arabic discourse across dialects and topics. Table 1 shows the key attributes of the dataset.

We categorized the data by dialect and domain using a combination of a prompt-based method and manual reviews. The texts already had preliminary topic labels based on the collection criteria; however, the dialects were not labeled. We used a prompt-based classification approach powered by the GPT-4o-mini LLM. The instructions were to output a dialect label per text and select the dominant dialect in case of mixed usage. The

prompt explicitly listed the targeted dialects and enforced consistent formatting. At the end, an Arabic speaker manually reviewed each domain and dialect label to resolve ambiguous cases such as domain-overlapping or dialectally mixed texts.

The dataset comprises six Arabic dialects—MSA, Gulf, Egyptian, Sudanese, Levantine, and Iraqi—as shown in Figure 2. It also spans seven domains—health, politics, education, online advertisements, sports, religion, and economy. The initial dataset consisted of 21,000 texts; however, after cleaning and filtering, the final dataset comprised 14,403 real texts. Raw data were pre-processed to ensure quality; this included duplicate removal to prevent model overfitting, empty-text removal (such as tweets containing only hashtags), and text normalization to remove URLs, usernames, emojis, and hashtags. The clean dataset was used as the foundation for deepfake generation. To better understand the structure of the dataset, Figure 3 illustrates the distribution of text samples across topics. Domains such as sports and politics exhibited higher representation, reflecting their popularity on social media.

3.2. Deepfake Data Generation. To simulate realistic misinformation, deepfake texts were generated via a prompt-based approach using the OpenAI API. Text was generated using GPT-4o-mini with the following parameters: temperature = 0.9, top-p = 1.0 (default), and max-tokens = ~4096 (default). This stage aimed to generate deceptive text that is similar to real-world misinformation while preserving the linguistic and thematic attributes of the original text. The prompt was designed to mimic user-generated posts across different domains. Each deepfake text was generated based on the corresponding real post, ensuring that it followed the same topic, tone, length, and dialect. The generation process employed multiple deception styles, including exaggeration, omission, mixed truth, and contradiction, which are common types of misinformation found on X. The final dataset contained 28,806 real and fake texts. Table 2 shows one sample of real text and its corresponding deepfake, with the type of deception used.

3.3. Model Architecture and Training. To detect deceptive Arabic text effectively, we adopted a transfer-learning approach using a pretrained BERT-base-uncased model as the baseline architecture, which is a stacked bidirectional transformer encoder⁸. This model was chosen for its deep bidirectional understanding of language context. Although this model was originally trained by Google on large-scale English-language data, its architecture can be effectively generalized to other languages after fine-tuning. The model was fine-tuned for a binary classification task to label each text sample as real or fake.

As illustrated in Figure 4, the model was fine-tuned for a binary classification task to label each text sample as real (1) or fake (0). Fine-tuning was conducted in the Hugging Face Transformers framework to achieve state-of-the-art performance. We used the AdamW optimizer, which decouples weight decay from gradient updates and helps to prevent overfitting—a crucial factor given the linguistic complexity of Arabic and limited dataset size. The learning rate was set to 2e-5, a value empirically shown to yield stable convergence in BERT-based fine-tuning without catastrophic forgetting of pretrained weights⁹. A binary cross-entropy loss function was applied since the output space was

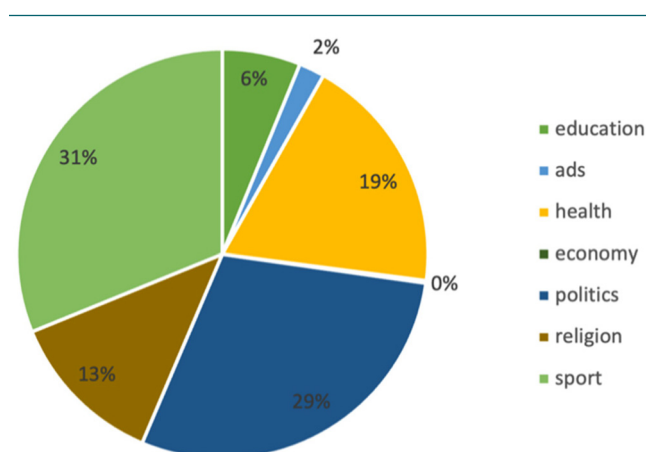
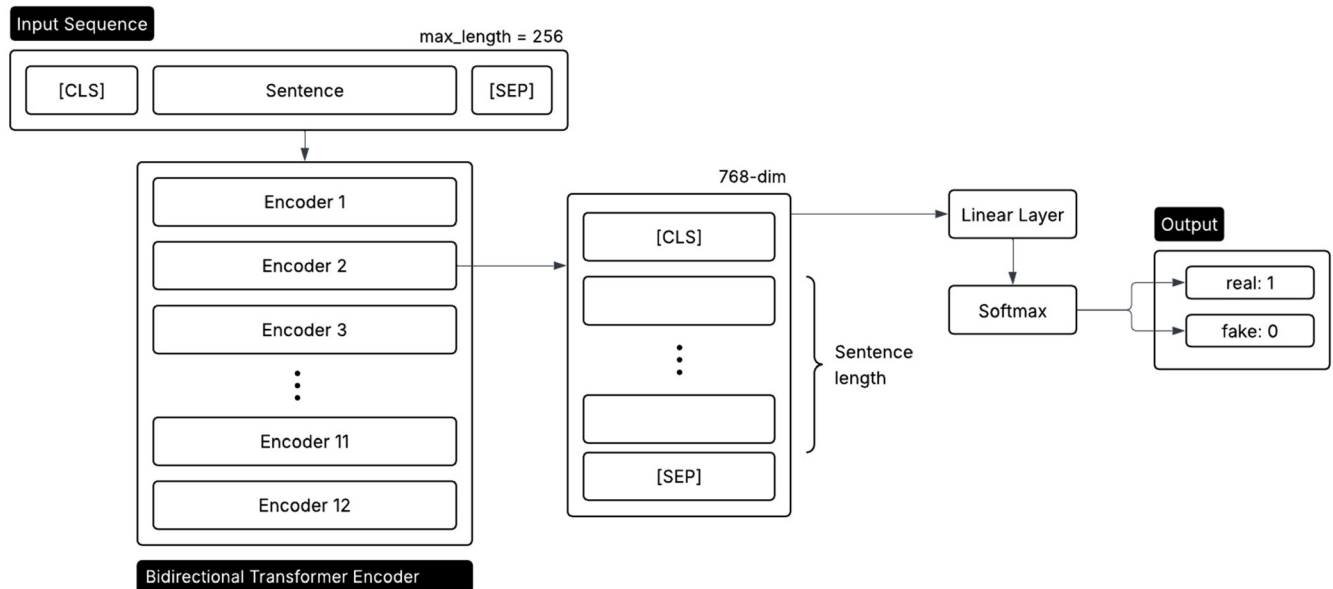
**Figure 3.** Distribution of the dataset across topics

Table 2. Real vs. deepfake Arabic text sample

Real text	Deepfake text	Deception type
أزمة التملك السكني تعكس فشل سياسة السلطة بسبب القمع	أزمة التملك السكني تعكس نجاح سياسة السلطة في تحسين الأوضاع بسبب الدعم الكبير الذي تقدمه للمواطنين.	Contradiction

**Figure 4.** BERT-base-uncased architecture for Arabic deceptive-text detection**Table 3.** Training configuration

Framework	Hugging Face Transformers
Optimizer	AdamW
Learning Rate	2×10^{-5}
Batch Size	16
Epochs	3
Loss Function	Binary cross-entropy
Label Encoding	{fake: 0, real: 1}

restricted to two mutually exclusive classes: fake = 0 or real = 1. All training configurations are shown in Table 3. The training was conducted on Google Colab using a high-performance T4 GPU environment, which enabled parallel computations, thus reducing training time. The model was trained on Arabic text samples, each labeled with its corresponding class (fake or real).

3.4. Evaluation Metrics and Validation. The model was evaluated using four metrics—accuracy, precision, recall, and F1-score. A confusion matrix was generated, which is a performance-evaluation tool used in classification tasks to visualize model predictions compared to actual values¹⁰. For our

binary classification problem, the matrix was structured as shown in Table 4, where

- TP (True Positives): Real tweets correctly identified as real.
- TN (True Negatives): Fake tweets correctly identified as fake.
- FP (False Positives): Fake tweets incorrectly predicted as real (also called a "Type I error").
- FN (False Negatives): Real tweets incorrectly predicted as fake (also called a "Type II error").

Accuracy provides an overall measure of correctness, whereas precision and recall offer deeper insights into the tendencies of Type I and Type II errors, where the cost of false negatives can be high.

To ensure reliable performance assessment, a stratified train-validation-test split was applied, maintaining an approximately 1:1 class ratio across all subsets. This helped preserve the class balance and prevent data leakage between splits. The data were split into 75% training, 15% testing, and 15% validation. Cross-domain validation was performed using four datasets, each representing a different data domain, to further assess the generalization of the model across varying linguistic and contextual settings.

4. RESULTS AND DISCUSSION

The fine-tuned BERT model performed well across all evaluation sets, as summarized in Table 5, demonstrating that transfer learning can be effective for detecting deception in Arabic text. The model achieved training, validation, and test accuracies of 93.7%, 93.2%, and 92.5%, respectively, with an F1 score of 92.5%. These

Table 4. Confusion matrix structure

		Predicted	
		Real (1)	Fake (0)
Actual	Real (1)	True Positive (TP)	False Positive (FP)
	Fake (0)	False Negative (FN)	True Negative (TN)

Table 5. *Evaluation Metrics*

Subset	Loss	Accuracy	Precision	Recall	F1
Training	0.1377	0.937236	0.937235	0.937236	0.937235
Validation	0.186762	0.932534	0.932561	0.932534	0.932525
Test	0.212243	0.925264	0.92553	0.925264	0.925248

Table 6. *Cross-domain validation results*

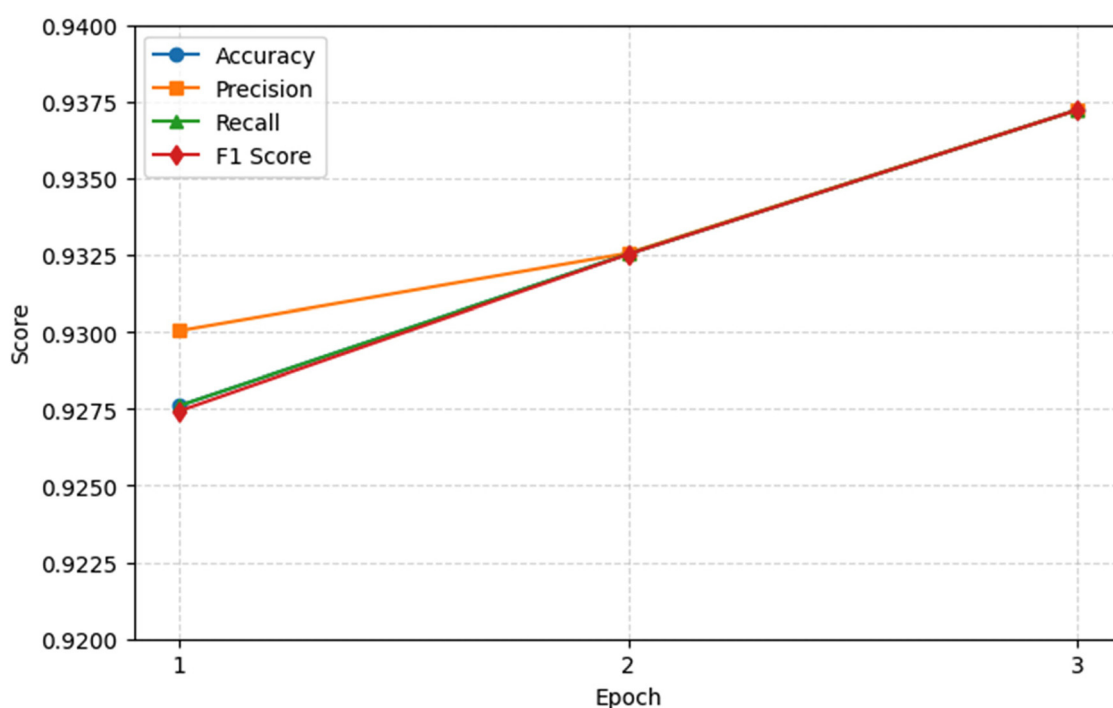
Sources	Accuracy	Precision (weighted)	Recall (weighted)	F1 (weighted)
entertainment	0.849417	0.857303	0.849417	0.848581
governmental	0.569704	0.691781	0.569704	0.495685
news	0.499614	0.494677	0.499614	0.351474
e-commerce	0.454203	0.493177	0.454203	0.414901

results across datasets indicate effective generalization and ability to capture linguistic cues associated with deception. The high performance confirms that even with a transformer-based architecture pretrained on English data, the model can adapt to Arabic linguistics through fine-tuning. Moreover, the close alignment between training and testing metrics suggests minimal overfitting, indicating that the model successfully learned the underlying patterns in the data. The learning curve presented in Figure 5 shows that all evaluation metrics increased steadily and uniformly over the three epochs. This indicates stable model learning and improvement. All scores had effectively converged by Epoch 2, suggesting that the model achieved high performance with minimal trade-offs between precision and recall.

A confusion matrix for the test set (Figure 6) shows a balanced distribution of true positives and true negatives with relatively few misclassifications, confirming the effectiveness of the model in distinguishing between deceptive and authentic Arabic text.

To further evaluate the generalization and robustness of the model, a cross-domain validation was conducted across four content domains—entertainment, government, news, and e-commerce—as shown in Table 6. The entertainment domain achieved the highest performance, with 84.9% accuracy and 0.85 F1 score, reflecting the ability of the model to detect deepfakes in conversational and emotionally expressive text. Other domains achieved significantly lower accuracy, such as e-commerce (45.4%).

This variation is attributed to the linguistic diversity and nature of the content in different domains. The data for the entertainment domain were obtained from YouTube. The comments and posts in X and YouTube typically use informal and expressive Arabic styles with identifiable stylistic patterns. In contrast, governmental and news data typically contain formal and factual language with limited emotional tone, making it hard for the model to distinguish between fake and real text. e-commerce demonstrated the lowest performance, likely due to the nature of

**Figure 5.** Learning curve across epochs

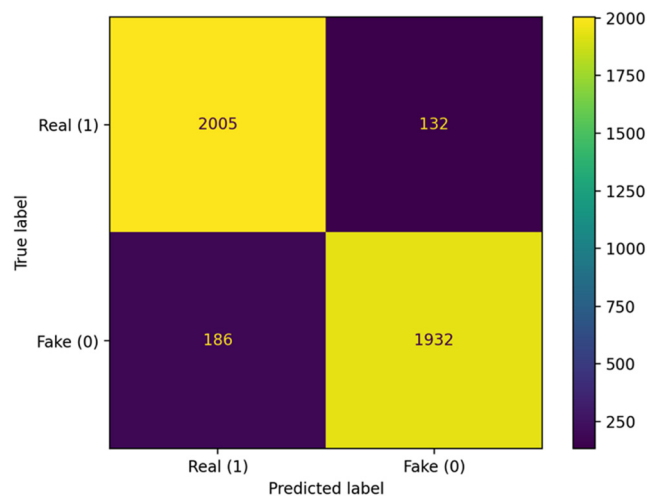


Figure 6. Confusion matrix for the testing dataset

the data. Content from e-commerce platforms such as Amazon consists of short product titles, often mixed with English phrases, and lack contextual depth. In comparison, data from X are contextually rich and linguistically varied. Hence, the model, which was fine-tuned on X data, could perform well on a similar type of expressive content. This indicates that the model can capture stylistic and lexical markers of deception more effectively in subjective and expressive contexts than in objective or factual ones, as shown in Figure 7.

A closer examination of the confusion matrices for the cross-domain validation in Figure 8 further clarifies this variation. The matrices for the news and e-commerce datasets illustrate the degradation in performance, showing predictions that are nearly random (approximately a 50/50 split between correct and incorrect classifications for each class).

The fine-tuned BERT model represents a significant advancement over existing benchmarks that typically focus on MSA in

isolated news domains^{1,2}. By successfully identifying deceptive markers across six dialects and seven domains, this approach demonstrates robustness superior to that of traditional models that require manual feature extraction for the complex Arabic morphology^{4,13}. Furthermore, the 92.5% F1-score of the model highlights the need for fine-tuning encoder-based architectures to overcome the performance failures observed in general-purpose tools such as GPTZero when processing intricate Arabic text^{11,12}.

One limitation was the reduced performance in code-mixed and English-mixed Arabic text. For example, tweets containing nonstandard spellings or repetitive expressions that were challenging for the tokenizer to handle reduced the classification reliability. Furthermore, dialect categorization presented some challenges, especially with Gulf Arabic. Owing to annotation difficulties, all Gulf variants, such as Kuwaiti and Bahraini, were grouped under Gulf. Consequently, the dataset comprises 28,806 samples, which is relatively limited for training and evaluating deep-learning models. The limited size of the dataset may constrain the generalizability and robustness of the model. Despite these limitations, the dataset represents a valuable step toward building a comprehensive Arabic deepfake-detection dataset spanning diverse dialects and domains.

5. CONCLUSIONS

This study investigated the detection of AI-generated Arabic text on social media by developing a comprehensive dataset spanning multiple domains and regional dialects. Experimental results validated the high quality of the proposed dataset, with the trained model achieving a robust 92% accuracy and a 92.5% F1 score. A significant finding of this study was the variation in performance across different data sources. The highest accuracy was observed in entertainment content from YouTube, suggesting that the model effectively identifies the stylistic and expressive mark-

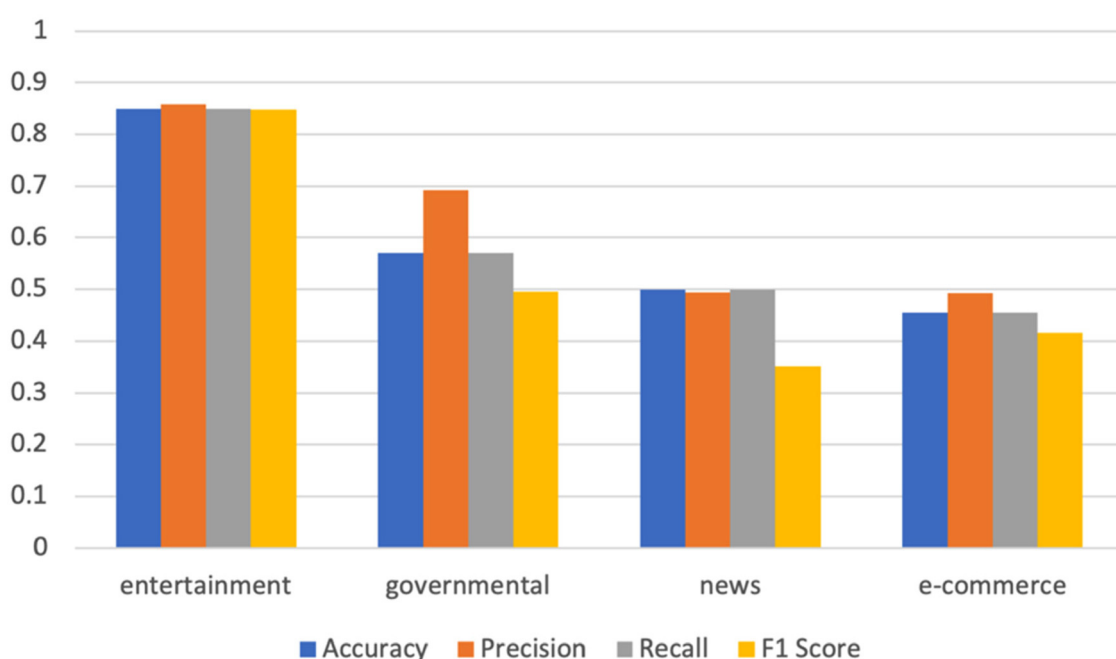


Figure 7. Performance comparisons across domains

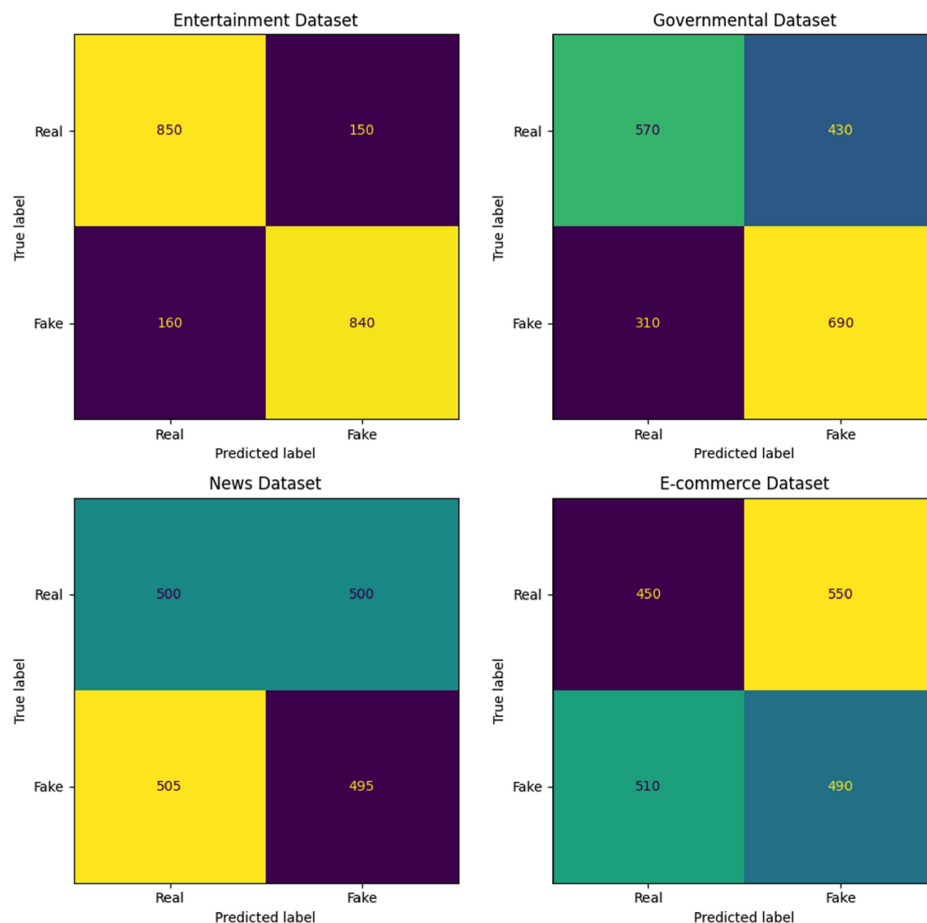


Figure 8. Confusion matrices on testing data for the four datasets

ers inherent in synthetic conversational Arabic. This highlights the critical need for incorporating diverse data sources, including social-media platforms and official governmental records, to ensure that detection frameworks can capture a broad spectrum of linguistic patterns and generalize successfully to unseen data. Although the use of BERT-base-uncased posed certain semantic constraints for the Arabic language, the success of transfer learning demonstrated that the dataset can support resilient and effective detection models. Consequently, this study provides a benchmark for the Arabic NLP community. Future work will focus on further expanding the dataset to include broader dialectal variations and specialized topics.

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Collection and Generation of Arabic E-Commerce Text Data: A Study on Deepfake Detection and Dataset Development

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ABSTRACT

Amazon is a major e-commerce platform and one of the primary online destinations for purchasing electronics. On such platforms, sellers use product titles to provide key descriptions of their items, making these titles the first elements that customers read and rely upon when deciding to buy. However, the growing use of automated text-generation tools has made it easier to create Arabic product titles that resemble genuine listings but may not accurately describe the product. These tools are often used to save time and reduce manual effort, as a large variety of products makes manual title writing time-consuming. This practice can reduce customer trust when the generated titles fail to reflect actual product properties. This study develops a machine learning model for detecting Arabic synthetic product titles on Amazon. The objective is to construct a dataset of real and synthetically generated Arabic smartphone titles and train a classifier capable of distinguishing organically written titles from template-generated synthetic texts. Real titles were collected from Amazon.sa, and synthetic titles were produced using a structure-aware template approach. A BERT-based binary classifier was fine-tuned, achieving training and testing accuracies of 99.1% and 98.3%, respectively, demonstrating strong in-domain performance. Synthetic titles were generated using a structured template-based pipeline rather than neural generative language models. Therefore, the findings are limited to template-generated synthetic content. This study provides a controlled framework for evaluating synthetic title detection in structured Arabic e-commerce contexts.

Keywords: Arabic text, deepfake detection, e-commerce, BERT model, machine learning, synthetic data generation

1. INTRODUCTION

E-commerce platforms, such as Amazon.sa, have become preferred destinations for purchasing consumer electronics across the Arab world because of the wide variety of available products and the trust established through consistent service and quality assurance. On these platforms, product titles are crucial because they compress brand, model, memory, color, and network specifications into the first piece of text that a customer reads, directly influencing search ranking and click-through behavior. The mass production of Arabic product titles that closely resemble authentic marketplace listings is possible using readily accessible AI text-generation tools. Sellers may adopt such tools to reduce manual effort and accelerate listing creation, particularly given the large volume of products available in modern e-commerce. The increasing ease of automated product title generation highlights the need to distinguish between organically written and synthetically generated titles on high-volume platforms. In this study, synthetic titles were generated using a structure-aware template-based approach rather than neural generative language models. Accordingly, the detection task focuses specifically on template-generated synthetic product titles and does not directly evaluate robustness against large-scale neural text generators. Figure 1 presents a diagram of the Arabic synthetic data generation and

detection process followed in this study. The contribution of this study lies in the controlled evaluation of template-based synthetic title detection within structured e-commerce contexts.

Previous studies have shown that machine-generated Arabic texts can closely mimic human-written Arabic, making automatic detection challenging. Nagoudi et al.¹ provided early evidence that synthetic Arabic news content can be automatically generated in the misinformation domain, highlighting the realism of the generated Arabic text and the need for reliable detection methods. Complementing this, Harrag et al.² Demonstrated that short-form Arabic texts, such as automatically generated tweets, can be identified using BERT-based models. This is particularly relevant because product titles are short, compressed sequences of attribute-dense texts.

More broadly, Alyoubi et al.³ reported strong deep learning performance for Arabic misinformation detection tasks while emphasizing linguistic challenges specific to Arabic, including orthographic variation, dialect diversity, and tokenization complexity. On the architectural side, Alnabrisi and Saad⁴ compared transformer-based models, such as BERT and RoBERTa, for Arabic synthetic text detection and observed competitive performance. Within the e-commerce domain, Alharthi et al.⁵ examined fabricated and deceptive Arabic reviews, highlighting credibility concerns in online marketplaces.

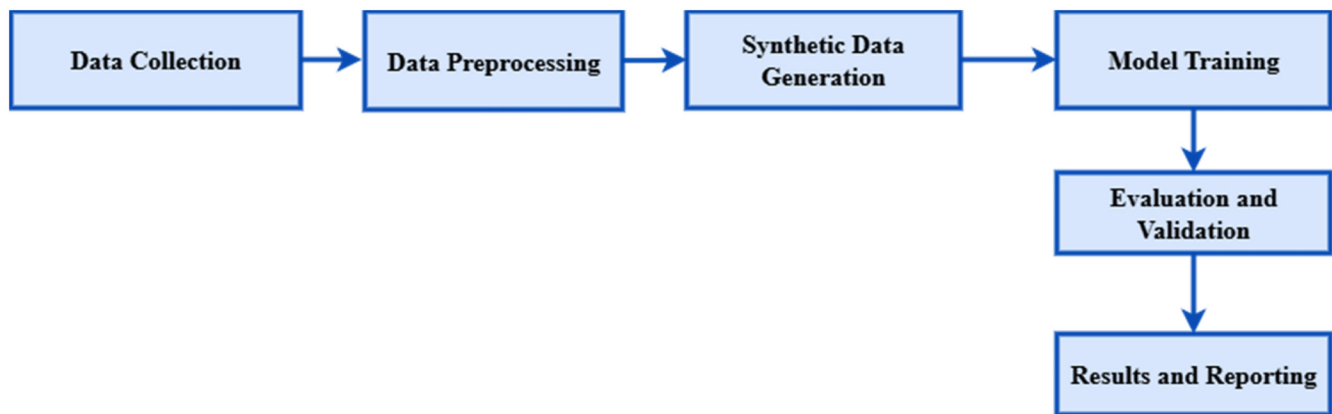


Figure 1. Workflow diagram of the Arabic synthetic data generation and detection process

Despite these recent studies, two practical gaps remain. First, in terms of domain, most Arabic synthetic text detection research focuses on news or social media content rather than on structured e-commerce product titles. Titles are short, formula-like, and specification-dense. In the case of electronics, product titles typically contain attributes such as brand, model, RAM/ROM, color, and network type. These structural characteristics differ substantially from narrative news articles or conversational social media posts and therefore require domain-specific modeling considerations. Second, previous studies often assumed the availability of synthetic examples without clearly describing how such data are generated. Few studies have provided transparent generation pipelines for producing realistic Arabic synthetic titles that preserve marketplace formatting while varying product attributes. Without structure-aware generation, reproducibility and systematic evaluation become more challenging. To address these gaps, this study constructed a paired real-synthetic dataset of Arabic smartphone titles collected from Amazon.sa and evaluated a classifier to distinguish synthetically generated titles from real marketplace titles. Synthetic titles were produced using a structure-aware templating approach that preserves typical marketplace ordering (brand name, model, key specifications, and color/variant) while substituting slot values from curated attribute lists. Light rephrasing and length/format validation were applied to ensure naturalness and to remove malformed or duplicate outputs. The final dataset consisted of 4,606 real titles and approximately 6,000 synthetic titles. Because the generation was not one-to-one, stratified splits and class weighting were used to mitigate class imbalance during training. The combined real and synthetic datasets were used to fine-tune a BERT-based binary classifier. The model performance was evaluated using accuracy, precision, recall, F1-score, and confusion matrices. The implementation was conducted using the HuggingFace Transformers library to support reproducibility. The contributions of this study are as follows:

1. Construction of an Arabic smartphone title dataset collected from Amazon.sa consisting of 4,606 cleaned real marketplace titles.
2. Development of a transparent, structure-aware synthetic title generation pipeline with controllable slot-based attribute substitution.
3. Empirical evaluation of synthetic-versus-real title classification using transformer-based models in an e-commerce setting.
4. Robustness analysis under distribution shift to assess model behavior on external Arabic corpora.

The remainder of this article is as follows. Section 2 describes the dataset collection process, synthetic generation rules, and preprocessing steps. Section 3 details the experimental setup, including model architecture, training configuration, and evaluation metrics. Section 4 presents the results and discussion, including a robustness evaluation under a distribution shift and practical implications. Section 5 concludes the study and outlines limitations and directions for future research.

2. METHODOLOGY

2.1. Dataset Collection and Preparation. Product titles were collected from Amazon.sa under the Mobile/Smartphone category using a lightweight web scraping tool that paginated publicly accessible category pages and extracted only visible product titles from each listing. This scraper accesses public URLs, implements fixed delays between requests to reduce server load, and does not capture personal or user-generated data. Only publicly visible product titles were collected; no reviews, seller metadata, or private information were accessed. Data were collected in a single snapshot, reflecting the marketplace conditions at that time. Non-phone items, such as accessories, bundles, and sponsored non-phone listings, were excluded. The cleaning steps included trimming whitespace, normalizing punctuation, removing empty rows and exact duplicates, and collapsing near duplicates (same brand/model/specifications) into a single entry. Common marketplace spellings for brands were preserved, and a consistent unit format (e.g., GB) was maintained. The resulting corpus contained 4,606 smartphone titles written primarily in Arabic, with occasional English brand names and specification terms (e.g., RAM, GB, 5G). This dataset served as the real class for the subsequent experiments. Table 1 presents representative examples of real and synthetic Arabic smartphone titles used in this study.

The accompanying figures provide a descriptive context of mobile/smartphone products. Figure 2 shows the brand distribution, illustrating the market coverage and representation across

Table 1. Representative real and synthetic Arabic smartphone titles

Type	Example Title
Real	، أسود G، 5GB، 256GB RAM، S238 سامسونج جالاكسي
Synthetic	، لون أسود G، ذاكرة 8 جيجابايت، سعة 256 جيجابايت، يدعم شبكة S235 سامسونج

major manufacturers. Figure 3 shows the RAM distribution, highlighting common memory configurations and specification patterns used in the titles. Figure 4 shows the proportion of 5G versus 4G mentions, reflecting the technology mix and generational characteristics of the devices represented in the dataset. These distributions characterize the common structural and lexical elements of marketplace titles and inform the synthetic generation process described in Section 2.2.

To further characterize the semantic structure of the collected titles, topic modeling was performed on a subset

of real Arabic smartphone titles using Latent Dirichlet Allocation (LDA). Three dominant topics were identified, reflecting recurring lexical patterns in the dataset (Table 2).

The extracted topics correspond to device descriptors, memory and connectivity specifications, and technical features such as camera and battery capacity. These results confirm the structured and attribute-dense nature of the smartphone product titles in the dataset and align with the statistical distributions presented earlier.

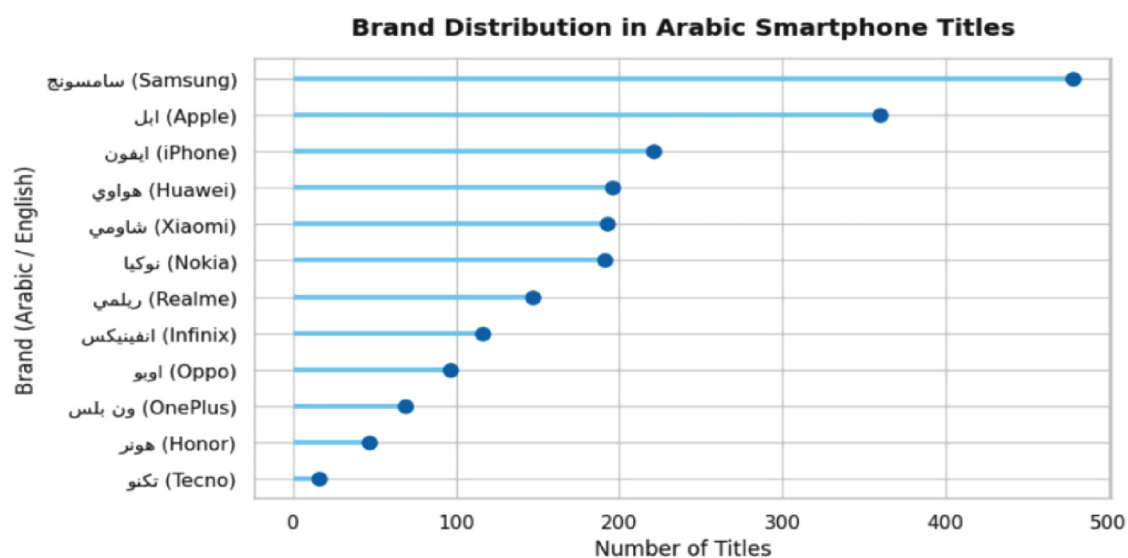
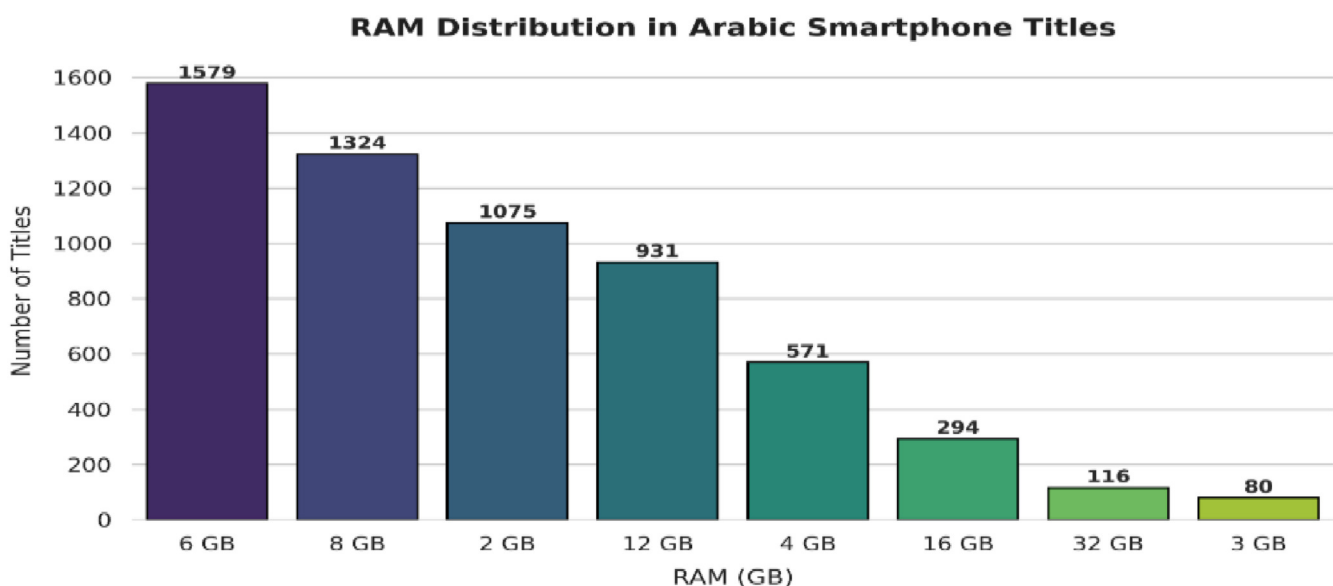
**Figure 2.** Brand distribution in the real Arabic smartphone title dataset, illustrating relative market coverage across major manufacturers**Figure 3.** RAM distribution showing the frequency of memory configurations mentioned in titles

Table 2. Topic modeling results for real Arabic smartphone titles

Topic	Representative Terms
Topic 1	اتصال, ثنائي, هاتف, RAM
Topic 2	جيجابايت, رام, ذاكرة, 5G, 256
Topic 3	كاميرا, بطارية, التخزين, تقنية

2.2. Data Generation (structure-aware templates).

Synthetic titles were generated using a structure-aware templating approach that mirrors the typical marketplace order of smartphone titles. Each template begins with the brand name and model/series, followed by key specifications (RAM/ROM, network type), and concludes with color or variant information. The template includes predefined slots for the brand, model, RAM, storage capacity, network type (4G/5G), and color. The slot values were drawn from curated attribute lists derived from real datasets to ensure realistic combinations and marketplace-consistent phrasing. Light connector rephrasing was applied to reduce repetitive phrasing, and length and format filters were used to remove malformed or duplicate outputs. Synthetic generation was not constrained to a one-to-one mapping with real titles; the final synthetic set contained approximately 6,000 titles compared to 4,606 real titles. To evaluate the alignment of basic structural signals, Table 3 compares real and synthetic titles in terms of 5G/4G mentions and title length statistics, and Figure 5 shows the length distributions for both sets. These comparisons ensured that the synthetic titles approximated the key structural characteristics of the real dataset. The slightly narrower dispersion observed in the synthetic set, with an interquartile range (IQR) defined as the difference between the 75th and 25th percentiles of 66 versus 75 for real titles, reflects the structured nature of template-based generation and may introduce regularity patterns that are not present in organically written titles. This characteristic is considered when interpreting the classification performance.

Table 3. Summary of real vs. synthetic titles

Metric	Real	Synthetic
Count (titles)	4,606	6,000
% 5G	10.38%	5.65%
% 4G	4.58%	5.52%
Median length (chars)	126	125
IQR length (chars)	75	66

2.3. Data Preprocessing.

Real and synthetic datasets were merged and labeled for binary classification (real vs. synthetic). In this study, the “synthetic” label refers exclusively to template-generated titles and does not imply factual inaccuracy or deceptive intent. Only light normalization was applied to preserve the marketplace-specific stylistic cues that may be informative for classification. The preprocessing steps included trimming whitespace, standardizing punctuation, ensuring consistent unit formatting, and removing duplicates. The dataset was divided into training, validation, and test sets using stratified sampling to maintain class balance. As a sanity check, preprocessing was performed to ensure that the structural characteristics of the titles were not distorted. Figure 5 shows similar length distributions for the real and synthetic sets (with medians of 126 and 125 characters, respectively). The synthetic set exhibited a slightly narrower dispersion (IQR: 66 vs. 75), reflecting the structural regularity introduced by the template-based generation process. This characteristic is considered when interpreting the model performance.

3. EXPERIMENTAL WORK

3.1. Model Architecture and Training.

A pretrained Bert-Base-Uncased model from the HuggingFace Transformers library was fine-tuned to distinguish between real and synthetic product titles. Transformer-based models were selected because they capture bidirectional contextual dependencies through self-attention mechanisms, enabling the modeling of interactions between specification tokens within compact, attribute-dense titles. Traditional machine learning approaches, such as term frequency-inverse document frequency (TF-IDF) with logistic regression, treat tokens independently and do not explicitly model contextual relationships, which are important in structured e-commerce titles containing brand names, specifications, and variants. Prior studies on short-text classification tasks have also demonstrated the strong empirical performance of the BERT family of models, further motivating their adoption for this task. Although Arabic-pretrained transformer models are available, BERT-Base-Uncased was selected because of its robustness in mixed Arabic-English environments and its ability to handle code-switching patterns commonly observed in e-commerce titles (e.g., RAM, GB, and 5G). This choice also facilitated reproducibility and comparability with previous short-text classification studies. The BERT-based architecture adopted in this study is shown in Figure 6.

The input titles were processed using the associated WordPiece tokenizer and truncated to a maximum sequence length of 256 tokens. The WordPiece tokenizer segments Arabic words

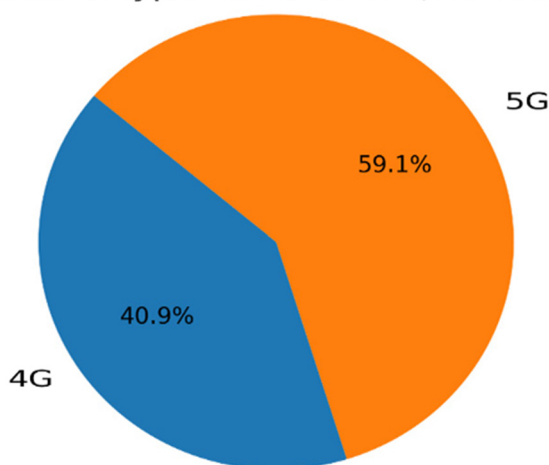
Figure 4. Distribution of 4G versus 5G mentions in the collected dataset

Figure 4. Distribution of 4G versus 5G mentions in the collected dataset

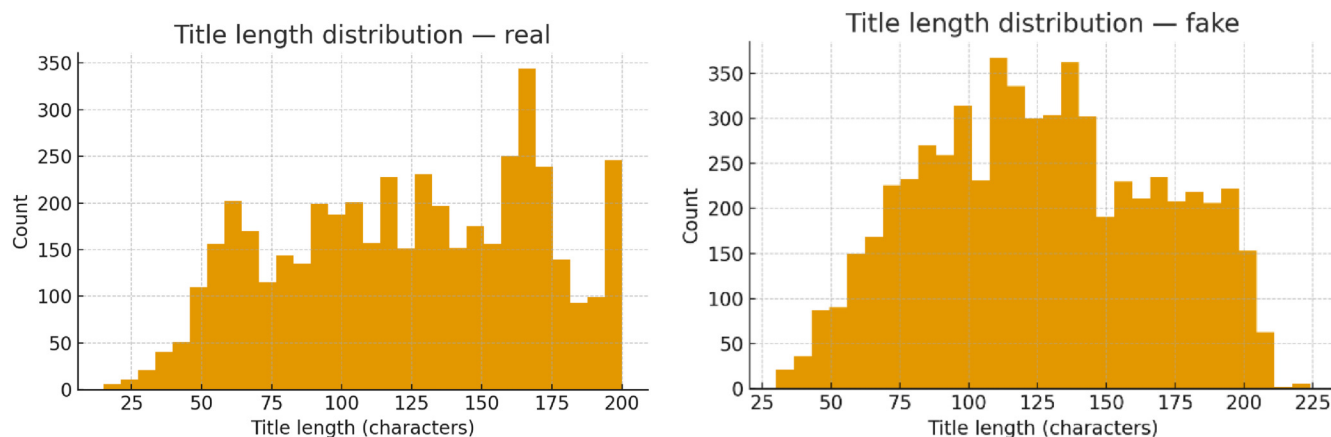


Figure 5. Title length distributions of real vs. synthetic Arabic smartphone titles

into subword units, allowing the model to handle morphological variations and unseen lexical forms commonly found in Arabic texts. Arabic product titles frequently include mixed Arabic–English technical terms (e.g., “RAM”, “5G”), and subword tokenization enables consistent representation of these hybrid expressions within the same embedding space. This approach improves robustness to spelling variations and formatting differences typical in marketplace listings. The final hidden representation corresponding to the [CLS] token (768-dimensional) was passed to a linear classification layer, followed by softmax activation to produce binary predictions (REAL = 1, SYNTHETIC = 0). Training was conducted using the AdamW optimizer with a learning rate of $2e-5$, batch size of 16, weight decay of 0.01, and up to 3 epochs. Mixed-precision (FP16) training was performed using a graphics processing unit. A random seed of 42 was used for reproducibility. Class imbalance was addressed using stratified data splits and a weighted cross-entropy loss. The best model was selected based on the validation F1-score, with an evaluation performed at the end of each epoch.

3.2. Evaluation Metrics. Performance was evaluated using accuracy, precision, recall, and F1-score for each class,

along with macro and weighted averages. Precision measures the proportion of predicted instances of a class that are correct, whereas recall reflects the proportion of true instances that are correctly identified. The F1-score provides a harmonic mean of precision and recall, offering a balanced assessment when class distributions are not perfectly uniform. Confusion matrices were used to analyze error patterns (REAL $\rightarrow$ SYNTHETIC versus SYNTHETIC $\rightarrow$ REAL) and to assess class-specific misclassification behavior. These metrics are appropriate for slightly imbalanced datasets and support consistent comparisons across training, validation, testing, and distribution-shift evaluations.

4. RESULTS AND DISCUSSION

4.1. Model Performance Overview. For the training split ($N = 7,424$), the classifier achieved an accuracy of approximately 0.991 with high scores for both classes (synthetic: $P = 0.9907$, $R = 0.9933$, $F1 = 0.9920$; real: $P = 0.9913$, $R = 0.9879$, $F1 = 0.9896$), as listed in Table 4. In the held-out test split ($N = 1,591$), the accuracy was approximately 0.983, with balanced class performance (synthetic: $P = 0.9791$, $R = 0.9911$, $F1 =$

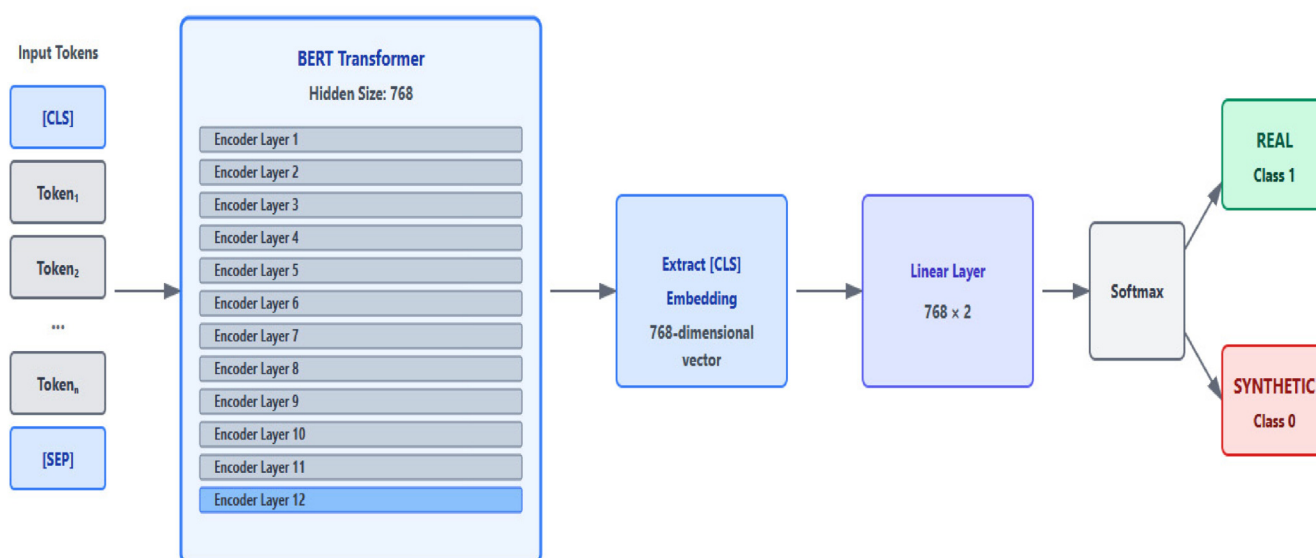


Figure 6. BERT-based architecture for real versus synthetic Arabic product title classification

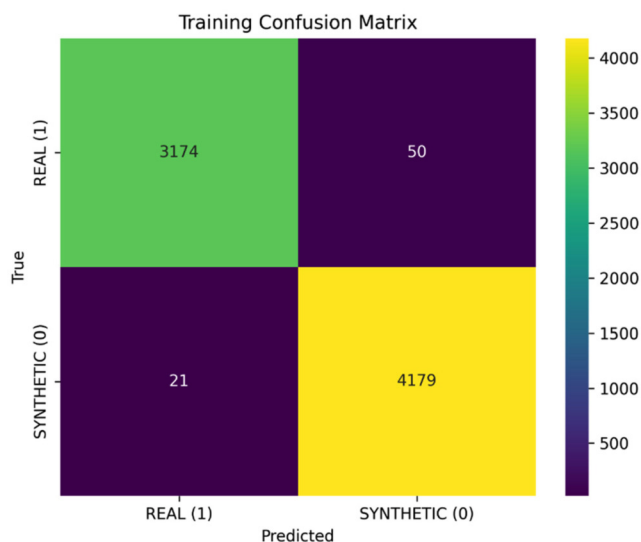


Figure 7. Training confusion matrix (REAL = 1, SYNTHETIC = 0). Counts: REAL→REAL = 3174, REAL→SYNTHETIC = 50, SYNTHETIC→REAL = 21, SYNTHETIC→SYNTHETIC = 4179 (N = 7,424)

0.9851; real: P = 0.9882, R = 0.9725, F1 = 0.9830). The small gap between the training and test performances suggests limited overfitting and stable in-domain generalization to unseen titles from the same distribution. To contextualize the performance of the transformer-based classifier, a traditional machine learning baseline using TF-IDF feature representations combined with logistic regression was implemented. The baseline achieved an accuracy of 91.0% on the held-out test split compared with 98.3% achieved by the BERT-based model. The baseline captures surface lexical patterns, but it does not model contextual dependencies between specification tokens within attribute-dense titles. The observed performance gap indicates that contextual modeling contributes to additional discriminative capacity beyond simple lexical frequency patterns. Here, precision (P) measures the proportion of predicted instances of a class that are correct, whereas recall (R) measures the proportion of correctly identified true instances. The convergence behavior of the model across epochs is shown in Figure 8.

4.2. Performance Interpretation. The test confusion matrix (Figure 7) shows a low number of misclassifications: 19 real titles were incorrectly classified as synthetic, and eight synthetic titles were misclassified as real. This indicates balanced performance across both classes, with high recall for synthetic titles (≈ 0.99) and slightly lower recall for real titles (≈ 0.97). The classifier demonstrated mild asymmetry in the error distribution,

favoring the detection of synthetic titles over the preservation of real titles. In practical deployment scenarios, such behavior may be acceptable in automated screening systems, where missing synthetic titles is considered less desirable than manually reviewing a small number of real titles flagged for verification. If different operational trade-offs are required, the classification threshold can be adjusted, or the class weights can be recalibrated to rebalance false positives and false negatives. The held-out test split confusion matrix is presented in Figure 9.

4.3. Error and Anomaly Analysis. Most misclassifications occur for titles that are very short, dominated by marketing-oriented phrases, or omit key specifications such as brand, model, or RAM/ROM information. These cases reduce the availability of structural and attribute-based cues on which the classifier can rely, increasing ambiguity between real and synthetic classes. This observation is consistent with the slightly narrower length dispersion observed in the synthetic set, reflecting the structured nature of the template-based generation. Although structure-aware templating improves realism, it may also introduce regularity patterns that influence the classifier's decision boundaries.

4.4. Comparison with Related Studies. To explore robustness under a distribution shift rather than to validate general synthetic text detection capability, the classifier trained on Amazon.sa smartphone titles was evaluated on four external Arabic corpora with distinct stylistic profiles. These corpora differ substantially from product titles in structure, length, and lexical composition and are therefore used as distribution-shift stress tests rather than as equivalent training domains. Table 5 summarizes performance across the Governmental, News, YouTube, and Twitter datasets. The results indicate that performance correlates with structural similarity to product titles. Short, attribute-sparse, yet title-like texts (YouTube and Twitter) show stronger transfer performance, whereas longer, claim-style prose (Governmental and News) yields lower accuracy. The confusion matrices in Figure 10 reveal a predominance of REAL → SYNTHETIC errors in Governmental and News corpora, consistent with distributional mismatch. These texts lack specification cues such as brand names, RAM/ROM indicators, and network labels (e.g., 5G), and differ substantially in length, syntax, and vocabulary. Consequently, the classifier trained on specification-dense product titles exhibited reduced robustness outside its native domain. These experiments were intended to analyze model behavior under structural and lexical shifts rather than to claim broad robustness to arbitrary AI-generated Arabic texts.

Table 4. Training classification report (BERT detector)

	precision	Recall	f1-score	support
Synthetic	0.990738542	0.993333333	0.992034241	4200
Real	0.991285403	0.987903226	0.989591425	3224
Accuracy	0.990975216	0.990975216	0.990975216	0.990975216
Macro avg	0.991011972	0.99061828	0.990812833	7424
Weighted avg	0.990976026	0.990975216	0.990973406	7424

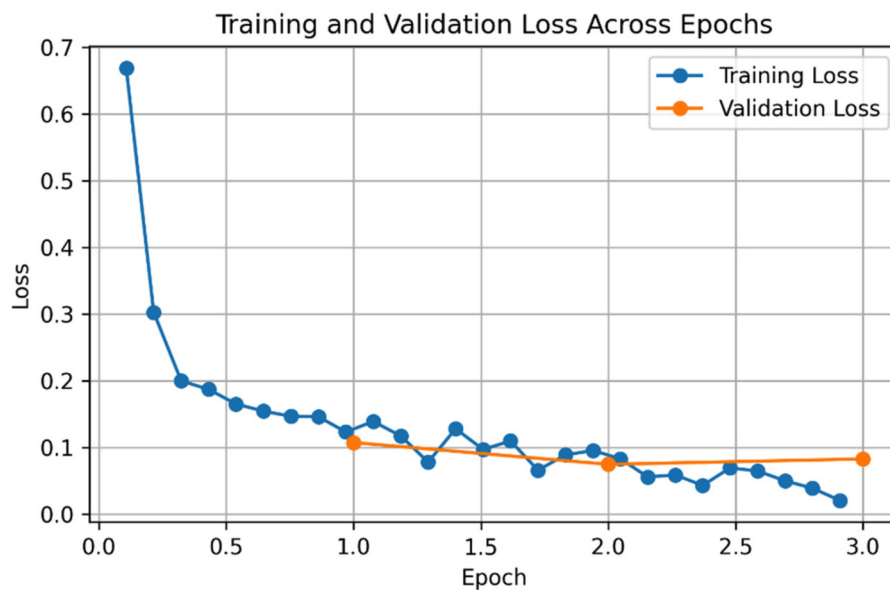


Figure 8. Training and validation loss across epochs during fine-tuning of the BERT-based classifier

Table 5. External datasets and distribution-shift evaluation results

test_dataset	n_test	accuracy	precision	recall	f1
Governmental	7704	0.6616	0.6624	0.6616	0.6606
News	6477	0.541	0.595	0.541	0.4648
YouTube	4456	0.8312	0.8548	0.8312	0.8284
Twitter	4255	0.7932	0.7943	0.7932	0.793

This evaluation highlights the domain-specific nature of learned representations and should not be interpreted as a general synthetic text detection capability across arbitrary Arabic text types.

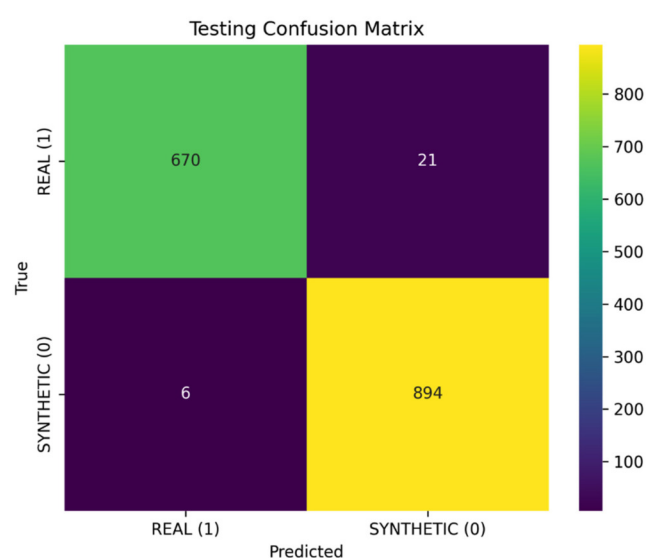


Figure 9. Confusion matrix on the held-out test split ($N = 1,591$) for the REAL (1) versus SYNTHETIC (0) classifier: $TP_{\text{real}} = 670$, $FN_{\text{real}} = 21$, $FP_{\text{synthetic}} = 6$, $TN_{\text{synthetic}} = 894$; overall accuracy $\approx 98.3\%$

4.5. Practical Implications. This detector can serve as an early screening tool for e-commerce. Titles predicted as synthetic may be flagged for manual review or used to prompt clarification of specifications (e.g., brand, model, RAM/ROM, network type). This screening can support quality control workflows in high-volume marketplaces without automatically rejecting legitimate listings.

4.6. Limitations and Future Work. This study focused on short, specification-dense smartphone titles collected from Amazon.sa; therefore, the results may not be generalizable to other product categories, platforms, longer descriptions, or alternative title formats. Marketplace naming conventions, specification formatting, and attribute ordering may evolve over time, which could affect model performance when applied to future marketplace snapshots. The labels distinguish synthetic from organically written titles and do not verify factual correctness. The synthetic set exhibits greater uniformity and may include combinations not typically used by sellers. Consequently, part of the strong in-domain performance may reflect sensitivity to generator-specific structural regularities introduced by the template-based generation process rather than the purely intrinsic characteristics of AI-generated Arabic text. Therefore, the reported performance should not be interpreted as evidence of robustness against modern neural generative language models without additional empirical validation on such data. The detector is trained exclusively on titles with a fixed input length,

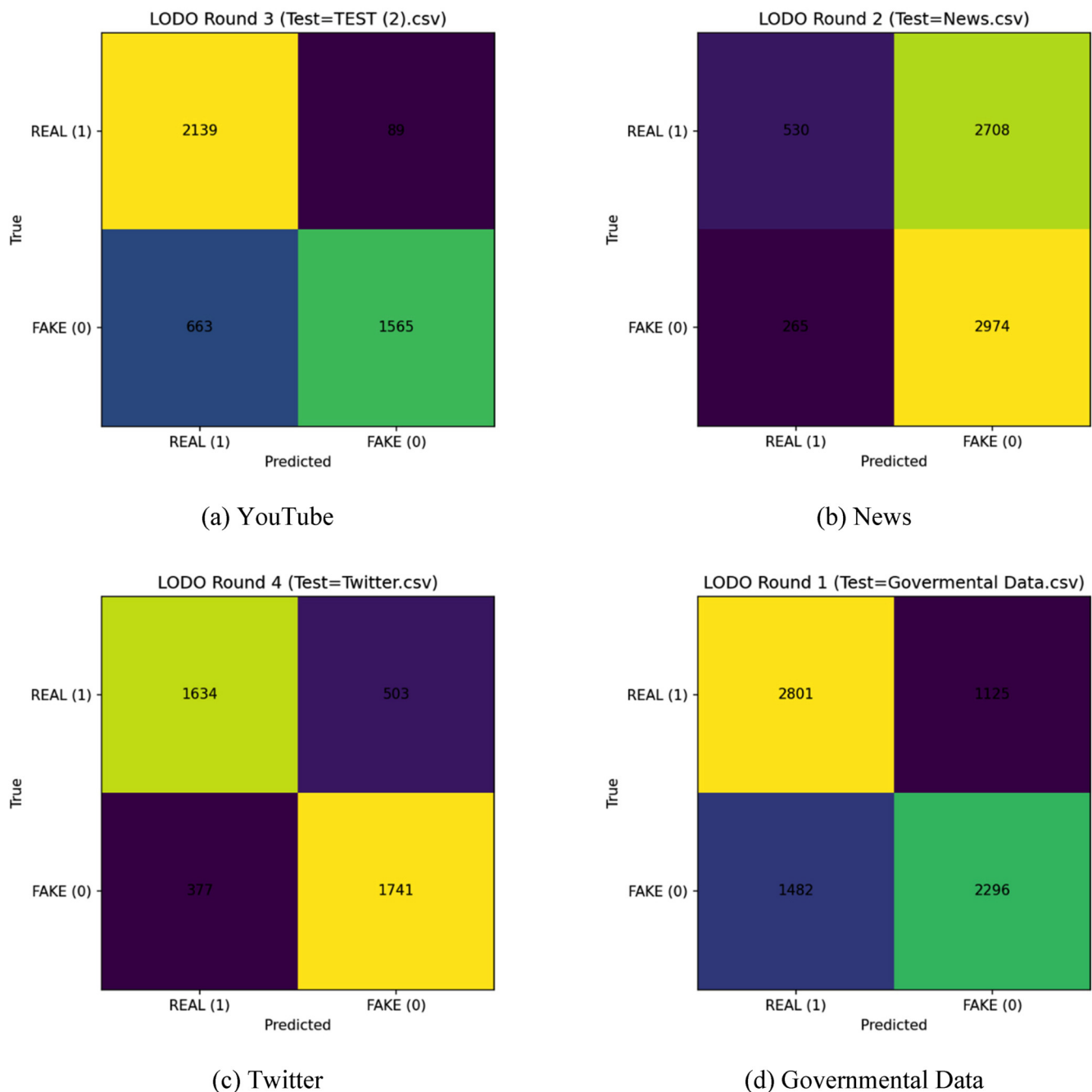


Figure 10. Cross-domain confusion matrices: (a) YouTube comments, (b) Twitter comments, (c) Governmental text, (d) News text

which may encourage reliance on surface cues such as “GB” or “5G.” Although this supports its performance within the domain, it reduces robustness for structurally different text types (e.g., news or formal statements). Future work may broaden coverage to include additional product categories, platforms, dialect variations, and temporal snapshots. Improvements may include stricter specification validation during generation, increased phrasing diversity, and realistic noise injection (e.g., typographical errors or spelling variants), as well as domain-adaptive training and threshold calibration strategies. Human evaluations of fluency and perceived authenticity, along with the public release of code and configuration details under responsible usage guidelines, would further enhance transparency and reproducibility.

5. CONCLUSIONS

This study investigated synthetic Arabic text generation and detection for e-commerce product titles, focusing on smartphone listings on Amazon.sa. A corpus of 4,606 real titles was collected and cleaned, and a structure-aware templating method was used to generate realistic synthetic titles. A BERT-based binary classifier was trained to distinguish between real and synthetic titles. The results indicate that structure-aware generation is effective for short, attribute-dense titles. By preserving the typical marketplace structure of product titles (brand, model, specifications, and variant) and systematically varying the slot values, the synthetic set approximated the real distribution in terms of length and specification cues, such as

5G/4G mentions. On the held-out test split of Amazon titles, the classifier achieved approximately 98.3% accuracy (training $\approx 99.1\%$), with low false positive and false negative rates, indicating strong in-domain separation between real and synthetic titles. Evaluation under distribution shift showed that performance decreases outside the e-commerce title domain, indicating domain-specific learning. This study addressed synthetic versus organically written title classification and did not evaluate factual correctness or deceptive intent. Moreover, the detection task focuses on template-generated synthetic titles and should not be interpreted as a comprehensive solution for detecting arbitrary AI-generated Arabic text produced by large-scale neural language models. Because the synthetic titles were generated using structured templates, some regularity patterns may have contributed to the strong in-domain performance. Furthermore, the dataset was limited to smartphone titles from a single platform and time snapshot, which may constrain cross-domain and temporal generalizability. Future work may expand data coverage to additional product categories and platforms, incorporate more diverse and specification-aware generation strategies with realistic noise patterns, and explore domain-adaptive training approaches to improve robustness and transferability. Human evaluation of fluency and perceived authenticity, as well as reproducibility initiatives, including code and template release under responsible usage guidelines, would further strengthen this line of research. Overall, this study demonstrates that structure-aware synthetic data supports the evaluation of Arabic title classification models in e-commerce contexts.

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Evaluation of Azure Pronunciation Assessment Tool for Arabic-Speaking Learners

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ABSTRACT

Accurate reading aloud is crucial for Arabic-speaking learners because minor errors can alter meaning or hinder understanding. This study evaluated the Microsoft Azure Pronunciation Assessment (PA) tool for modern standard Arabic using the KSU Arabic Speech Database. We focused on male speakers recorded in silent rooms. We used the KSU database's varied prompts words, phrases, and sentences to test Azure PA at the word, phoneme, and sentence levels. Because Azure PA is a closed source, we approximated its scoring by deriving equations for the Accuracy, Completeness, and Fluency metrics. We showed that a simple weighted combination closely matched the Pronunciation scores. We also applied a standard audio preprocessing pipeline (channel selection, denoising, pre-emphasis, silence trimming, and loudness normalization) to measure its impact. With preprocessing, for male speakers in the KSU database under the no-reference mode, Accuracy increased from 91.74% to 95.33%, Fluency from 60.84% to 97.84%, Completeness from 97.16% to 100.0%, and Pronunciation from 73.64% to 96.26%. The number of decoded word tokens increased fivefold. After preprocessing, all the consonant classes reached 90% accuracy, although the glottal segments remained weak. Sentence-level tests showed that Azure PA originally captured only brief fragments of long recordings. After preprocessing, it covered a greater portion of each sentence and recovered more of the target text. These results demonstrate both the strengths and limitations of Azure PA as a diagnostic tool for Arabic pronunciation based on KSU data.

Keywords: Arabic, audio preprocessing, automatic speech recognition (ASR), computer-assisted language learning (CALL), pronunciation assessment, speech scoring

1. INTRODUCTION

Advances in AI and technology have rendered traditional language schools less relevant. The focus has shifted to bridging language gaps, especially in speech, by using speech-to-text technology, an approach now adopted by companies such as Apple in their earphones. Automated speech and language technologies are being increasingly used to support language learning by providing fast and scalable feedback on spoken performance. A particularly important application is pronunciation assessment, in which learners need feedback not only on what they say (the transcript) but also on how accurately individual speech sounds are produced. Existing studies on Arabic speech recognition often report aggregate error metrics, such as word error rate (WER) and character error rate (CER); however, these measures are limited for diagnostic analysis because they treat recognition errors as equally important and do not reveal segment-level pronunciation behavior, such as performance on dentals, emphatics, and pharyngeals (see Table 1)¹. A previous study tested Microsoft Azure Pronunciation Assessment (PA) on three children's datasets in Arabic and found that when automatic speech recognition (ASR) was used for evaluation without supplying a reference word to the tool, most of the recognized

words were incorrect in the majority of datasets, and using audio preprocessing to fix some gaps led to higher and more accurate scores. This study used the Azure PA tool on the King Saud University (KSU) dataset to test the strengths and weaknesses of its ASR technology. The dataset features many young adult native Arabic speakers reading texts, answering questions, and pronouncing words with distinct phonemes. Identifying gaps will help improve Arabic speech-to-text technology.

2. RELATED WORK

Automatic pronunciation assessment (APA) systems, such as Krajka's English for Kids², exist for young English learners. However, computer-assisted language learning (CALL) tools for Arabic remain underdeveloped³. This section reviews Arabic speech datasets and summarizes their features and limitations. Reliable mispronunciation detection for Arabic learners requires high-quality speech datasets that include detailed demographics, varied recording conditions, and diverse pronunciations. Our previous study tested Azure PA, a cloud-based Microsoft service designed for CALL, teacher feedback, and automated oral-skill assessment. We evaluated its ability to recognize beginner-level

Table 1. Phoneme-level segment types and corresponding letters

Segment Type	Example Arabic Letters	Description
Emphatics	ص، ض، ط، ظ	“Heavy” consonants produced with pharyngealization
Pharyngeals	ع، ح	Produced deep in the throat
Uvulars	خ، غ	Produced near the uvula
Glottals	ه، ء	Produced in the glottis
Velars	ك، ق	Back of the tongue
Dentals/Alveolars	ش، ت، د، س، ز، ن، ل	Front of the tongue
Labials	ب، م، ف	Lips
Vowels	ا، و، ي	Basic vowels or glides

reading in children by comparing the ASR scores with and without a reference text. Azure PA scores the pronunciation accuracy (correctness of sounds), fluency (smoothness and rhythm), completeness (coverage of expected words), and overall pronunciation at the phoneme, word, and sentence levels. It can be integrated into educational platforms through its application programming interface (API).

2.1. Objectives. To characterize Azure PA for Arabic beyond aggregate WER/CER metrics and quantify how input conditioning affects reliability, this study aims to

- benchmark Azure PA on the KSU Arabic Speech Database using its built-in ASR-based scoring across multiple prompt types;
- quantify the effects of standardized audio preprocessing/conditioning on the PA metrics (Accuracy, Fluency, Completeness, Pronunciation) and score stability;
- measure the ASR coverage improvements after preprocessing (e.g., increased decoded tokens/words and more complete hypotheses for long prompts);
- analyze segment/phoneme-category performance (e.g., dentals, emphatics, pharyngeals, glottals) to identify systematic strengths and weaknesses; and
- identify consistent failure patterns and summarize practical guidance for reliably deploying Azure PA for Arabic assessment/CALL tools.

3. METHODOLOGY

3.1. Dataset Review. Potential datasets were reviewed to select the most suitable one for this study. Table 2 summarizes all the reviewed datasets.

(a) Arabic speech mispronunciation detection dataset (ASMDD) The ASMDD contains single-word recordings from 100 Egyptian children (aged 2–8 years), supporting word-level mispronunciation benchmarking⁴.

(b) QCRI aljazeera speech resource (QASR) QASR provides 2,041 h of multi-dialect Arabic broadcast speech with transcripts, mainly for transfer learning and dialect modeling⁵.

(c) KSU arabic speech database The KSU Arabic Speech Database includes sentences and words of more than 300 speakers and recorded in diverse environments, thereby capturing pronunciation variability⁶.

(d) Multi-Genre broadcast challenge 3 (MGB-3) MGB-3 covers 16 h of Egyptian Arabic from YouTube, spanning many genres⁷.

(e) Children arabic utterances for mispronunciation detection This dataset includes 16 Arabic words pronounced in quiet settings by 27 Egyptian children (aged 7–12 years). It supports error-pattern studies⁸.

(f) Dataset for speech recognition to support arabic phoneme pronunciation With 28 Arabic phonemes pronounced 10 times by 89 children, this dataset supports phoneme-level modeling⁹.

(g) Arabic voice recognition (down syndrome children) This dataset features speech from 37 children (27 with Down syndrome and 10 with speech disabilities) and is useful for testing articulation diversity¹⁰.

(h) Arabic pronunciation assessment for saudi arabian students (APASAS) This corpus for Saudi elementary children (ages 6–15) included 503 participants and 33 h of validated audio. It is the largest pronunciation assessment dataset for Saudi students^{11,12}.

(i) Common voice arabic dataset Common Voice Arabic contains volunteer speech, mostly from adults, but lacks mispronunciations and is less suitable for word-level benchmarking¹³.

3.2. KSU Arabic Speech Database. In this study, the KSU Rich Arabic Speech Database was used as the main evaluation corpus. The KSU database provides recordings from hundreds of modern standard Arabic speakers and diverse prompts, including digits, words, sentences, and Q&A. Its comprehensive phonetic coverage enabled us to analyze the performance of Azure PA across challenging segment classes. The database uses clean pronunciations of young adult speakers to minimize confounding factors. Other datasets focus on children’s speech, small vocabularies, or uncontrolled recordings, making them less suitable for precise analysis. By contrast, KSU database’s controlled Multi environment and multichannel recordings provide consistent, high-quality data, supporting a robust evaluation and establishing it as an ideal choice for our study. Therefore, the other datasets were used as supplementary references.

3.3. Mispronunciation Detection in Children with Azure Pronunciation Assessment. Our earlier study systematically evaluated Microsoft Azure’s pronunciation assessment system for Arabic-speaking children using three datasets:

Table 2. Comparison of databases

Database	Speakers	Dialect	Prompts	Sampling rate	Environment
ASMDD	100 children (2–8)	Egyptian	100 words	44.1 kHz	Quiet
QASR	– (2000 h)	Multi-dialect	Broadcast news	16 kHz	Studio / field
KSU Arabic Speech DB	>300	MSA, mixed accents	Digits, words, sentences	48 kHz	Quiet, office, cafeteria
MGB-3	– (16 h)	Egyptian	YouTube shows	16 kHz	Noisy, real-world
Children Arabic Utterances	27 children	Egyptian	16 words	–	Quiet
Phoneme Pronunciation DB	89 students	Arabic learners	28 phonemes × 10	16 kHz	Classroom
(Down-syndrome)	37 children	Mixed Arabic	Letters, words, numbers	–	Controlled
APASAS	503 students	Saudi MSA	Sentences, paragraphs	–	School
Common Voice Arabic	>1000 adults	Mixed Arabic	Read sentences	16 kHz	Home / mobile

Egyptian children’s word-level recordings, recordings from children with Down syndrome, and Arabic pronunciation assessments for Saudi students. We compared reference scoring (aligned to the prompt) with no-reference scoring (grading Azure’s own ASR output), and found that the reference text and phoneme-level scoring produced clearer and more accurate results, especially for early readers. By contrast, the no-reference mode often assigned high scores to incorrect or out-of-vocabulary words.

We also introduced standardized audio preprocessing, which improved the word-level scores and brought Azure’s proficiency ratings closer to teacher assessments, particularly for beginners. However, even after conditioning, Azure PA struggled with Arabic-specific contrasts, such as emphatics, pharyngeals, uvular /ق/, interdentals, and final clusters. Therefore, this study serves as a key reference for comparing Azure PA with other engines and highlights its capabilities and limitations in cloud-based Arabic reading support for pronunciation assessment. It can improve mispronunciation detection for diverse groups and guide interventions for difficult segment types.

3.4. Overview of the Evaluation Pipeline. This study evaluated Microsoft Azure PA, a tool that scores how spoken words match the expected pronunciation, for modern standard Arabic using recordings from the KSU Arabic Speech Database. The end-to-end workflow is shown in Fig. 1, where KSU database audio is selected and submitted to Azure PA, and the returned ASR (software converting speech to text) hypothesis and scoring outputs are aggregated for downstream analyses (examining how specific sound groups perform, how much of each prompt is recognized, and the types of errors made).

3.5. Dataset and Audio Selection (KSU Arabic Speech Database). We used the male subset of the KSU Arabic Speech Database (Sessions 2 and 3; LDC2014S02), which is organized as session → speaker → environment. Each speaker/environment includes multiple prompt categories (e.g.,

word lists, fixed sentences, paragraph reading, and responses), enabling evaluation across short and long utterances and diverse phonetic content.

To reduce confounding from channel quality and recording variability, we focused on high-quality Yamaha_Mixer recordings from controlled environments (e.g., Silent_Room). All selected .flac files were batch converted to mono WAV files while preserving the dataset folder structure for consistent automated processing.

3.6. Azure Pronunciation Assessment Scoring Model.

Azure PA is a closed-source cloud service built on Azure Speech-to-Text. It runs the ASR and then computes the Accuracy, Fluency, Completeness, and Pronunciation scores at the sentence, word, and phoneme levels. Because its implementation is not public, we treated the PA as a black box and approximated its behavior using Microsoft’s official metric descriptions.

(a) Accuracy: GOP-style scoring from phonemes upward Microsoft states that “Syllable, word, and full text accuracy scores are aggregated from phoneme-level accuracy scores.” Therefore, we modeled Accuracy as a goodness-of-pronunciation (GOP)-type score in Equation 1:

$$\text{GOP}(p) = \frac{1}{T_p} \sum_{t \in T_p} \log \left(\frac{P(q_t = p | O_t)}{\max_{p'} \cdot} \right). \quad (1)$$

The simplified equation is expressed in Equation 2:

$$\text{Accuracy} = \left(\frac{\text{Number of Correct Phonemes}}{\text{Total Expected Phonemes}} \right) \times 100. \quad (2)$$

(b) Completeness: coverage ratio over the reference text Completeness only measures how the reference script is pronounced, and not its clarity (Equation 3):

$$\text{Completeness} = \left(\frac{\text{Number of Matched Words}}{\text{Total Reference Words}} \right) \times 100. \quad (3)$$



Figure 1. Complete workflow of data ingestion, Azure PA inference, and analysis

(c) **Fluency: timing-based penalties** Fluency penalizes unnatural rhythms, pauses, hesitation, and irregular rates. We approximate this because Azure's penalty system is not public (Equation 4).

$$\text{Fluency} = 100 - (W_1 \times \# \text{Pauses} + W_2 \times \# \text{Hesitations} + W_3 \times \text{RateDeviation}) \quad (4)$$

(d) **Overall Pronunciation score: weighted combination of sub-scores** Pronunciation is a combined score, heavily weighted toward the lowest sub-metric, based on a weighting of 0.6, 0.2/0.2 weighting (equation 5):

$$\text{PronScore} = 0.60s_0 + 0.20s_1 + 0.20s_2. \quad (5)$$

3.7. Audio Preprocessing (Overview). To improve robustness and reduce variability owing to recording conditions and silent artifacts, we applied a standardized audio conditioning pipeline before submitting the recordings to Azure PA (see Fig. 2). Each file was processed using bandpass filtering and noise gating, pre-emphasis, voice activity detection (VAD) based trimming, loudness normalization, and resampling. This preprocessing was applied uniformly across the evaluated subset to increase the decoding stability and improve the reliability of phoneme-level scoring. Full parameter settings and an ablation-style comparison (before and after pre-processing) are reported in the Experiments section.

4. EXPERIMENTS

4.1. Test Setup. We used the male subset of the KSU Rich Arabic Speech Database (Sessions 2 and 3, LDC2014S02), totaling 29.5 GB of audio. The data were organized by session, speaker, and environment (Office or Silent_Room), each containing text-category folders. Each folder contained recordings from Mic_CreativeSB.flac (medium quality) and Yamaha_Mixer.flac (high quality). We analyzed only the high-quality YamahaMixer recordings from controlled environments.

For this study, we focused on the high-quality mixer channel under controlled conditions, and therefore, only used the Yamaha_Mixer track from the Silent_Room (or office) environment.

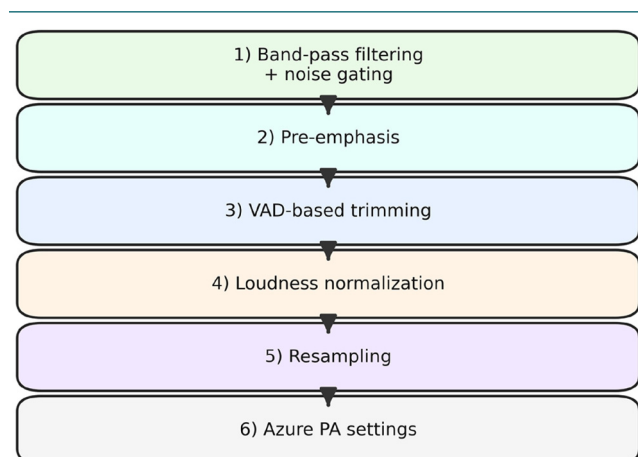


Figure 2. Preprocessing pipeline applied prior to Azure PA

Each environment included 10 text-category folders designed to ensure phonetic richness. Each speaker/session/environment had the following characteristics:

- SAAB_sentences_1 and 2: Continuous readings of sub-lists. SAAB_sentences_1 is common across speakers, and SAAB_sentences_2 is randomly assigned, enabling the assessment of long, phonetically dense material.
- Fixed_Sentences: Two short, accent-sensitive sentences for dialect discrimination.
- Numbers: Recordings of digits 0–9 were included because these numbers are common in real-life scenarios.
- Common_Words_1 & 2: Ten high-frequency familiar words per list covering most Arabic letters.
- Paragraphs_1 & 2: Two long paragraph readings—one prose and one Qur'anic—both letter-complete.
- Phonetic_Distinctive_Words_1 & 2: Lists of words emphasizing nasals, fricatives, and vowels to probe difficult contrasts.
- Common_List: Shared, phonetically balanced sentence prompts for most speakers.
- Random_List: Additional phonetically balanced sentences assigned to subsets of speakers.
- Questions_1 & 2: Recordings of volunteers answering simple spoken prompts and providing semi-spontaneous conversational speech.

For Azure integration, each Yamaha_Mixer.flac file was batch converted to a mono WAV format, preserving the folder structure. A Python script scanned these files, extracted metadata, and ran two Azure Speech passes: (1) ASR to obtain a hypothesis transcript, and (2) Pronunciation Assessment using the ASR result as a reference. All scores and breakdowns were aggregated for a systematic evaluation, thus eliminating the need for manual transcription. All experiments used Azure Speech locale Arabic-Saudi Arabia (ar-SA) with consistent PA settings:

- 100-point grading scale
- Phoneme-level granularity (to support segment-level diagnostics)
- Miscue detection enabled
- InitialSilenceTimeoutMs = 4000 ms to reduce early cutoff and improve decoding continuity on longer files

We evaluated Azure PA under two scoring modes:

- With-reference mode: Prompt/reference text was provided (for tasks with a target script), enabling alignment-based scoring and word/phoneme feedback.
- No-reference (ASR-driven) mode: Azure's ASR hypothesis was used as the reference, enabling transcript-free large-scale processing, but potentially inflating scores when ASR produced incorrect words.

4.2. Experimental Conditions. We ran two main conditions: (C1) Raw audio → Azure PA and (C2) Preprocessed audio → Azure PA, where preprocessing followed the steps in Fig. 2 (band-pass/noise gating, pre-emphasis, VAD trimming, loudness normalization, resampling). Azure was configured consistently across runs (local ar-SA, 100-point scale, phoneme granularity, miscue detection, and extended initial-silence timeout).

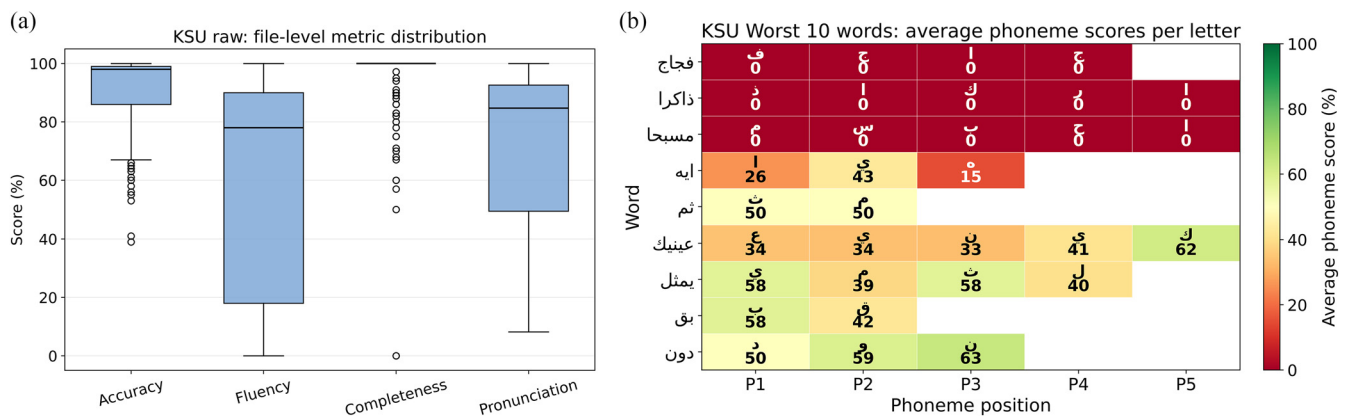


Figure 3. Azure Pronunciation Assessment results: (a) metric scores; (b) worst 10 words, average phoneme (per letter) scores

4.3. Procedure and Outputs. For each file, the pipeline (Fig. 1) submitted audio to Azure and logged (i) the ASR hypothesis and (ii) PA scores (Accuracy, Fluency, Completeness, Pronunciation) with word/phoneme-level details. We aggregated the results per condition and analyzed the performance according to prompt type and Arabic segment classes (Table 1).

5. RESULTS

5.1. Numerical & Graphical Results. As shown in Fig. 3 (a), without reference, the KSU database mean scores were 91.74% Accuracy, 60.84% Fluency, 97.16% Completeness, and 73.64% Pronunciation. Accuracy clustered above 90%, reflecting clean acoustics rather than perfect script adherence.

Fluency varied significantly (from 0 to 100), averaging 60.84%, likely because of Azure's sensitivity to pauses and hesitation, especially in long or conversational passages.

Completeness reached nearly 100% across most files, with the ASR hypothesis serving as the reference for evaluation.

Pronunciation averaged 73.64%, between the Accuracy/Completeness and Fluency scores, closely matching the predicted score distribution. This means that the distribution of

these three variables is similar to what is suggested, but not at the decimal point level.

In Fig. 3(b), words like "فجاج" always received 0 Accuracy and an Omission error, meaning Azure could not align any token to the reference. The same occurred for "ذاكرا" and "مسبحا".

For "ثم", the phoneme scores were low (15%–40%), which is usually labeled as Mispronunciation, as shown in Fig. 4 (a). This highlights the Azure PA's weakness in glottal-heavy interjection.

"ثم" scored near 100%, reflecting Azure's strength on dental, labial, and vowel segments, although performance can decline in fast speech due to merging with adjacent words.

"عينيك" contains pharyngeal, vowel, nasal, and velar sounds, revealing gaps in Azure's handling of pharyngeal–vowel–nasal patterns.

The word "بق" mostly came from a wrong ASR assumption in "أصابكم بق؟"; an example of ASR output is "أصابكم بق؟". The full audio text was "رأيت قذيفا، على واستعظم الإنسان، لماذا أخطأ"، "وآل يرث ملكنا، كن هنا فهل كانت حلب إمارة"، "أدم، سيشكروننا في ندوة، من غضب لعلمهم، قابلهم وأصبر، لا لم يبق زوجها"، but the ASR output cut it by a huge margin, reducing it to only "أصابكم بق؟". This behavior was observed in many, if not most, cases, suggesting that ASR struggles with long audio texts.

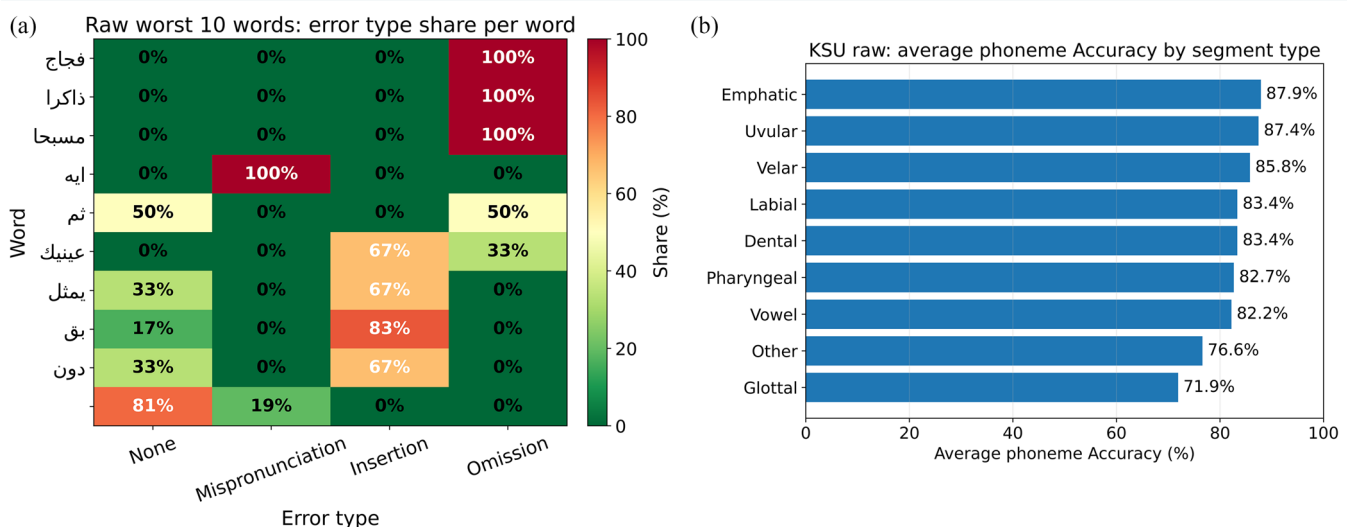


Figure 4. Azure Pronunciation Assessment results: (a) error type for the worst 10 words; (b) average pronunciation accuracy scores by phoneme segment type

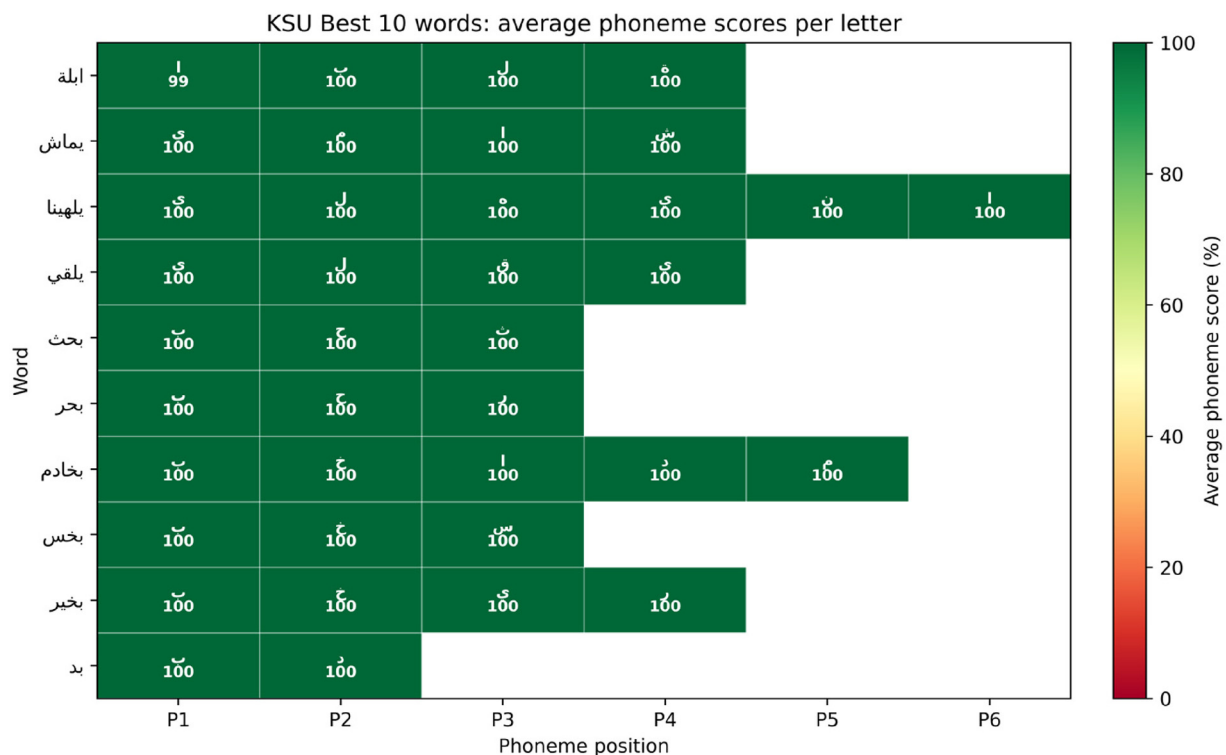


Figure 5. KSU database average phoneme scores (per letter) for the best 10 words

This example is unique because it consists of many unrelated sentences with short pauses. Consequently, ASR took the first sentence it recognized and stopped too early, after a small pause from the reader. Moreover, as it presented the output of the same text, it always left out the first sentence, "فهل كانت حلب إمارة"، and took the second one, "رأيت قذيفا".

Figure 5 shows the words with the highest phoneme scores, but most are false positives (e.g., "يماش ابله") that do not exist in the original sentences. This indicates that Azure PA is unreliable for long sentences without a reference text. Some correct words, such as "بحر" (/b/, vowel, /h/, /r/), received 100% scores, showing that Azure PA can reliably recognize all phonemes in simple words, even for difficult consonants such as /h/.

In summary, Azure PA performs best on lexically salient and stressed words, avoiding glottally heavy or very short structures, and achieves high phoneme scores even for difficult consonants. Many errors in the "worst words" are due to alignment and prosodic reduction rather than the inability of the model to recognize consonants.

5.2. Proposed Improvements. Five main acoustic/phonetic issues degrade Azure PA for children's speech. We addressed loudness variation, low signal-to-noise ratio (SNR), and clipping by applying loudness normalization (−23 LUFS/dBFS RMS) and peak clamping. The HVAC/handling

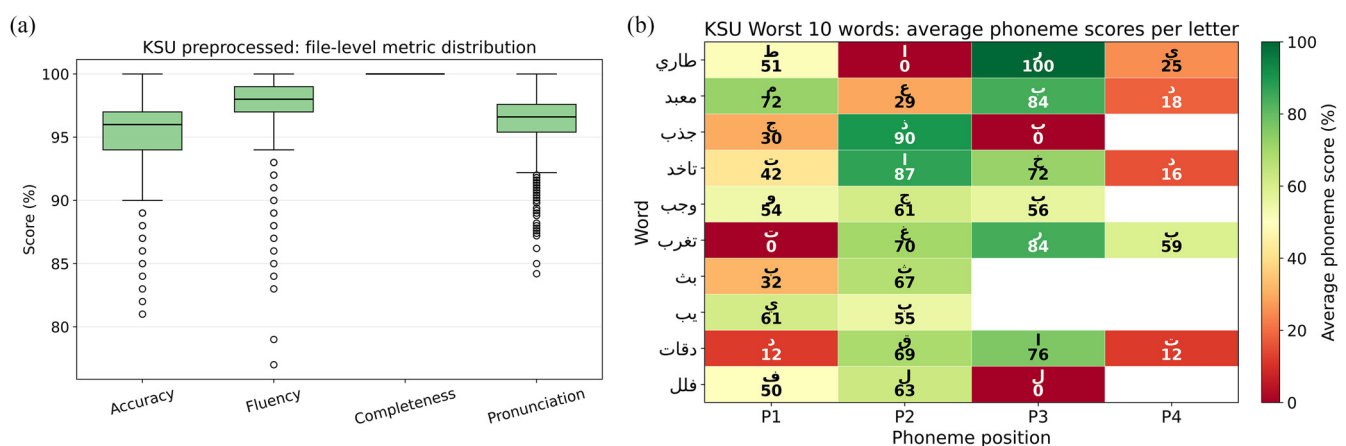


Figure 6. Azure Pronunciation Assessment results with preprocessing: (a) metric scores; (b) average phoneme (per letter) scores for the worst 10 words

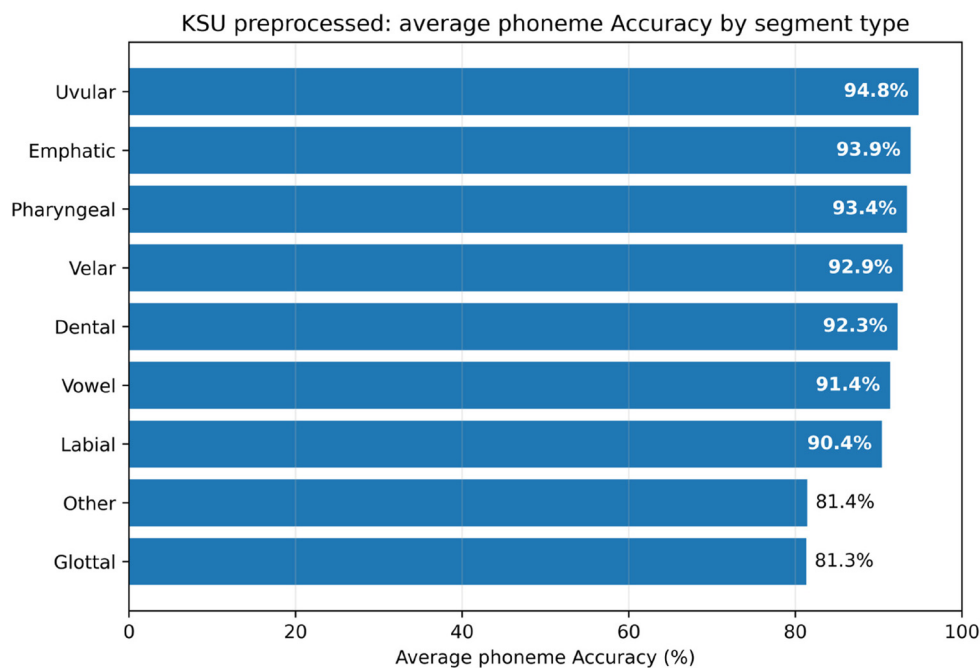


Figure 7. KSU database with preprocessed average pronunciation accuracy scores by phoneme segment type

noise was reduced using a Butterworth band-pass filter (80–7000 Hz) and spectral gating, thereby improving the SNR for low-energy consonants. To correct high-frequency fricative underestimation ($/s, \int, \theta, f/$), we applied pre-emphasis ($\alpha = 0.97$) and used a fricative-safe VAD to retain low-energy sounds (Equation 6).

$$y[n] = x[n] - \alpha x[n-1] \quad (6)$$

Audio preprocessing steps included pre-emphasis ($\alpha = 0.97$, 3–8 kHz), a 4th-order Butterworth band-pass filter (80–7000 Hz), spectral gating, loudness normalization (−23 LUFS/dBFS RMS, peak clamp), WebRTC-VAD (20 ms, aggressiveness = 2, +120 ms hangover, 200 ms min, <150 ms gap), 16 kHz resampling, and setting Azure PA InitialSilenceTimeoutMs to 4000 ms.

5.3. Validation. After preprocessing, the scores improved to 95.33% for Accuracy, 97.84% for Fluency, 100.00% for Completeness, and 96.26% for Pronunciation, with Fluency showing the greatest gain. This confirms that the earlier disfluency was mostly due to recording artifacts and silences rather than speaker issues. Fig. 6 (a) shows that Accuracy and Fluency clustered near the top. Completeness was always nearly 100%, and Pronunciation closely tracked the other metrics. These results validated the KSU database corpus and our preprocessing. Azure PA consistently achieved high scores with conditioned audio, confirming that the subsequent analyses reflected Azure PA's true performance.

The lowest-scoring words in Fig. 6 (b) highlight specific Azure PA challenges. For "طاري", consonants were recognized reasonably ط (51%), ر (100%), but the long vowel ا (0%) and final ي (25%) were under-scored, likely due to vowel reduction in natural speech. In the word "معبد", ر (72%) and ب (84%), but the pharyngeal ع (29%) and final د (18%) were problematic, showing Azure's general difficulty with pharyngeals and word-final stops,

which can be blurred or devoiced. For "تغرب", the initial ت was missed (0%), غ (70%), ر (84%) and ب (59%) were detected, pointing to challenges with word-initial stops, especially if spoken quickly or joined to a previous word.

Figure 7 shows that after preprocessing, the phoneme accuracy improved for all segment types. Most classes now exceeded 90% accuracy, with the uvular, emphatic, and pharyngeal segments showing substantial gains. Glottal remained the weakest but also improved. This suggests that the previous variability was mainly due to channel and silence artifacts, and not model limitations.

For the sentence-based KSU database material, Fig. 8 (a, b, c, d) demonstrates that after preprocessing, Azure PA processed many more audio files than with the raw recordings. The total decoded word count increased from approximately 14,000 to over 74,000 after preprocessing because Azure analyzed each file more deeply and produced more complete transcripts. The ASR coverage charts confirmed that more files yielded more usable hypotheses. For the "target sentence" figures, the improvement was clear in both key scripts. For Text 1 (the long chain "... كن هنا فهل", "كانت حلب إمارة", "رأيت قنيفة", "على واستعظم الإنسان", "لماذا أخطأ آدم", "أصابكم يق؟", "أصابعكم يق؟", "فهل كانت حلب إمارة", "رأيت قنيفة", "قابلهم وأصبر", "كن هنا", etc.), the raw ASR often collapsed the entire waveform into a brief fragment like "أصابعكم يق؟". After preprocessing, a dramatic jump in detections occurred, and nearly every clause in Text 1 ("كن هنا", "فهل كانت حلب إمارة", "رأيت قنيفة", "قابلهم وأصبر", etc.) was now recovered in many more files. Azure followed the reader through pauses and extracted most of the scripted material. For Text 2 ("الحظة من فضلك السلام عليكم", "لا", "نعم", "لا أدري", "شكرا", "الله أعلم", "قريباً"), the improvement was even more pronounced. Detection counts increased from a few hundred to over 3,000, with big gains for nearly every prompt, especially "الحظة من فضلك", "نعم", "لا", and "السلام عليكم". The previously missed or partially decoded tokens now appeared reliably and repeatedly.

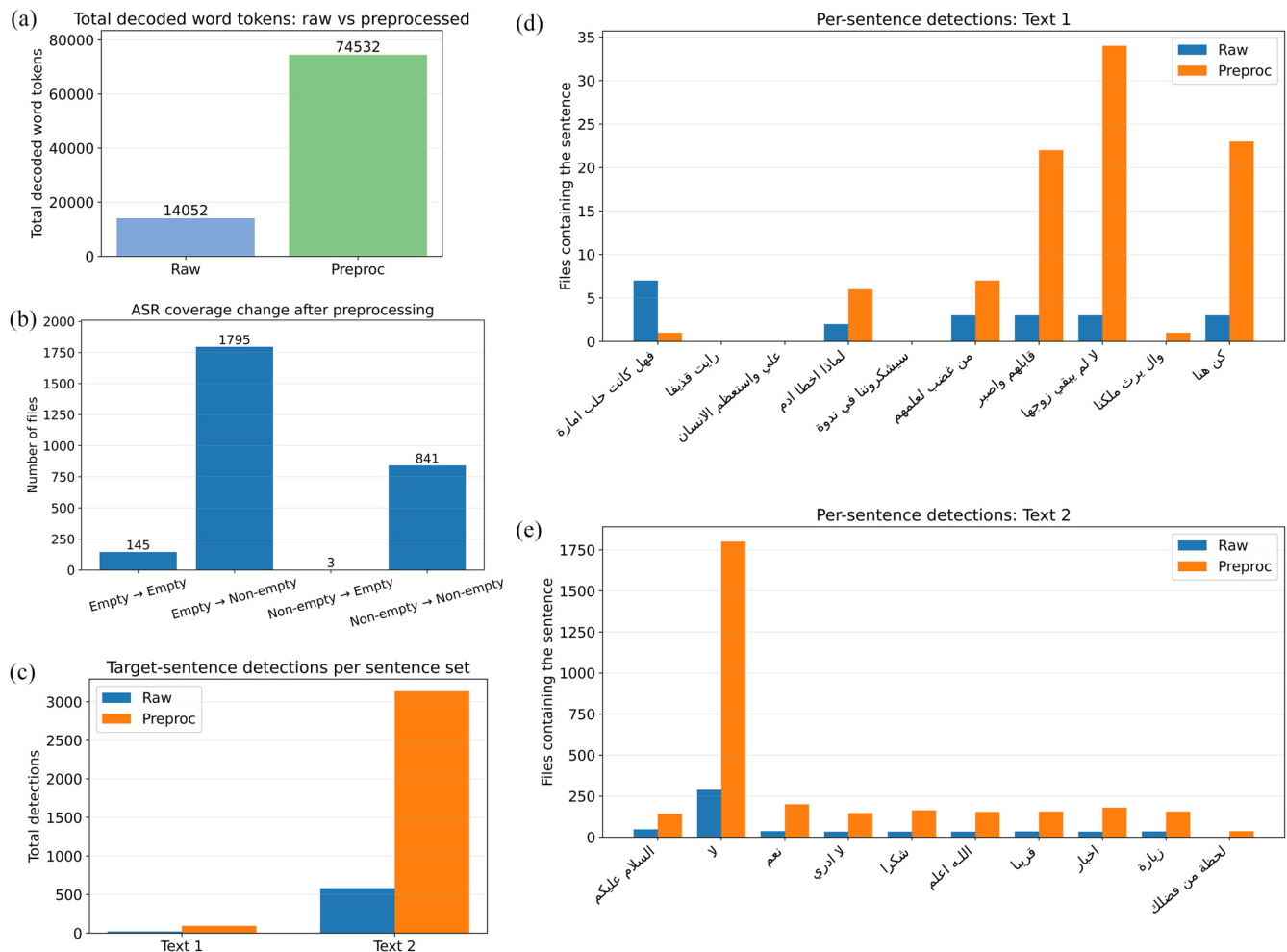


Figure 8. Azure Pronunciation Assessment results on APASAS dataset with and without preprocessing: (a) with reference; (b) without reference

Overall, these results show that preprocessing transforms Azure PA performance, from capturing only short fragments to analyzing and transcribing a much larger portion of each recording, resulting in outputs that more closely match the full KSU database sentence prompts.

6. DISCUSSION

Interpretation of preprocessing gains. The consistent improvement after preprocessing suggests that Azure PA reliability depends strongly on input conditioning. Because Azure is trained primarily on fluent adult speech, normalizing the bandwidth, silence, and loudness reduces mismatches and improves decoding continuity, particularly for longer utterances.

No-reference (ASR-driven) scoring limitation. In the no-reference mode, Azure PA scores can be inflated when the ASR hypothesis is incorrect because the assessment is partially aligned to the system's own transcript. Therefore, high Completeness/Pronunciation values should be interpreted alongside coverage and error-type indicators rather than as direct evidence of correct lexical recognition.

Segment-class implications. The segment-class analysis (Table 1) provides diagnostic insight beyond WER/CER-style reporting

by highlighting which Arabic sound groups remain challenging (e.g., emphatics/pharyngeals/glottals), supporting targeted improvements in Arabic pronunciation feedback and CALL settings.

Generalizability. These findings are limited to a controlled subset (KSU database, adult male speakers, selected channels/environments, and ar-SA locale) and may not be generalizable to children, disordered speech, noisy mobile recordings, or other dialect locales/engines.

7. CONCLUSION

This study evaluated Microsoft Azure PA using the KSU Arabic Speech Database, focusing on high-quality male recordings to isolate the system behavior. We reverse-engineered Azure PA's scoring, modeling Accuracy, Completeness, and Fluency, and found a simple weighted combination that closely matched the reported Pronunciation scores. Audio preprocessing was essential; on raw audio, Azure PA often decoded only short fragments, resulting in low Fluency and Pronunciation scores. With preprocessing, the decoded words increased fivefold, scores stabilized in the high-90% range, and the system captured more target sentences. Segment-level analysis showed strong performance for uvular, emphatic, and pharyngeal consonants, but persistent

weaknesses for glottal consonants and certain word types. Overall, Azure PA with preprocessing is a valuable tool for segment-level diagnostics in Arabic pronunciation, although users must be aware of its limitations in certain phoneme segments, reduced words, and long passages. Future work should extend this analysis to other speaker groups and explore hybrid systems that combine Azure PA with custom Arabic phoneme models to obtain more robust feedback.

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Simulation-Based Modeling and PID control optimization for quadcopter UAV using genetic algorithm

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ABSTRACT

Quadcopters are widely used in modern applications; however, maintaining a stable hover and accurate path following remains challenging owing to their nonlinear dynamics. In this study, an efficient simulation-based control framework was developed, in which a nonlinear model was derived using the Newton–Euler method and subsequently linearized via feedback linearization. In MATLAB/Simulink, two proportional–integral–derivative tuning methods—manual tuning and a genetic algorithm (GA) with a population size of 30 and up to 30 generations—were employed to design the controller. Manual tuning achieved an integral square error (ISE) value of 0.03316, whereas the GA-based approach generated an ISE of 0.030056, corresponding to an average improvement of 13.9%. Furthermore, the GA-based tuning produced a smoother system response with reduced overshoot, thereby enhancing the quadcopter stability and trajectory tracking, and contributing to more reliable real-world flight performance.

Keywords: quadcopter UAV, PID controller, genetic algorithm (GA), feedback Linearization, trajectory tracking

1. INTRODUCTION

A quadcopter is an unmanned aerial vehicle (UAV) equipped with four rotors and is widely used in both military and civilian applications. Several methods have been employed to model quadcopters, including the Newton–Euler method, the Euler–Lagrange formulation, and aerodynamic modeling^{1,2}. As a quadcopter operates with six degrees of freedom (6-DoF), stabilizing the system remains a challenging task. Its motion can be categorized into translational movement along the x , y , and z axes, and rotational movement about roll (ϕ), pitch (θ), and yaw (ψ) axes. The aerodynamic forces acting on a quadcopter during forward flight significantly influence its stability, as reported in³. A proportional-derivative (PD) controller combined with a feedback linearization strategy (FBL) has been used to control and stabilize quadcopter systems while achieving trajectory tracking⁴. A comprehensive analysis of quadcopter mathematical models, including both nonlinear and linear representations, forms the foundation for developing and implementing effective control strategies. Among various control techniques, the proportional–integral–derivative (PID) controller is most widely used for quadcopter systems^{5,6}. The FBL technique transforms a nonlinear quadcopter system into an equivalent linear system, thereby simplifying controller design. Furthermore, FBL has been integrated with linear quadratic regulator (LQR) control to achieve optimal stabilization of the Euler angles and to minimize trajectory tracking⁷.

A comparison of LQR, PID, and LQR-PID controllers in terms of vertical position and vertical speed, based on system

performance characteristics such as overshoot, settling time, and rise time, indicates that the PID controller provides superior performance in achieving the optimal vertical speed. However, the LQR controller demonstrates the best capability for achieving optimal stability⁸. Most existing studies treat nonlinear compensation and PID tuning as separate problems. In this study, feedback linearization and genetic algorithm (GA)-based PID tuning were combined and evaluated within a unified framework, with a direct comparison to manual tuning.

To enhance trajectory tracking and address hover instability, an LQR controller combined with Lyapunov theory was applied to achieve optimal longitudinal stability of the quadcopter, while minimizing a cost function associated with controller energy consumption⁹. The results reported in⁹ demonstrate that the LQR controller effectively stabilizes the system and reduces energy consumption, even in the presence of disturbances.

Manual tuning of the PID parameters has been applied based on simulation results to improve system speed and accuracy¹⁰. The H-shaped quadcopter is modeled using the Newton–Euler method, as described below:

An additional strategy for optimizing PID parameters in H-shaped quadcopters is the use of a GA, which also aims to minimize the cost function¹¹. In¹², PID parameters were optimized using two approaches: GA and ant colony (ACO) method. The study demonstrates the capability of GA to effectively select optimal parameters, resulting in improved settling time for Euler angles when using 60 generations and a population size of 50. However, the results in¹² indicate that ACO achieves a shorter settling time compared to GA. This comparison suggests that,

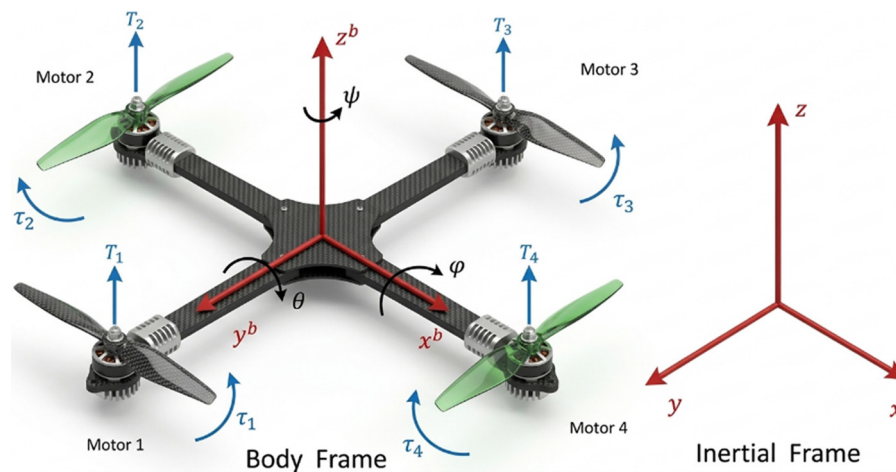


Figure 1. Quadcopter freebody diagram¹³

while GA is effective due to its global search capability, ACO may provide better performance in certain scenarios owing to its local search efficiency. In this context, the PID controller is commonly selected due to its simplicity and ease of implementation. By contrast, the LQR controller requires full-state measurements.

Many control techniques have been proposed for quadcopter systems. However, most existing studies either focus only on complex controller designs or do not provide a unified comparison between manual tuning and intelligent optimization methods. Therefore, developing a practical and efficient approach to improve stability and trajectory tracking remains a challenge. In this study, a GA is employed for PID tuning due to its capability for global search and its effectiveness in handling nonlinear optimization problems. The novelty of this study lies in the integration of feedback linearization with GA-optimized PID control, along with a direct comparison to manual tuning. The main objective is to enhance quadcopter stability and tracking performance through an efficient simulation-based control strategy.

This study contributed to the field of UAV control. This represents an improvement in the stability of the quadcopter by

implementing a control strategy. Newton–Euler equations were applied to model the nonlinear dynamics of the system, as shown in Section 2, and linearized by FBL to enable a state-space representation suitable for controller synthesis.

This study focused on validating a UAV system by applying simulation methods to ensure the validity of the derived mathematical models and control strategies. The primary goal is to design a UAV system that performs perfectly in real life. A PID controller was designed and tested under different conditions to optimize the trajectory tracking and system robustness.

This study evaluated two tuning methods: manual tuning and GA tuning. The simulation results obtained under different situations show a smoother transient response of the GA and an enhancement of the hover stability and trajectory tracking precision.

This study seeks to provide an understanding of mathematical modeling, control design, and optimization methodologies to optimize quadcopter flying performance. Using traditional control methods with optimization methodologies, the proposed system aims to achieve precise control and maximum responsiveness to changing conditions.

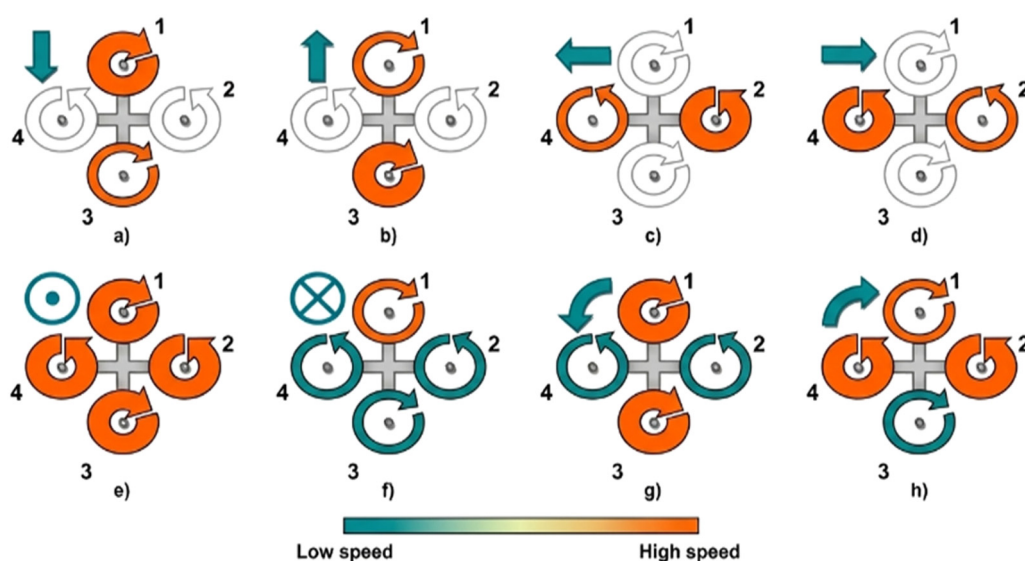


Figure 2. Quadcopter movements¹⁵

Table 1. Physical parameters of the quadcopter¹⁴⁻¹⁷

Parameter	Symbol	Value	Unit
Total mass	m	1.2	kg
Arm length (center to motor)	L	0.23	m
Moment of inertia (x-axis)	I_x	0.021	$\text{kg} \cdot \text{m}^2$
Moment of inertia (y-axis)	I_y	0.021	$\text{kg} \cdot \text{m}^2$
Moment of inertia (z-axis)	I_z	0.037	$\text{kg} \cdot \text{m}^2$
Thrust coefficient	b	2.98×10^{-6}	$\text{N} \cdot \text{s}^2$
Drag coefficient	d	1.14×10^{-7}	$\text{N} \cdot \text{m} \cdot \text{s}^2$
Gravitational acceleration	g	9.81	m/s^2

The main contributions of this study are the development of a quadcopter model by applying Newton–Euler and linearizing it using FBL, tuning PID gains using GA and manual tuning using the same Simulink block diagram, and comparing them based on integral square error (ISE) values. The remainder of this paper is organized into five sections. Section 2 describes the physical structure of a quadcopter. Section 3 begins by presenting nonlinear modeling and then linear modeling. The optimization of the best PID controller to improve the performance of the system is discussed in Section 4. The results are presented and discussed in Section 5 after a simulation using MATLAB and Simulink. Finally, a summary is presented in Section 6.

2. QUADCOPTER MODELING

The modeling of a quadcopter requires an analysis of the dynamic torques and forces of vehicle flight. The quadcopter moves freely in 6-DoF space and its motion can be characterized by 6-DoF: (x, y, z) are translations and (ϕ, θ, ψ) are rotations. These phenomena must be incorporated into modeling based on the correct physical principles for proper design and analysis of the control law.

To model the system, the Newton–Euler method, which works according to Newton’s second law, must be applied¹³.

As with any system modeling, some assumptions must be made for the quadcopter to simplify the model¹³.

1. The quadcopter holds a symmetrical structure.
2. A proportional relationship exists between the squared value of the rotor speed and the thrust.
3. The analysis of one rotor is enough because all rotors are coinciding.

Additionally, small-angle assumption facilitated the linearization of the quadcopter model under hovering conditions, thereby reducing the multiple-input multiple-output (MIMO) nonlinear system to four independent single-input single-output (SISO) systems¹⁴.

These assumptions simplify the modeling process while preserving the essential dynamics of the quadcopter. A symmetrical structure is assumed because most small UAV quadcopter frames are designed and built with equal arms and balanced layouts. The thrust produced by each rotor was assumed to increase with the square of its speed. This follows how real propellers work because spinning faster pushes much more air and creates much more lift. Because the quadcopter is built with a symmetric shape, all four rotors are identical. Therefore, analyzing a single rotor is sufficient.

The next step was to specify the physical parameters of the quadcopter and develop a mathematical model for the system based on its nonlinear and linear characteristics. Nonlinear systems exhibit a non-proportional response to applied inputs, making their behavior difficult to predict. However, a nonlinear system can be simplified using FBL to develop a practical controller. The following two sections describe the nonlinear model of the quadcopter UAV, followed by the linear model applied to develop the controller.

2.1. Physical Structure and Parameters. The most important step in understanding quadcopters is understanding their physical structures. It plays a crucial role in maintaining stability and overall performance. The quadcopter contained four rotors designed to be positioned at equal distances from the center of the mass of the UAV body. The rotors were divided into groups of two, with one group rotating counterclockwise and the other clockwise, driven by four motors, as shown in Figure

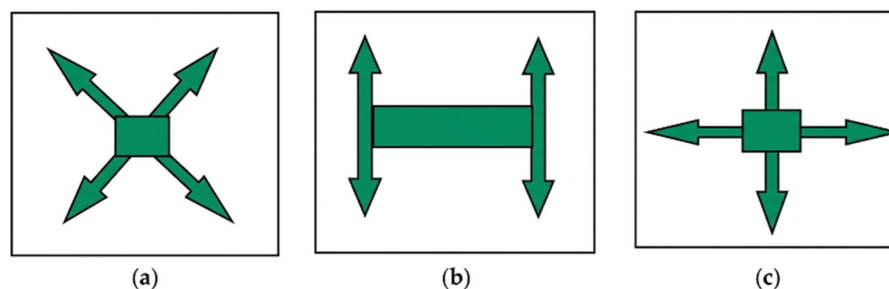
**Figure 3.** Different physical structures of quadcopter¹⁶

Table 2. Variables applied in the nonlinear model and input mapping

Variable	Definition	Units
$y, z; \dot{x}, \dot{y}, \dot{z}; \ddot{x}, \ddot{y}, \ddot{z}$	Quadcopter UAV position, velocity, and acceleration in inertial frame	m, m/s, m/s ²
$\varphi, \theta, \psi; \dot{\varphi}, \dot{\theta}, \dot{\psi}; \ddot{\varphi}, \ddot{\theta}, \ddot{\psi}$	Roll, pitch, and yaw angles, angular rates, and angular accelerations	rad, rad/s, rad/s ²
m, g	Vehicle mass and gravitational acceleration	kg, m/s ²
I_x, I_y, I_z, I_R	Moments of inertia about body axes and rotor inertia	kg·m ²
L	Half motor-to-motor distance (arm length)	m
u_1-u_4	Control inputs: thrust (u_1), roll (u_2), pitch (u_3), yaw (u_4)	N, N·m
b, d	Thrust and drag (moment) coefficients	N·s ² , N·m·s ²
$\Omega_1 - \Omega_4, \Omega_r$	Rotor angular speeds and net reaction term	rad/s
$\mathbf{U} = [U_1 U_2 U_3 U_4]^T$	Input vector (equivalent to $[u_1, u_2, u_3, u_4]^T$)	–

1. Studying the mechanical design of a quadcopter is important before deriving a mathematical model or applying a controller to a UAV system.

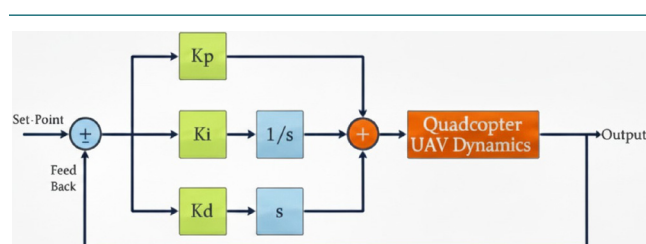
Figure 1 illustrates the physical structure of a quadcopter consisting of four rotors. To balance the quadcopter UAV flight, the two rotors rotate in opposite directions. As shown in Figure 1, rotors 2 and 4 rotate counterclockwise, whereas rotors 1 and 3 rotate clockwise. When the rotors rotate, aerodynamic reaction forces generate torque on the quadcopter body.

As Figure 2 illustrates, there are eight possible cases for the quadcopter to move, resulting from differential rotor speeds. Differences in the rotor thrust lead to vertical motion and rotation around the roll, pitch, and yaw axes.

Figure 3 illustrates the three physical structures of the quadcopter: X, H, and +. Although these configurations differ in shape, they share the same basic symmetry used in the modeling assumptions of this study. Because the focus here is on control rather than mechanical design, the same control approach is applied to all configurations.

As this study was based purely on simulations, the physical parameters of the quadcopter were assumed using typical values commonly reported for small quadcopter UAVs in the literature, to ensure that the model represented a realistic quadcopter configuration and that the simulation results were meaningful and reproducible. The primary physical parameters used in this study are listed in Table 1. Furthermore, only physical parameters that directly influence the system dynamics and controller design were considered in this study.

2.2. Nonlinear Dynamic Model. The relationship between the forces and torque generated by the rotors and the motion of the quadcopter are presented using a nonlinear model of the quadcopter UAV.

**Figure 4.** PID controller block diagram of quadcopter¹⁴

Abbasi & Mahjoob¹⁷ started by focusing on the three Euler angles, which are the roll angle (ϕ), the pitch angle (θ), and the yaw angle (ψ). The final nonlinear equations of the quadrotor positions with Euler angles are written as follows:

$$\ddot{x} = -(\cos \phi \sin \theta \cos \psi + \sin \phi \sin \psi) \cdot \frac{u_1}{m} \quad (1)$$

$$\ddot{y} = -(\cos \phi \sin \theta \sin \psi + \sin \phi \cos \psi) \cdot \frac{u_1}{m} \quad (2)$$

$$\ddot{z} = g - (\cos \phi \cos \theta) \cdot \frac{u_1}{m} \quad (3)$$

$$\dot{\phi} = \theta \dot{\psi} \left(\frac{I_y - I_z}{I_x} \right) - \frac{I_R}{I_x} \dot{\theta} g(u) + \frac{L}{I_x} u_2 \quad (4)$$

$$\dot{\theta} = \dot{\phi} \dot{\psi} \left(\frac{I_z - I_x}{I_y} \right) - \frac{I_R}{I_x} \dot{\phi} g(u) + \frac{L}{I_y} u_3 \quad (5)$$

$$\dot{\psi} = \dot{\theta} \dot{\phi} \left(\frac{I_x - I_y}{I_z} \right) + \frac{1}{I_z} u_4 \quad (6)$$

These equations describe the motion of the quadcopter in space. When the quadcopter tilts, a component of the thrust is redirected laterally, resulting in motion along x and y axes. The equation shows that the drone moves up or down depending on the balance between the total thrust and gravity. The Euler angle equations describe the rotational dynamics of the quadcopter. When an imbalance in thrust occurs between opposing rotors, the quadcopter undergoes rolling or pitching motion. The yaw motion originates from the twisting effect created by the spinning rotors. The inertia terms indicate how difficult it is for a drone to change its rotation.

This approach has been applied to model a quadcopter¹⁷. The following equations show the input of a quadcopter UAV²:

$$\begin{aligned} u_1 &= b (\Omega_4^2 - \Omega_2^2) \\ u_2 &= b (\Omega_3^2 - \Omega_1^2) \\ u_3 &= d (\Omega_4^2 - \Omega_2^2 - \Omega_3^2 - \Omega_1^2) \\ u_4 &= b (\Omega_1^2 + \Omega_2^2 + \Omega_3^2 + \Omega_4^2) \end{aligned} \quad (7)$$

These inputs are derived from the rotor speed. Changing the motor speed changes the lift and creates a turning force. We used the square of the rotor speed because spinning faster pushes more air and produces greater thrust.

A quantitative link between the input ($\mathbf{U}$) and the speed of the rotor (Ω) as well as the disturbance equation can be shown by the

following as¹⁸:

$$\begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{bmatrix} = \begin{bmatrix} b & b & b & b \\ -b & -b & b & b \\ -b & b & b & -b \\ -d & d & -d & d \end{bmatrix} \begin{bmatrix} \Omega_1^2 \\ \Omega_2^2 \\ \Omega_3^2 \\ \Omega_4^2 \end{bmatrix} \quad (8)$$

$$\Omega_r = \Omega_4 + \Omega_2 - \Omega_1 - \Omega_3 \quad (9)$$

This matrix shows how each rotor contributes to the quadcopter's movement. The opposite rotors work in pairs, and the signs indicate whether they help or oppose each other. The last row uses the drag coefficient because the yaw motion originates from the twisting effect of the propellers.

Table 2 defines each variable derived in the mathematical nonlinear model.

2.3. Linearization via Feedback Linearization. To facilitate the controller design, the nonlinear quadcopter model was transformed into an equivalent linear form using feedback linearization. To obtain identical results for the converted input and output, input-output linearization was used. It involves multiple differentiations of the output before the point where the input is found¹⁹. Other linearization methods exist, such as small-angle approximations or Jacobian-based linearization around the hover point; however, these methods only work in a very limited area and neglect several nonlinear effects. FBL was preferred because it avoids these limitations and offers a clearer input-output structure for later PID designs.

$$\dot{x} = f(x) + g(x)u \quad (10)$$

$$y = h(x) \quad (11)$$

$f(x)$ is a nonlinear system, $g(x)$ is the input dynamics, and the control input (u) is assigned to a state vector (x''). y represents the controlled variable (CV) with a nonlinear function $h(x)$. Eqs. 10–14 are applied to linearize the system, as presented in¹⁷ and¹⁹.

The following formula shows the frequent differentiation of the output variable, where y'' is defined in Table 2, and $L_f h(x)$ and $L_g h(x)$ represent the Lie derivatives of the output function $h(x)$ along the system dynamics $f(x)$ and the control input vector $g(x)$, respectively.

$$\dot{y} = L_f h(x) + L_g h(x)u \quad (12)$$

The formula of higher-order systems can be represented as follows:

$$y^{(r)} = L_f^r h(x) + L_g L_f^{r-1} h(x)u \quad (13)$$

Here, $y^{(r)}$ represents the required order of differentiation of the output for feedback linearization. The expression $L^r h(x)$ the repeated Lie derivative of $h(x)$ along $f(x)$ applied r times, while $L_g L^{r-1} h(x)$ denotes the Lie derivative of $h(x)$ along $g(x)$ after being differentiated $r-1$ times along $f(x)$, which forms part of the feedback linearization process.

To convert the system into a linear form, (14), which is presented as the input, must be substituted into (10) to eliminate

nonlinearity.

$$u = \frac{1}{L_g L_f^{r-1} h(x)} \left(-L_f^r h(x) + v \right) \quad (14)$$

In the linearized model, v denotes the transformed linear control input introduced through the FBL process.

The controlled variable can then be expressed as follows, where v is the new linear control input:

$$y^{(r)} = v \quad (15)$$

$$y = \begin{bmatrix} Z \\ \phi \\ \theta \\ \psi \end{bmatrix} \quad (16)$$

Linearized vertical dynamics:

$$\ddot{z} = v_z \quad (17)$$

v_z corresponds to the new control input associated with the vertical motion along the z -axis. Linearized rotational dynamics as v_ϕ , v_θ , and v_ψ represent their corresponding linear control inputs:

$$\ddot{\phi} = v_\phi, \quad \ddot{\theta} = v_\theta, \quad \ddot{\psi} = v_\psi \quad (18)$$

The previous approaches in Eqs. 15–18 were used in¹⁹. After linearizing the system, the state-space representation of the input can be expressed as follows²:

$$\dot{x} = Ax + Bu \quad (19)$$

A and B represent the state and input matrices, respectively.

The state space representation of the output as C is the output matrix:

$$y = Cx \quad (20)$$

The state variables are the following:

$$x = [\phi \ \dot{\phi} \ \theta \ \dot{\theta} \ \psi \ \dot{\psi} \ z \ \dot{z}]$$

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad B = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

3. CONTROL SYSTEM DESIGN (PID)

After obtaining the mathematical model, the next step is to develop control strategies for the nonlinear dynamics of the

Table 3. Variables applied in the PID controller design and Euler angle dynamics

Variable	Definition	Units
$u(t)$	Control signal (PID controller output)	N·m
K_p K_i	Proportional gain constant Integral gain constant	– s – 1
K_d	Derivative gain constant	s
$e(t)$	Tracking error between desired and actual angle	rad
$desired(t)$	Desired Euler angle input	rad
$actual(t)$	Measured or actual Euler angle	rad
U_ϕ, U_θ, U_ψ	Control torques for roll, pitch, and yaw axes	N·m
$\Phi(s), \Theta(s), \Psi(s)$	Laplace-transformed roll, pitch, and yaw angles	rad
s	Complex frequency variable in Laplace domain	rad s – 1
b	Thrust coefficient (from rotor model)	N·s ²
T_x, T_y, T_z	Torque produced about each rotational axis	N·m
I_x, I_y, I_z	Moments of inertia about body axes (repeated here for clarity)	kg·m ²

Table 4. Comparison between GA and DE²⁴

Feature	GA	DE	UAV Relevance
Optimization type	Population-based	Differential updates	Global search for nonlinear system
Convergence rate	Moderate, stable	Faster, consistent	GA avoids premature convergence
Reliability	High	Very high	GA reliable for dynamic models
Performance (MSE, IAE)	Nearly equal to DE	Slightly better in some cases	Both ensure low error
Parameter sensitivity	Low	High	GA easier to tune
Implementation	Simple	Parameter dependent	GA easier in Simulink
Overall suitability	Robust, flexible	Efficient, sensitive	GA best balance for quadcopter UAV PID

quadcopter UAV. Control methods such as PID control, and feedback linearization are widely used due to their effectiveness in handling system complexity and achieving high performance. These controllers stabilized the quadcopter under various flight conditions.

The PID controller is the most common controller used for a quadcopter owing to its effectiveness in controlling the roll, pitch, and yaw Euler angles.

Figure 4 illustrates the process of combining each part of the PID controller with the quadcopter in a feedback loop. The PID controller was utilized, as shown in the following equations²⁰:

$$u(t) = K_p e(t) + K_i \int_0^t e(t) dt + K_d \frac{de(t)}{dt} \quad (21)$$

In this study, the same PID gains were used for the roll, pitch, and yaw axes to maintain a clear and consistent comparison between the tuning methods. The use of identical gains enables the effect of the tuning approach to be observed without being affected by axis-specific adjustments. Although the axes have different inertial properties, this assumption is reasonable for a comparative analysis and makes the methodology straightforward.

where the error is represented as²⁰:

$$e(t) = desired(t) - actual(t) \quad (22)$$

By controlling only the Euler angles, some terms in their equations were eliminated as follows:

$$\ddot{\phi} = \frac{U_2}{I_{xx}} \quad (23)$$

$$\ddot{\theta} = \frac{U_3}{I_{yy}} \quad (24)$$

$$\ddot{\psi} = \frac{U_4}{I_{zz}} \quad (25)$$

Applying the Laplace transform to the Euler angles helps extract the characteristics of the system more easily using MATLAB.

$$\frac{\Phi(s)}{U_2(s)} = \frac{lb}{I_{xx}s^2} \quad (26)$$

$$\frac{\Theta(s)}{U_3(s)} = \frac{lb}{I_{yy}s^2} \quad (27)$$

$$\frac{\Psi(s)}{U_4(s)} = \frac{ld}{I_{zz}s^2} \quad (28)$$

To reduce the time required to tune the PID parameters, the quadcopter was divided into four axes: roll, pitch, yaw, and altitude. This division process facilitates independent tuning of parameters for each axis while neglecting the inherent coupling effects present in the real system. Additionally, it aids in analyzing the influence of the control gains on the system response. Subsequently, the PID gains were tuned. The quadcopter response

was evaluated using step and sinusoidal inputs, particularly for GA-based tuning. The goal was to achieve a smooth and stable response with minimal overshoot. The primary performance metric used for tuning was the ISE value, which quantifies the deviation of the system response from the reference signal. The settling time and overshoot were also verified to ensure that the controller did not react too slowly or aggressively. The same evaluation criteria were applied to both manual tuning and GA-based methods.

The PID gains were tuned to achieve a stable response with an acceptable rise time, settling time, and overshoot. Adjustments are made based on the system response to reference inputs to responsiveness and dampening rather than following a strict tuning sequence.

Applying a PID controller to the quadcopter establishes a closed-loop system that enables prediction of key performance characteristics, such as the peak time, rise time, settling time, and overshoot, which indicate the system's stability. Table 3 defines each variable applied to design the PID controller.

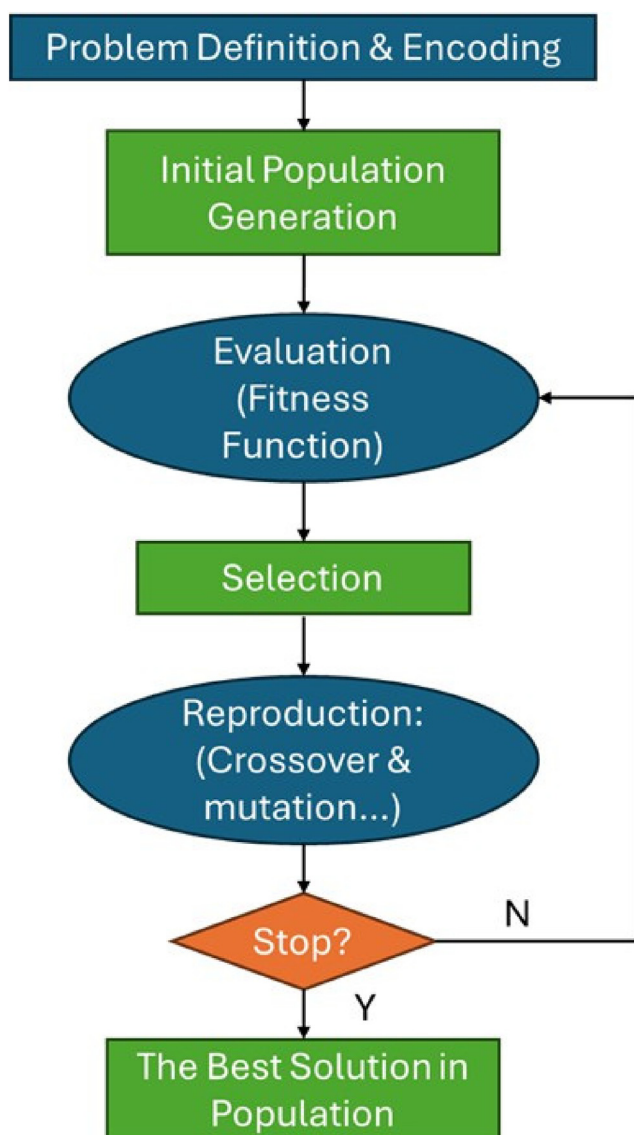


Figure 5. Genetic Algorithm flowchart²⁵

4. GENETIC ALGORITHM FOR PID OPTIMIZATION

The GA is an evolutionary optimization technique inspired by natural selection. It is particularly suitable for designing PID controllers for complex systems and handling large nonlinear search spaces, as it reduces the likelihood of being trapped in local minima. Therefore, GA is an appropriate choice for such applications²¹.

Several recent studies, as presented in²², have also shown that GA-based tuning enhances quadrotor stability and tracking, which supports the approach used in this work; additionally, GA is an easy algorithm to apply and less sensitive to tuning settings than other evolutionary methods, which makes it a practical option for UAV PID tuning²³.

A comparison between two evolutionary algorithms, GA and differential evolution (DE), was performed to investigate their high capabilities in PID parameter tuning. As reported in²⁴, both methods demonstrated similar performance in minimizing the mean squared error (MSE) and integral of absolute error (IAE) for higher-order systems; however, the GA was simpler to apply and less sensitive to tuning parameters. Based on these features, GA is a practical choice for systems in which robustness and adaptability are critical. Table 4 summarizes the comparison investigated between GA and DE.

For the GA, the fitness function is the ISE. As mentioned in Section 3, the GA parameters were selected based on the ISE value to ensure stable and repeatable optimization results. The PID gains were constrained to positive values within bounded ranges to prevent unrealistic or unstable solutions, whereas the population size and number of generations were fixed throughout the optimization process.

The GA is a practical choice for quadcopter control, as it can search for a suitable combination of PID gains and handle the nonlinear nature of UAV dynamics. This demonstrates that it is a useful method for determining gain values that produces stable and smooth responses in simulations.

Figure 5 illustrates the five steps involved in the operation of the GA.

- Initialization: The start involves generating a chromosome that represents a collection of PID gain values.
- Selection: After operating the fitness function, which reduces the error of unreal PID gains, the best values were selected.
- Crossover: It is about using parents, which are a set of chromosomes, and mixing them to have offspring. This is similar to the biological process of merging, which offers a vast solution space for researchers.
- Mutation: The offsprings are manipulated randomly to discover new regions of solution space.
- Termination and Evaluation: The last step is to choose the optimal solution after a specified number of generations, after which the algorithm reaches the end and stops.

5. SIMULATION SETUP AND SCENARIO DESCRIPTION

Two tuning methods are used to optimize the PID parameters. The first method involves manual tuning, whereas the second employs GA.

Table 5. Manual PID tuning values for three trials

Trial	K_p (Manual)	K_i (Manual)	K_d (Manual)
1	1.5	3.9	16.0
2	1.9	3.6	17.5
3	2.5	2.9	18.5

5.1. Manual PID Tuning. The outputs are generated from the control inputs processed by the linear model through its transfer function representation. The ODE45 solver provides a numerical solution to the state-space equations, enabling simulations of the system. This block diagram shows the feedback loop for every control variable, with each PID controller tuned manually by the operator such that the ISE decreases over time.

Figure 6 illustrates a closed loop of a quadcopter control system in Simulink. The entire system works based on four PID controllers developed to control the attitude and altitude. The error signal to the PID controller is defined according to the difference between the actual output and input signals.

Table 5 lists the values of the proportional (P), integral (I), and derivative (D) gains, which were applied to optimize the attitude and altitude performance. The PID parameters are tuned based on the stability of the system. Because the controlled variables are connected in the same closed loop, there is no difference in the values of the PID gains, and this equalization produces a similar response for the fourth controlled variable. However, each trial showed a different stability and tracking trajectory based on the overshoot performance.

Figure 7 illustrates trial 1, where a step input has been applied to the quadcopter UAV system and the PID gains, which are selected after several trials for Φ , Θ , Ψ , and Z , showed a high steady-state error as well as a failure to predicting the future error based on the rate of change of it. Additionally, there is a high overshoot in the system response, which significantly affects the stability of the quadcopter.

Table 6. Performance metrics of manual PID tuning

Trial	Rise time T_r (s)	Settling time T_s (s)	Overshoot OS (%)
1	0.55	2.8	3.0
2	0.50	2.5	2.5
3	0.45	2.2	2.0

The same process was applied, as shown in Figure 8; however, different PID gain values were applied to improve the stability of the quadcopter system. It could be seen that a slight minimization occurred for the overshoot as well as the steady-state error. However, the optimal system performance has not yet been achieved.

In Trial 3, as Figure 9 demonstrates, the updated PID gains contribute to minimizing the current error as well as the steady-state error and predicting the future error based on its rate of change. Even though the simulation can be different from reality, the chosen values of the parameters result in good performance of the system with high stability and accuracy.

Table 6 shows that manual tuning is able to stabilize the system, but the response changes noticeably from one trial to another. While the rise time is generally short, the settling time and overshoot remain relatively high. This behavior reflects the trial-and-error nature of manual tuning, where small changes in gains can lead to different levels of performance.

5.2. GA-Based Tuning. In this section, the system faces a new sine input to test its ability to maintain stability with a low overshoot.

Table 7 lists the GA parameters used to tune the PID gains in the three trials. The mutation operation was adaptively handled using MATLAB's built-in mutation-adapt-feasible function of MATLAB, which automatically adjusts the mutation value during the optimization process instead of using a fixed probability value.

Figure 10 present the best solution of the ten-generation process, and they show a little oscillation in the system; however,

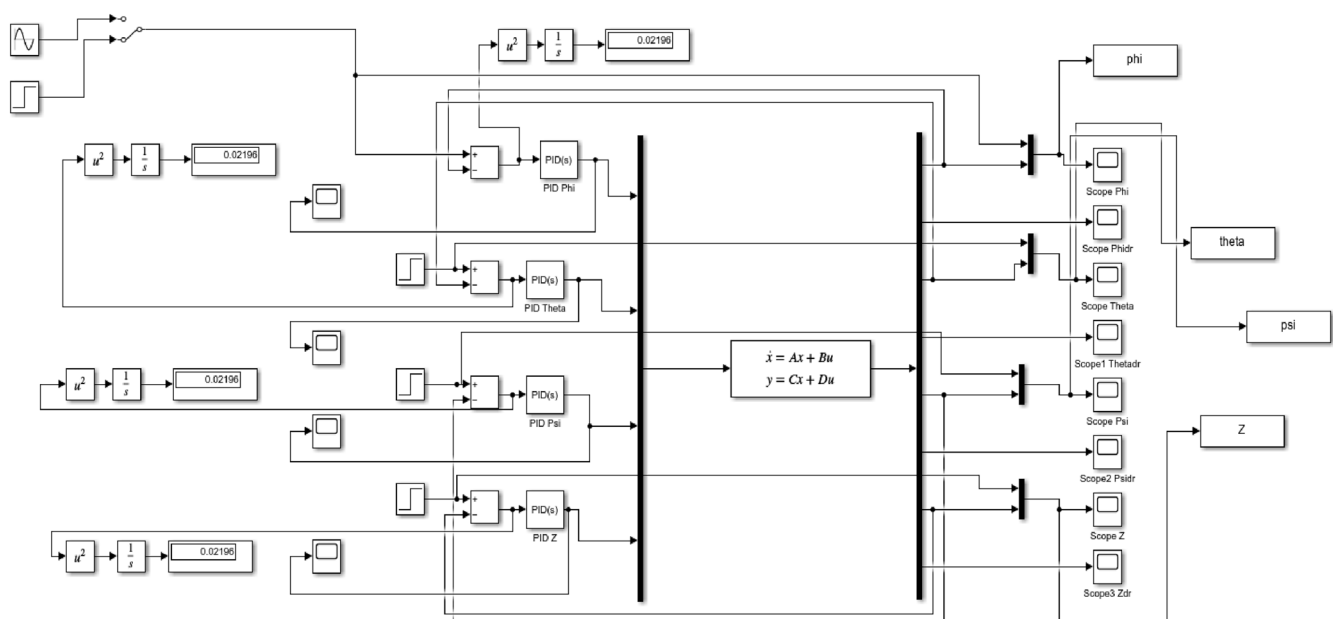
**Figure 6.** SIMULINK block diagram

Table 7. Genetic Algorithm parameters used for PID optimization

GA Parameters	Value
Population Size	30
Crossover Probability	0.8
Mutation	Adaptive (auto-adjusted)
Generations	10, 20, 30

it took less time compared to a large number of generations process.

Figure 11 shows the response of the control variable with respect to the number of generations, which was 20. Slight improvements in the overshoot and settling time performance of the system were observed between $G = 10$ and $G = 20$. It showed better results regarding the error; however, it took more time compared to ten generations.

A better result is illustrated in Figure 12, which shows a more evolved solution than the previous two solutions. The optimal fitness value was reached as 0.030056. This solution is not the

most optimal solution; however, it shows a better performance of the GA in tuning the PID gains instead of tuning them manually, which may require more human effort. In Figure 12 d, the quadcopter rises quickly to 1 m in nearly 1 s, then oscillates slightly after 6 s, but returns to the steady state smoothly. It could be seen from Figures 10a, 11a, and 12a, that the roll angle kept its performance similar to the other angles in each trial, even though it received a different input.

As listed in Table 8, the population value was fixed at 30, and the system performance was tested based on different generations (10, 20, and 30) to configure how the GA is evolving and gives better values of PID gains and ISE. Population represents the number of solutions per generation. Usually, an increase in the PID gain results in a lower efficiency and affects the response of the system owing to noise; however, in our case, the GA reached the optimal point, so a large increase in the PID parameters did not occur, as shown. The best fitness value was obtained in the last trial because the algorithm required a longer time to generate optimal results.

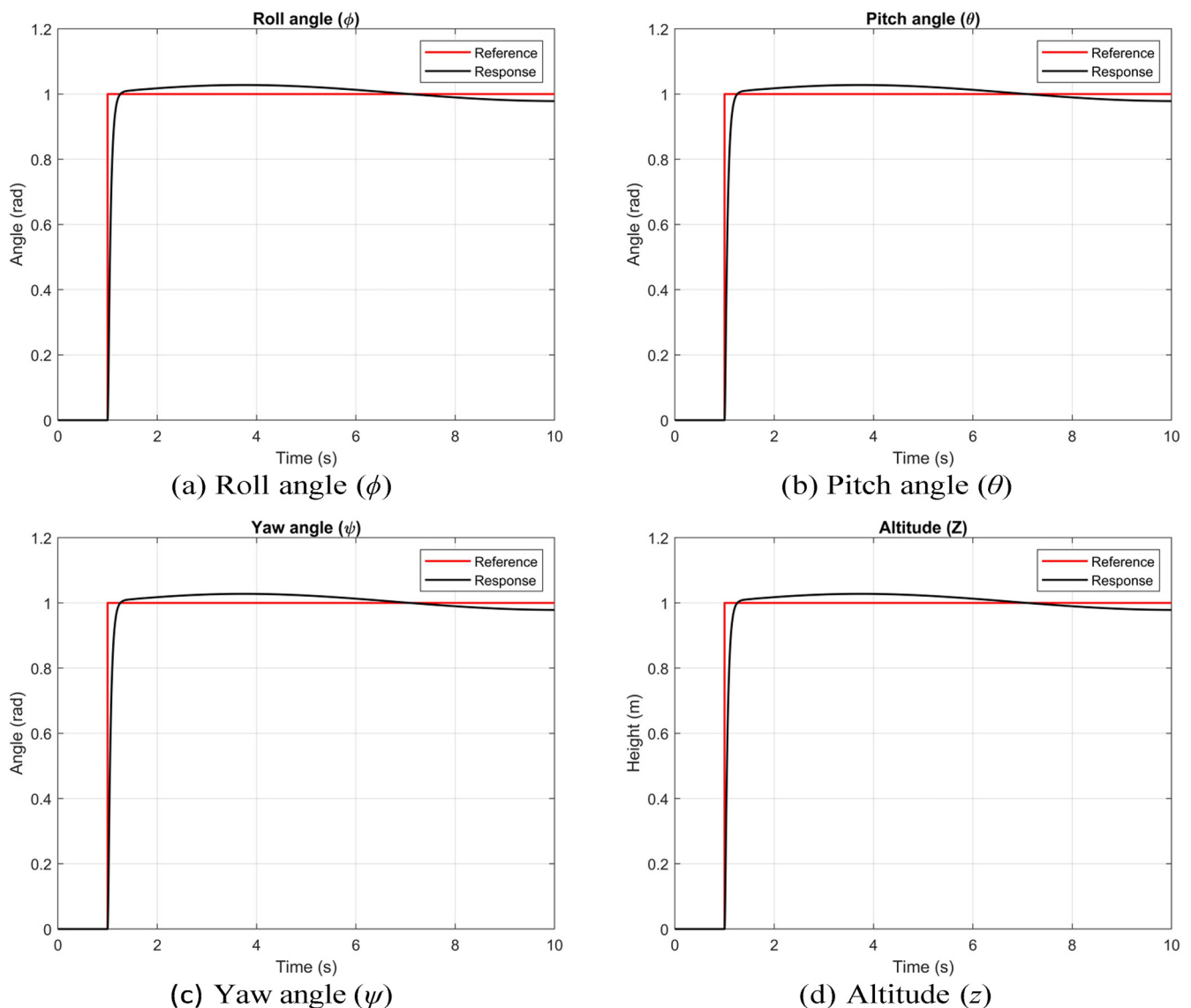
**Figure 7.** Quadcopter responses of attitude and altitude for trial 1

Table 8. GA optimization results for different numbers of generations

Trial	Population Size	Generations	K_p (All)	K_i (All)	K_d (All)
1	30	10	2.2142	3.5205	19.8439
2	30	20	2.9508	3.2705	19.9689
3	30	30	2.9801	2.9893	19.9913

Table 9. Performance metrics of GA-tuned PID

Trial	Rise time T_r (s)	Settling time T_s (s)	Overshoot OS (%)
1	0.35	1.5	1.5
2	0.30	1.3	1.3
3	0.28	1.1	1.0

Table 9 shows that, compared to the manual tuning method, the GA achieved a more stable response. It can be noticed that the rise time is reduced to nearly 0.3 s, and the settling time decreases to 1–1.5 s, which is almost half of the manual values. A less

aggressive system response is produced as the overshoot value is reduced to 1% at the last trial. The enhancement of the system's performance demonstrates that the GA method results in better PID gains, which provide a faster and more stable performance for all four axes.

5.3. Disturbance Tests and Scenario Evaluations. To ensure that the GA performed better than the trial-and-error method, different scenarios and disturbances were applied to both methods.

Figure 13 illustrates a scenario in which the best manually tuned PID gains for altitude were tested by applying a rectangular disturbance. It could be seen that Figure 13 b shows the response, as it results in high overshoot and an unstable system.

Table 10 lists the values of T_r , T_s , and OS for manual tuning. High values were obtained when a disturbance was applied to the system.

In Figure 14, four scenarios were applied to test the adaptation of the system while flying. Each figure shows the rising and landing times of the quadcopter. Figure 14 a shows a scenario in

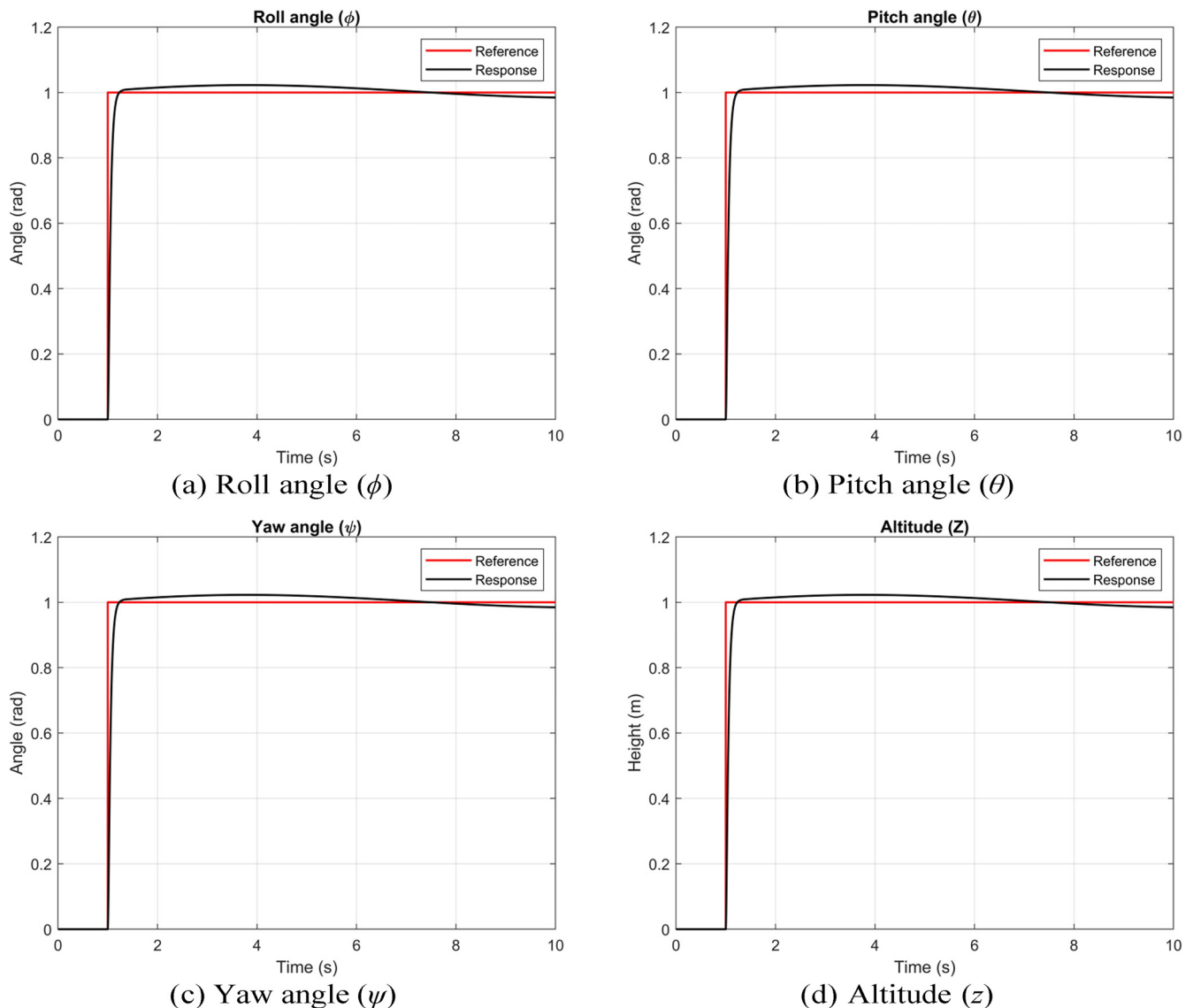
**Figure 8.** Quadcopter responses of attitude and altitude for trial 2

Table 10. T_r , T_s , and OS for manual tuning

Metric	Value
Rise time T_r (s)	0.35
Settling time T_s (s)	8.00
Overshoot (%)	8%

which the quadcopter UAV takes off at 1 s until it reaches 1 m, stays at the same level for 5 s, and then lands at ground level.

Another scenario is illustrated in Figure 14 b, where the quadcopter performs a two-time takeoff to reach a level of 1 m and then lands. The two takeoff and landing processes were repeated every 2 s and ended at 8 s.

Between takeoff and landing, the quadcopter remained at the same level for 2 s. In scenario 3, the quadcopter UAV takes off at 1 s to reach the level of 1 m and stays for 1 s more. It repeats the same process every 1 s until 10 s, however, every 1 s it flies almost 0.25 m more. Finally, it landed at 10 s, as presented in the Figure 14 c.

The last scenario in Figure 14 d consists of 5 phases: take-off (0 s–1 s), hovering at 1 m (1 s–3 s), climb to 2 m and staying at the same level (3 s–5 s), descent to 1 m (5 s–9 s), and landing to the ground level phase (9 s–10 s). Each scenario was applied to the system based on Trial 3, which exhibited the best performance of the three trials. For each scenario, a good performance was observed, despite a slight overshoot.

Once the scenarios and input disturbances are applied to the same PID gains of the manual tuning method, the GA-tuned PID gains are evaluated by applying the same process.

Figure 15 shows that the same input disturbance was applied to the best altitude PID gains for the GA. However, better performance for the GA altitude response was observed.

Table 11 summarizes that the GA under a disturbance shows lower values of T_r , T_s , and OS, confirming that the GA outperforms the manual tuning method.

Figure 16 illustrates four cases in which the system can adapt to different scenarios that were also applied to a manually tuned system. Each scenario is explained in section 5.1. Overall, there was

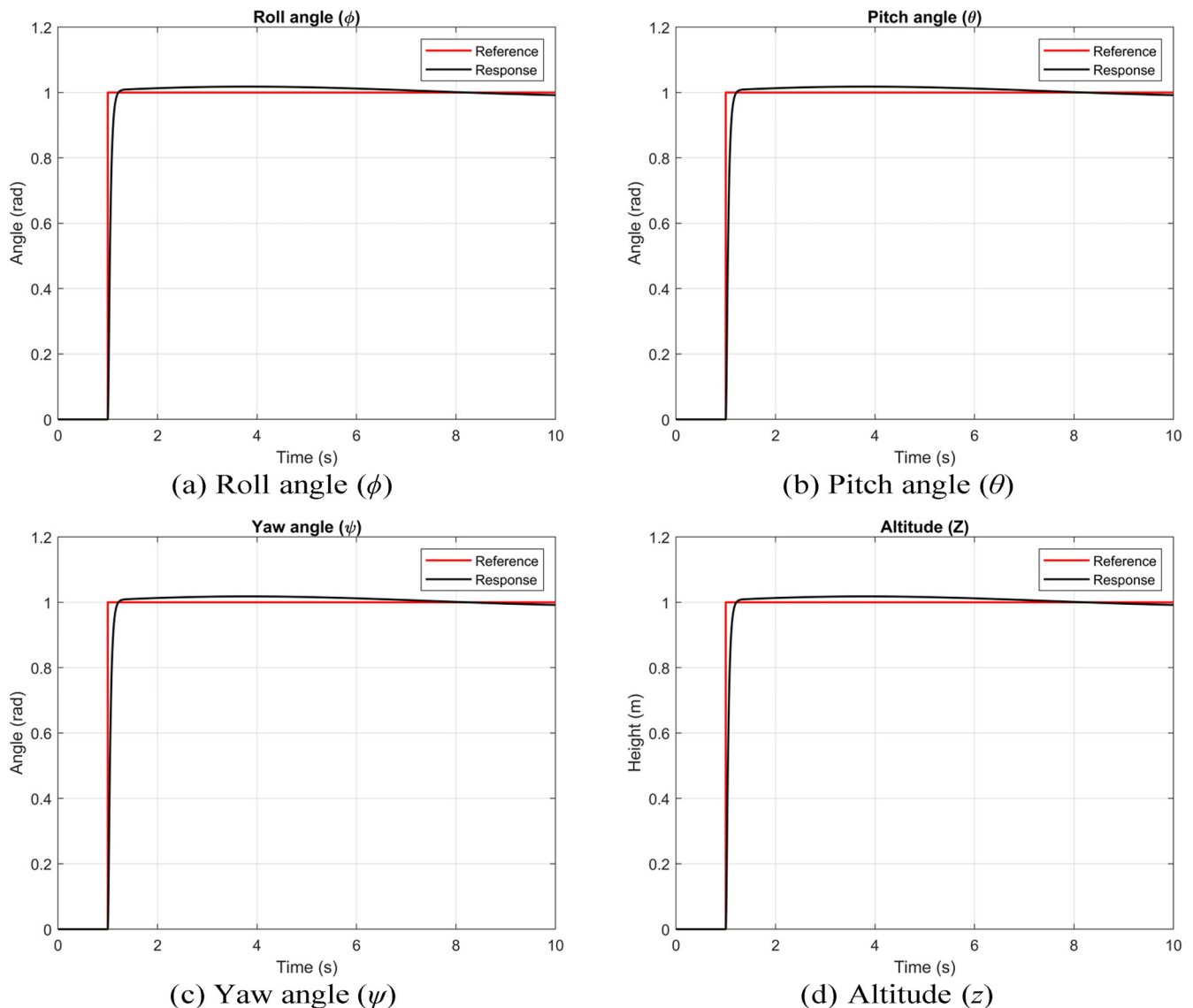
**Figure 9.** Quadcopter responses of attitude and altitude for trial 3

Table 11. T_r , T_s , and OS for GA tuning under disturbance

Metric	Value
Rise time T_r (s)	0.30
Settling time T_s (s)	7.50
Overshoot (%)	7%

no significant difference among the four cases regarding the performance of the system as it reached the optimal point. However, it was confirmed that increasing the number of generations to 30 assists in minimizing the overshoot and confirming the damping efficiency of the controller.

The four scenarios focused on the z direction; therefore, most of the changes were only in altitude. Although the roll, pitch, and yaw controllers remained stable, they were not fully challenged by the horizontal movement or path tracking. This means that the scenarios show how the quadcopter handles vertical changes, but do not reflect full trajectory tracking. To achieve a x - y path, tests are required to evaluate all axes together to achieve an x - y path.

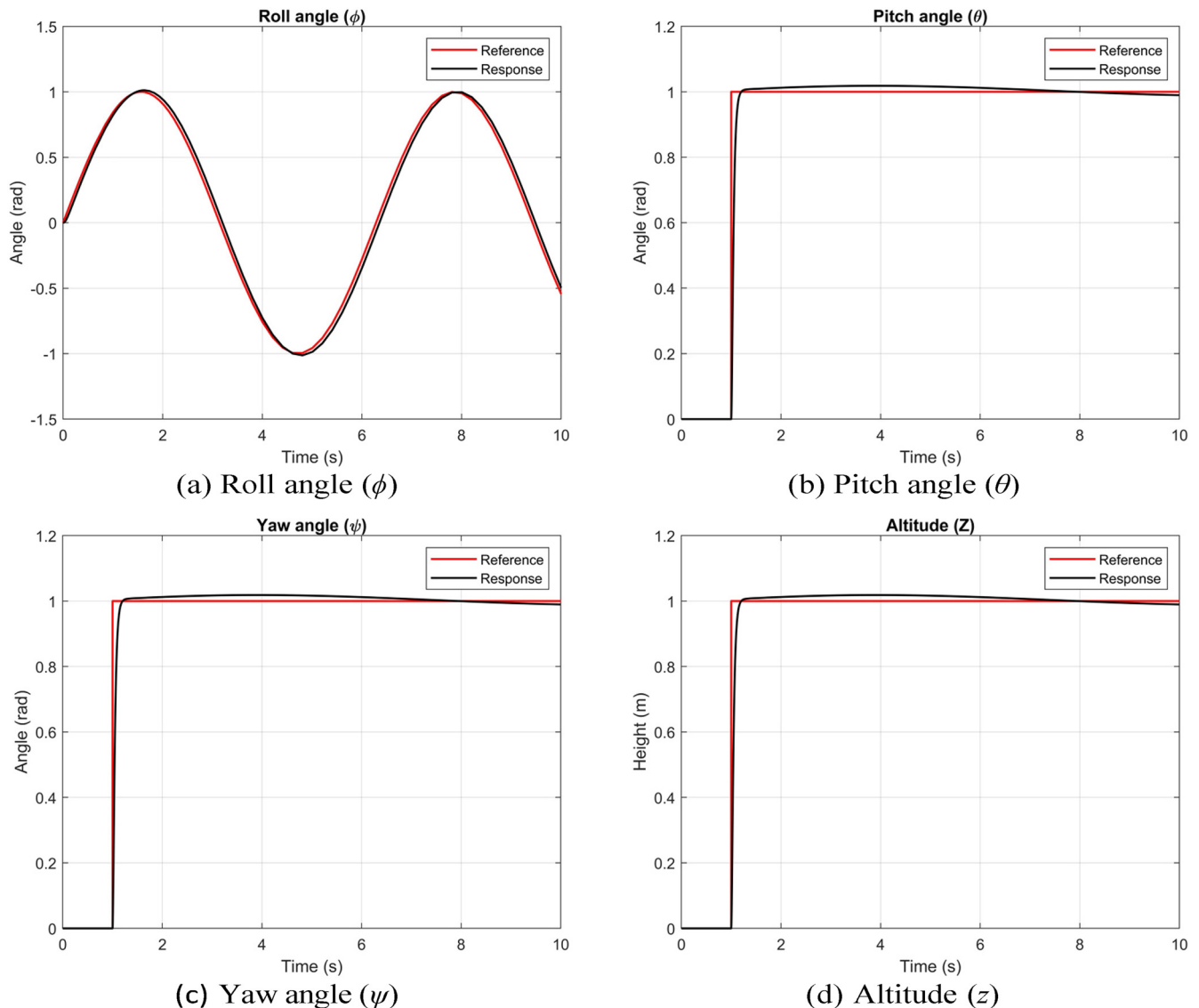
Table 12. Comparison between manual and GA tuning based on ISE performance

Trial	ISE (Manual)	ISE (GA)	Improvement (%)
1	0.03919	0.03140	19.9
2	0.03543	0.03101	12.5
3	0.03316	0.030056	9.3
Average	–	–	13.9

Table 13. Runtime comparison for best PID gains

Method	Search effort	Best result obtained at	Total tuning time
Manual tuning	≈10 simulations	Trial 3	≈10 minutes
GA tuning (best run)	$P = 30, G = 30$ (≈900 evals)	≈30 minutes Trial 3	(or more)

5.4. Comparative Analysis. After obtaining the ISE values for both methods, a comparison was conducted as follows:

**Figure 10.** Quadcopter responses of attitude and altitude under $G = 10$

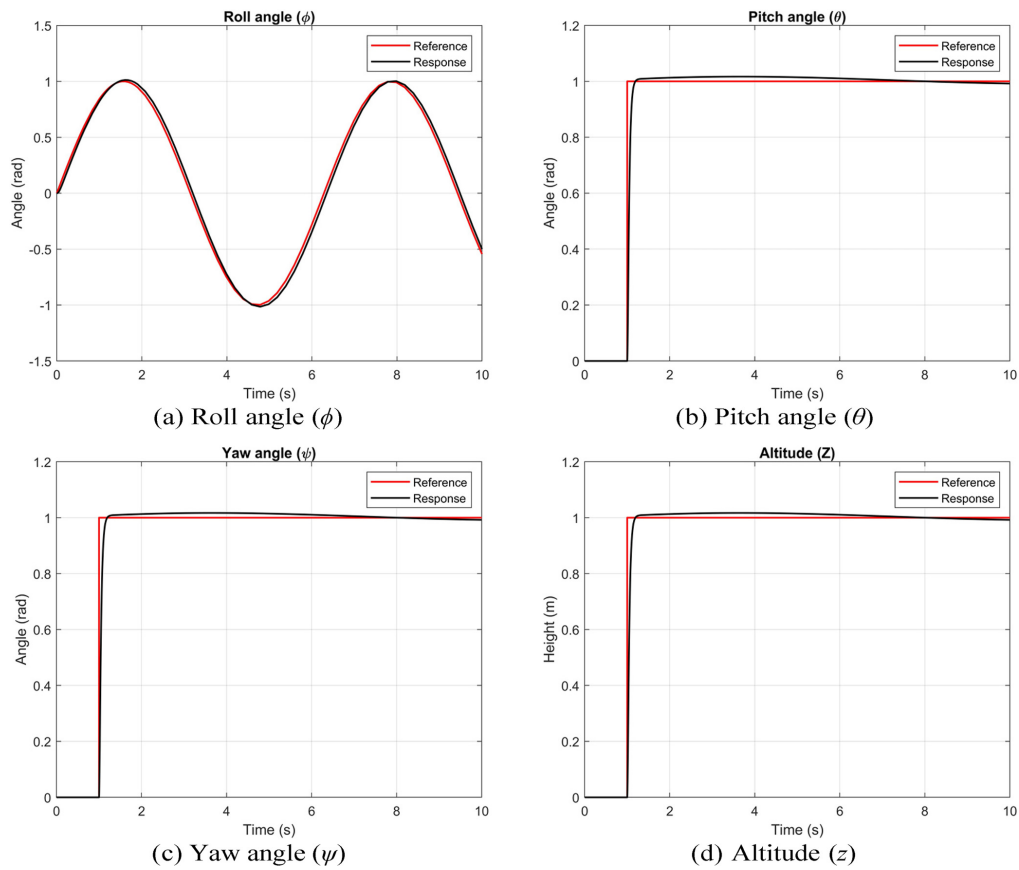


Figure 11. Quadcopter responses of attitude and altitude under $G = 20$

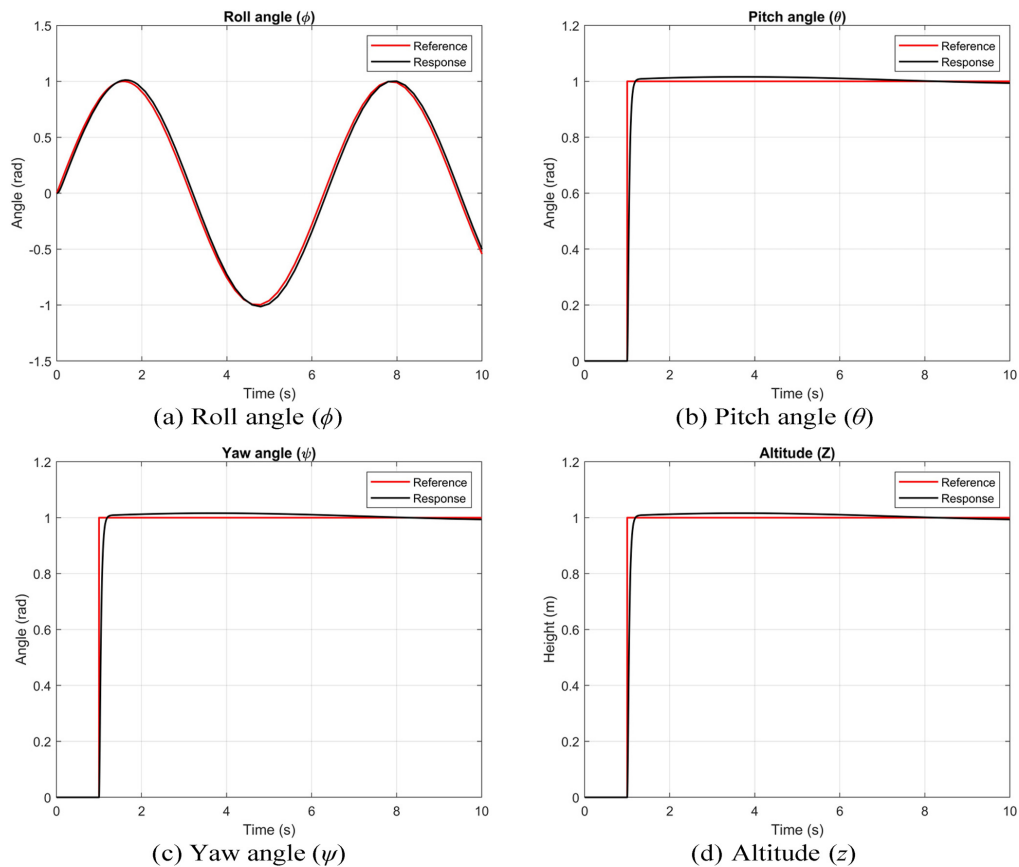
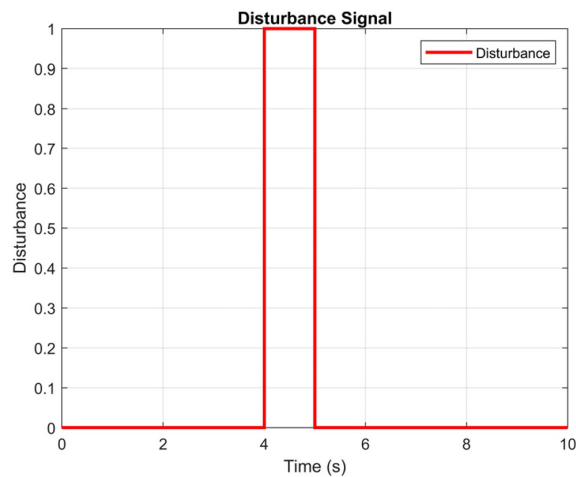
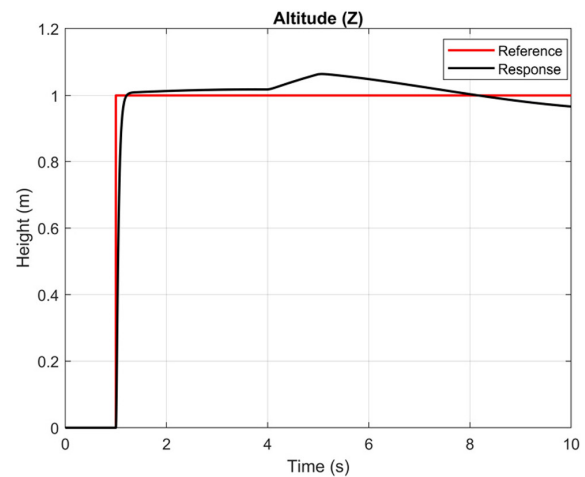


Figure 12. Quadcopter responses of attitude and altitude under $G = 30$

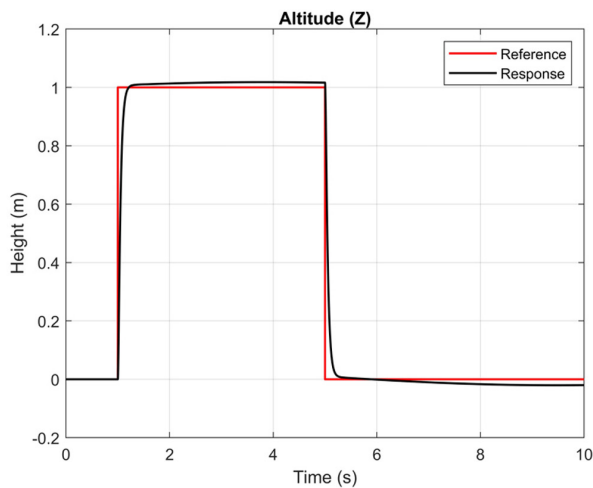


(a) Disturbance (Input) signal.

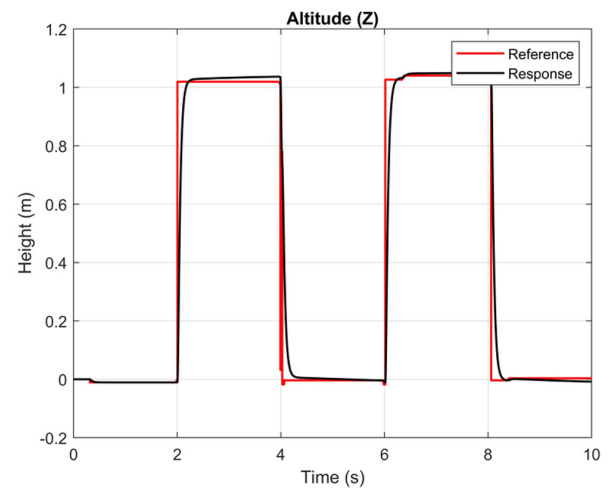


(b) Manual tuning under disturbances.

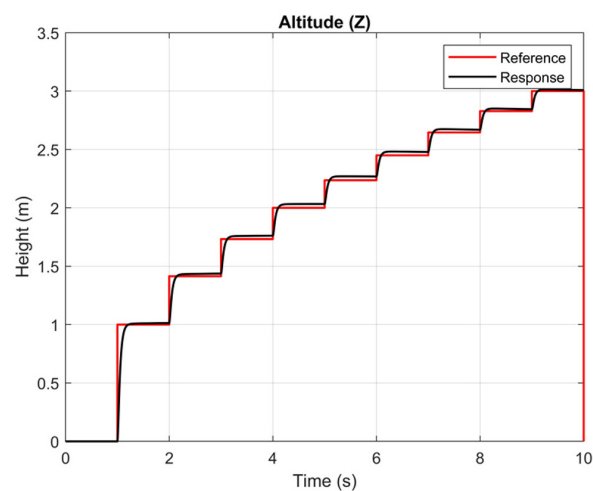
Figure 13. Manual tuned quadcopter response of altitude tested by disturbance input



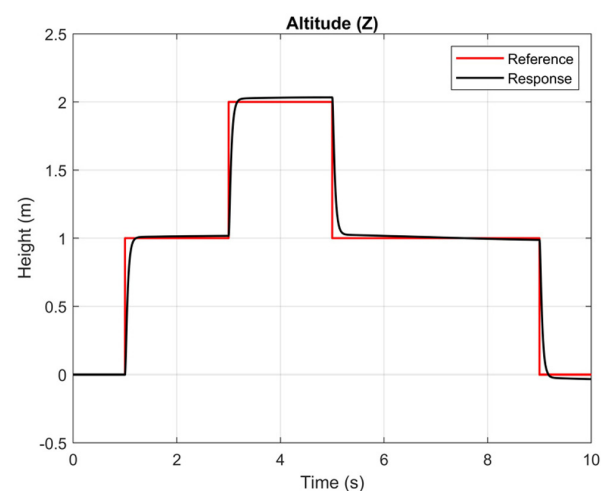
(a) Scenario 1: Take-off and landing using PID controller (Altitude z)



(b) Scenario 2: Take-off and landing using PID controller (Altitude z)



(c) Scenario 3: Takeoff and landing using a PID controller (altitude z)



(d) Scenario 4: Takeoff and landing using a PID controller (altitude z)

Figure 14. Quadcopter responses of altitude tested by four scenarios

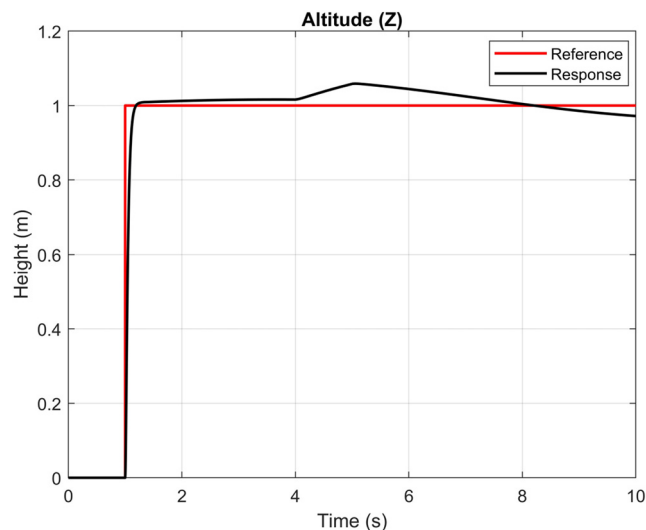
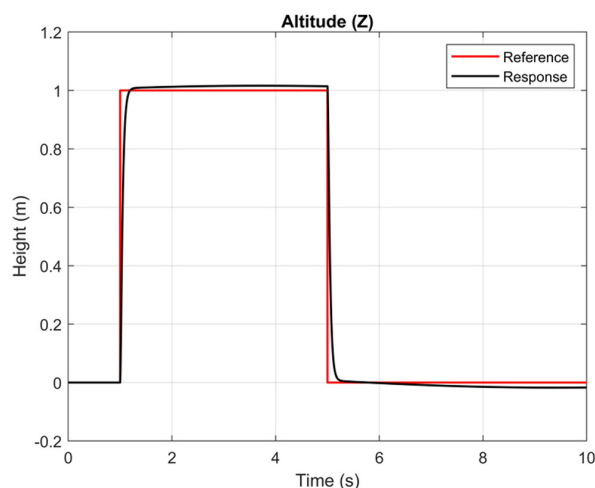


Figure 15. GA tuning under disturbance

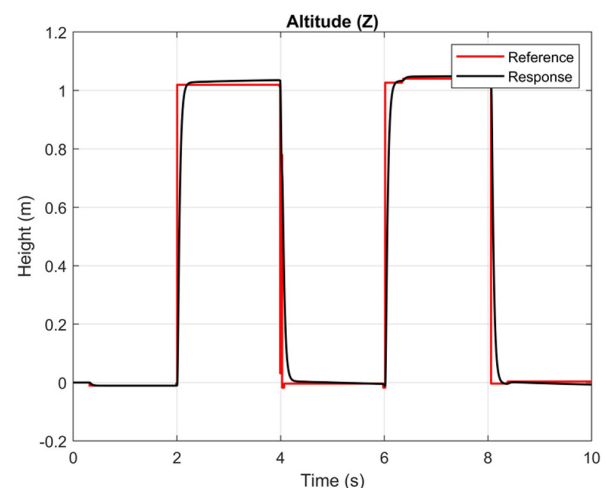
Table 12 shows that the GA-tuned controller consistently achieves lower ISE values than manual tuning across all trials. This indicates that the GA-selected gains allow the system to follow the reference signal more closely and with less variation between runs. The improvement is observed in all cases, which suggests that GA provides a more reliable tuning approach than manual adjustment. Notably, the GA-derived PID parameters are specific to this quadcopter model and the simulation scenarios applied to it, so they might not fit a different frame or flight regime. However, the tuning procedure is general. Changing the model parameters with the GA regenerating PID gains will show the same workflow that is applied to obtain suitable PID gains.

Figure 17 shows the GA convergence curve for the best ISE value in Trial 3. The ISE increases rapidly in the early generations, from 0.0315 to nearly 0.0302, and then stabilizes after 15–20 generations. By the end of the run, the best ISE value of 0.030056 was reached, indicating near convergence.

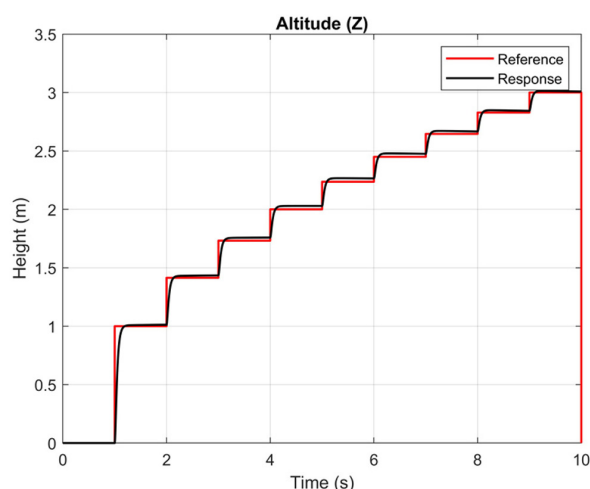
Table 13 shows that the computational time of GA-based PID tuning is evaluated by its fitness. Moreover, GA spends a longer time than the manual tuning method to generate the best PID gains because of its 900 evaluations. Conversely, the manual-



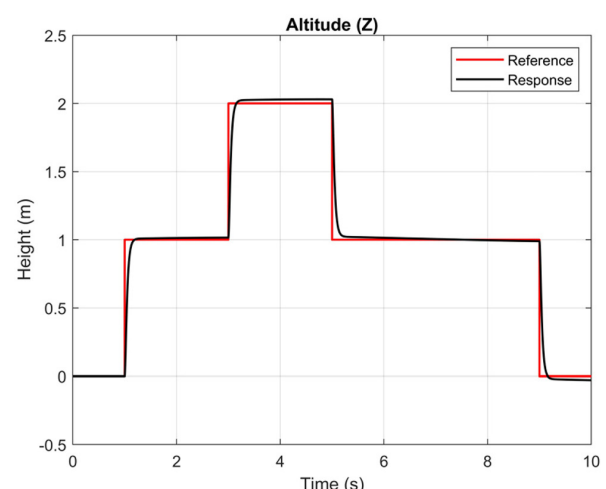
(a) Scenario 1: Take-off and landing using the PID controller (altitude z)



(b) Scenario 2: Take-off and landing using the PID controller (altitude z)



(c) Scenario 3: Takeoff and landing using a PID controller (altitude z)



(d) Scenario 4: Take-off and landing using the PID controller (altitude z)

Figure 16. Altitude responses of the quadcopter under GA-PID control for $G = 30$

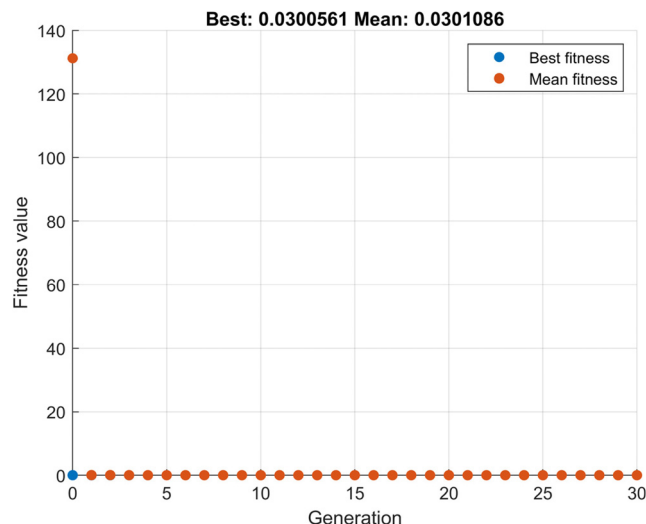


Figure 17. GA convergence curve showing best and mean ISE versus generation

based PID tuning does not use generations, but rather depends on trial-and-error, which is the reason for it to be faster than the GA. Although the GA is slower, it offers a more systematic and repeatable way to tune the controller than manual tuning.

6. CONCLUSION

This study focused on modeling and controller design of a quadcopter system to enhance hover stability and trajectory tracking performance. The nonlinear dynamics were derived by modeling the quadcopter system using the Newton–Euler method and further applying the FBL to obtain a suitable state-space representation for the input and output.

In MATLAB/Simulink, two PID tuning methods were applied: manual and GA. The comparison shows that GA-based tuning yields smoother responses and more consistent behavior than manual tuning. This suggests that a systematic optimization approach can reduce the uncertainty associated with trial-and-error adjustments.

Importantly, the results presented in this work are based on simulations and do not account for practical effects, such as real external disturbances. In addition to being simulation based, this study relied on simplified assumptions. For example, inter-axis coupling and sensor noise are not explicitly modeled, and parameters such as mass and inertia are assumed to be constant, which may affect the applicability of the tuned gains to real flight conditions. Therefore, future work should focus on the real-time implementation and experimental validation of an actual quadcopter platform.

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Enhancing 2-DOF Helicopter MIMO System Control using ZOA-Tuned Single Neuron PID Algorithm

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ABSTRACT

Traditional proportional–integral–derivative (PID) controllers are broadly employed in engineering. However, they perform poorly in complex, non-linear systems, and the single-neuron PID (SNPID) has been proposed as an alternative. Few studies have applied SNPID controllers to multi-input multi-output (MIMO) systems, and none has implemented this control technique experimentally on a 2-DOF helicopter—a system that is both complex and nonlinear. In this study, the SNPID settings were optimally computed using the Zebra Optimization Algorithm (ZOA). The proposed SNPID controller was compared with a conventional PID controller, with both controllers tuned by the ZOA to ensure a fair assessment. Real-time results indicate that the SNPID controller achieves greater stability and more accurate reference tracking than the PID controller, with an integral square error (ISE) of 4.7101×10^{-4} versus 5.7751×10^{-4} for the PID controller. Furthermore, when disturbances occur, the SNPID controller returns to the reference signal, whereas the PID controller cannot. These findings provide evidence that SNPID controllers outperform conventional PID controllers in MIMO systems.

Keywords: proportional–integral–derivative (PID) control, single-neuron PID (SNPID), two-degree-of-freedom (2-DOF) helicopter, multi-input multi-output (MIMO) systems; Zebra Optimization Algorithm (ZOA), real-time control

1. INTRODUCTION

Numerous industrial applications make extensive use of proportional–integral–derivative (PID) control owing to its simple structure and robustness.¹ However, traditional PID controllers have fixed coefficients, which can reduce their performance or even cause instability in dynamic, nonlinear systems.^{2,3} To address this limitation, artificial neural networks (ANNs) have been proposed, as they can handle complex and dynamic systems by updating their weights. However, ANNs incur computational overhead and require substantial processing time owing to the training of many weights.^{1,4} Moreover, stability depends on network size and the number of training iterations.⁵ To combine the simplicity of a traditional PID controller and the adaptivity of an ANN, the single-neuron PID (SNPID) controller has been introduced. It constitutes the basic unit of a neural network in which PID coefficients are optimized by an ANN.⁶ Numerous studies have investigated SNPID controllers with different optimization methods—for example, radial basis function (RBF),⁷ extended Kalman filter (EKF),⁵ and fuzzy logic¹—though these have been primarily applied in single-input single-output (SISO) applications.

In this study, an SNPID controller was evaluated on a two-degree-of-freedom (2-DOF) helicopter MIMO system, which is a complex, nonlinear system with coupling effects. Although the SNPID controller has been tested on a 2-DOF helicopter using only simulation,⁸ to the best of our knowledge, no real-time

results have been reported for controlling a 2-DOF helicopter. The following are this study's primary contributions:

1. The SNPID controller parameters are tuned using the Zebra Optimization Algorithm (ZOA).
2. A real-time platform is used to test and assess the performance of the SNPID controller for the 2-DOF helicopter MIMO system, representing the first such demonstration reported in the literature.

The rest of this document is structured as follows: Section 2 presents the 2-DOF helicopter MIMO system. Section 3 describes the proposed control algorithm. Section 4 presents the ZOA. The findings and discussion are presented in Section 5, and the conclusions are presented in Section 6.

2. THEORY: 2-DOF HELICOPTER MIMO SYSTEM

In this study, the Quanser 2-DOF helicopter (known as Aero 2) was used as a dual-rotor helicopter, as shown in Figure 1 (a). The free-body diagram of the helicopter is shown in Figure 1 (b). This model allows for rotation about the z-axis and y-axis; therefore, only yaw and pitch movements are possible. The following is the expression for the equations of motion:

$$J_p \ddot{\theta} + D_p \dot{\theta} + K_{sp} \theta = \tau_p, \quad (1)$$

$$J_y \ddot{\psi} + D_y \dot{\psi} = \tau_y. \quad (2)$$

The torques τ_p and τ_y acting on the pitch and yaw axes are expressed as follows:

$$\begin{cases} \tau_p = K_{pp}V_p + K_{py}V_y \\ \tau_y = K_{yp}V_p + K_{yy}V_y \end{cases}, \quad (3)$$

where J_p denotes the total moment of inertia for pitch, D_p denotes the pitch damping coefficient, K_{sp} denotes the pitch stiffness, K_{pp} denotes the torque thrust gain from the pitch rotor, K_{py} denotes the cross-torque thrust parameter between the pitch and yaw, V_p denotes the pitch voltage, and V_y denotes the yaw voltage.

3. CONTROL ALGORITHMS

3.1. PID Controller. The PID controller is entirely dependent on the error signal $e(k)$, which is calculated at the discrete time instant k , expressed as follows:

$$e(k) = r(k) - y(k), \quad (4)$$

where $r(k)$ is the desired reference signal and $y(k)$ is the actual output. The discrete-time PID digital form is expressed as follows:

$$u(k) = K_p x_1 + K_i x_2 + K_d x_3, \quad (5)$$

where x_1 , x_2 , and x_3 are defined as:

$$\begin{cases} x_1 = e(k) - e(k-1) \\ x_2 = e(k) \\ x_3 = e(k) - 2e(k-1) + e(k-2) \end{cases}. \quad (6)$$

Here, x_1 denotes the proportional component, x_2 denotes the integral component, and x_3 denotes the derivative component. Furthermore, K_p , K_i , and K_d denote gain coefficients that govern the stability and performance of the system. These coefficients vary from system to system, so therefore require a tuning method to obtain optimal values.

3.2. Adaptive Single-Neuron PID. The proposed controller is an adaptive SNPID controller. It has the same simple structure as the PID controller (5) but differs in how K_p , K_i , and K_d are adaptively computed, along with the weights w_1 , w_2 , and w_3 . The weights are computed as follows:

$$\begin{cases} w_1 = w(k-1) + \eta_p e(k) u(k-1) x_1 \\ w_2 = w(k-1) + \eta_i e(k) u(k-1) x_2 \\ w_3 = w(k-1) + \eta_d e(k) u(k-1) x_3 \end{cases}. \quad (7)$$

where η_p , η_i , and η_d denote the learning rates that govern the changes in the corresponding weight coefficients w_1 , w_2 , and w_3 , respectively. These equations define the self-learning mechanism that produces the real controller output $u(k)$, expressed as follows:

$$u(k) = u(k-1) + K \sum_{i=1}^3 w'_i(k) x_i. \quad (8)$$

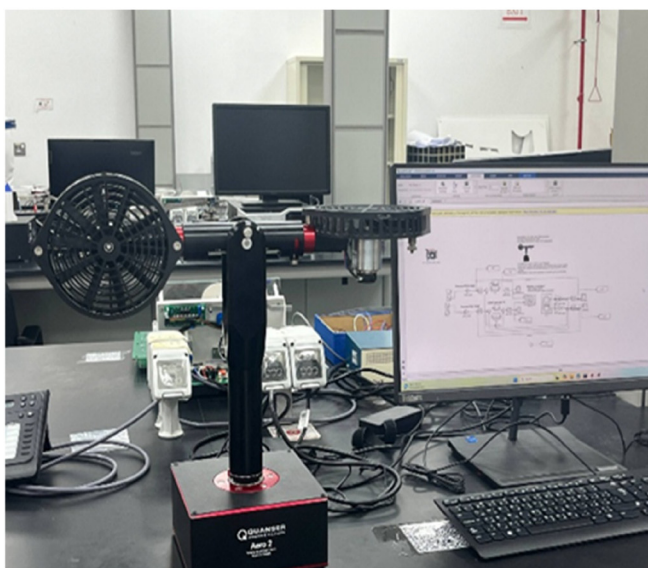
In (8), the controller uses the previous output ($u(k-1)$) and an incremental term. K denotes the scaling coefficient of the adaptive SNPID controller, and w'_i denotes the normalized weights, defined as follows:

$$w'_i(k) = \frac{w_i}{\sum_{i=1}^3 |w_i(k)|}. \quad (9)$$

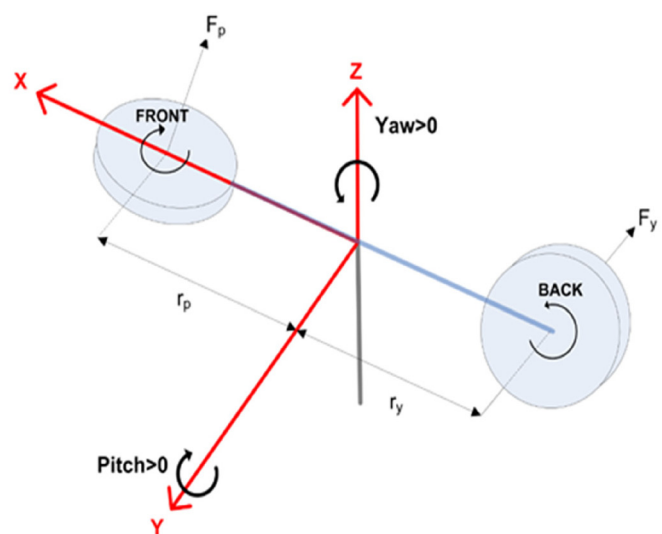
Figure 2 shows the SNPID controller implemented in MATLAB. The controller parameters are computed using the ZOA, as described in the following section.

4. ZEBRA OPTIMIZATION ALGORITHM

Zebras are African animals that can run at high speeds when threatened. They exhibit two main behavioral traits in nature: food acquisition and formulating a safety plan against predators.¹⁰ These two behaviors inspired the development of the ZOA. The mathematical representation of the ZOA population



(a)



(b)

Figure 1. (a) 2-DOF helicopter in the lab; (b) free-body diagram⁹

is expressed as follows:

$$X = \begin{bmatrix} X_1 \\ \vdots \\ X_i \\ \vdots \\ X_N \end{bmatrix}_{N \times M} = \begin{bmatrix} x_{(1,1)} & \cdots & x_{(1,j)} & \cdots & x_{(1,M)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{(i,1)} & \cdots & x_{(i,j)} & \cdots & x_{(i,M)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{(N,1)} & \cdots & x_{(N,j)} & \cdots & x_{(N,M)} \end{bmatrix}, \quad (10)$$

where X denotes the zebra population, X_i denotes the search agent of the i^{th} zebra, $x_{i,j}$ denotes the value for the j^{th} problem dimension of the i^{th} zebra, N denotes the number of search agents (zebras), and M denotes the dimensionality of the optimization problem. Each search agent represents a possible solution to the problem; consequently, the proposed values can be used to evaluate the objective function, expressed as follows:

$$F = \begin{bmatrix} F_1 \\ \vdots \\ F_i \\ \vdots \\ F_N \end{bmatrix}_{N \times 1} = \begin{bmatrix} F(X_1) \\ \vdots \\ F(X_i) \\ \vdots \\ F(X_N) \end{bmatrix}_{N \times 1}, \quad (11)$$

where F denotes the vector containing all F_i , which are the objective functions corresponding to X_i . The ZOA selects the lowest value in minimization or the highest value in maximization when comparing the objective function values. This strategy is repeated at each iteration. The two zebra behaviors are used to update the ZOA search agents; accordingly, the ZOA passes through two phases:

1. Food acquisition

Table 1. PID coefficients

Coefficient	Direction	Value
K_p	Pitch	999.15
K_i	Pitch	3.8995
K_d	Pitch	999.64
K_p	Yaw	959.12
K_i	Yaw	6.1865
K_d	Yaw	999.34

2. Safety plan against predators.

4.1. Phase 1: Food Acquisition Behavior. Zebras devote 60%–80% of their time to searching for their preferred food, which in many cases is grass. In the ZOA, the best search agent is called the pioneer zebra (PZ), which leads other agents toward its position in the search space. The mathematical formulation of the food acquisition phase is given in (12), and the updating condition is given in (13).

$$x_{(ij)}^{new,P_1} = x_{(ij)} + r(PZ_j - I \cdot x_{(ij)}), \quad (12)$$

$$X_i = \begin{cases} X_i^{new,P_1}, & F_i^{new,P_1} < F_i \\ X_i, & \text{else,} \end{cases} \quad (13)$$

where X_i^{new,P_1} denotes the new position of the i^{th} zebra for phase 1, $x_{(ij)}^{new,P_1}$ denotes its j^{th} dimension, $I = \text{round}(1 + \text{rand})$, with rand is an arbitrary number in the interval $[0, 1]$, F_i^{new,P_1} represents the objective function value, PZ_j represents the pioneer zebra in its j^{th} dimension, and r represents a random number in the interval $[0, 1]$.

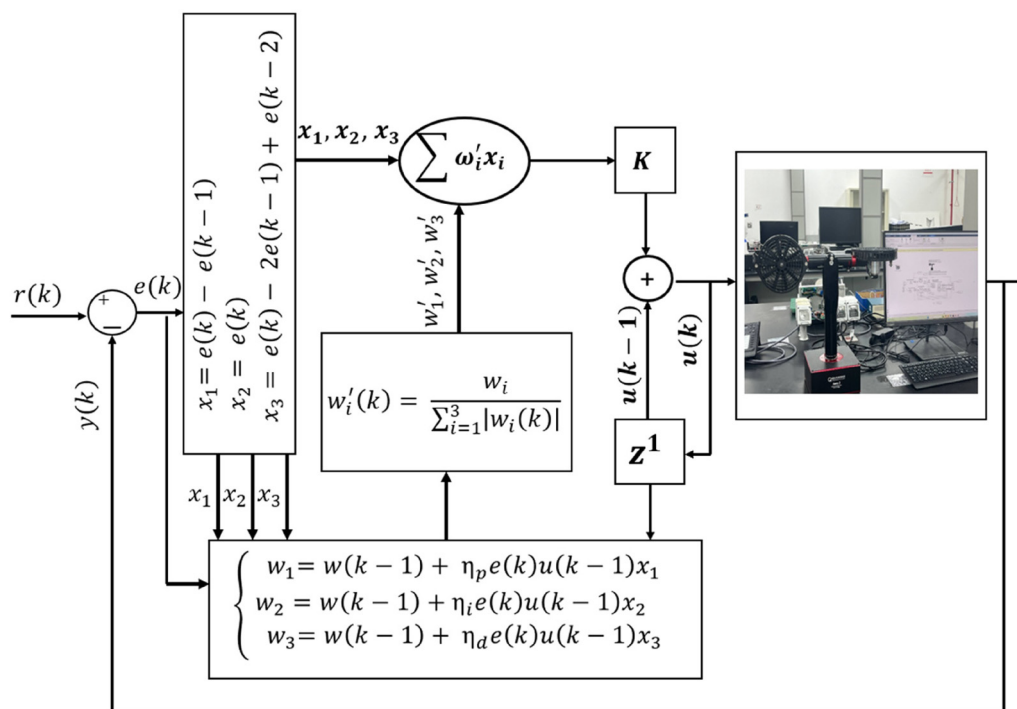


Figure 2. Schematic of the SNPID controller in MATLAB

4.2. Phase 2: Safety Plan Against Predators. While zebras graze, they face threats from various predators—for example, lions, leopards, hyenas, cheetahs, and wild dogs—with lions representing the primary threat. Zebras counter these threats through one of two strategies:

1. If the threat is a lion, the zebra attempts to escape.
2. If the predator is of another species, particularly a smaller one, the zebra would choose to confront and frighten it.

The two strategies are expressed mathematically in (14), and the updating condition is given as (15):

$$x_{(ij)}^{new,P_2} = \begin{cases} S_1 : x_{(ij)} + R(2r - 1) \cdot \left(1 - \frac{t}{T}\right), P_s \leq 0.5 \\ S_2 : x_{(ij)} + r(AZ_j - I \cdot x_{(ij)}), \text{ else,} \end{cases} \quad (14)$$

$$X_i = \begin{cases} X_i^{new,P_2}, & F_i^{new,P_2} < F_i; \\ X_i, & \text{else,} \end{cases} \quad (15)$$

where S_1 corresponds to the lion-threat scenario, S_2 corresponds to the other-predator scenario, X_i^{new,P_2} denotes the new position of the i^{th} zebra for phase 2, $x_{(ij)}^{new,P_2}$ denotes its j^{th} dimension, F_i^{new,P_2} denotes its objective function value, t denotes the current step number, T denotes the total number of iterations (maximum number of iterations), R denotes a constant equal to 0.01, P_s denotes the probability of selecting a strategy, generated randomly in the interval $[0, 1]$, and AZ_j denotes the position of a

Table 2. SNPID coefficients

Coefficient	Direction	Value
K	Pitch	853.65
η_p	Pitch	0.0198
η_i	Pitch	0.0066
η_d	Pitch	0.0733
K	Yaw	858.19
η_p	Yaw	0.0672
η_i	Yaw	0.0047
η_d	Yaw	0.0534

randomly selected zebra designated as the attacked zebra in the j^{th} dimension.

5. RESULTS AND DISCUSSION

In this section, the PID and SNPID controllers are applied to the experimental platform. The coefficients for both controllers are tuned by the ZOA to ensure a fair comparison. Figure 3 shows the ZOA flowchart used to tune both controllers, in which the integral square error (ISE) is used as the objective function. In this study, the ISE is configured such that the ZOA minimizes the sum of the tracking errors on the pitch angle, e_p , and yaw

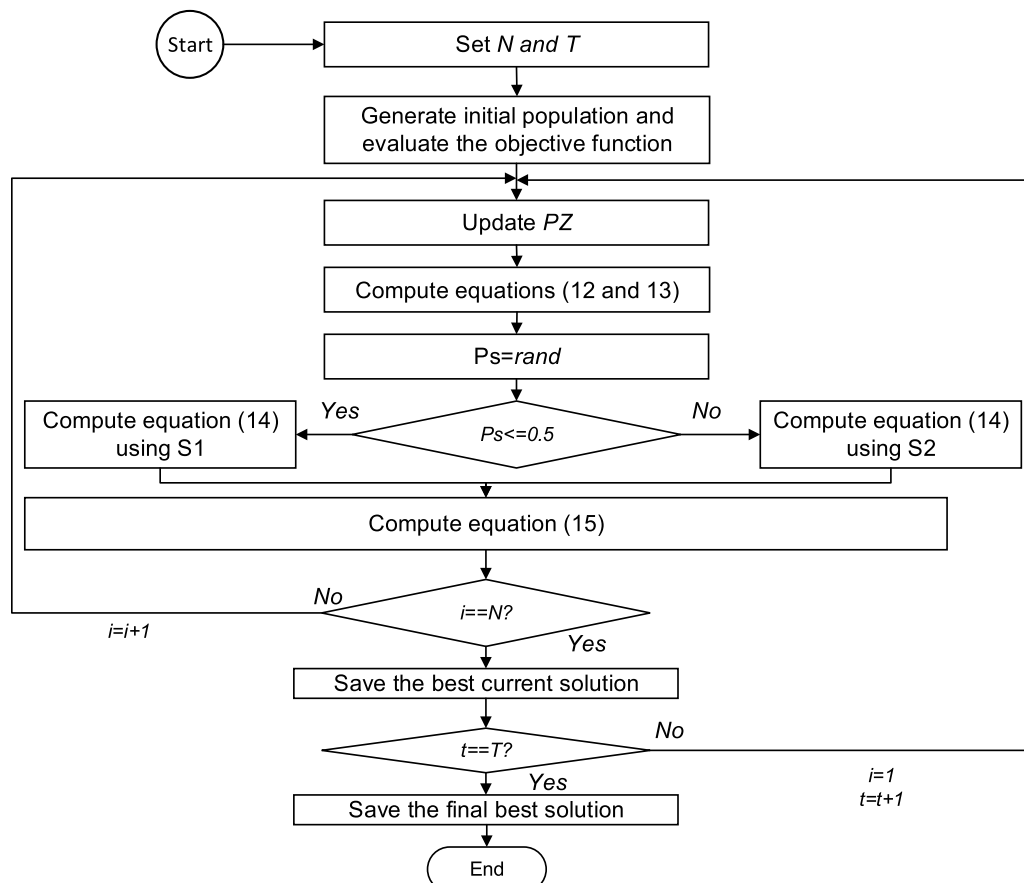


Figure 3. ZOA flowchart

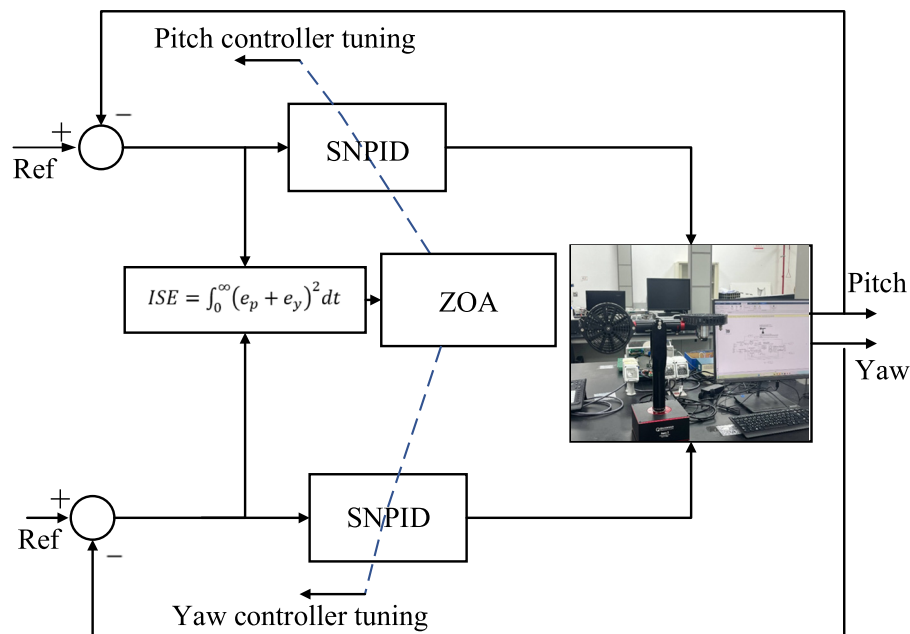


Figure 4. ISE computation

angle e_y . That is, the following ISE formulation is used: $ISE = \int_0^\infty (e_p + e_y)^2 dt$.

Figure 4 illustrates the computation of the ISE for the proposed SNPID controller. Incorporating the total error in the pitch and yaw angles into the objective function implies that the ZOA must reduce the total error while accounting for the coupling effects. The system parameters and simulations were implemented using MATLAB R2024a. The ZOA optimization was performed offline; the resulting controller parameters were then used to obtain real-time results online.

5.1. Turing Coefficients. The PID coefficients (K_p , K_i , and K_d) were first optimized using the ZOA with $N = 100$ and $T = 30$. Figure 5 shows the convergence curve for the optimization process. The optimized coefficient values for both the pitch and yaw directions are listed in Table 1. To ensure a fair comparison, the optimized PID coefficients were used as initial values in the SNPID controller, the remaining coefficients (K , η_p , η_i and η_d), were then optimized using the same algorithm. The

resulting ISE convergence curve is shown in Figure 6, and the corresponding coefficient values are presented in Table 2.

5.2. Experiments. In this experiment, the 2-DOF helicopter platform was used, as shown in Figure 1 (a), and the system was tasked with tracking a sinusoidal reference function. Figure 7 (a) and Figure 7 (b), show the pitch and yaw angle responses, respectively, with time on the x -axis. The SNPID controller achieves an ISE of 4.7101×10^{-4} compared with 5.7751×10^{-4} for the PID controller, demonstrating superior reference tracking.

Figure 7(c) and Figure 7(d) show the corresponding control signals; it is observed that the SNPID controller maintains a more consistent control signal, whereas the PID controller exhibits a more aggressive signal with larger oscillations. This suggests that the PID controller is more susceptible to noise than the SNPID controller, confirming that the SNPID controller is more stable in noisy environments. Similar performance was observed when the reference amplitude was increased to 30° : the ISE for the SNPID

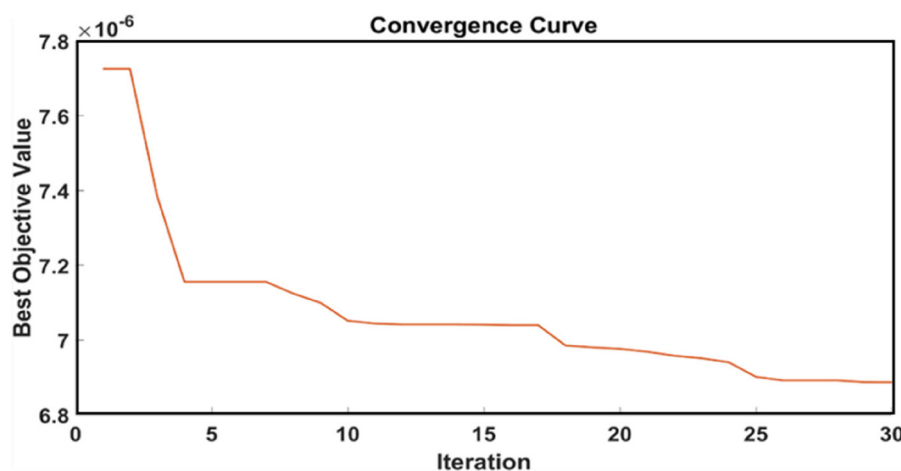


Figure 5. Integral square error of the Zebra Optimization Algorithm for PID coefficient tuning

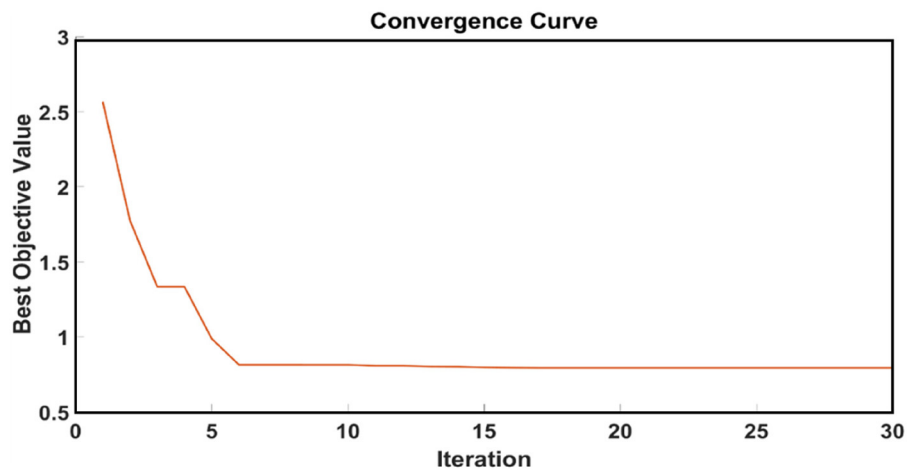


Figure 6. Integral square error of the Zebra Optimization Algorithm for SNPID coefficient tuning

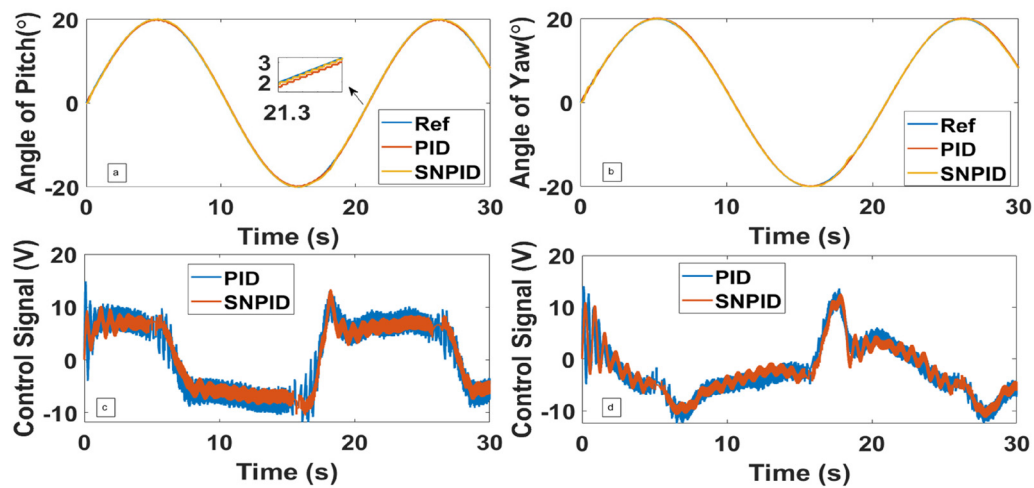


Figure 7. Sinusoidal reference tracking with an amplitude of 20° and a frequency of 0.05 Hz: (a) pitch response; (b) yaw response; (c) control signal for pitch; and (d) control signal for yaw

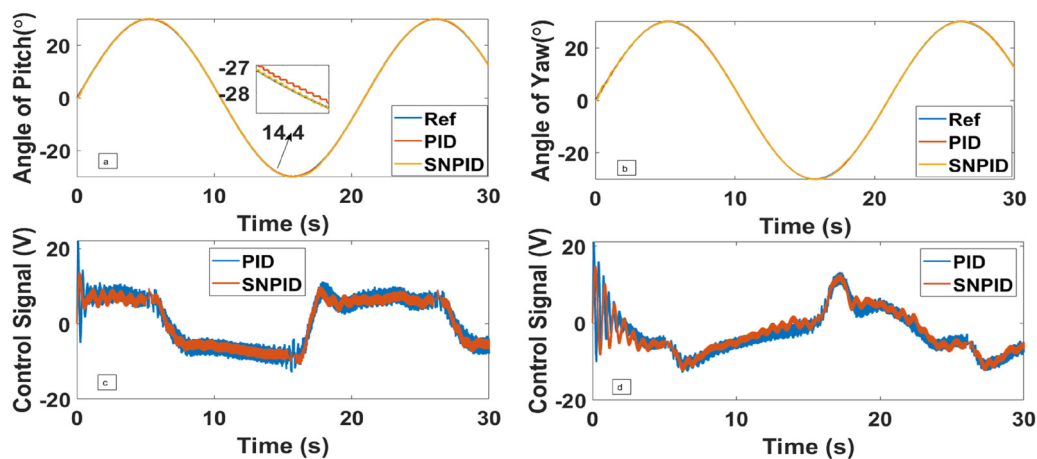


Figure 8. Sinusoidal reference tracking with an amplitude of 30° and a frequency of 0.05 Hz: (a) pitch response; (b) yaw response; (c) control signal for pitch; and (d) control signal for yaw

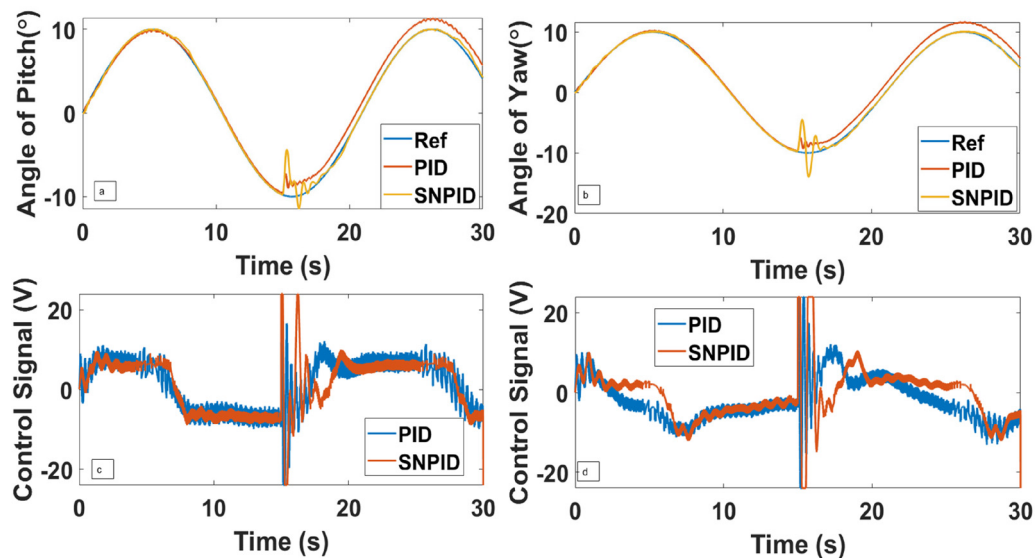


Figure 9. Sinusoidal reference tracking with an amplitude of 10° and a frequency of 0.05 Hz, subject to an internal disturbance in pitch and yaw with a magnitude of 10° : (a) pitch response; (b) yaw response; (c) control signal for pitch; and (d) control signal for yaw

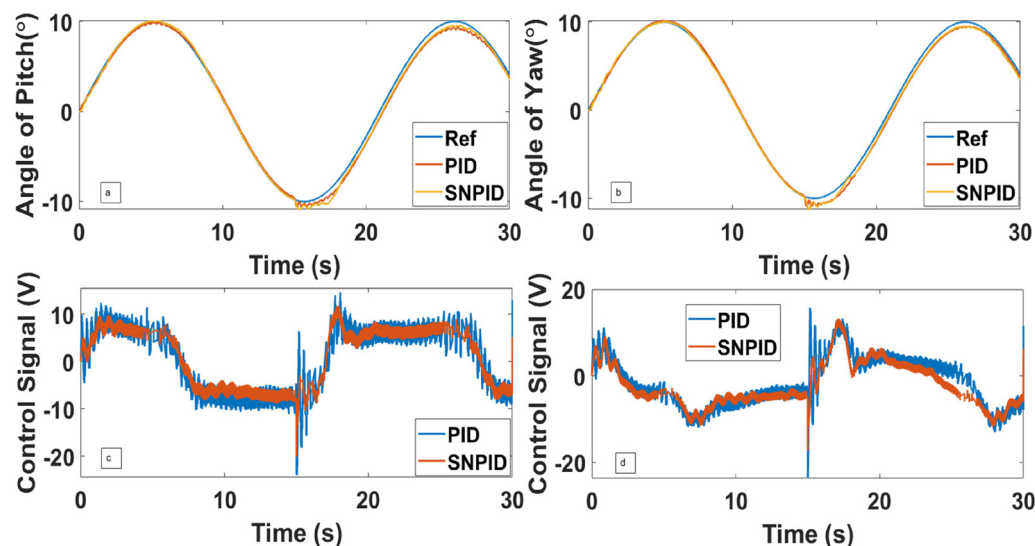


Figure 10. Sinusoidal reference tracking with an amplitude of 10° and a frequency of 0.05 Hz, subject to an external disturbance in yaw with a magnitude of 0.01 V: (a) pitch response; (b) yaw response; (c) control signal for pitch; and (d) control signal for yaw

controller was 5.4964×10^{-4} compared with 6.3272×10^{-4} for the PID controller. The SNPID controller continued to demonstrate the greatest stability and lowest tracking error, as shown in Figure 8.

Figure 9 presents results for a sinusoidal reference signal with an amplitude of 10 subject to an internal disturbance introduced at $t = 15$ s and persisting to the end of the trial. The ISE for the SNPID controller is 0.0075 compared with 0.018 for the PID controller, representing a substantially lower tracking error. When the disturbance was applied, the PID controller failed to return to the reference signal. By contrast, the proposed SNPID controller immediately rejected the disturbance and recovered the reference signal.

Figure 10 presents results for a sinusoidal reference signal with an amplitude of 10 subject to an external disturbance introduced at $t = 15$ s and persisting to the end of the trial. The ISE for the SNPID controller is 5.5053×10^{-4} compared with $6.1735 \times$

10^{-4} for the PID controller. When the disturbance was applied, the SNPID controller remained stable and provided more accurate tracking than the PID controller, as confirmed by the ISE values. However, neither controller fully recovered the original reference signal.

6. CONCLUSIONS

This study evaluated the performance of the SNPID controller in controlling an aerodynamic MIMO system. The results demonstrate that the SNPID controller exhibits a superior ability to track the reference signal in MIMO systems and to recover tracking after a disturbance, compared with the PID controller. These findings confirm the applicability of the proposed controller to MIMO systems in industrial applications, owing to its simple structure, making it a strong and practical competitor to the conventional PID controller. However, the selection of the initial

weights affects the performance of SNPID. Therefore, future work will focus on developing methods to reduce this effect or to design these weights optimally.

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Experimental Modeling and Control of a DC Servo Motor Based on System Identification: A Comparative PID with Policy Iteration

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ABSTRACT

Direct current (DC) servo motors are essential in industrial automation and robotics, where precise position and speed control are critical; however, they require high-performance control strategies. This study investigates an experimental framework for the modeling and control of a DC servo motor using system identification and quantitatively compares a traditional Ziegler–Nichols (ZN)-tuned proportional-integral-derivative (PID), a traditional linear quadratic regulator (LQR), and the proposed adaptive policy iteration on an identified model. A second-order transfer function derived from the closed-loop step-response data showed good agreement with the measured dynamics. Experimental results indicated that the real-time PID controller achieved the fastest rise time but exhibited a larger overshoot and weaker robustness to parameter variations compared with other strategies. The optimal LQR design provided improved damping and stability margins, significantly reducing the overshoot at the cost of a slightly slower response. The proposed adaptive-policy-iteration approach demonstrated superior adaptability, convergence of online near-optimal gains, reduced control effort, and improved trajectory tracking under varying conditions. The findings present the system-identification framework as a practical solution for deriving accurate models for industrial servo motors. Additionally, this study highlights trade-offs in tracking performance; the proposed adaptive policy iteration improves the transient response compared to traditional PID and LQR methods, but at the cost of a slightly increased overshoot.

Keywords: Direct current servo motor, proportional-integral-derivative controller, linear quadratic regulator controller, policy iteration, system identification

1. INTRODUCTION

Owing to their excellent controllability, wide speed range, and predictable dynamic behavior, direct current (DC) servo motors are indispensable in modern industrial automation, robotics, and precision mechatronic systems. DC motors have been effectively deployed in demanding applications, including robotic manipulators, computer-numerical-control machining centers, and aerospace actuation systems. These applications necessitate both the accurate mathematical modeling of motor dynamics and the design of high-performance control strategies that can achieve precise tracking, disturbance rejection, and robust operation under varying conditions.

Proportional-integral-derivative (PID) controllers remain the most widely adopted solution in the industry because of their simplicity and ease of implementation¹. However, PID controllers are limited by their sensitivity to system-parameter changes and suboptimal transient performance under varying operating conditions². Recent studies have explored advanced tuning techniques, including genetic algorithms, particle-swarm optimization (PSO), fuzzy logic, and machine learning-based adaptive PID schemes, to overcome these drawbacks and enhance robustness^{3–8}.

Parallel to PID advancements, optimal control methods, such as linear quadratic regulators (LQRs), have gained prominence owing to their systematic design approach, which minimizes the quadratic cost function to balance state regulation and control effort. LQR controllers offer superior damping and robustness compared with PID controllers, making them suitable for high-precision applications. Recent studies have demonstrated the integration of LQRs with embedded platforms and hybrid designs that combine LQRs with disturbance observers for improved resilience^{9–12}.

The latest developments in motor control involve adaptive and learning-based strategies, particularly reinforcement learning (RL) and policy-iteration algorithms. These approaches enable online optimization without requiring complete system models, making them highly effective in time-varying and uncertain environments. Policy iteration-based adaptive controllers have shown promising results in achieving near-optimal performance while reducing control effort and improving trajectory tracking^{13–15}. Furthermore, deep RL techniques have demonstrated adaptability and fault tolerance in complex motor-control tasks, bridging the gap between theoretical optimality and practical implementation^{16,17}.

In addition to learning-based strategies, recent studies have demonstrated the effectiveness of metaheuristic optimization for the proportional-integral (PI) control of DC-motor drives. Aldhaif Allah and Mohamed proposed an adaptive-velocity PSO scheme for the offline tuning of the cascaded PI controllers of a permanent-magnet DC-motor drive in light electric vehicles, achieving improved transient behavior and reduced steady-state errors compared with classical PSO-based tuning¹⁸. Motivated by this approach, the present study complements optimization-based tuning by combining the experimental system identification of a laboratory DC servo motor with a unified comparison of a Ziegler–Nichols (ZN)-tuned PID baseline, traditional LQR design, and the proposed online policy-iteration controller under same identical plant dynamics. The present study offers an analysis among three control techniques: (i) ZN-tuned PID, (ii) LQR, and (iii) adaptive policy iteration, assessed using an identified transfer-function model of an experimental DC servo motor to overcome the aforementioned restrictions. The controls are developed and evaluated under the same specified conditions and uniform reference situations, which facilitates an equitable and replicable evaluation of tracking performance and control effort, while accurately representing the operations of a realistic laboratory plant using information-driven models.

1.1. Research Gap and Contributions. Despite the extensive literature on DC-motor control, several research gaps remain:

- Limited comparative analysis: Few studies have provided rigorous experimental comparisons of the classical, optimal, and adaptive-control methods on the same hardware platform under identical operating conditions.
- Theory-practice gap: Many advanced control methods have been validated only in simulations and lack experimental verifications that account for real-world nonlinearities, measurement noise, and hardware constraints.
- Educational accessibility: Advanced control techniques are often presented with mathematical complexities that limit their adoption in undergraduate laboratories despite their practical utility.

This study makes the following novel contributions to the literature to address these research gaps:

1. Comprehensive experimental framework: Development of a complete experimental methodology for DC servo-motor system identification and control design using standard laboratory equipment accessible to undergraduate and graduate control laboratories.
2. A data-driven input-output model of the considered DC motor is extracted and adopted as a unified test plant for regulator synthesis and comparative analysis.
3. Three control strategies (PID, LQR, and the proposed adaptive policy iteration) are designed, compared, and evaluated under identical conditions to enable a meaningful performance comparison.
4. Detailed methodology: Step-by-step procedures are provided for system identification, controller design, and experimental implementation, making the work reproducible and pedagogically valuable.

1.2. Paper Organization. The remainder of this paper is organized as follows. The mathematical model of the DC servo motor is introduced in Section 2. The traditional control strategies used for comparison are presented in Section 3, including the traditional PID controller with ZN analytical tuning and the traditional LQR controller. Subsequently, the proposed adaptive LQR control based on policy iterations is described in Section 4. The experimental setup, data-acquisition procedure, and system identification used to derive the motor transfer-function model are discussed in Section 5. Section 6 presents a simulation study that provides a comparative evaluation of the traditional PID, traditional LQR, and proposed adaptive controllers using the identified model. Section 7 concludes the paper.

2. DC-MOTOR MATHEMATICAL MODEL

The electrical dynamics of a permanent-magnet DC motor in an armature-control configuration are governed by the armature-circuit equation, while the mechanical dynamics follow Newton's second law applied to the rotor. Under the common assumption that the electrical time constant is considerably smaller than the mechanical time constant, the motor dynamics from the input voltage $V(s)$ to the output position $\theta(s)$ can be approximated by a second-order transfer function:

$$\frac{\theta(s)}{V(s)} = \frac{k_m}{s(\tau_m s + 1)}, \quad (1)$$

where $\theta(s)$, $V(s)$, k_m , and τ_m are the output position, input voltage, motor-torque constant, and motor time constant, respectively.

Equation (1) represents a second-order system with one pole at the origin (owing to the integration from the velocity to the position) and one pole in the left half-plane. The standard second-order transfer-function form is:

$$T(s) = K \frac{\omega_n^2}{s^2 + 2\omega_n \zeta s + \omega_n^2}, \quad (2)$$

where ω_n , ζ , and K are the natural frequency, damping ratio, and DC gain, respectively.

3. TRADITIONAL CONTROL STRATEGY

This section reviews the conventional control strategies employed in this study to provide a clear baseline for comparison with the proposed method. Specifically, the traditional PID controller (including its control law and ZN analytical tuning) and LQR controller are presented as conventional benchmarks for DC servo-motor position control.

3.1. Traditional PID-Controller Design and Implementation. Traditional PID control remains one of the most widely deployed feedback-control strategies in industrial practice owing to its simple structure and ease of implementation. This section presents the design and tuning of the traditional PID controller for the DC servo motor, including the PID control law and ZN analytical-tuning approach. The corresponding experimental implementation and performance evaluation are presented in Section 5.

3.2. Traditional PID-Control Theory. The traditional PID controller computes a control signal $u(t)$ based on the tracking error $e(t) = r(t) - y(t)$, where $r(t)$ is the reference (setpoint) and $y(t)$ is the measured output. The control law comprises three components with distinct roles:

$$u(t) = K_p e(t) + K_i \int_0^t e(t) dt + K_d \frac{de(t)}{dt}, \quad (3)$$

where, K_p , K_i , and K_d are the proportional, integral, and derivative gains, respectively.

The challenge in PID-controller design is selecting the three gains (K_p , K_i , K_d) to achieve the desired balance among the competing performance objectives: fast rise time, minimal overshoot, short settling time, and zero steady-state error.

3.2.1. Traditional ZN analytical tuning. Although manual tuning provides valuable insights, it is time-consuming and dependent on operator experience. The traditional ZN method offers a systematic analytical approach for determining PID gains based on either open-loop step-response characteristics or closed-loop stability margins.

This approach determines the ultimate gain K_u (the proportional gain that produces sustained oscillations) and ultimate period T_u (the oscillation period at the stability boundary). The PID gains are computed as follows:

$$K_p = 0.6K_u, K_i = \frac{2K_p}{T_u}, K_d = \frac{K_p T_u}{8}. \quad (4)$$

Modern optimal control is formulated in the state-space framework, where the system dynamics are defined as follows:

$$\dot{x}(t) = Ax(t) + Bu(t) \quad (5)$$

$$y(t) = Cx(t) + Du(t). \quad (6)$$

For the DC servo motor, the state vector $x = [x_1 \ x_2]^T$ comprises the position (x_1) and velocity (x_2), and A , B , C , and D are the system matrices. The traditional LQR problem seeks a state-feedback control law:

$$u(t) = -Kx(t) \quad (7)$$

that minimizes the infinite-horizon quadratic cost function:

$$J = \int_0^\infty (x^T Q x + u^T R u) dt, \quad (8)$$

where $Q \geq 0$ is a symmetric positive semi-definite state-weighting matrix, and $R > 0$ is a scalar control-weighting parameter. Matrix Q penalizes state deviations (a large Q forces states to remain near zero), whereas R penalizes control effort (a large R encourages smaller control signals).

4. PROPOSED ADAPTIVE LQR CONTROL (POLICY ITERATION)

The traditional LQR design provides a systematic approach to compute an optimal state-feedback gain when an accurate model of the plant is available. To improve adaptability under modeling uncertainty or changing operating conditions, this section

presents the proposed adaptive-policy-iteration approach, which learns an approximately optimal feedback gain online for a continuous-time LQR problem.

In contrast to traditional control methods, optimal control optimizes the performance index during the control process while achieving the control goal. For optimal control design, a critical step is to resolve the derived optimal control equation, for example, the algebraic Riccati equation (ARE) or Hamilton–Jacobi–Bellman (HJB) equation. In this section, we develop a policy-iteration algorithm to solve the LQR problem online without using knowledge of the internal dynamics of this system. A flowchart of the algorithm is presented in Figure 1. For further information and the proof of this algorithm, please refer to the previous study¹⁴.

Considering the linear time-invariant dynamical system described by Eqs. (5)–(6), and the quadratic cost function to be minimized, as expressed in Eq. (8), the solution to this optimal control problem, determined by Bellman’s optimality principle, is given by Eq. (7), with:

$$K = R^{-1} B^T P. \quad (9)$$

K is obtained after P , where matrix P is obtained by solving the ARE:

$$A^T P + PA - PBR^{-1}B^T P + Q = 0. \quad (10)$$

We now develop a policy-iteration algorithm. Let K be a stabilizing gain for Eq. (5), and assume (A, B) is stabilizable, such that $\dot{x} = (A - BK)x$ is a stable closed-loop system. The corresponding cost function is given by

$$J = \int_0^\infty (x^T Q x + u^T R u) dt = x^T P x \quad (11)$$

and satisfies the HJB equation:

$$x^T Q x + u^T R u + \frac{\partial J}{\partial x} (Ax + Bu) = 0. \quad (12)$$

Substituting $J = x^T P x$ and $u = -Kx$:

$$x^T (Q + K_i^T R K_i + (A - BK)^T P_i + P_i (A - BK_i)) x = 0. \quad (13)$$

For a given K_i , a Lyapunov equation is used to solve for P_i :

$$(A - BK_i)^T P_i + P_i (A - BK_i) = -(K_i^T R K_i + Q). \quad (14)$$

The control law is updated as follows:

$$K_{i+1} = R^{-1} B^T P_i. \quad (15)$$

This approach is repeated until convergence:

$$K_{i+1} \approx K_i \Rightarrow K^* = R^{-1} B^T P^*. \quad (16)$$

From a computational perspective, the proposed adaptive-policy-iteration approach is lightweight because it operates on a low-order linear state-space model and relies on matrix operations of small dimensions. Unlike actor–critic or deep reinforcement-learning methods, which require function approximation and extensive training data, the policy-iteration algorithm updates the control gain through iterative solutions of Lyapunov-type equations. Thus, this algorithm is suitable for

real-time implementation on standard control hardware. Stability and safety during online learning are ensured by initializing the algorithm with a stabilizing feedback gain and performing incremental policy updates without injecting random exploration signals into the control input. Consequently, the closed-loop system remains stable throughout the learning process while gradually improving its performance. Compared with modern learning-based controllers, the proposed policy-iteration method offers a transparent and computationally efficient alternative for linear systems, making it particularly attractive for safety-critical applications that require stability, interpretability, and predictable behavior.

5. EXPERIMENTAL SYSTEM IDENTIFICATION

Accurate mathematical modeling is a prerequisite for systematic controller design. This section describes the experimental apparatus, data-acquisition procedures, and system-identification methodology employed to derive the transfer-function model of a DC servo motor from laboratory measurements. This section also summarizes the experimental closed-loop responses used to support controller tuning and validation.

5.1. Experimental Setup and Equipment. The experiments were conducted at the Control Systems Laboratory of King Fahd University of Petroleum and Minerals. The experimental apparatus comprised a complete servo-motor training system with integrated position- and velocity-measurement capabilities. Table 1 summarizes the key hardware components.

The DCM150F servo motor was a permanent-magnet DC motor with armature control, which is typical of the configuration used in laboratory servo trainers. The armature voltage of the motor served as the control input, the angular position was measured using a potentiometer, and the angular velocity was obtained from the tachogenerator output. The SA150D servo amplifier provided power amplification with current-limiting protection.

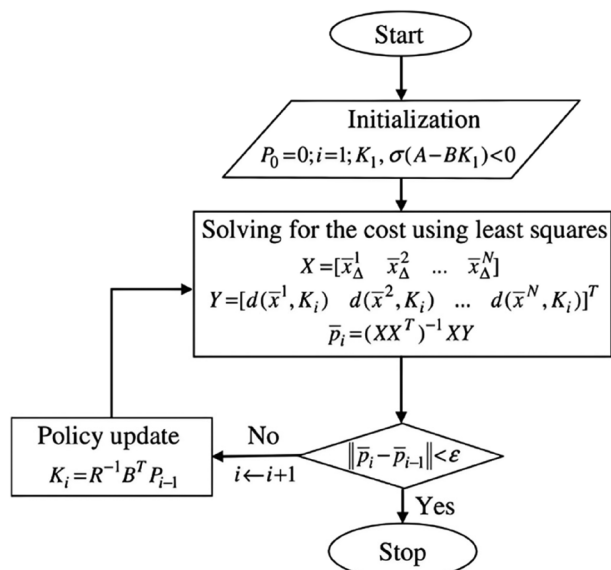


Figure 1. Continuous-time linear policy-iteration algorithm¹⁴

The closed-loop experimental configuration is illustrated in Figure 2. The system implemented position feedback control, in which the reference position (setpoint) was compared with the measured output position to generate an error signal. This error signal passed through the control elements (initially configured as a simple proportional gain for system identification) before being amplified and applied to the motor armature. A closed-loop configuration was essential for stable operation and enabled the investigation of both open-loop motor dynamics and closed-loop system behavior.

To gain an intuitive understanding of the additional PID action and to validate the physical-system behavior, a manual tuning experiment was conducted using the PID150Y hardware unit shown in Figure 3, which was integrated into the servo trainer. This unit provided an independent adjustment of the proportional, integral, and derivative gains using front-panel potentiometers.

5.2. Data-Acquisition Procedure. For system identification, a step-input experiment was designed to excite the dominant system dynamics while maintaining operation within the linear region. The systematic procedure steps are illustrated in Figure 4.

5.3. System Identification: Transfer Function. The DC motor was subjected to step inputs under a closed-loop position control. The experimental apparatus utilized standard laboratory hardware, and all signals were logged using a MATLAB interface. The experiment was repeated thrice to ensure repeatability and to assess measurement consistency. The identified dynamic parameters exhibited minimal variation across the trials, indicating stable system behavior within the operating region. The resulting second-order model was validated by comparing its simulated step response with the experimental data, showing close agreement in the rise time, settling time, and overshoot.

Figure 5a shows a representative step response obtained from the closed-loop system, displaying both the input voltage step and the resulting output position trajectory. Critical dynamic parameters were extracted from this step response and are summarized in Table 2.

From these values, the following second-order transfer function was obtained:

$$T(s) = \frac{6.543}{s^2 + 4.743s + 6.543} \quad (17)$$

The identified system model guided the implementation of standard PID controllers using hardware (PID150Y module) and MATLAB simulations. The experimental tuning followed a classical sequential approach:

- **Case 1 – Proportional Control Only (P):**

Starting with $K_i = 0$ and $K_d = 0$, the proportional gain gradually increased from zero until the closed-loop response exhibited a reasonable speed with an acceptable overshoot. Figure 5b shows the resulting step response.

- **Case 2 – Proportional-Integral Control (PI):**

To maintain the proportional gain from Case 1, an integral action was introduced by slowly increasing K_i from zero. The integral gain was adjusted to eliminate the steady-state error observed

Table 1. Servo-Motor Components

Component Number	Component Name	Model/Type
1	Servo amplifier	SA150D, Feedback Instruments, England
2	Servo motor	DCM150F, Feedback Instruments, England
3	Power supply	PS150E, Feedback Instruments, England
4	Attenuator unit	AU150B, Feedback Instruments, England
5	Operational amplifier	OU150A, Feedback Instruments, England
6	Tachometer	GT150X, Feedback Instruments, England
7	Pre-amplifier unit	PA150C, Feedback Instruments, England
8	Output angular potentiometer	OP150K, Feedback Instruments, England
9	Input angular potentiometer	IP150H, Feedback Instruments, England
10	Data-acquisition system	National Instruments DAQ, National Instruments, US
11	Software environment	MATLAB R2023b, MathWorks, US

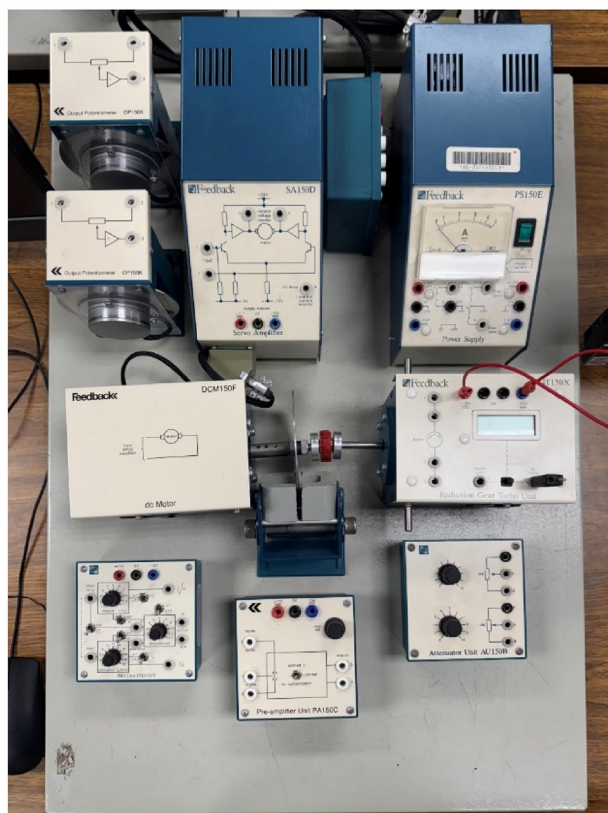
in the P controller while monitoring for excessive overshoot or oscillations. Figure 5c presents the improved response.

• Case 3 – Full PID Control:

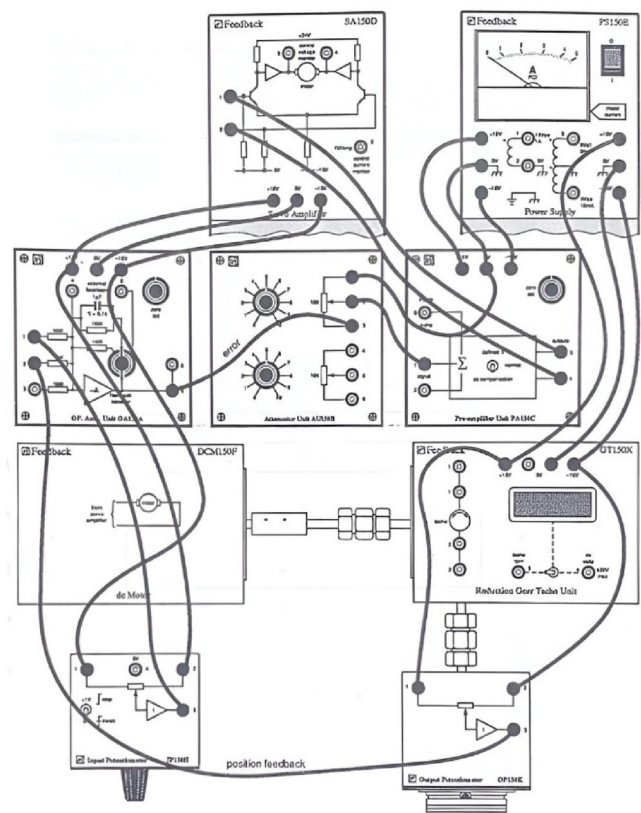
With the P and I gains fixed from Case 2, a derivative action was added by increasing K_d from zero. The derivative gain was tuned to reduce overshoot and improve damping without introducing excessive noise sensitivity. Figure 5d shows the final PID response.

Table 3 presents the performance characteristics extracted from each experimental configuration.

The experimental-tuning results indicate distinct performance characteristics for P, PI, and PID controllers. The P controller achieved the fastest rise time but exhibited a significant overshoot (14.73%) and a small steady-state error, confirming its ability to provide rapid corrective action without eliminating offsets. The PI controller successfully removed the steady-state error and reduced the overshoot. However, this was at the cost of slightly slower rise and settling times, reflecting the tradeoff introduced by the integral action. In contrast, the PID controller delivered the best overall performance, combining zero steady-state error with minimal overshoot (2.52%) and the shortest settling



(a)



(b)

Figure 2. Closed-loop position experiment: (a) experiment components, (b) experimental setup

Table 2. Summary of Experimentally Obtained System Parameters

Parameter	Symbol	Value	Units
Peak time	T_p	1.241	s
Settling time (2%)	T_s	1.687	s
Rise time (10%–90%)	T_r	1.033	s
Percent overshoot	PO%	4.279	%
Damping ratio	ζ	0.927	—
Natural frequency	ω_n	2.558	rad/s
DC gain	K	1.00	—

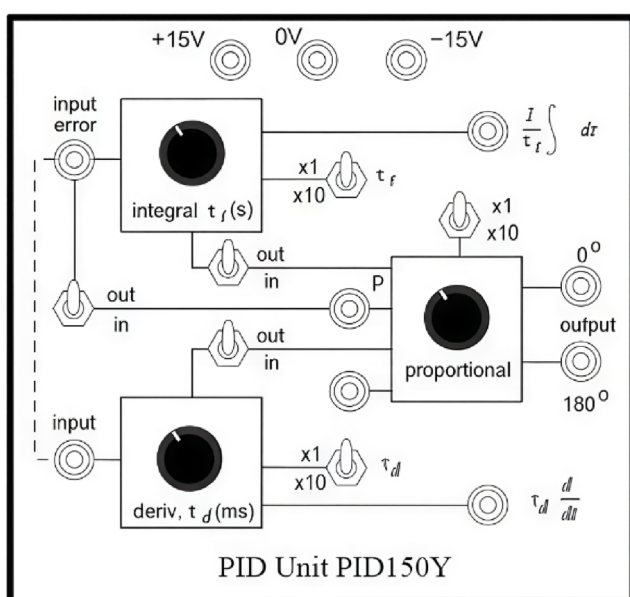
time, demonstrating the effectiveness of the derivative action in enhancing system stability and damping.

6. SIMULATION STUDY

Using the experimentally identified plant model, MATLAB simulations were conducted to compare the traditional PID controller using the ZN method, the traditional LQR controller, and the proposed adaptive-policy-iteration controller.

6.1. Traditional PID Control. This subsection evaluates the traditional PID controller in a simulation using the experimentally identified transfer-function model. The PID gains were determined using the ZN method, and the resulting closed-loop step response was used as a baseline for comparison with the traditional LQR and proposed adaptive controllers.

The ultimate gain and period can be computed for the identified system with $\omega_n = 2.558$ rad/s and $\zeta = 0.927$ from the stability analysis. By applying the Routh–Hurwitz criterion to the closed-loop characteristic equation with proportional gain only, a stability boundary occurred at $K_u = 3.33$, corresponding to $T = 2$ s. Figure 6 shows the simulated step responses for the P, PI, and PID controllers tuned using the ZN method. These responses closely matched the experimental results shown in Figure 5,

**Figure 3.** Front panel and signal terminals of the PID-controller module (PID150Y)

validating both the identified model and tuning methodology. Notably, the aggressive transient behavior observed in the experimental and simulated responses in Figure 5b–d and Figure 6, including the fast rise time and noticeable overshoot, is consistent with the characteristics of ZN-based tuning. This behavior reflects the intentional design philosophy of the ZN rules, which prioritizes rapid responses at the expense of reduced robustness margins. The close agreement between the experimentally observed responses and expected ZN behavior further validates the correctness of the experimental setup and tuning implementation. Table 4 lists the gains obtained for the three controllers (P, PI, and PID).

6.2. Traditional LQR Control. The state-space representation of the identified transfer function can be expressed in the following controllable canonical form:

$$\dot{x} = \begin{bmatrix} 0 & 1 \\ -6.543 & -4.743 \end{bmatrix} x + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u \quad (18)$$

$$y = [6.543 \ 0]. \quad (19)$$

Utilizing the state-space system from Eq. (18), an LQR was designed to minimize the cost function, balancing the state deviations and control effort:

$$Q = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}, R = [0.5] \quad (20)$$

Therefore, the traditional LQR cost function can be defined as follows:

$$J = \int_0^\infty (x_1^2 + 2x_2^2 + 0.5u^2) dt \quad (21)$$

Solving the Riccati equation yielded the following state feedback gain:

$$K = [3.74 \ 4.90]$$

The weighting matrices Q and R were selected based on the physical characteristics of the DC servo motor and desired closed-loop performance. The position and velocity states were weighted unequally in Q , with the velocity state x_2 assigned a higher penalty to suppress oscillations, damp rapid motion, and reduce overshoot, while maintaining accurate position tracking. The control weighting R was chosen to balance the control effort and response speed; in particular, a relatively smaller R encouraged the controller to act more aggressively, improving the rise and settling times without causing excessive actuator activity. These values were determined through iterative experimentation in MATLAB, where several combinations of Q and R were evaluated to achieve an appropriate tradeoff among the response speed, control effort, and overshoot. The effectiveness of the selected weighting matrices was reflected in the resulting time-domain response, which exhibited smooth transient behavior, improved damping, and reduced overshoot compared with the traditional PID controller. The final selection provided a fast and well-damped response with minimal steady-state error. Figure 7a shows the traditional LQR step response, and Figure 7b shows the state responses.

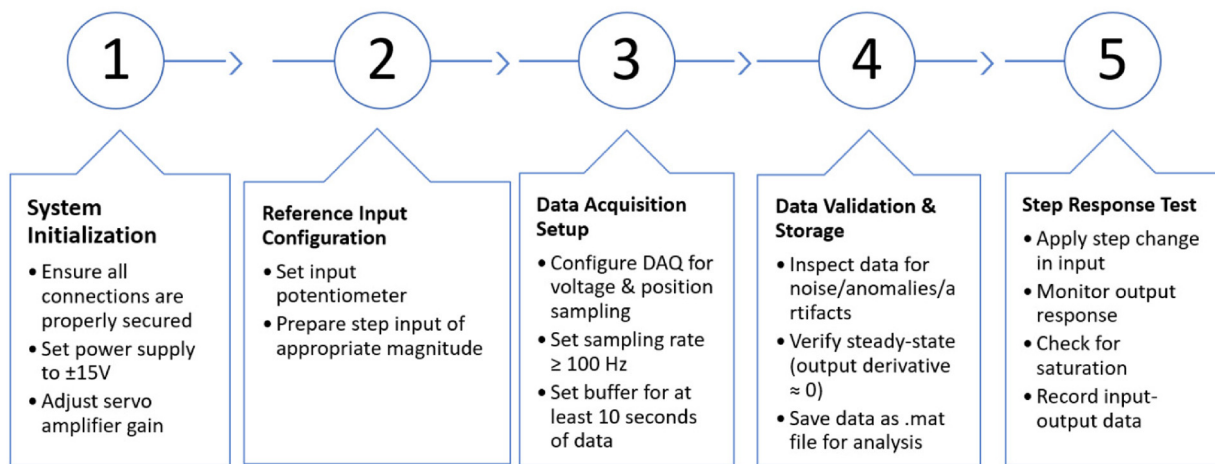


Figure 4. Steps of the systematic procedure

A continuous-time policy-iteration algorithm was implemented to achieve real-time optimality under uncertain conditions. The algorithm alternates between policy evaluation (Lyapunov-equation solution) and improvement (gain adjustment) as follows:

$$\begin{aligned}
 & (A - BK_i)^T P_i + P_i (A - BK_i) \\
 & = - (K_i^T R K_i + Q) \\
 & K_{i+1} = R^{-1} B^T P_i.
 \end{aligned} \tag{22}$$

The iterative update trajectory, cost-matrix convergence, and closed-loop pole migration are shown in Figure 8a-d. The proposed adaptive controller not only achieved LQR-level performance but also displayed a rapid adjustment capability for changing motor parameters.

Figure 9 and Table 5 provide a direct simulation-based comparison of the three control strategies: the traditional PID controller tuned using the ZN method, the traditional LQR controller, and the proposed adaptive controller. The traditional PID

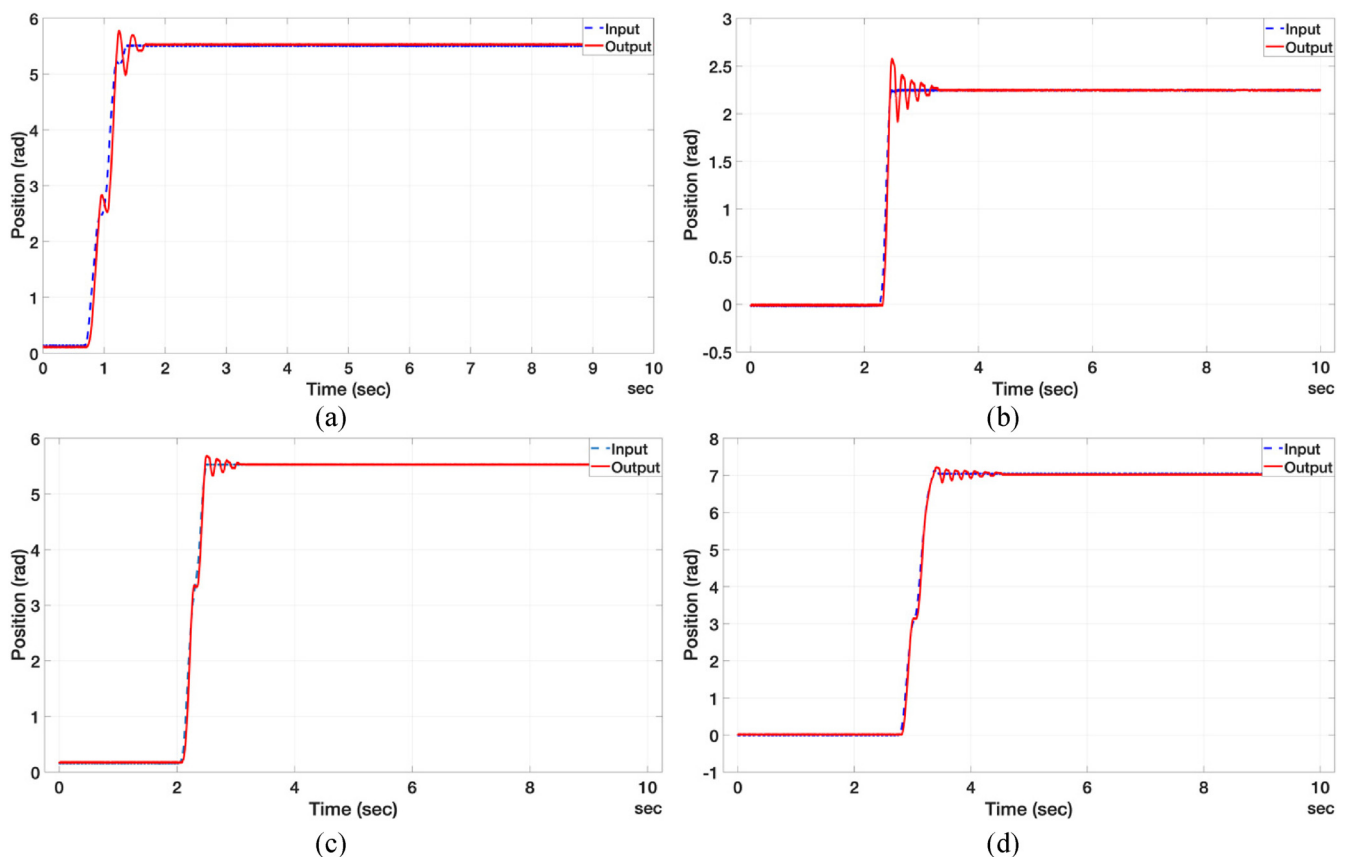
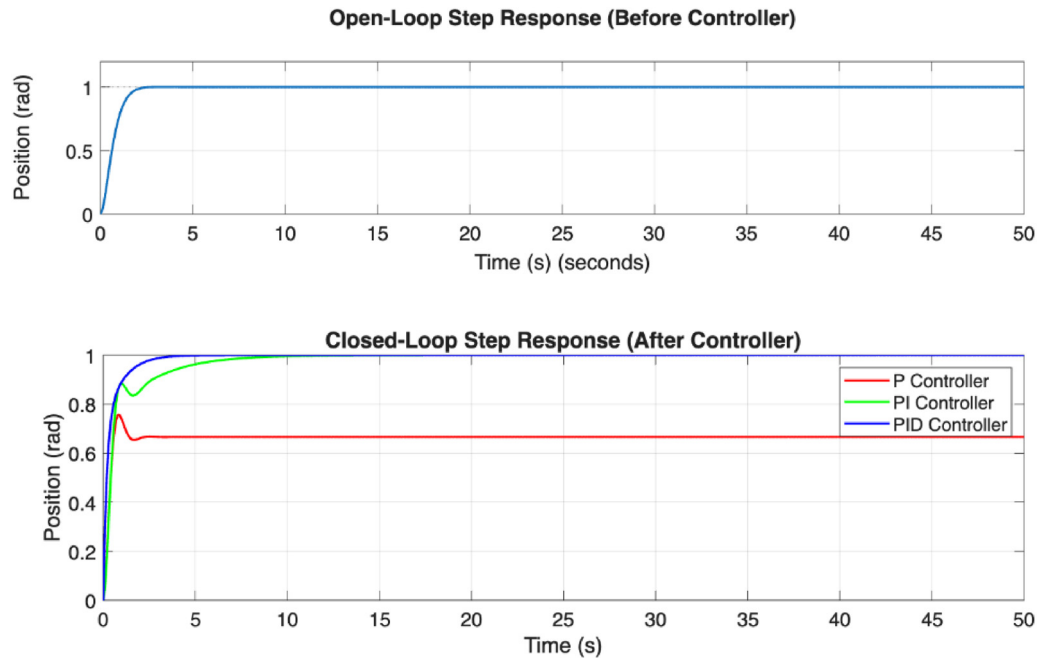


Figure 5. Experimental results with traditional PID controller: (a) step input response, (b) response with P controller, (c) response with PI controller, and (d) response with PID controller

Table 3. Summary of Experimental PID-Tuning Performance

Controller	Rise Time (s)	Settling Time (s)	Overshoot (%)	S.S. Error
P	0.132	1.016	14.7336	0.01227
PI	0.141	1.086	2.951	0
PID	0.133	0.985	2.5178	0

**Figure 6.** PID tuning with ZN method**Table 4.** ZN PID Gain Values

Controller / Gain	K_P	K_I	K_D
Case 1 (P)	2	-	-
Case 2 (PI)	1.8	1.08	-
Case 3 (PID)	2.4	2.4	0.6

ZN controller achieved a faster rise time (1.0519 s) than the traditional LQR controller (1.2984 s); however, it required a longer settling time (2.5455 s versus 2.2548 s), reflecting the typical

tradeoff between the faster initial response and damping. In contrast, the proposed adaptive controller provided the best overall transient performance, yielding the shortest rise time (1.0271 s) and settling time (1.7066 s). Compared with the traditional LQR, the proposed adaptive controller improved the rise and settling times by approximately 20.9% and 24.3%, respectively, and by approximately 2.36% and 33.0%, compared with the traditional PID ZN controller. All three controllers achieved approximately zero steady-state error, and the overshoot remained negligible (PID and LQR showed ~0% overshoot, whereas the proposed

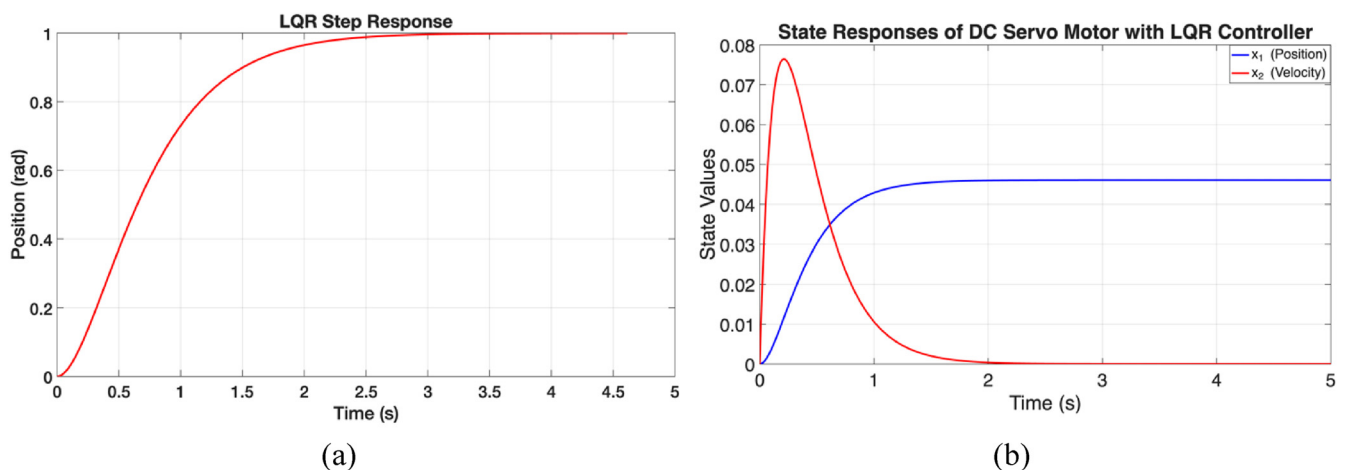
**Figure 7.** Simulation under traditional LQR: (a) step response with LQR, (b) state responses under LQR

Table 5. Performance Comparison between the Traditional PID ZN, Traditional LQR, and Proposed Adaptive LQR

Controller	Rise Time (S)	Settling Time (S)	Overshoot (%)	S.S. Error
Traditional PID ZN	1.0519	2.5455	<0.01	0
Traditional LQR	1.2984	2.2548	0	0
Proposed Adaptive	1.0271	1.7066	0.0429	0

adaptive controller exhibited a very small overshoot of approximately 0.0429%). Overall, the results confirm that the proposed adaptive strategy improved convergence speed while maintaining good damping and steady-state accuracy relative to both traditional baseline controllers.

7. CONCLUSION

This study presents a comprehensive experimental framework for DC servo-motor modeling and control using traditional PID, traditional LQR, and the proposed adaptive-policy-iteration strategy. A second-order transfer function was accurately identified from closed-loop experiments, providing a reliable basis for controller design. Comparative evaluation using the experimentally identified model revealed that PID control offers simplicity and a fast response but can be sensitive to parameter variations,

whereas LQRs achieve systematic optimality and superior damping at the cost of a slower rise time. The proposed adaptive-policy-iteration approach demonstrated the most advanced capabilities, including online gain updating and improved transient responses, making it highly suitable for time-varying systems. Overall, the results confirmed that the controller selection should align with application-specific requirements: PID for quick implementation, LQR for robust optimal performance, and adaptive methods for dynamic environments. While the proposed framework provides a comprehensive comparative evaluation, the study is limited to a single DC servo motor platform and primarily linear model-based analysis under nominal operating conditions. These limitations motivate further investigation into real-time adaptive implementation, disturbance-aware control design, and extension to nonlinear or higher-order modeling frameworks. Future work will further investigate these directions, including disturbance rejection, constraint-aware control,

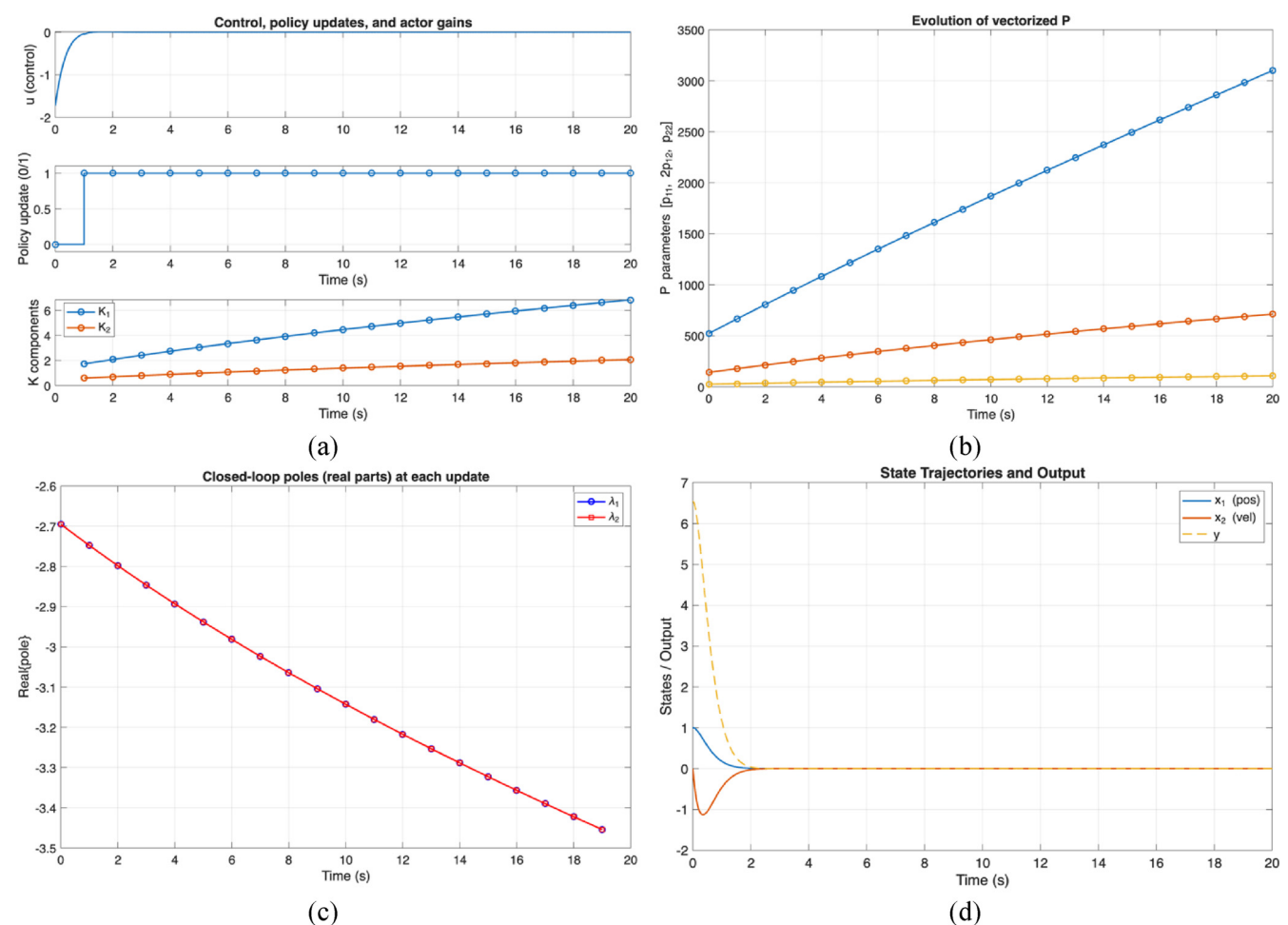


Figure 8. Proposed adaptive online LQR control: (a) control, policy updates, and actor gains, (b) evaluation of vectorized P, (c) closed loop (real parts) at each update, and (d) state trajectories and output

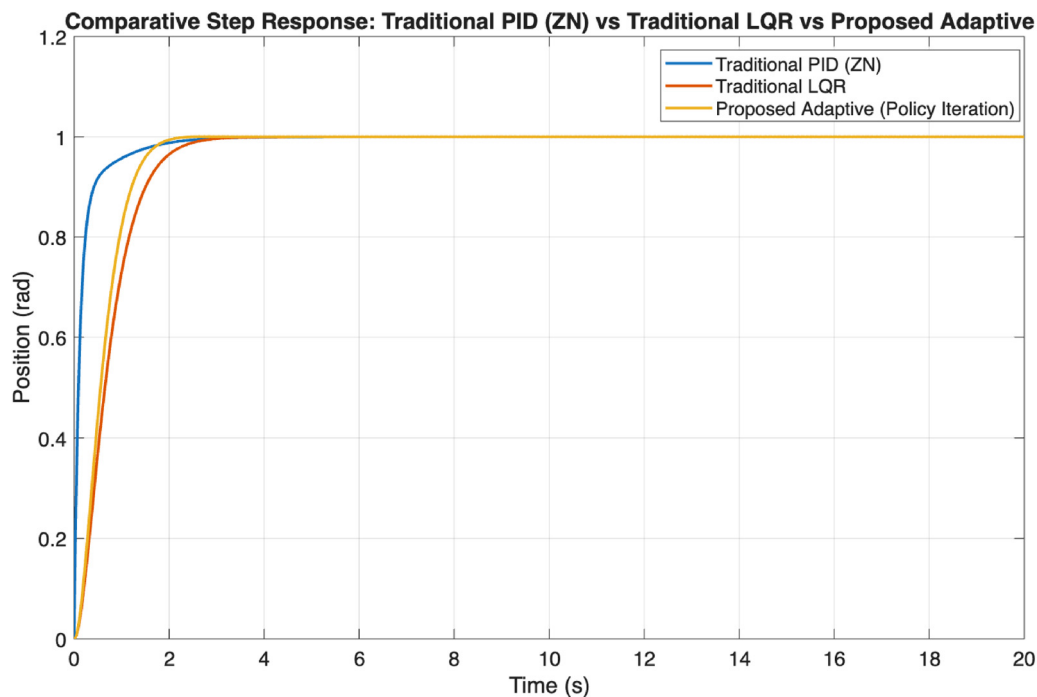


Figure 9. Comparison of all controllers: traditional PID controller tuned using ZN method, traditional LQR controller, and proposed adaptive LQR controller

and integration of reinforcement learning techniques to enhance adaptability and industrial applicability.

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Techno-Economic Optimization of a Grid-Tied Photovoltaic System for Schools in Saudi Arabia

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ABSTRACT

The educational sector in Saudi Arabia represents a significant portion of the national energy load, with government-constructed buildings accounting for approximately 13% of the total consumption, largely driven by air conditioning demands in the harsh climate of the Eastern Province. This project investigates the techno-economic feasibility of integrating a grid-tied photovoltaic (PV) system into a standard elementary school in Dammam to reduce operational costs and align with the renewable energy targets of Saudi Vision 2030.

Using HelioScope for physical design and HOMER Pro for economic optimization, a 149 kWp solar PV system was modeled for the “Al Madinah Al Munawwarah School.” Although initially modeled to evaluate hybrid configurations, the optimization demonstrated that a strictly grid-tied PV system was the most viable. The design utilized the building rooftop and football court structure to overcome space constraints, deploying 240 high-efficiency panels. The simulation results indicate that the proposed system generates sufficient energy to reduce the grid reliance of the school from 100% to 52.1%, reducing the peak demand during active academic hours.

The techno-economic analysis reveals a levelized cost of energy (LCOE) of 0.23 SAR/kWh, which is significantly lower than the governmental tariff of 0.32 SAR/kWh. The project demonstrates strong financial viability with a net present cost (NPC) reduction of 15% compared with the base case, a simple payback period of 7.5 years, and an internal rate of return (IRR) of 12.6%. Replicating this model could significantly relieve the municipal grid, validating the strategic advantage of school rooftops for decentralized generation.

Keywords: grid-tied photovoltaic, HOMER Pro, school energy profiling, distributed generation, Saudi Vision 2030, techno-economic analysis

1. INTRODUCTION

The educational sector in Saudi Arabia represents a major portion of government facilities, contributing significantly to the national energy demand. According to Alshibani¹, government-constructed buildings account for approximately 13% of the total energy consumption in Saudi Arabia. The majority of this consumption is driven by air conditioning (AC) due to the harsh hot and humid climate of the Eastern Province.

This project utilizes the “Standard Reference School” profile derived from real-world datasets of 352 operating schools to design a hybrid renewable energy system (HRES). The goal is to lower the specific energy consumption and reduce operational costs under the governmental tariff of 0.32 SAR/kWh.

1.1. Literature Review. Driven by the Vision 2030 goals, the integration of renewable energy into public facilities has gained significant traction within the Saudi Arabian research community. Recent state-of-the-art research has emphasized the necessity of decarbonizing the educational sector. Alshibani (2020) established foundational energy consumption patterns for Saudi schools and identified air conditioning as the primary

load driver, with a 97% correlation with total usage¹. Building on this, Almasri et al. (2025) conducted an updated techno-economic analysis of Saudi government schools, reporting that energy use intensity (EUI) typically ranges between 20.4 and 38.8 kWh/m²/yr, concluding that achieving “zero-bill” status is technically feasible but requires significant retrofitting².

Furthermore, state-of-the-art 2024 research in Buraidah City focused on the “zero-bill” concept for schools, finding that surplus generation during weekends and summer breaks is critical for offsetting the high costs of peak operational hours³. This is further supported by a comprehensive 2024 study by Imam et al., which validated the techno-socioeconomic feasibility of widespread solar photovoltaic (PV) integration across Saudi Arabia, emphasizing that grid-tied configurations significantly outperform off-grid setups in urban environments because of the elimination of expensive battery storage requirements⁴.

Recent optimization studies in 2025 using the HOMER Pro engine also confirmed these findings. Almohammadi and Allouhi (2025) conducted a techno-economic assessment of grid-connected solar PV systems in the Saudi building sector and established that optimized distributed generation architectures

are highly effective at lowering both the levelized cost of energy (LCOE) and greenhouse gas emissions⁵. Similarly, studies on grid-connected PV systems in other regions of Saudi Arabia have demonstrated promising economic indicators. Research conducted at Al Baha University optimized a hybrid grid/PV system to achieve a cost of energy (COE) of approximately 0.29 SAR/kWh, validating the economic advantage of renewable integration over standard grid tariffs⁶.

Despite these recent advancements, a research gap remains regarding localized, highly specific techno-economic optimization mapped to the distinct operational constraints of the Eastern Province. This project bridges this gap by proposing a grid-tied PV system explicitly tuned to this region. To achieve this goal, this study utilized statistical mean data from Alshibani¹ to establish an accurate baseline electrical load profile for a standard reference school. Building upon this baseline, HelioScope was employed to physically design and maximize the solar array output across the available rooftop area. Finally, HOMER Pro was used to conduct a rigorous techno-economic optimization aimed at minimizing the net present cost (NPC) and reducing the heavy air-conditioning consumption of the facility^{7,8}.

2. METHODOLOGY AND SYSTEM DESIGN

The design methodology bridges statistical load findings with simulation tools, utilizing the multistep workflow shown in Figure 1 to assess the technical and economic viability¹.

2.1. Site Selection and Load Assessment. All facility parameters and statistical load profiles utilized in this section were derived directly from billing data encompassing 352 public schools in the Eastern Province. The site parameters are detailed in Table 1, establishing a statistical baseline rooftop envelope of 1,524.5 m² and indicating high cooling demands. However, for the specific installation site at Al Madinah Al Munawwarah Elementary School in Dammam (latitude 26.419°, longitude 50.047°), the analysis revealed an actual usable rooftop area of approximately 1,244.8 m². This actual usable space was utilized for the physical PV array design and was aligned closely with the statistical average. The energy consumption metrics established a mean annual baseline of 410,968 kWh/yr, heavily driven by an AC capacity of 160.12 TR.

2.2. Solar Design in Helioscope. The solar PV system was designed to maximize the available 1,244.8 m² of actual usable rooftop space established in the site analysis. To minimize shading effects and avoid structural obstructions, the PV system was divided between the football court rooftop structure (160 panels) and the main school building (80 panels), as shown in Figure 2. The system utilizes 240 PV modules (Canadian Solar CS6.1-72TB-620H) and two Huawei SUN2000-65KTL-M0 inverters, with 6 mm² copper cabling to mitigate resistive losses. The system losses and technical specifications are detailed in Figures 4 and 5.

2.3. Load Profiling in HOMER Pro. An electrical load profile was constructed using HOMER Pro to reflect specific academic schedules. High-load active hours (07:00–13:00) cover classes, whereas passive hours (14:00–06:00) represent base loads when the building is unoccupied.

The annual consumption was distributed across the year to account for three critical factors:

1. **Weekly Cycles:** Consumption peaks during weekdays and drops significantly during weekends.
2. **Academic Calendar:** Consumption is drastically reduced during the summer break (July–August) when the facility is non-operational.
3. **Weather Impact:** High consumption rates are modeled during the hot summer school months owing to peak AC usage, whereas winter months reflect lower consumption owing to reduced cooling requirements.

The resulting seasonal profiles are shown in Figure 6. The key load metrics derived from this model are summarized as follows:

- **Average Daily Consumption:** 1,156 kWh/d
- **Average Load:** 48.17 kW
- **Peak Load:** 385.41 kW
- **Load Factor:** 0.12

2.4. Hybrid System Optimization in HOMER Pro. An initial comprehensive model was developed, which included a

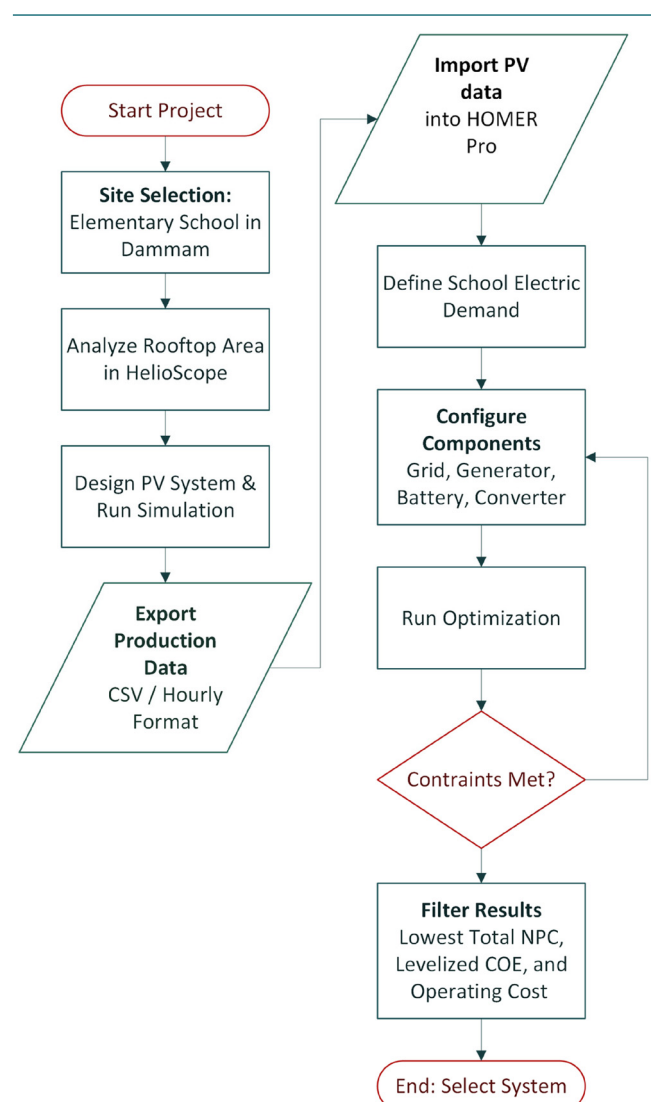


Figure 1. Hybrid system design workflow

Table 1. Standard Reference School Profile (Mean Values)

Parameter	Value	Description
Location	Eastern Province	Hot & humid climate (high latent load).
Total Built Area	4,165.6 m ²	Average gross floor area of the sample.
Total Roof Area	1,524.5 m ²	Available envelope for PV installation.
AC Conditioned Area	817.7 m ²	Only 19.6% of the school is actively cooled.
Building Age	32.8 years	Indicates prethermal code construction.
Occupancy	381 Students	Plus ~28 staff members.
Mean Annual Energy	410,968 kWh/yr	The foundational baseline for this project.
AC Capacity	160.12 TR (Tons Refrigeration)	Primary driver of load (R=0.97).
Net Energy Use Intensity (EUI)	502 kWh/m ² /yr	Calculated based on conditioned area (817 m ²).
Peak Load Driver	Cooling	Increases exponentially with consumption.
Current Tariff	0.32 SAR/kWh	Governmental rate.

utility grid, a diesel generator, battery storage, and the electrical load, as shown in Figure 7. The PV component was coupled directly to the AC bus because the imported production data accounted for the inverter efficiencies.

Although the term "hybrid energy system" was used during the initial modeling phase, the optimization constraints revealed that adding battery storage or diesel generation created an unnecessary financial burden for this specific load profile without providing proportional benefits. Consequently, these components were excluded, and a strictly grid-tied PV system was selected as the optimal configuration.

2.5. Model Formulation and Techno-Economic Assumptions. Techno-economic optimization relies on minimizing the NPC and LCOE. The NPC is expressed as follows:

$$NPC = \frac{C_{ann,tot}}{CRF(i, N_{proj})}, \quad (1)$$

where $C_{ann,tot}$ represents the total annualized cost, i is the real discount rate, N_{proj} is the project lifetime, and CRF is the capital recovery factor. The LCOE is defined as:



Figure 2. Proposed PV system layout on the school rooftop and football court

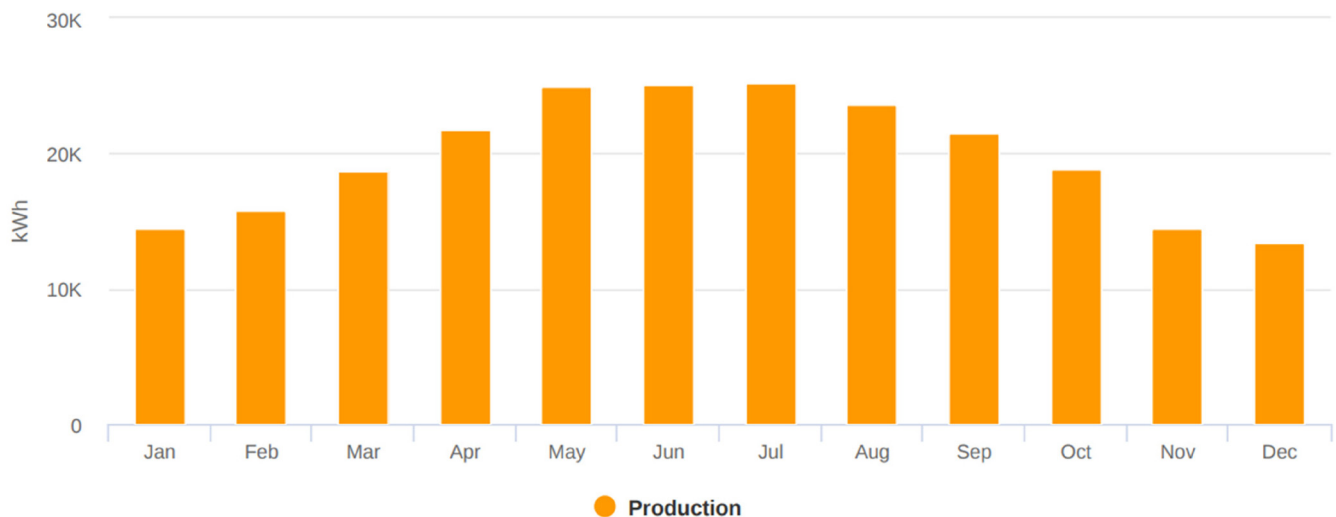


Figure 3. Simulated monthly energy production

$$LCOE = \frac{C_{ann,tot}}{E_{served}}, \quad (2)$$

where E_{served} represents the total electrical load served by the system annually.

The accuracy of these financial outputs relies heavily on the input of baseline economic parameters into the simulation. Table 2 outlines the key techno-economic assumptions used to model the system over its projected lifespan.

3. RESULTS AND DISCUSSION

Following the comprehensive simulation in HOMER Pro, a detailed analysis was conducted to evaluate the technical and economic feasibility of the proposed grid-tied PV system. The proposed design emerged as a superior solution, achieving the lowest cost among all the design alternatives. Table 3 presents a

core techno-economic comparison between the current base case and the optimized proposed case.

The calculated LCOE for the proposed system is 0.23 SAR/kWh, representing a 28% reduction compared with the standard governmental tariff of 0.32 SAR/kWh. This aligns with recent findings in the literature demonstrating that distributed renewable systems in Saudi Arabia could achieve a COE significantly lower than the national grid rate³. To visualize the financial viability of the project over its 25-year lifespan, a cumulative cash flow analysis was performed (Figure 8). The break-even point occurs at approximately 7.5 years, after which the system generates net positive savings.

3.1. Economic Sensitivity. This economic analysis relied on key baseline assumptions, including tariff stability at 0.32 SAR/kWh, a fixed 8% nominal discount rate, and current PV capital expenditure. Fluctuations in these parameters, such as potential tariff structural reforms by the utility provider, changes

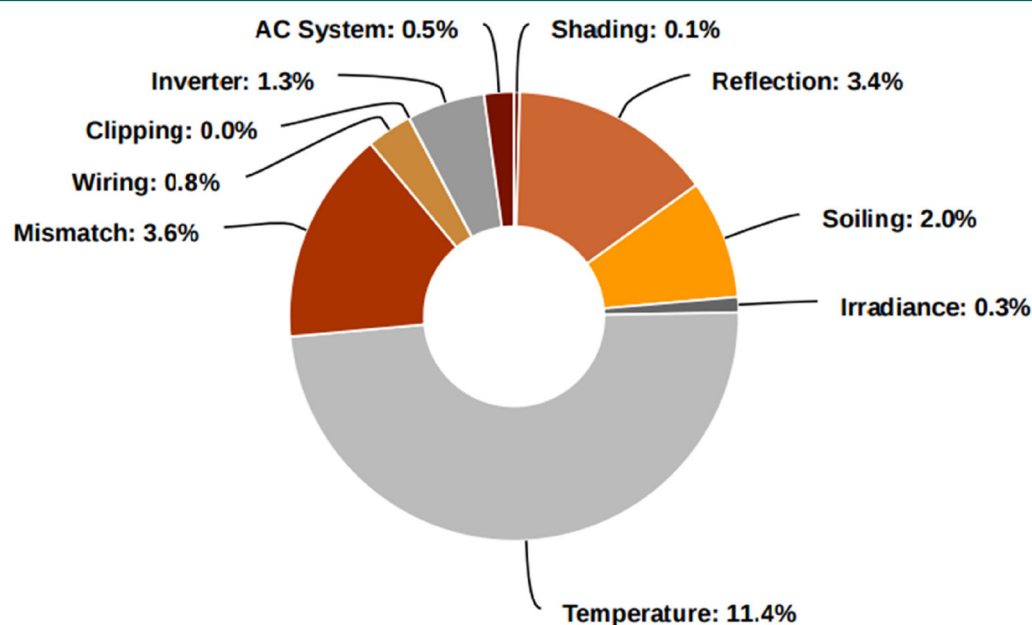


Figure 4. System loss diagram

Table 2. HOMER Pro Key Economic and System Assumptions

Parameter	Value	Unit	Description/Justification
Project Lifetime	25	Years	Standard operational lifespan for PV systems.
Grid Tariff	0.32	SAR/kWh	Fixed governmental rate for public facilities.
Nominal Discount Rate	8	%	Standard baseline opportunity cost for energy investments
Expected Inflation Rate	2	%	Typical long-term macroeconomic assumption.
Annual Capacity Shortage	0	%	Appropriate for a grid-tied system with full utility backup.
PV System Capital Cost (CAPEX)	371,975	SAR	Aggregated turnkey cost for the 149 kWp system derived from HelioScope sizing (approx. 2,496 SAR/kW).
PV System O&M (OPEX)	96,960	SAR	Estimated lifetime operations and maintenance budget (equating to standard ~1% of CAPEX annually).

Table 3. Techno-Economic Comparison

KPI	Base Case (Grid Only)	Proposed Case (Grid-tied PV)
Annual Consumption	410,968 kWh	260,429 kWh (Grid Purchase)
Grid Purchase	100%	52.1%
Annual Bill	131,510 SAR	83,337 SAR
Net Present Cost (NPC)	1,738,729 SAR	1,470,731 SAR
Payback Period	N/A	7.51 years
Return on Investment	N/A	9.3 %
Internal rate of return	N/A	12.6 %

Note: "Annual Consumption" in the proposed case represents the energy purchased from the grid. This difference was compensated for by the PV system.

in the national discount rate, or variations in PV component pricing, could significantly alter the resulting NPC and LCOE, thereby impacting the payback period of the system.

The technical performance was further detailed by comparing the load of the facility against solar generation. Figure 9 shows

the time-series relationship between consumption and production, and the seasonal and hourly performances of the solar array are visualized in the data map shown in Figure 10. A key finding of this study is the grid purchase frequency, as shown in Figure 11. The system successfully offsets 47.9% of the annual load; however, the remaining 52.1% grid reliance is largely inevitable owing to the "passive hours" (nighttime) when solar generation is zero. Integrating battery storage to capture this load was evaluated during the HOMER optimization but was deemed economically inefficient because the NPC was significantly increased without providing proportional returns.

Furthermore, the heatmap of the energy sold to the grid shown in Figure 12 highlights a strategic advantage unique to educational facilities: the summer break. In July and August, the school exports the vast majority of its generation to the municipal grid. This coincides precisely with the peak national demand period in the Eastern Province, suggesting that schools can act as distributed generation nodes to support the grid when it is most stressed.

Finally, this study evaluates the ecological benefits of renewable energy integration. Figure 13 outlines the environmental impact, detailing the reduction of 160 tons of CO2 emissions

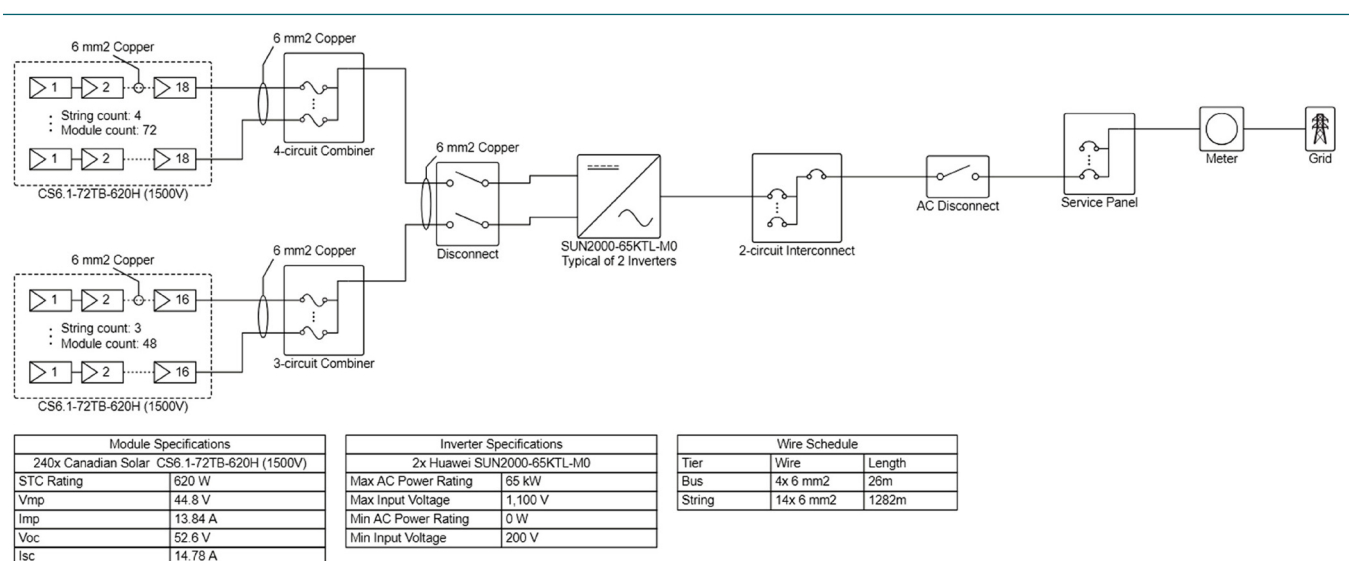


Figure 5. Single line diagram of the proposed PV system

- **Average Daily Consumption:** 1,156 kWh/d
- **Average Load:** 48.17 kW
- **Peak Load:** 385.41 kW
- **Load Factor:** 0.12

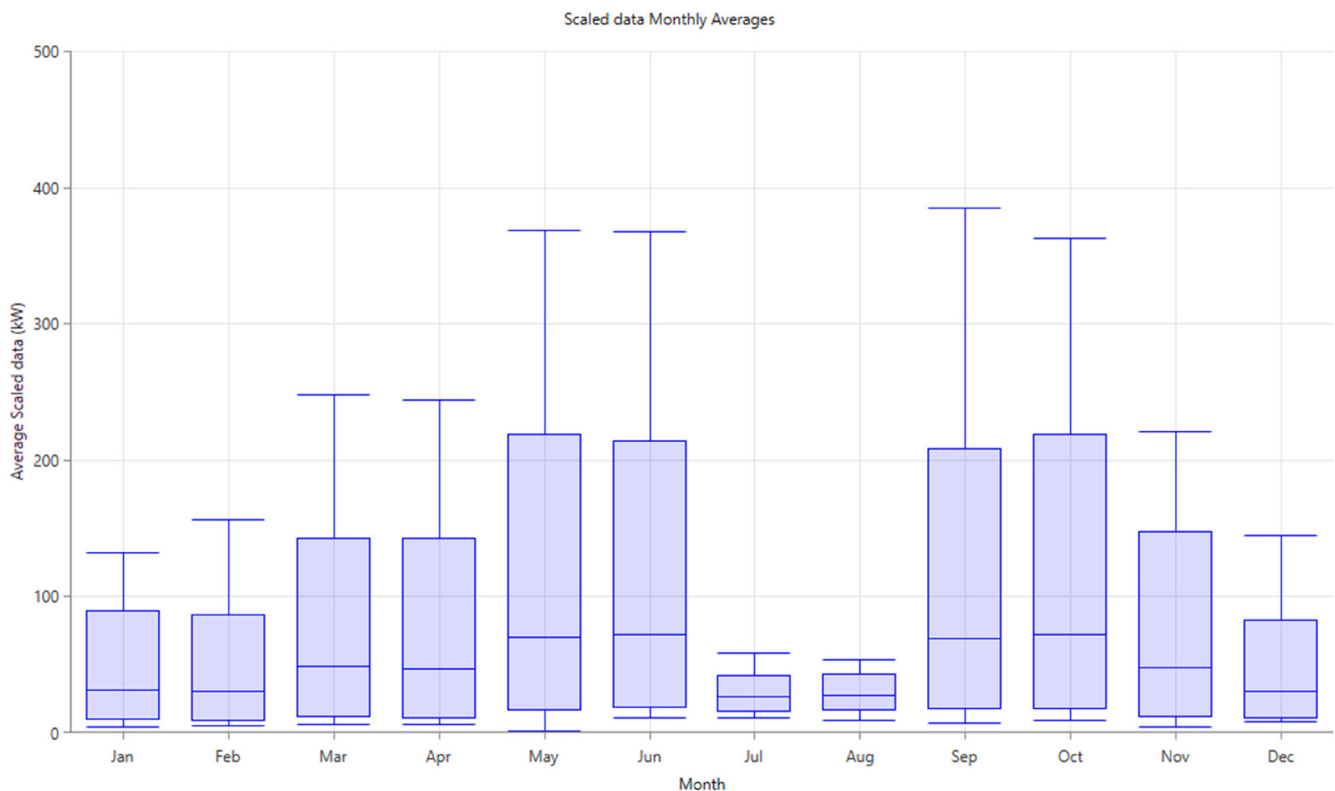


Figure 6. Monthly seasonal electrical load profile

annually, demonstrating how localized grid-tied systems can directly contribute to the broader decarbonization targets of the Saudi Green Initiative.

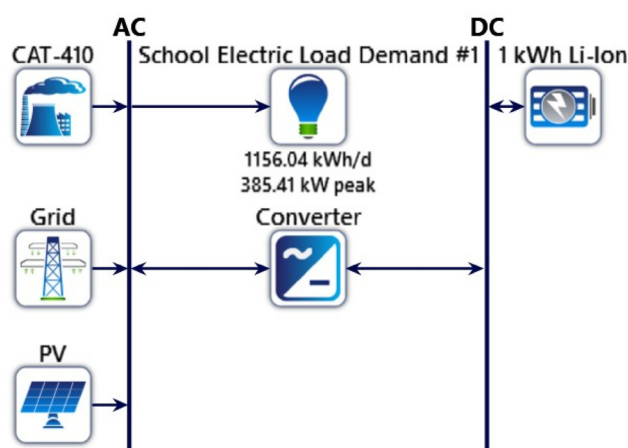


Figure 7. HOMER Pro system schematic

4. CONCLUSIONS

This study validated the techno-economic feasibility of integrating grid-tied solar PV systems into educational facilities in the Eastern Province of Saudi Arabia. For the modeled standard elementary school, a 149 kWp rooftop system reduced grid reliance from 100% to 52.1%, presenting a highly compelling financial case with a payback period of 7.5 years and an IRR of 12.6%. Ecologically, the system avoids significant carbon emissions and directly supports the Saudi Green Initiative.

4.1. Limitations and Scalability. To illustrate the macro-level impact, theoretically scaling this specific 149 kWp design across 100 standardized schools in the region could yield an annual municipal grid relief of approximately 15 GWh and save more than 4.8 million SAR in utility costs. However, although educational buildings utilize standardized architectural designs that theoretically make this model highly replicable, a critical limitation is the inherent variability among existing infrastructures. Differences in the available unshaded roof areas, localized load profiles, building ages, and regional climate disparities must be carefully assessed before broadly projecting these results across all schools.

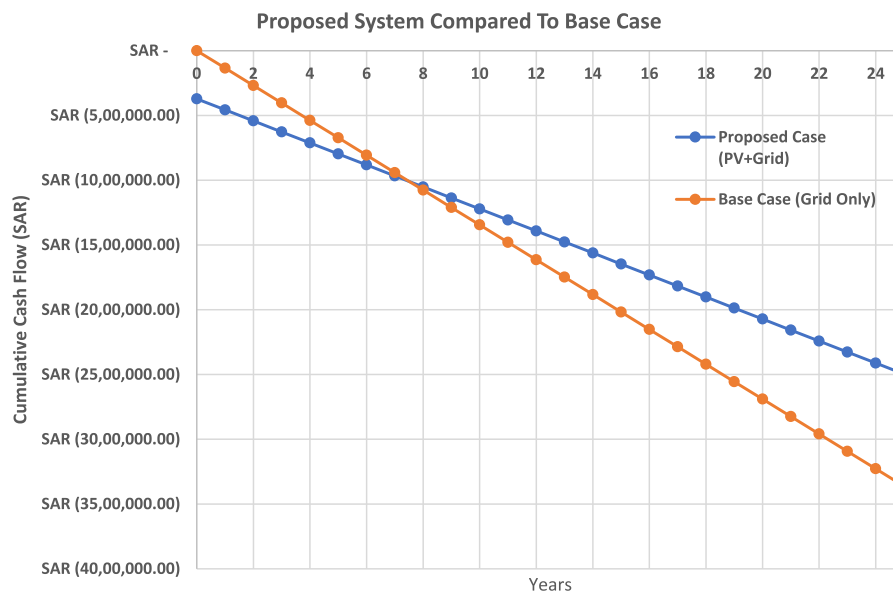


Figure 8. Cumulative cash flow analysis

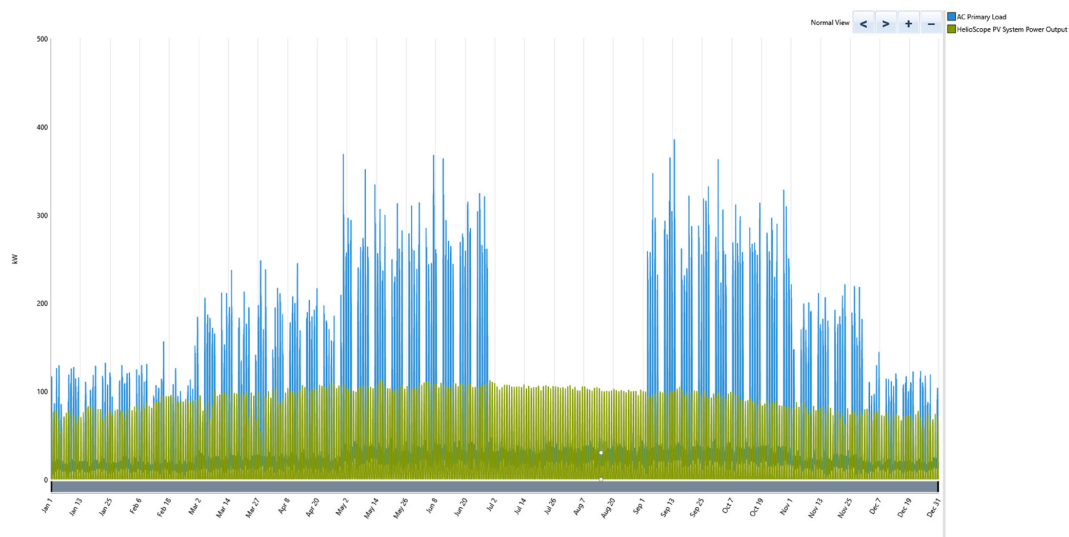


Figure 9. Time series comparison of electrical consumption vs. solar production

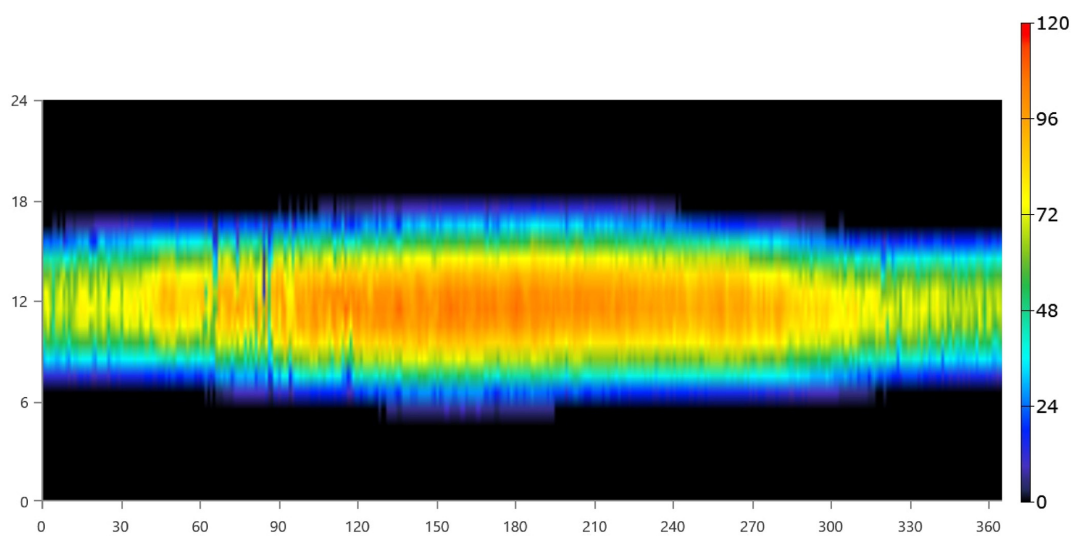


Figure 10. Heat map of PV power output (kW)

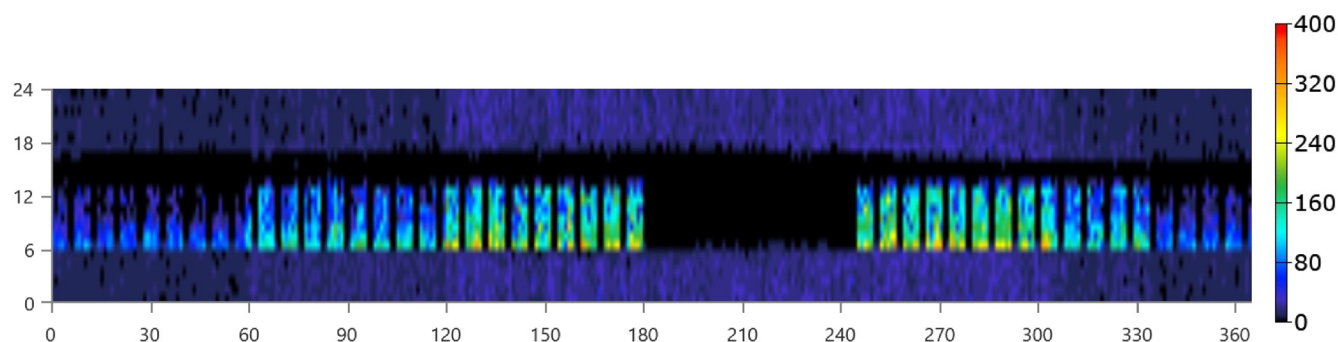


Figure 11. Heatmap of grid energy purchases (kW)

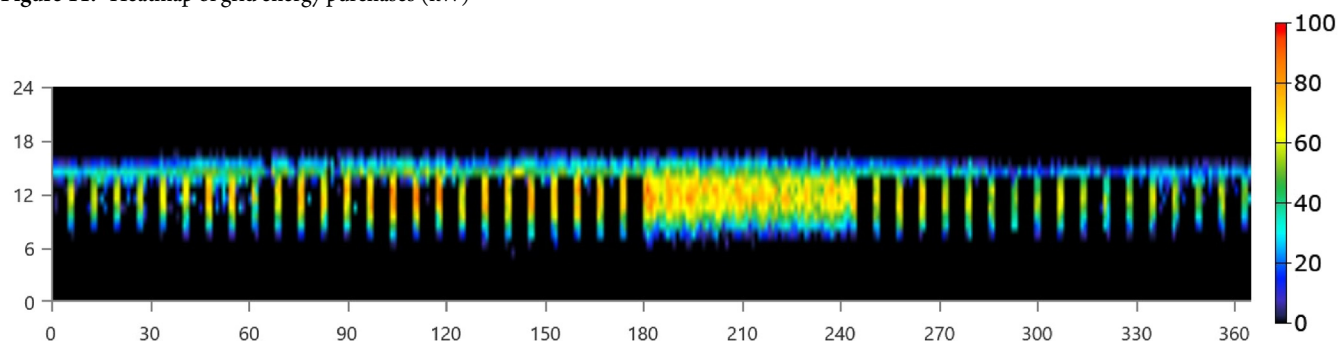


Figure 12. Heatmap of energy sold to the grid (kW)



Figure 13. Environmental impact and emissions reduction summary

4.2. Future Work. Future research should investigate the impact of implementing dynamic energy-efficient retrofits (e.g., upgrading HVAC infrastructure or building envelopes) in tandem with PV deployment to further reduce the initial required solar capacity and drive schools closer to the true zero-bill status.

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Monitoring Carbonate Levels in Saline Water Using Electrical Resistivity in Carbonate Formations

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ABSTRACT

Geologic carbon capture and sequestration (CCS) is a well-established method for storing large amounts of CO₂. However, monitoring the dissolved carbonate species associated with solubility trapping remains challenging. This study evaluated whether electrical resistivity (ER) can detect the carbonate-rich brines formed during solubility trapping, rather than focusing solely on freephase CO₂. Potassium carbonate (K₂CO₃), a highly conductive tracer, was examined within Austin Chalk limestone cores saturated with solutions ranging from 0.1 to 5 wt% in deionized water (DI) and synthetic produced water (PW). Fluid-only tests showed minimal resistivity variation across a wide range of frequencies (12 Hz–10 kHz), but the resistivity decreased significantly with increasing carbonate concentration. In DI solutions, resistivity dropped from approximately 5.27 Ω·m at 0.1 wt% to 0.16 Ω·m at 5 wt%. When introduced into the Austin Chalk matrix (porosity ~25%–27%), the bulk resistivity increased owing to the resistive nature of the rock, but the inverse relationship between resistivity and carbonate concentration remained consistent. For example, in the K₂CO₃ + PW system at 1 kHz using the 4-electrode setup, resistivity decreased from 1.81 Ω·m at 0.1 wt% to 1.50 Ω·m at 5 wt%. Frequency-dependent trends were also observed; higher frequencies (10 kHz) consistently yielded lower resistivities than low-frequency measurements (12 Hz), particularly in rock-saturated systems. Overall, these results establish a quantitative basis for applying electrical geophysical methods to monitor the changes in carbonate concentrations in carbonate reservoirs and support improved long-term CO₂ containment strategies.

Keywords: electrical resistivity, carbonate monitoring, austin chalk, potassium carbonate, produced water, porosity

1. INTRODUCTION

Climate change is a major environmental challenge of the 21st century, with measurable impacts observed across both environmental and engineered systems, including rising land and ocean temperatures, glacier retreat, sea-level rise, and ecosystem degradation¹. The primary driver of these changes is the accumulation of greenhouse gases (GHGs) in the atmosphere, particularly carbon dioxide (CO₂), which is largely emitted in fossil fuel combustion and industrial activities². Although CO₂ is naturally present and plays an essential role in maintaining Earth's radiative balance, elevated atmospheric concentrations enhance the greenhouse effect and accelerate global warming³. Long-term observations indicate that the global mean sea level has risen at an average rate of approximately 1.8 mm/year since 1961, and more than 3 mm/year since the early 1990s, primarily because of thermal expansion and melting of ice masses⁴. Because CO₂ is the dominant GHG emitted by human activities, carbon management technologies are needed along with the use of renewable energy. Hence, the global climate policy focuses on emission reduction, with numerous countries committed to achieve a net-zero target by the mid-century⁵. International climate frameworks, therefore, emphasize deep decarbonization pathways⁶.

Among the available mitigation strategies, geological carbon capture and sequestration (CCS) has emerged as a mature and scalable technology capable of reducing emissions from large stationary sources, such as power plants, cement industries, and refineries². In CCS operations, the captured CO₂ is compressed and injected into deep geological formations, including saline aquifers, depleted hydrocarbon reservoirs, and unmineable coal seams⁷. Once injected, CO₂ can be immobilized through multiple trapping mechanisms, including structural, residual, solubility, and long-term mineral trapping⁸. Deep saline aquifers, in particular, offer the largest global storage capacity and are therefore considered one of the most promising long-term storage options⁹. Although the engineering feasibility of CO₂ injection has been widely demonstrated, monitoring the long-term stability and geochemical evolution of the stored CO₂ remains a critical challenge. Solubility trapping involves the dissolution of CO₂ into formation brine, forming carbonic acid that dissociates into bicarbonate (HCO₃⁻) and carbonate (CO₃²⁻) ions¹⁰. These dissolved carbonate species alter the pore-fluid chemistry, ionic strength, and potential reservoir properties through dissolution–precipitation reactions¹¹, highlighting the importance of developing monitoring tools capable of detecting carbonate-rich fluids rather than focusing solely on free-phase CO₂.

The electrical resistivity method is a noninvasive geophysical approach for characterizing subsurface fluid distribution and has long been applied in hydrogeology and petroleum engineering¹². In relatively clean carbonate systems, the bulk resistivity is largely controlled by the pore-fluid conductivity and porosity, as described by Archie's foundational relationship¹². Therefore, variations in ionic composition and salinity directly influence the electrical response, suggesting that resistivity measurements may be sensitive to the dissolved carbonate species generated during CO₂ solubility trapping. Early investigations established the dependence of resistivity on saturation and salinity, which formed the basis for modern petrophysical interpretation¹². More recent studies have extended these concepts to CCS monitoring, primarily focusing on detecting free-phase CO₂ plumes because of their high resistivity relative to that of formation brines¹⁴. Although effective for tracking plume migration, this approach is inherently less sensitive to dissolved carbonate ions, which are a key mechanism for long-term CO₂ storage.

Experimental studies have revealed that saturating carbonate rock samples with CO₂-saturated brines causes changes in the rock properties. Mineral dissolution experiments demonstrated that calcite-rich formations are highly reactive under CO₂ storage conditions, leading to measurable changes in porosity and

permeability⁸. Additional work investigating acid-driven wormholing processes highlighted how fluid chemistry evolution influenced both the mechanical behavior and petrophysical properties of carbonate rocks¹³. Recent studies on rock properties under CO₂ storage conditions have suggested that salinity in CO₂-saturated brines affects wormhole formation and rock stiffness, thus showing the importance of monitoring dissolved carbonate species in addition to the supercritical CO₂ phase¹⁵. However, these studies have focused more on core flooding, geochemical modeling, and mechanical tests, whereas electrical geophysical tests have received limited attention.

Austin Chalk is a highly porous Upper Cretaceous formation commonly used as an analog for carbonate reservoirs because of its relatively simple mineralogy and consistent petrophysical characteristics. Micropetrographic and X-ray diffraction (XRD) analyses indicate that Austin Chalk is composed predominantly of calcite with minimal clay or dolomite content, thereby reducing surface conduction effects and allowing the fluid-controlled electrical behavior to be more clearly isolated¹⁶. Recent geo-electrical investigations of carbonated brine injection in carbonate aquifers have demonstrated the potential of electrical methods for monitoring CO₂ storage. However, the reported frequency dependence and electrode configuration responses are

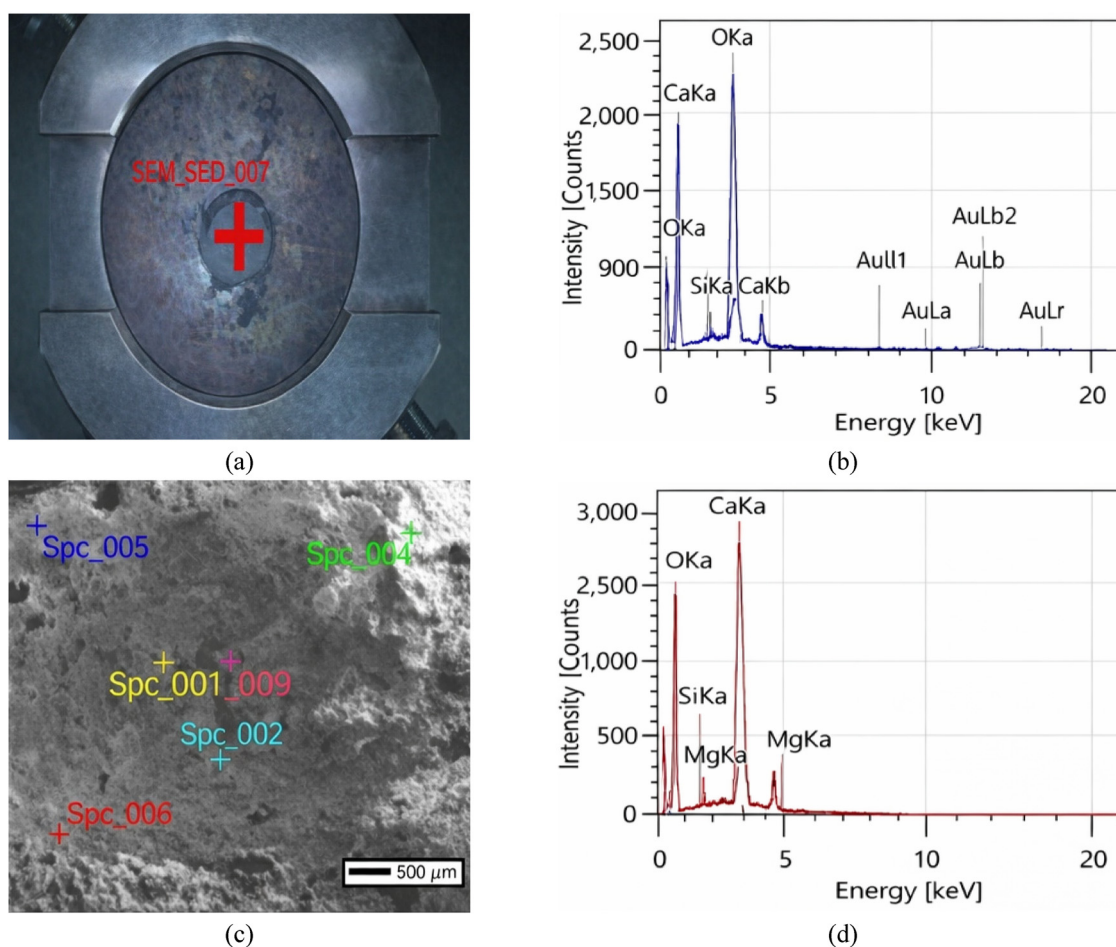


Figure 1. Scanning electron microscope (SEM) images and energy-dispersive X-ray spectroscopy (EDS) analyses of the Austin Chalk carbonate sample. (a) Core holder and SEM sampling location. (c) SEM micrograph showing analyzed spots. (b) and (d) Representative EDS spectra indicating the dominant elemental composition of the carbonate matrix. Modified after Helmi et al. (2025)¹⁴

Table 1. *Material and fluid properties*

Material	Description	Initial Porosity (%)
Austin Chalk	Limestone (>90% Calcite)	25–27
Formation Age	Upper Cretaceous	-
Permeability	8–15 mD	-
UCS	2500–3000 psi	-
Homogeneous	No	-
PW Base	High-salinity Brine	-
DI Base	Deionized Water	-
Additive	Potassium Carbonate (K_2CO_3) (0.1–5 wt%)	-

inconsistent across experimental setups¹⁴. These inconsistencies raise questions regarding the measurement precision and practical limits of resistivity monitoring in carbonate reservoirs.

Despite the extensive body of CCS research, only a limited number of studies have systematically evaluated whether electrical resistivity can be used to monitor carbonate-rich fluids quantitatively. Most existing studies rely on NaCl brines or live CO_2 systems, where the influences of the carbonate concentration, measurement frequency, and electrode configuration remain poorly constrained¹⁴. As a result, a clear knowledge gap exists regarding the detectability limits and reliability of electrical resistivity for monitoring solubility-trapping processes in carbonate formations such as Austin Chalk.

This study addresses that gap by evaluating the resistivity response to controlled carbonate concentrations using potassium carbonate (K_2CO_3) as a surrogate carbonate source. The use of K_2CO_3 allows precise control of dissolved carbonate levels under laboratory conditions, which is difficult to achieve using pure CO_2 because of phase behavior and solubility limitations. Experiments were conducted in deionized water (DI) and synthetic produced water (PW) over a concentration range of 0.1–5 wt%, with measurements at 12 Hz, 1 kHz, and 10 kHz. The investigation was extended to rock–fluid systems using Austin Chalk cores with well-characterized porosity and mineralogy to evaluate the influence of the rock matrix on bulk resistivity. By isolating the fluid chemistry effects from rock-controlled parameters, this study established a quantitative baseline for assessing the feasibility of electrical resistivity as a monitoring tool for carbonate-rich fluids associated with CO_2 solubility trapping.

2. METHODOLOGY

2.1. Materials and Brine Preparation. The brines used in this study were prepared using analytical-grade K_2CO_3 dissolved in both DI and PW. Austin Chalk limestone sister cores were selected as the rock samples for all rock–fluid interaction experiments and were cut to uniform dimensions (length: 2.8 inches, ~7.11 cm; diameter: 1.5 inches, ~3.8 cm) to ensure consistency across all measurement frequencies.

Two fluid systems were prepared to simulate different reservoir baselines:

1. DI: Used as a control to isolate the rock–fluid interaction.

2. Synthetic PW: Prepared to mimic the complex chemistry of deep-formation brines. The composition per liter of DI was: 53.668 g NaCl, 8.515 g $MgCl_2 \cdot 6H_2O$, 18.817 g $CaCl_2 \cdot 2H_2O$, and 1.351 g Na_2SO_4 .

Analytical-grade potassium carbonate (K_2CO_3) was added to these base fluids at varying concentrations: 0.1, 0.25, 0.5, 0.75, 1, 2, 3, 4, and 5 wt%. The comprehensive physical and mineralogical properties of the materials and fluids, including the initial porosity and mechanical strength of the Austin Chalk, are summarized in Table 1.

Figure 1 shows the mineralogical composition and microtexture of the Austin Chalk limestone samples as determined by scanning electron microscopy–energy dispersive X-ray spectroscopy (SEM–EDS) characterization. As can be observed, the calcite-dominated carbonate matrix is accompanied by only minor accessory phases, confirming the relative mineralogical simplicity of the rock and minimizing the influence of clay-related surface conduction on the electrical measurements.

2.2. Test Workflow . Experiments were conducted using a custom hydrostatic core holder equipped with two to four electrode arrays for the rock–fluid system. This configuration minimizes contact resistance, which is critical for measuring conductive saline fluids. The experimental workflow is illustrated in Figure 2, representing the sequential analysis of both the fluid system and the integrated rock–fluid system. The procedure involves four key stages:

1. Fluid characterization: Measurement of density, viscosity, pH, resistivity of bulk fluids, and temperature. Baseline resistivity measurements at frequencies of 12 Hz, 1 kHz, and 10 kHz with multi concentrations of K_2CO_3 solutions (DI or PW) were established for the fluid system to verify the electrical properties of the brine before core introduction.
2. Core saturation: Vacuum-saturation of dry sister limestone cores with K_2CO_3 solutions (DI or PW with multi concentrations).
3. Porosity analysis: The gravimetric porosity of each core was calculated by comparing the dry and wet weights, ensuring that the samples were fully saturated. 1
4. Resistivity measurement: The resistivity was measured at frequencies of 12 Hz, 1 kHz, and 10 kHz using two- and four-electrode systems.

Table 2. *Austin chalk core properties and calculated porosity*

Sample Environment	Concentration (wt%)	Dry Weight (g)	Wet Weight (g)	Porosity (%)
Austin Chalk + DI	0.1	180.66	201.20	25.37
Austin Chalk + DI	5.0	175.55	197.67	26.16
Austin Chalk + PW	0.1	175.75	198.50	26.45
Austin Chalk + PW	5.0	177.87	199.98	25.11

3. EXPERIMENTAL WORK

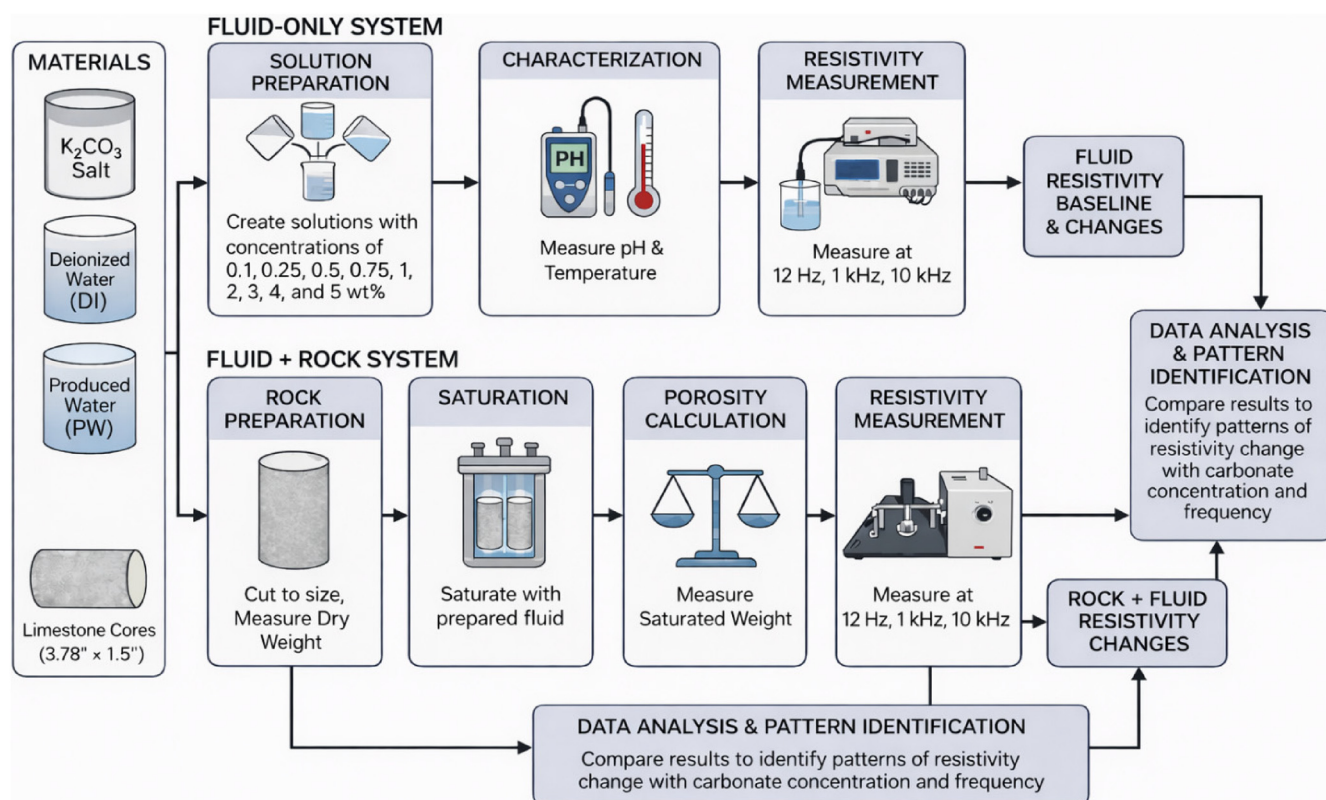
3.1. Fluid-only system. For the fluid-only system measurements, K_2CO_3 brines solutions were prepared in DI and PW under ambient temperature and pressure. Solutions with various concentrations (0.1, 0.25, 0.5, 0.75, 1, 2, 3, 4, and 5 wt%) were prepared to examine how the resistivity varied with increasing salt content. Prior to the readings, the temperature and pH of each solution were recorded. The resistivity was then measured using a benchtop dip-cell resistivity meter at three frequencies—12 Hz, 1 kHz, and 10 kHz—for DI.

3.1.1. Fluid + rock system. To evaluate the interaction between the K_2CO_3 brine solutions and Austin Chalk, cylindrical core samples were cut to approximately 2.8 inches in length and 1.5 inches in diameter. The end faces were leveled to ensure a proper fit within the benchtop resistivity setup. The dry weight of each sample was measured. The samples were then vacuumed according to their pore structures and saturated over four to five nights.

After saturation, the wet weight of each core was recorded and used to calculate the gravimetric porosity based on the dry and saturated masses. Resistivity measurements were then carried out

using the two- and four-electrode configurations at 12 Hz, 1 kHz, and 10 kHz under the same conditions applied during the fluid-only phase. The physical properties and calculated porosities of the Austin Chalk cores are summarized in Table 2.

3.2. Instrumentation. All instruments were calibrated before testing to minimize measurement uncertainty and ensure repeatability across frequencies and fluid systems. In addition, all experiments were carried out on an integrated benchtop measurement platform designed to ensure accurate and repeatable characterization of the electrical and physicochemical properties in both fluid-only and rock–fluid systems, as shown in Figure 3. Baseline resistivity measurements were first determined for the prepared brines using the benchtop dip-cell resistivity setup, as illustrated in Figure 3 (a), before introducing the rock samples to isolate the fluid-controlled electrical behavior. Core saturation was conducted in a vacuum chamber, as shown in Figure 3 (b), to ensure that the rock pore spaces were fully occupied with fluids and that the air content, which is known to introduce substantial uncertainty in the resistivity measurements of porous rock, was kept at a minimum. Bulk resistivity measurements were performed using a high-precision impedance analyzer, shown

**Figure 2.** Workflow for detecting carbonate levels

in Figure 3 (c), which can be operated in both two- and four-electrode configurations. The precision of the impedance analyzer can be set at $\pm 0.05\%$, covering a frequency range of 12 Hz to 200 kHz. This allowed for a systematic evaluation of the frequency-dependent effects and electrode configuration sensitivity. The four-electrode configuration was used to reduce electrode polarization and resistance, particularly in highly conductive brines, whereas the two-electrode configuration was used for a comparative assessment of the robustness of the measurements.

The fluid chemistry was continuously monitored using a benchtop electrochemical meter, as illustrated in Figure 3 (d), with the capability to measure pH, oxidation–reduction potential (ORP), and temperature with a resolution of ± 0.01 pH units. This ensured that changes in electrical response could be understood in the context of well-controlled chemical conditions,

especially considering the highly alkaline nature of the K_2CO_3 solutions. The densities and kinematic viscosities of the carbonate brines were measured using a calibrated viscometer, as shown in Figure 3 (e). This instrument measures density and kinematic viscosity simultaneously, and is useful in assessing changes in these properties with increasing concentrations of carbonate. Gravimetric measurements were performed using a semi-micro analytical balance, as shown in Figure 3 (f), with a resolution of 0.01 mg. This balance was used to accurately prepare the concentrations of K_2CO_3 and to measure the dry and saturated masses of the core used to calculate porosity. This instrumentation suite was used to control and measure the electrical, chemical, and physical properties, and to ensure that changes in resistivity could be attributed to changes in the frequency and concentration of the carbonate solutions rather than experimental uncertainty.



Figure 3. Experimental setup for carbonate brine characterization: (a) solution resistivity device; (b) vacuum saturation chamber for Austin Chalk cores; (c) GW Instek LCR 821 for resistivity measurements; (d) Hanna Instruments device for pH, redox potential, and temperature; (e) Anton Paar viscometer for viscosity and density; and (f) A&D GR semi-microbalance for solution preparation and porosity verification

Table 3. Electrical and pH measurements of K_2CO_3 in deionized water

Concentration	pH	Res_12 Hz	Res_1 kHz	Res_10 kHz
0.1	11.17	5.2711305	5.315967	5.315546
0.25	11.44	2.1985041	2.18080105	2.18088525
0.5	11.56	1.150287775	1.1748847	1.17533517
0.75	11.65	0.8058361	0.83961714	0.8414527
1	11.68	0.66918371	0.70668639	0.708364075
2	11.84	0.31378814	0.34663456	0.34716081
3	11.93	0.2632513	0.26571415	0.26664035
4	12	0.19581973	0.19784053	0.198865665
5	12	0.162865955	0.164343665	0.165194085

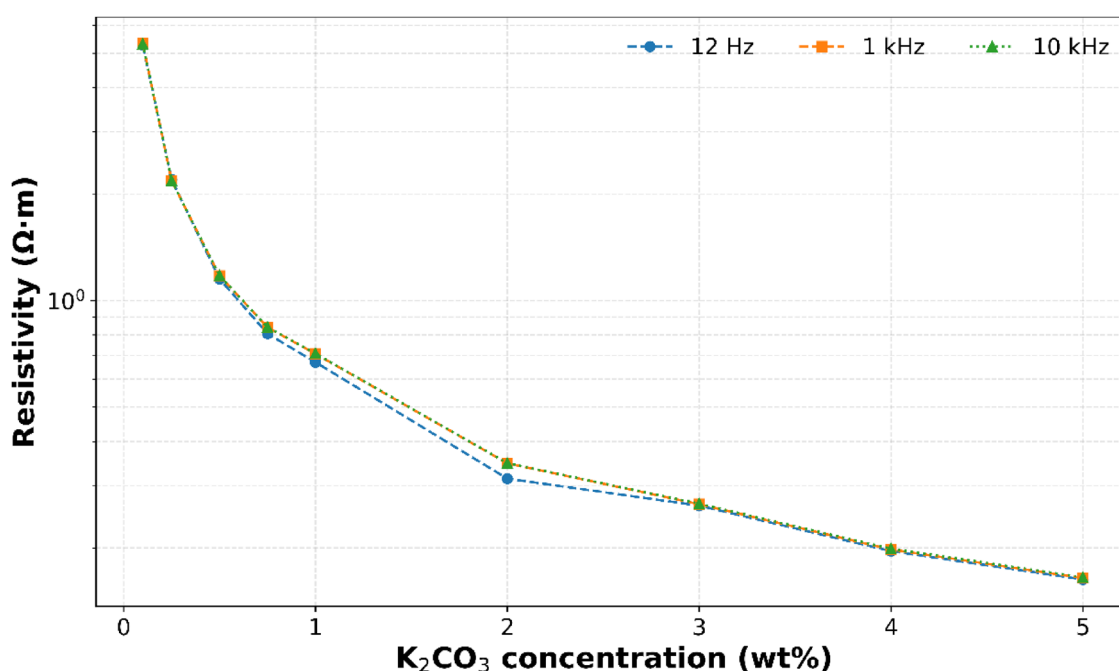
4. RESULTS AND DISCUSSION

The results of this study demonstrate the sensitivity of the ER method to varying carbonate concentrations and solvent types within Austin Chalk limestone. The following sections analyze the resistivity trends across fluid-only systems and saturated rock–fluid systems.

4.1. Fluid-only Resistivity Trends. The electrical resistivity of the K_2CO_3 solutions, both DI and PW, exhibited a significant, non-linear decrease as concentration increased from 0.1 to 5 wt%. This trend is fundamental for monitoring geochemical reactions and CO_2 –brine–rock interactions in deep saline aquifers. As detailed in Table 3, the resistivity of the DI system at 1 kHz decreased rapidly from 5.316 $\Omega \cdot m$ at 0.1 wt% to 0.164 $\Omega \cdot m$ at 5 wt%, representing a substantial reduction of approximately 96.9%. This high-contrast geophysical signature, illustrated in Figure 4, tracks the resistivity response across the tested concentration range. In addition, Figure 4 shows that the pure fluid resistivity values remained nearly identical across the tested frequency spectrum of 12–10 kHz.

By contrast, the PW system characterized in Table 4 and Figure 5 maintained a significantly lower baseline resistivity due to its inherent high salinity, with values decreasing from 0.087 $\Omega \cdot m$ at 0.1 wt% to 0.066 $\Omega \cdot m$ at 5 wt%. Although the relative change in the PW system was dampened compared to that in the DI system, both environments demonstrated a clear inverse relationship between the carbonate concentration and resistivity across the tested range. This comparison is highlighted in Figure 6, which shows that the high ionic strength of the host brine acted as a conductive mask, reducing the relative signal of the added K_2CO_3 . The physical properties of the PW solvent also showed measurable shifts, with the baseline density recorded at 0.1 wt% and a slight increase in viscosity from 1.13 to 1.15 cP, as depicted in the profiles in Figure 7.

Furthermore, the pH measurements presented in Tables 3 and 4 reflect a marked increase in alkalinity with increasing carbonate enrichment. In the DI system, the pH rose from 11.17 to 12.0, whereas in the PW system, it increased from 8.02 to 10.83. As illustrated in Figure 8, these pH shifts serve as critical secondary

**Figure 4.** Electrical resistivity as a function of K_2CO_3 concentration in deionized water at different frequencies

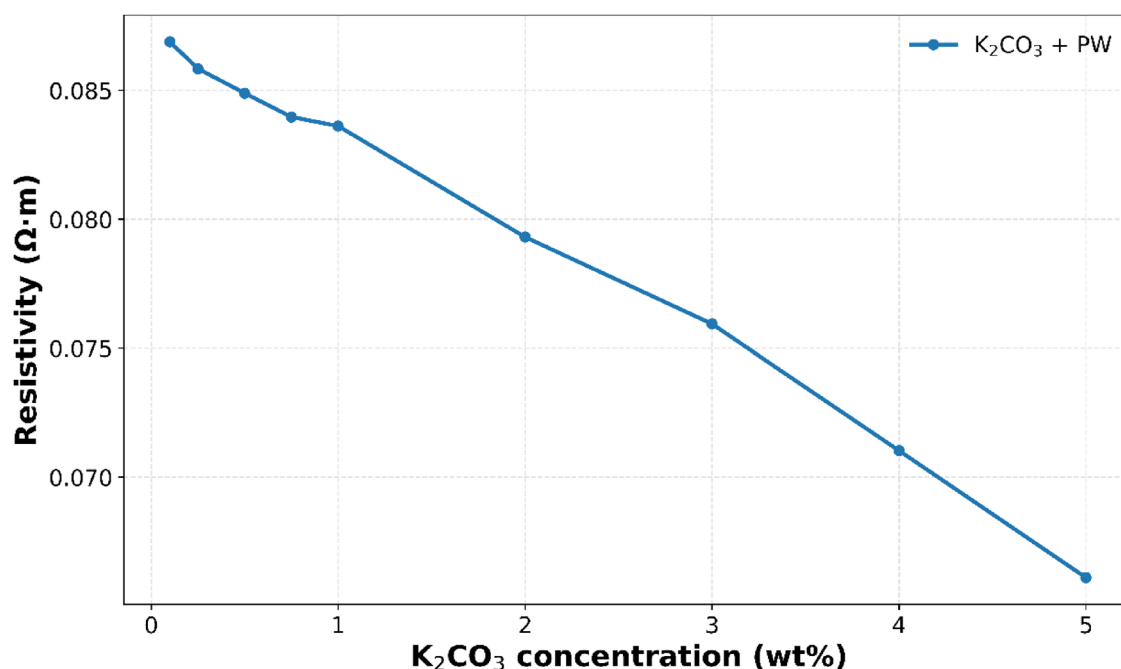


Figure 5. Electrical resistivity as a function of K₂CO₃ concentration in produced water

indicators for detecting geochemical equilibrium shifts during the carbon sequestration processes. The correlation between increasing pH and decreasing resistivity provides a robust framework for multiparameter reservoir monitoring.

4.2. Austin Chalk Saturated Core Results. The bulk resistivity in the Austin Chalk cores (porosity ~25%–27%) decreased in line with the fluid-only systems; however, the measured values were higher because the limestone matrix was resistive and reduced the pore volume available for the ionic current flow. A comparison of the 4-electrode measurements in Table 5 with the 2-electrode measurements in Table 6 shows that the

2-electrode setup reports a higher resistivity at every tested frequency for each brine type. For example, at 0.1 wt% K₂CO₃ in DI at 1 kHz, the 2-electrode configuration recorded 81.647 Ω·m (Table 6), whereas the 4-electrode setup recorded a significantly lower value, 65.921 Ω·m (Table 5). This discrepancy is attributed to the inclusion of the contact resistance and electrode polarization in the 2-electrode setup, whereas the 4-electrode configuration isolates the true bulk properties of the saturated rock.

The sensitivity of these electrical signatures to the carbonate levels is heavily influenced by the background fluid

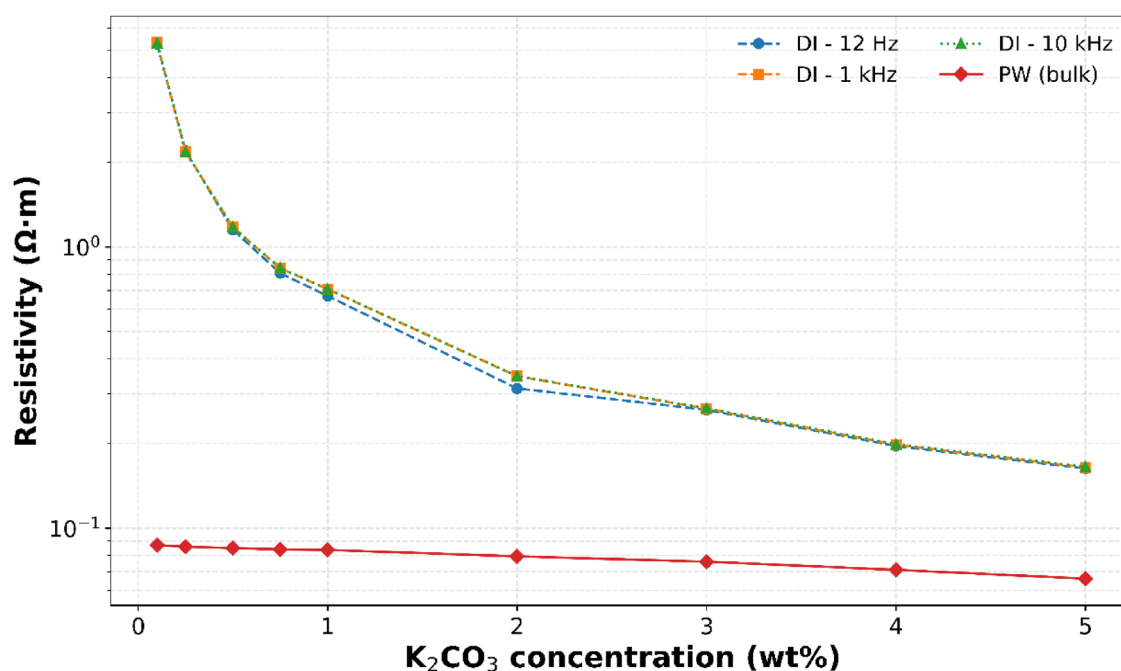


Figure 6. Comparison of electrical resistivity across varying K₂CO₃ concentrations for deionized water and produced water solvents

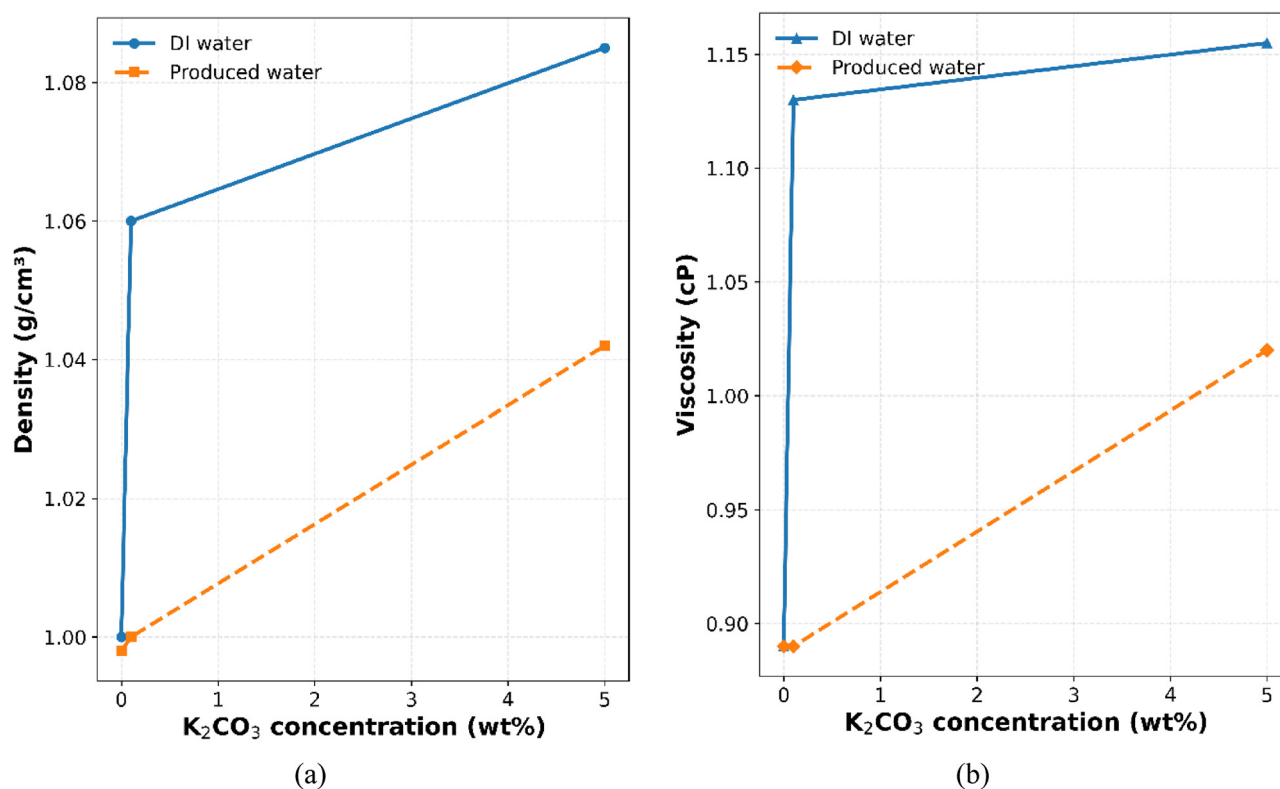


Figure 7. Variation of (a) density and (b) viscosity of deionized water and produced water with varying concentrations of K_2CO_3 (0.1 and 5 wt%)

environment. In the DI-saturated Austin Chalk, increasing the K_2CO_3 concentration led to a substantial resistivity drop from 65.921 to 1.072 $\Omega \cdot m$ (at 1 kHz, 4e), indicating high diagnostic sensitivity in low-salinity aquifers. Conversely, as can be observed in Table 5, the PW environment demonstrated a much more attenuated response, with resistivity values only shifting from

1.815 to 1.496 $\Omega \cdot m$. This behavior confirms that the high initial ionic strength of PW acts as a conductive mask that dampens the relative impact of additional carbonate ions. Furthermore, the data in Table 5 highlights the frequency-dependent response or dispersion. At 0.1 wt% concentration, the bulk resistivity drastically declines from 80.605 $\Omega \cdot m$ at 12 Hz to 66.040 $\Omega \cdot m$ at

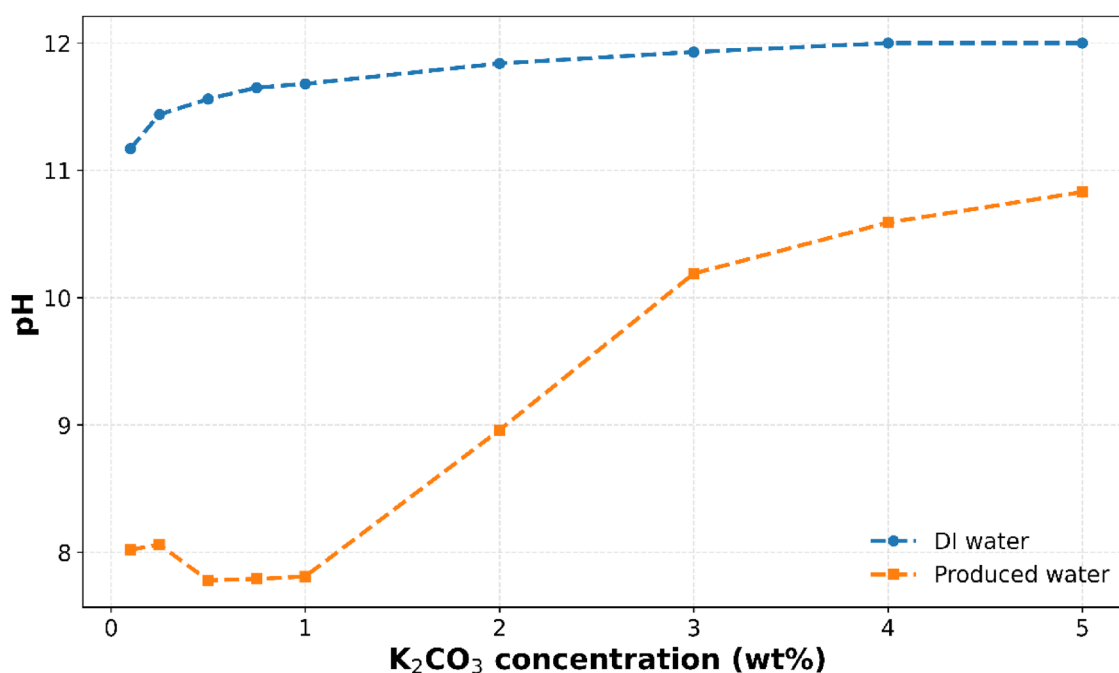


Figure 8. Variation of pH of deionized water and produced water with varying concentrations of K_2CO_3 (0.1 and 5 wt%)

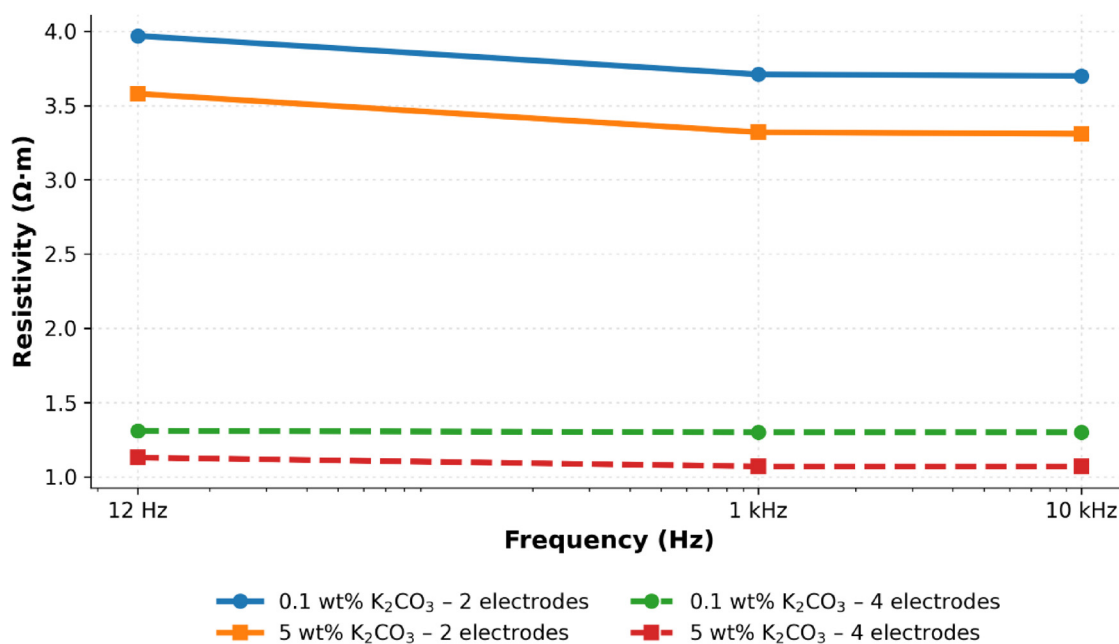


Figure 9. Comparative analysis of 2- and 4-electrode resistivity measurements for Austin Chalk samples across frequencies from 12 Hz to 10 kHz. The samples were saturated with DI containing 0.1 and 5 wt% K₂CO₃ to illustrate the discrepancy between measurement techniques at varying salinity levels

10 kHz. This sharp reduction indicates that at higher frequencies, the electrical signal is better able to bypass the polarization barriers at the rock–fluid interface and within the narrow pore throats of the limestone. In the PW-saturated system, the dispersion follows a similar pattern, dropping from 3.266 to 1.110 Ω·m at the same frequencies. Collectively, these results demonstrate that while electrical resistivity is a robust indicator of carbonate levels, the most accurate characterization is achieved using 4-electrode measurements and accounting for the frequency-dependent behavior of the specific host aquifer fluid.

The patterns shown in Figures 9 and 10 support the numerical differences observed between the 2- and 4-electrode methods. Figure 9 shows that in a low-salinity DI solution, the 2-electrode approach overestimates the resistivity at low frequencies because ions accumulate at the electrode–fluid interface and cause electrode polarization. However, the 4-electrode setup largely avoids this artifact by separating the electrodes used to drive the current from those used to measure the voltage. Figure 10 shows that the high ionic strength of PW lowers the bulk resistivity; however, a consistent difference remains between the two

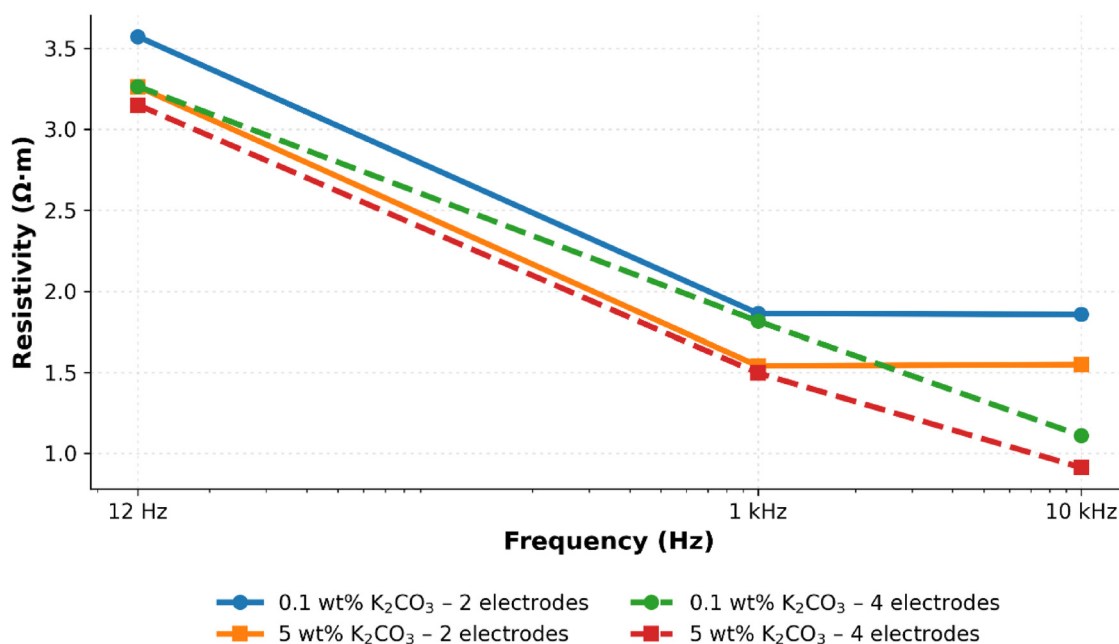


Figure 10. Comparative analysis of 2- and 4-electrode resistivity measurements for Austin Chalk samples across frequencies from 12 Hz to 10 kHz. The samples were saturated with produced water containing 0.1 and 5 wt% K₂CO₃ to illustrate the discrepancy between measurement techniques at varying salinity levels

Table 4. Electrical and pH measurements of K_2CO_3 in produced water

Concentration	pH	Res
0.1	8.02	0.086880973
0.25	8.06	0.08583691
0.5	7.78	0.084889643
0.75	7.79	0.083963056
1	7.81	0.08361204
2	8.96	0.079302141
3	10.19	0.075930144
4	10.59	0.071022727
5	10.83	0.066093853

measurement methods. This gap indicates that the contact resistance contributes meaningfully, even when the background brine salinity is high. Collectively, these results show that a 4-electrode setup is needed to measure the true frequency-dependent dispersion of the Austin Chalk because it reduces the artifacts that can mask carbonate concentration changes in a standard 2-electrode system.

4.3. Mechanistic Interpretation of Resistivity Behavior. The observed non-linear decrease in resistivity with increasing K_2CO_3 concentration reflects enhanced ionic conductivity within the pore fluid. This behavior is consistent with the fundamental relationship between the fluid conductivity and resistivity in porous media established by Archie's law¹². Furthermore, the observed resistivity reduction aligns with recent geoelectrical evaluations of CO_2 storage, which demonstrate that increased ionic strength from carbonate species significantly enhances bulk conductivity¹⁴. This sensitivity is further influenced by the salinity of the host brine, because high-salinity environments can act as a conductive mask that dampens the electrical signature of the added carbonate species, a phenomenon observed in recent studies on CO_2 -brine-rock interactions¹⁵. At low concentrations, the increase in carbonate ion availability significantly improves the charge transport pathways, resulting in rapid resistivity reduction. However, above approximately 3 wt%, the resistivity trend becomes relatively stable, suggesting that the conductive pathways approach saturation, and additional ions contribute less effectively to bulk electrical transport. The limited frequency dependence observed in the fluid-only systems indicates that

conduction is dominated by ionic mobility rather than by interfacial polarization effects within the tested frequency range. In rock-fluid systems, the Austin Chalk matrix introduces tortuosity and geometric constraints that increase bulk resistivity while preserving the inverse relationship between carbonate concentration and electrical response.

4.4. Challenges and Scaling of CO_2 Monitoring Experiments. Pure CO_2 was not used in the current study because of the complexities involved in maintaining a stable dissolved CO_2 concentration. In its place, potassium carbonate, K_2CO_3 , was employed owing to its stable chemical properties, which could simulate the effects of the carbonate-rich aqueous solution in a subsurface reservoir. The solubility of K_2CO_3 in water produces carbonate ions, which influence the ionic conductivity in the same manner as the dissolved CO_2 , that is, HCO_3^- and CO_3^{2-} . However, in a real subsurface reservoir, the dissolved CO_2 causes geochemical reactions, including reduction of pH, dissolution of minerals, and precipitation, which also influence the electrical properties. The current study showed the strong influence of carbonate concentration on the electrical properties. In future studies, CO_2 injection experiments will be performed to assess the applicability of the proposed method for CCS monitoring in real reservoir conditions.

5. CONCLUSIONS

This study demonstrated that ER can detect controlled K_2CO_3 concentration changes in both fluid-only and carbonate rock systems, thus providing a potential monitoring pathway for solubility-trapped CO_2 . The main conclusions are as follows:

- The test specimens showed uniform electrical properties, validating the experimental setup.
- The solvent used significantly affects the resistivity, with DI leading to larger changes than the high-salinity PW.
- Electrode configuration is important; four-electrode setups better capture the true bulk resistivity.
- Frequency influences rock-fluid systems due to interfacial polarization. For example, the resistivity of DI-saturated Austin Chalk (0.1 wt%) dropped from 80.6 $\Omega \cdot m$ at 12 Hz to 66.0 $\Omega \cdot m$ at 10 kHz, whereas fluid-only systems remain frequency-independent.

Table 5. Bulk resistivity of Austin Chalk cores (4-electrode system)

Sample Environment	Concentration (wt%)	At 12 Hz (4e) $\Omega \cdot m$	At 1 kHz (4e) $\Omega \cdot m$	At 10 kHz (4e) $\Omega \cdot m$
Austin Chalk + DI	0.1	80.605	65.921	66.040
Austin Chalk + DI	5.0	1.126	1.072	1.074
Austin Chalk + PW	0.1	3.266	1.815	1.110
Austin Chalk + PW	5.0	3.151	1.496	0.913

Table 6. Bulk resistivity of Austin Chalk cores (2-electrode system)

Sample Environment	Concentration (wt%)	At 12 Hz (2e) $\Omega \cdot m$	At 1 kHz (2e) $\Omega \cdot m$	At 10 kHz (2e) $\Omega \cdot m$
Austin Chalk + DI	0.1	83.249	81.647	80.884
Austin Chalk + DI	5.0	3.584	3.318	3.310
Austin Chalk + PW	0.1	3.573	1.863	1.857
Austin Chalk + PW	5.0	3.264	1.540	1.549

- ER is highly sensitive at low K₂CO₃ concentrations (<3 wt%) but stabilizes at higher concentrations.

This study adds evidence to the research aimed at strengthening monitoring methods for carbon sequestration and describing the geochemical properties of subsurface reservoirs. Future research should focus on long-term studies of geochemical durability, dynamic flow conditions, and true CO₂-brine systems to evaluate field-scale geophysical tests and computational modeling. These steps will help extend the results to other settings and refine real-time monitoring approaches for high-salinity aquifers.

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Video Based Sperm Motility Grading and YOLOv8 Detection: A Tracking-Free Approach to Automated Semen Analysis

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ABSTRACT

This paper presents a unified deep learning framework for automated sperm counting and motility assessment using Computer-Aided Semen Analysis. Conventional semen analysis is predominantly manual, making it time consuming, subjective, and susceptible to inter-observer variability, whereas existing automated systems often struggle in the presence of debris and morphological abnormalities. To address these limitations, the You Only Look Once version 8 (YOLOv8) Nano object detection model was fine-tuned using carefully annotated clinical data to accurately detect and count only valid sperm cells that are characterized by the presence of both the head and tail, while effectively suppressing non-sperm objects in noisy and unclean semen samples. In addition, a tracking-free approach for motility assessment is proposed by reformulating the problem as a video-level regression task. Instead of relying on computationally expensive and error-prone tracking-by-detection pipelines, the proposed method predicts the overall sperm motility directly from video sequences by modeling global optical flow patterns and temporal dynamics. To achieve this, three spatiotemporal deep learning architectures were developed and systematically compared: a convolutional neural network (CNN)-based optical flow model, CNN-long short-term memory (LSTM) temporal model, and semi-supervised 3D autoencoder designed to learn latent motion representations from limited labeled data. All models were trained and validated on a real-world dataset acquired from a private fertility clinic, reflecting clinically relevant imaging conditions. The experimental results demonstrated that the proposed framework achieved robust sperm detection and reliable motility estimation (with the CNN-LSTM model achieving the best performance). The proposed approach offers an effective alternative to manual analysis.

Keywords: automated semen analysis, semen count, motility, deep learning, YOLOv8

1. INTRODUCTION

Male infertility has emerged as a significant global health concern, with sperm concentration and motility being recognized as the primary biomarkers for clinical diagnosis and fertility prognosis. Driven by the rising prevalence rates, the urgency to counter this issue is further underscored by recent longitudinal assessments reporting a significant decline in sperm concentration over the last five decades¹. In the wake of significant advancements in automated technologies, the World Health Organization has reaffirmed manual microscopic evaluation as the “gold standard” for semen analysis². This continued reliance is largely attributed to the absence of standardization in conventional Computer-Aided Semen Analysis (CASA) systems, which fail to properly identify sperm cells from other similar cellular artifacts such as leukocytes and cellular debris in a medical sample^{3,4}. In response to these limitations, modern deep learning (DL) frameworks have demonstrated superior ability to suppress biological artifacts and debris, ensuring that automated counts are accurate even in noisy or unclean clinical environments⁵.

The advent of DL has paved the way for overcoming these shortcomings by facilitating effective learning directly from

microscopic images⁶ and videos⁷. Within the context of sperm detection, the You Only Look Once (YOLO) model has been recognized as the foremost detection technique, owing to its ability to process data in real time⁸. Although preceding models have successfully detected sperms within scanned images, they often require considerable processing power, thus hindering their use in edge computing⁹. Recent studies have identified YOLO version 8 (YOLOv8) as an improved version that includes an anchor-free detection head and an enhanced fusion technique to effectively boost detection accuracy under noisy conditions. The evolution of YOLO architecture, culminating in the anchor-free detection head of YOLOv8, has significantly improved the ability of DL models to detect small objects in noisy environments¹⁰. This study focused on the YOLOv8 Nano model¹¹. To rationalize the need for this reduced architecture, the goal was to not only accelerate detection processing but also to ensure that this model has the ability to maintain high detection accuracy¹². Our contribution lies in the fine-tuning of the YOLOv8 Nano architecture using carefully annotated data to enhance its capability to accurately detect and count only valid sperm cells, which are characterized by the presence of both the head and tail, while effectively suppressing non-sperm objects and biological

artifacts. This approach enables rapid inference while preserving high detection accuracy, even in unclean or abnormal semen samples, where debris, cells, or morphological irregularities may otherwise lead to misclassification.

Notably, a critical gap remains in the automation of motility assessments. The prevailing DL paradigm typically relies on "tracking-by-detection," where the system must detect, identify, and link every individual sperm cell across hundreds of consecutive frames to calculate kinematic parameters. Although conceptually straightforward, this approach is computationally expensive and prone to identity-switching errors when the trajectories of the sperms intersect (i.e., occlusion occurs) or when detection fails within a single frame. Furthermore, the training of robust trackers requires datasets with exhaustive frame-by-frame coordinate annotations, which are scarce and expensive to generate. To overcome these bottlenecks, this study developed a unified resource-efficient framework that decouples counting from motility analyses. Instead of relying on error-prone object tracking, a holistic video regression task was used for motility assessment. By analyzing global optical flow patterns and temporal dynamics, the developed model could predict the overall motility percentage directly from video sequences. This approach aligns with the aggregate metrics provided by legacy CASA systems¹³; moreover, it also leverages the feature-learning characteristics of deep neural networks to handle noise and occlusion more effectively.

A custom dataset curated from a private fertility clinic was used in this study, ensuring that the developed models were trained and validated on real-world data characterized by varying contrasts and particulate noise, rather than idealized public datasets. The contributions of this study are threefold, which are as follows:

1. **Robust Counting:** YOLOv8 Nano was fine-tuned to accurately detect sperm cells in high-debris environments without explicit negative-class annotation.
2. **Efficient Motility Grading:** A regression-based motility framework that eliminates the need for frame-level tracking labels is proposed.
3. **Architectural Comparative Analysis:** Three distinct spatiotemporal architectures were evaluated: a convolutional neural network (CNN) with optical flow for explicit motion modeling, CNN–long short-term memory (LSTM) model for capturing long-term temporal dependencies, and semi-supervised 3D Autoencoder designed to extract latent motion features from limited labeled data.

2. METHODOLOGY

All experiments were conducted in a standardized DL environment using Python 3.12.12 and the PyTorch framework to ensure technical precision and full reproducibility. The YOLOv8 models were implemented using the Ultralytics 8.4.12 library. All model training and testing were performed on a Linux-based server equipped with an NVIDIA Tesla T4 GPU to maintain a consistent computational performance across all architectures. The framework was structured around two primary tasks: sperm

counting through object detection and sperm motility analysis using a comparative study of three distinct DL architectures.

2.1. Data Collection and Preparation. The data for this study were obtained from a custom set of patient sperm videos and images recorded by a fertility physician. The preparation process was divided into two parts to separately handle the counting and motility.

For the sperm counting, five frames were extracted from 32 videos (160 images in total); then, the images were manually labeled using Roboflow, as shown in Figure 1. Bounding boxes were only placed around valid sperm cells that clearly showed both a head and tail. This is important for helping the model learn the difference between a real sperm and other objects, such as white blood cells. To ensure that the performance of the model was evaluated fairly and prevent data leakage, the dataset was split into training, validation, and test sets in 80:10:10 ratio. Then, data augmentation techniques, such as rotation and flipping, were applied to make the dataset larger and more diverse, increasing the total training pool to 400 images.

A total of 279 videos were used for the motility task. Each video contained 30 frames and was paired with a motility percentage recorded by a doctor. The dataset was partitioned into 80% for training and 20% for testing to maintain consistent evaluation across all motility architectures.

2.2. Sperm Counting Model: YOLOv8. The YOLOv8 model was selected for the sperm counting task in this study because it is a well-known model for real-time object detection and provides high precision for small objects. The model uses convolutional layers integrated within a modified Cross Stage Partial backbone, utilizing Cross Stage Partial with two convolution flow modules to extract rich spatial features from the input images. Unlike classical multistage detection algorithms, YOLOv8 is a single-stage detector that analyzes the entire image in a single pass by concurrently predicting the bounding boxes and computing the confidence scores for the detected sperm cells. The total sperm count was derived by aggregating the individual detections that exceeded a specific confidence threshold, thereby improving the overall reliability of the system for rapid clinical applications.

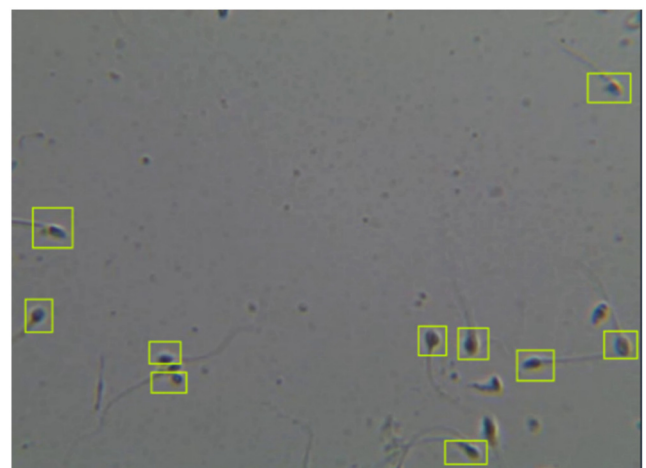


Figure 1. Manually labeled sperm cell image

2.3. Sperm Motility Architectures. To evaluate sperm motility, three different DL architectures were compared, each offering a different approach for processing temporal data. These included a CNN with optical flow (Model A), a CNN-LSTM hybrid model (Model B), and an autoencoder with latent feature regression to analyze compressed representations of movement (Model C). A comparison of these three models aided in determining the strategy that best captured the complex dynamics of sperm cells.

2.3.1. Model A: CNN with Optical Flow. The first approach used a CNN with an optical flow model. This method calculated the motion vectors between consecutive frames to capture temporal information rather than relying solely on static image features. These optical flow maps, which represented the direction and speed of movement, were then processed using a CNN to classify the motility grade. This technique enabled the model to track fast-moving sperm with high accuracy by focusing specifically on movement patterns.

2.3.2. Model B: CNN-LSTM. The second approach used a hybrid CNN-LSTM architecture designed to process raw video sequences directly. In this model, a time-distributed CNN served as a spatial feature extractor that converted individual video frames into dense feature vectors. These vectors were then fed sequentially into the LSTM network. The LSTM component is important for capturing long-term temporal dependencies, enabling the system to remember the historical trajectory of a sperm cell and classify its motility based on the temporal evolution of its movement.

2.3.3. Model C: 3D Autoencoder with Latent Feature Regression. In the third model, a two-stage semi-supervised architecture was used to handle the issue of limited labeled data. This method separated learning from motility predictions.

● **Stage 1: Unsupervised spatiotemporal feature learning:**

The first stage focused on unsupervised spatiotemporal feature learning. By employing a 3D convolutional autoencoder, compressed representations of sperm motion patterns were directly extracted from the raw video data. The architecture of the first stage comprises the following:

- **Encoder:** The encoder network processes the input video sequence using 3D convolutional layers to extract spatiotemporal features, and downsamples the data into a compact latent vector via global average pooling.
- **Decoder:** The decoder attempts to reconstruct the original optical flow sequence from a latent vector. The model was trained to minimize the reconstruction loss [mean squared error (MSE)], forcing the latent vector to capture the most essential dynamics of sperm movement.

● **Stage 2: Supervised motility regression:**

Once the autoencoder was trained, the encoder was frozen and used as a feature extractor. The learned latent vectors that encapsulated the high-level motion characteristics of each sample were fed into a separate multilayer perceptron (MLP) regressor. This lightweight regression network was trained to map the latent features directly to the motility percentage, effectively leveraging the robust features learned during the unsupervised stage.

3. EXPERIMENTAL WORK

This section describes the experimental procedures used to implement, train, and test the sperm count and motility models. The following subsections describe the detailed configurations of these models.

3.1. Experimental Setup for Sperm Counting. The sperm counting model was trained by fine-tuning YOLOv8 to the carefully annotated clinical data. The specific configuration is as follows:

- **Model Architecture:** The YOLOv8 Nano model was used for its lightweight architecture.
- **Input Resolution:** Images were processed at a resolution of 640×640 pixels.
- **Training Duration:** The model was trained for 50 epochs, which was sufficient to provide loss convergence ability without overfitting.
- **Batch Size:** A batch size of eight was selected.

3.2. Experimental Setup for Sperm Motility. To assess the temporal analysis capabilities of DL frameworks, the aforementioned three models were evaluated on the same dataset. They all shared a common dataset split: training 80% and testing 20%. The detailed configuration is described subsequently.

3.2.1. Model A: CNN with Optical Flow. The first model used a dense optical flow with a 3D CNN. The implementation information includes the following.

- **Input Processing:** The dense optical flow was computed using the Farneback algorithm. The input sequence comprised 30 frames, with each frame resized to 128×128 pixels.
- **Normalization:** Flow vectors were normalized to $[0, 1]$ values using MinMax normalization.
- **Architecture:** The model used 3D convolutional layers (32, 64, and 128 filters) with rectified linear unit (ReLU) activation to extract spatiotemporal motion features.
- **From Motion to Prediction:** To translate the complex motion patterns into a single result, a global average pooling 3D layer was used to condense the data, which were then fed into a 64-unit fully connected (dense) layer, followed by a final output neuron to calculate the motility percentage.
- **Regularization:** To prevent overfitting, L2 regularization was performed on the convolutional and dense layers, and a dropout layer (0.5) was applied to the prefinal output.
- **Training Settings:**
 - **Optimizer:** Adam.
 - **Loss Function:** MSE.
 - **Epochs:** 50.
 - **Batch Size:** 8.

3.2.2. Model B: CNN-LSTM. In the second model, a hybrid CNN and LSTM network was used. Unlike the 3D CNN, this model treated optical flow frames sequentially to determine temporal dependencies. The input shape was (30, 128, 128, 2), which denotes the sequence length (30), spatial dimensions (128×128), and flow vectors (2 represents (x, y)).

- **Spatiotemporal Architecture:**

- **Time-Distributed CNN:** Spatial features of each frame were encoded by attaching TimeDistributed wrappers to the Conv2D layers (16 and 32 filters). Each convolutional block was followed by MaxPooling2D and BatchNormalization to reduce the dimensionality and normalize the activations, respectively.
- **Sequence Modeling:** To bridge the spatial and temporal components, a global average pooling 2D layer was used to condense the spatial features of each individual frame into a vector. These vectors were then fed into an LSTM layer with 64 units, which enabled the model to learn the temporal dependencies and motion patterns across the 30-frame sequence.
- **Regression Head:** The LSTM output entered a fully connected dense layer (64 units) with ReLU activation, followed by a dropout layer (0.3) and single neuron output for motility prediction.

- **Training Configuration:**

- Optimizer: Adam.
- Loss Function: MSE.
- Epochs: 50.
- Batch Size: 8.

3.2.3. Model C: 3D Autoencoder. The third model used a 3D Convolutional autoencoder with a semi-supervised approach. First, the model learned unannotated data to a compressed feature of sperm motion patterns, followed by a regression network in which the learned features were assigned motility scores.

- **Input Configuration:** The input comprised 30 optical flow frames. For the 3D reconstruction process, the spatial resolution was downsampled to 64 × 64 pixels.

- **Autoencoder Architecture:**

- **Encoder:** To capture the spatiotemporal features, the encoder used three Conv3D blocks (32, 64, and 128 filters). This sequence was followed by MaxPooling3D after each block, which downsampled the spatial dimensions. A GlobalAveragePooling3D layer was subsequently used to extract a compact latent feature vector.
- **Decoder:** The decoder attempted to reconstruct the original optical flow sequence using mirrored Conv3D and UpSampling3D layers, culminating in a sigmoid activation function.
- **Unsupervised Training:** In this stage, the model was trained as an autoencoder to reconstruct the input optical flow sequences. By forcing the decoder to rebuild the original data using mirrored Conv3D and UpSampling3D layers, the model learned to condense complex movements into a meaningful latent space. This step is essential because it allows the encoder to capture robust patterns of sperm motion independently before manual labels are introduced for regression.

- **Motility Regression:**

- After training, the encoder was frozen and used to extract the latent features from the dataset.

- A separate MLP regressor (dense layers of 64 and 32 units with dropout) was trained on these latent features for 80 epochs to predict the final motility percentage.
- This two-step process allows the model to leverage robust feature learning even with limited labeled data.

4. RESULTS AND DISCUSSION

The experimental results demonstrated the efficacy of using YOLOv8 for object detection and the comparative strengths of the three models used for motility analysis, which are presented in detail subsequently.

4.1. Sperm Counting Results (YOLOv8). The YOLOv8 model was evaluated using a test dataset to determine its precision in detecting and counting sperm cells of varying densities. The evaluation yielded promising results with the model achieving a mean absolute error (MAE) of 2.9. This low error indicated that, on average, the model prediction deviated from the manual count by an expert by approximately three sperm cells per image. Furthermore, the root mean squared error (RMSE) was calculated to be 3.66, confirming that the model maintained consistent performance without significant outliers or extreme failures in detection.

In terms of total population analysis across the tested batch, the ground-truth manual count identified 315 sperm cells, whereas the YOLOv8 model successfully detected 355 cells. The evaluation yielded precision, recall, and mean average precision at 0.50 intersection over union (mAP@50) of 0.641, 0.714, and 0.668, respectively. The difference in total counts is likely a tradeoff; while the model occasionally missed overlapping or faint sperm cells (affecting recall), it also tended to pick up certain circular biological artifacts or debris as potential detections (affecting precision). Despite these minor misclassifications in noisy clinical samples, the MSE remained low at 13.4, reinforcing the reliability of the system as a tool for clinical screening. To provide a clearer picture of how these metrics were calculated, a detailed breakdown of true positives, false positives, and false negatives is presented in Table 1.

The YOLOv8 model was robust against background noise and other biological artifacts. The sample image (Figure 2) shows several spherical objects (white blood cells) among the sperm. Because of their similarity in size, traditional image processing methods are prone to identifying these round cells as sperm heads. The proposed model demonstrated the ability to differentiate real sperms from these particulate artifacts. The model produced bounding boxes for only objects presenting the typical sperm morphology with confidence scores ranging from 0.69 to 0.80, indicating a filter for circular debris and other non-sperm cells based on the final model results (Figure 2). This narrow-spectrum detection capability is crucial for preventing false positives and obtaining clinically meaningful semen sample counts.

4.2. Model Evaluation for Sperm Motility. To assess sperm motility, the three DL models were evaluated. The objective was to identify the method that can most effectively capture the spatiotemporal dynamics of sperm movement given the limited dataset size. The performance of each model was evaluated

Table 1. Confusion Matrix Breakdown for Sperm Detection

Metric	Value	Description
Ground Truth (Instances)	315	Total actual sperm cells identified by an expert
True Positives (TP)	225	Correctly identified sperm cells (recall * instances)
False Positives (FP)	130	Objects wrongly identified as a sperm (debris/artifacts)
False Negatives (FN)	90	Actual sperm cells missed by the model
Total Detections	355	Total number of bounding boxes generated by the model (TP + FP)

using the MSE and RMSE to measure the variance in predictions, as well as the MAE to determine the average deviation from the manual ground truth in percentage points.

4.2.1. Model A: CNN with Optical Flow Results. Model A was evaluated to assess its ability to predict motility based on immediate pixel displacement. This model yielded the second strongest performance among the tested models, achieving a MAE of 10.47%. This indicates that, on average, the motility prediction of the model deviated from the manual expert assessment by approximately 10 percentage points. Moreover, the model recorded MSE and RMSE of 183.02 and 13.53, respectively, reflecting its capability in effectively handling the variance in sperm movement speeds.

From Figure 3, we can observe that the training process exhibits considerable volatility in the initial stages, which is characterized by sharp spikes in the validation loss. After approximately 30 epochs, the model stabilizes, demonstrating successful convergence. The superior performance of this model is due to the Farneback algorithm, which explicitly computes motion features, allowing the network to focus more on the movement dynamics rather than static image noise.

4.2.2. Model B: CNN-LSTM Results. Model B achieved the highest performance among all tested models. The evaluation yielded an MAE of 9.32%, significantly outperforming the pure CNN approach. The MSE was 159.78, with a corresponding RMSE of 12.64.

As shown in Figure 4, the training process exhibits rapid convergence. The CNN-LSTM loss curve drops sharply within the first 10 epochs and stabilizes quickly. This stability suggests that

the LSTM component successfully captured long-term temporal dependencies in the sperm movement. By effectively modeling the historical trajectory of the optical flow vectors, the model could distinguish between consistent progressive motility and random motion more accurately than that achieved using only frame-by-frame analysis. The low MAE of 9.32% confirms that combining spatial feature extraction with temporal sequence modeling provides the most robust approach for automated motility assessment.

4.2.3. Model C: Autoencoder with Latent Regression Results. Model C used a semi-supervised approach, achieving an MAE of 11.35%. The MSE was 194.94, with an RMSE of 13.96.

The performance of these two stages is supported by the training curves. Figure 5 shows the unsupervised training of the autoencoder. The reconstruction loss (MSE) decreases smoothly and aligns closely with the validation loss, indicating that the model successfully learned to compress the complex spatiotemporal dynamics of the sperm videos into a compact latent representation without overfitting.

Figure 6 shows the training results of the MLP regressor on these extracted features. The curve demonstrates a significantly rapid convergence, dropping to a low error rate within the first 10 epochs. This suggests that the latent features learned by the autoencoder were highly discriminative and robust, effectively summarizing the motion patterns in a manner that made the regression task straightforward for the MLP.

4.3. Discussion and Comparative Analysis. The comparative evaluation of the three models revealed critical insights

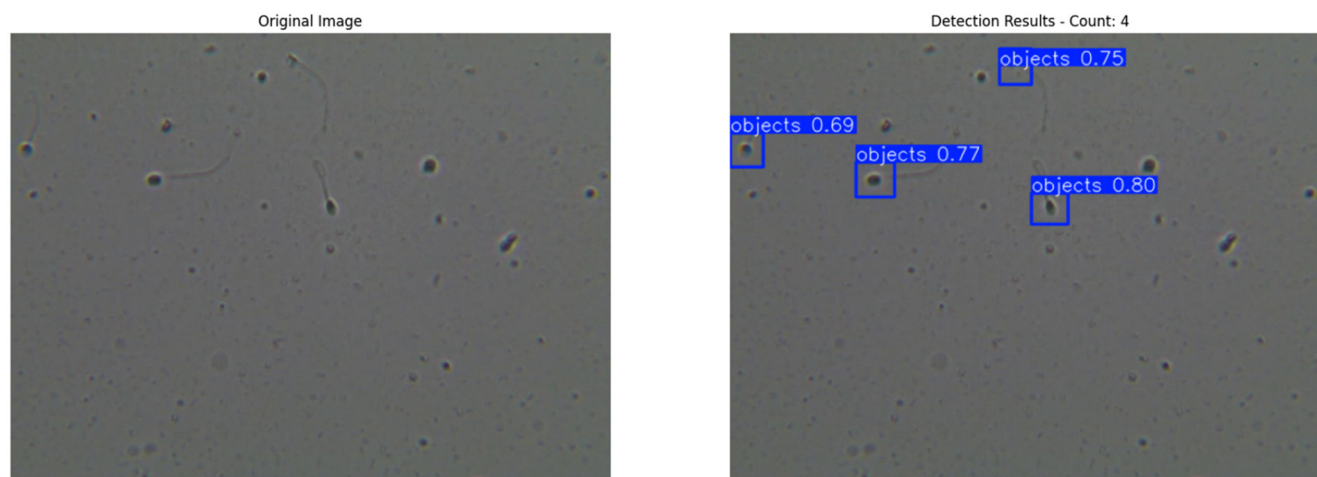
**Figure 2.** Example of sperm detection: Original and detection results

Table 2. Performance Comparison of Motility Analysis Models

Model Architecture	MAE	RMSE	MSE
Model A: CNN + Optical Flow	10.47%	13.53	183.02
Model B: CNN-LSTM	9.32%	12.64	159.78
Model C: Autoencoder + MLP	11.35%	13.96	194.94

into the effective modeling of sperm motility. A summary of the performance metrics is presented in Table 2.

4.3.1. Analysis of Results.

- **Superiority of Spatiotemporal Modeling:** Model B achieved the highest accuracy, with the lowest MAE of 9.32%. This performance demonstrates that when appropriately optimized with global average pooling to prevent overfitting, the LSTM network successfully captures the long-term temporal dependencies of sperm movement.
- **Robustness of Explicit Motion Features:** Model A remained highly competitive, securing the second-best performance with an MAE of 10.47%. This confirms that explicitly calculating motion vectors using the Farneback algorithm provides a clean, noise-free input signal. While it lacks the long-term memory of the LSTM, the direct correlation between optical flow intensity and motility grade proves to be a reliable and computationally efficient method for general motility assessment.
- **Viability of Semi-Supervised Learning:** Model C yielded an MAE of 11.35%. Although it ranked third, its performance validates the potential of unsupervised feature learning. The autoencoder successfully compressed complex video data into meaningful latent representations without requiring frame-level labels. This suggests that in clinical scenarios where expert annotation is scarce or expensive, a semi-supervised approach remains a scientifically valid and effective alternative.

4.3.2. Advantages of tracking-free regression. Beyond individual model performance, this framework establishes the viability of a tracking-free approach to motility analysis. Traditional CASA systems often fail during "identity switching" or presence of occlusions in high-density samples. By framing motility as a global video-level regression task, the proposed method

remained robust against these common tracking errors while significantly reducing computational overhead. This efficiency can facilitate high-speed analysis on low-cost clinical hardware and edge devices, offering a practical advantage over more hardware-intensive tracking pipelines.

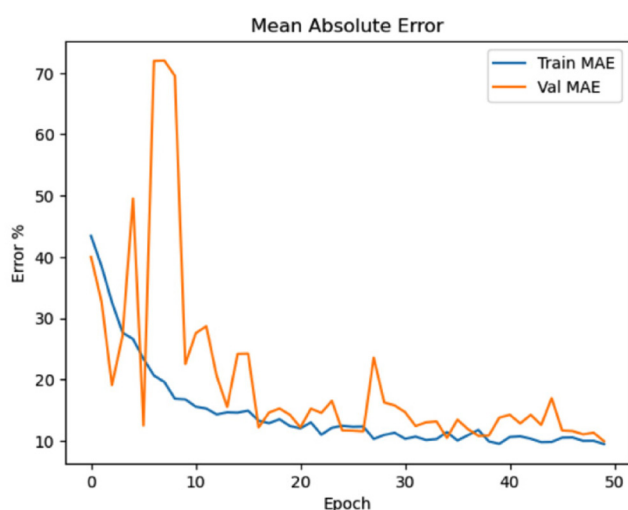
4.3.3. Strategic advantages of a tracking-free approach. Beyond individual model metrics, this framework demonstrates the clear benefits of moving away from traditional sperm tracking. Standard systems often fail in crowded samples owing to overlapping paths. By analyzing motility as a global, video-level regression task, the proposed method avoids these common errors while significantly lowering the computational burden. This efficiency facilitates high-speed analysis even on budget-friendly clinical hardware.

5. CONCLUSIONS AND FUTURE WORK

5.1. Conclusion. This study explored the application of advanced DL models to enhance the accuracy and efficiency of CASA, thereby addressing the critical limitations of subjective manual evaluation. It primarily focused on two main components of fertility diagnostics: sperm counting and motility. In particular, the YOLOv8 model was fine-tuned for sperm detection, and a comparative analysis was conducted on three different models (CNN with optical flow, CNN-LSTM, and semi-supervised autoencoder) to evaluate temporal movement dynamics. The results demonstrated that YOLOv8 achieved superior performance in sperm counting, with an MAE of 2.9. A significant advantage of this model is its robustness against background noise, as it successfully distinguished sperm cells from non-sperm biological artifacts such as leukocytes and round cells. This capability addresses a major deficiency of traditional threshold-based techniques, which often struggle with noisy, low-contrast clinical samples.

In motility analysis, the comparative study revealed that the CNN-LSTM model was the most effective approach, achieving the lowest MAE of 9.32%. This finding suggests that combining spatial feature extraction with temporal sequence modeling allows the system to capture long-term movement trajectories more effectively than using only frame-by-frame analysis. The CNN with optical flow model also demonstrated a robust performance with an MAE of 10.47%, confirming that explicitly calculating motion vectors provides a clean and reliable signal for motility grading. Meanwhile, the semi-supervised autoencoder showed promising results with an MAE of 11.35%, validating the potential of unsupervised feature learning in scenarios where labeled medical data are scarce. Collectively, these findings reinforce the feasibility of integrating AI-driven tools into clinical practice to offer a standardized, objective, and reproducible alternative to manual analysis.

5.2. Future Work. Although the proposed models demonstrated a strong baseline performance, several avenues for technical optimization and clinical expansion remain unexplored. Future research should prioritize the systematic evaluation of different iterations within the YOLOv8 family. Although the current study utilized the nano variant for its real-time efficiency, subsequent work should benchmark medium and large versions

**Figure 3.** Training and validation MAE for the CNN optical flow model

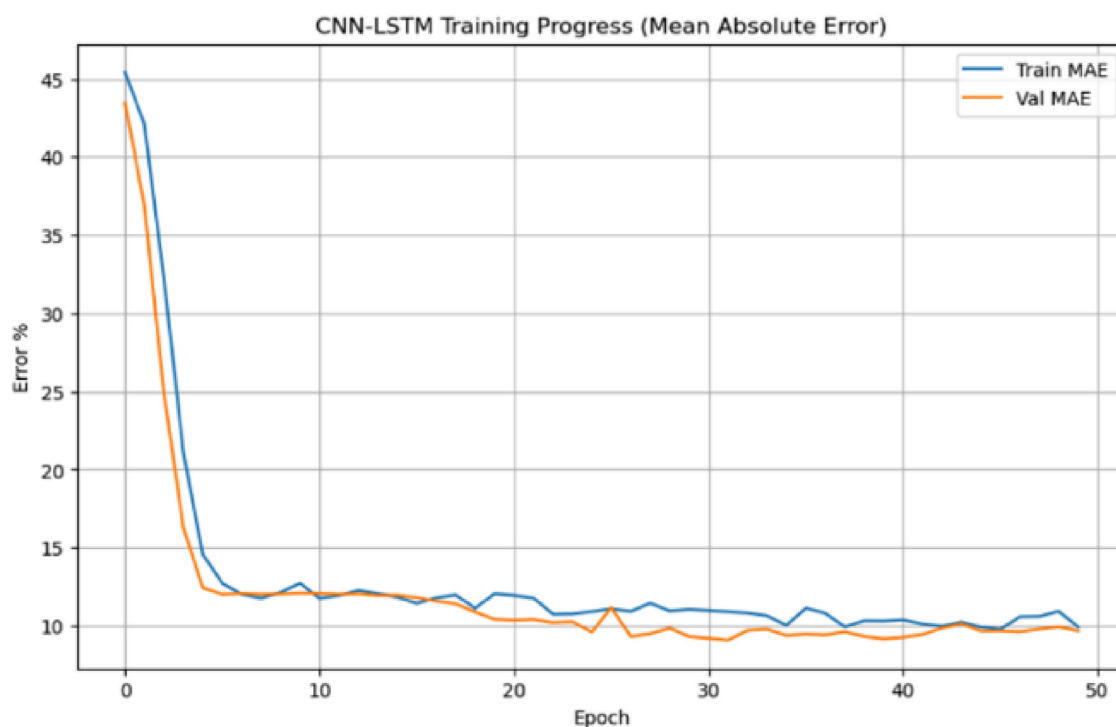


Figure 4. Training and validation MAE for the CNN-LSTM model

to quantify the tradeoffs between computational latency and detection precision. This comparative analysis will serve as a foundation for a cost-benefit analysis, aiding in the identification of the optimal architecture for specific use cases, such as deploying high-accuracy models on cloud servers versus lightweight models for edge devices and tablet-based microscope interfaces.

To further address the challenges of detecting small, densely packed sperm cells, the integration of Slicing Aided Hyper Inference, which is an open-source framework that has been designed to significantly improve the detection and segmentation of small or dense objects in high-resolution images, will be crucial. This technique involves partitioning high-resolution microscopic images into overlapping slices during the inference stage, allowing the model to detect small objects with greater visual fidelity before merging the results. Concurrently, this pipeline

is enhanced using super-resolution preprocessing. By employing DL-based upscaling techniques to increase the resolution of raw video feeds before analysis, the system can recover fine morphological details from lower-quality optical hardware, thereby improving the overall robustness of both counting and motility assessments.

Beyond these technical optimizations, the next phase of this research should prioritize external validation and patient-level generalization. Because the current dataset was derived from a single clinical source, future studies should incorporate multi-center data to ensure the robustness of the framework across different laboratory settings and optical hardware. We also intend

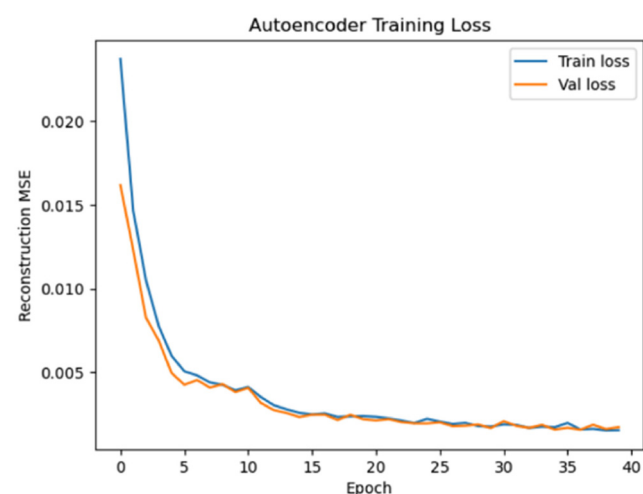


Figure 5. Autoencoder Training Loss (MSE)

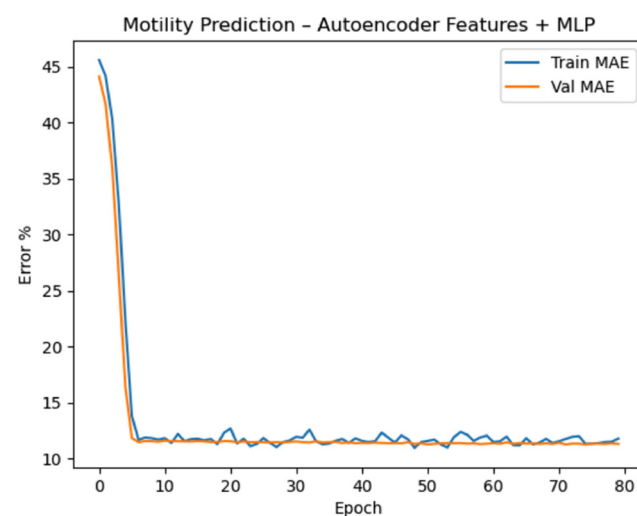


Figure 6. Motility prediction error (MAE) for the MLP regressor trained on extracted latent features

to conduct a more rigorous statistical analysis, including the calculation of confidence intervals for all performance metrics and a direct comparison with established computational baselines. By expanding the dataset to include a wider diversity of patient samples, we aim to transition this exploratory proof-of-concept into a clinically validated tool that is ready for real-world diagnostic deployment.

Finally, future iterations should aim to create a comprehensive diagnostic tool by incorporating sperm morphology classification to detect head and tail defects directly in the detection pipeline. Long-term studies comparing the outputs of the AI system with manual counts will be essential to validate the broader applicability of these advanced computer vision techniques in routine fertility diagnostics.

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Investigating the Fouling Tendency of Polyelectrolyte Complex Membranes

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ABSTRACT

Aqueous phase separation (APS) is a sustainable method for fabricating polymeric membranes without using toxic organic solvents. In this study, membranes were prepared using poly(sodium 4-styrene sulfonate) (PSS) and polyethyleneimine (PEI) via a pH-shift-induced APS. The membranes were tested for organic fouling using bovine serum albumin (BSA) as a model foulant in a dead-end filtration setup. The pure water flux, flux recovery ratio (FRR), reversible fouling ratio (RFR), irreversible fouling ratio (IFR), and total fouling ratio (TFR) were evaluated over three filtration cycles. The initial water flux was $255 \text{ Lm}^{-2}\text{h}^{-1}$ at 1 bar. After exposure to BSA, the flux significantly decreased to approximately 19% of its original value after three cycles. The FRRs remained low (0.19–0.31), while the IFRs were high (0.69–0.81), indicating dominant irreversible fouling. UV-vis analysis showed unstable rejection behavior, including negative rejection values in later cycles, likely due to insufficient cleaning and concentration polarization. The results show that although the PSS-PEI APS membranes exhibited high initial flux, their fouling resistance toward BSA was limited under the tested conditions.

Keywords: fouling, aqueous phase separation, membrane, water treatment, polyelectrolyte complexes

1. INTRODUCTION

Aqueous phase separation (APS) has gained significant research attention in recent years as a sustainable alternative to traditional membrane fabrication methods.^{1–8} Unlike nonsolvent-induced phase separation (NIPS), APS avoids the use of toxic organic solvents such as N-methyl-2-pyrrolidone (NMP). Several recent studies have demonstrated that APS can produce microfiltration, ultrafiltration, and nanofiltration membranes with controlled pore sizes and competitive performance compared with the NIPS membranes.^{2,4,9}

In APS, oppositely charged water-soluble polyelectrolytes are combined to form water-insoluble polyelectrolyte complexes. This can be achieved by varying the pH or salt concentration. In pH-shift-induced APS, the polymers are first mixed under conditions where complexation is prevented (for example, at a high pH where the weak polyelectrolyte is uncharged).³ After casting, immersion in an acidic bath causes protonation of the weak polyelectrolyte, leading to immediate complex formation and membrane precipitation. By adjusting parameters such as the polymer concentration and bath pH, the membrane structure and pore size can be tuned.⁹

One of the most widely studied pH-shift-induced APS membrane systems is the polyelectrolyte pair of poly(sodium 4-styrene sulfonate) (PSS) and polyethyleneimine (PEI), or commonly referred to as PSS-PEI. The advantage of the PSS-PEI system is that the phase inversion and polyelectrolyte

complexation is achieved by a mild pH shift, i.e., from a pH of approximately 12 to a pH of approximately 4.^{7,10} In this system, PEI acts as the weak polyelectrolyte ($\text{pK}_a \approx 8.5$), while PSS is a strong polyelectrolyte that remains charged over a wide pH range. Phase inversion typically occurs when the pH is shifted from approximately 12 to 4. Previous studies reported PSS-PEI ultrafiltration membranes prepared with different monomer mixing ratios with water permeabilities of approximately 40–200 LMH $\cdot \text{bar}^{-1}$ and bovine serum albumin (BSA) rejection ranging from 36% to 98%.¹⁰ However, the fouling behavior of PSS-PEI membranes has not been systematically studied.

Membrane fouling is one of the main challenges in filtration processes.^{11,12} Fouling reduces water flux owing to the deposition of particles, organic matter, microorganisms, or inorganic compounds on the membrane surface or inside the pores.¹² Fouling can occur through several mechanisms depending on the type of molecule, for example, pore blocking, adsorption inside the pores, or formation of a cake layer on the surface (Figure 1).

For water filtration systems, particulate fouling (Figure 1a) occurs in two ways: inside the pores, which decreases the diameter for the water flux, and other types that decrease the water flux from the top of the membrane by creating a layer, in extreme cases a cake layer, that prevents the water from entering the membrane smoothly, with particles such as silt clay that are generally $>100 \mu\text{m}$. Inorganic fouling (Figure 1b) occurs when dissolved inorganic compounds or elements, such as iron, are absorbed by the membrane surface, forming particles that are generally 10

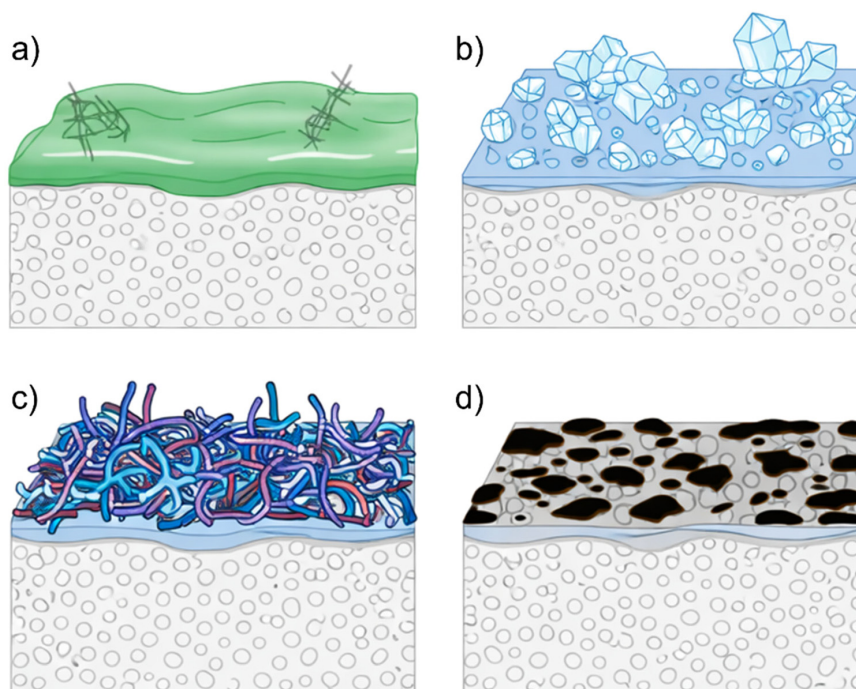


Figure 1. Schematic showing different types of fouling: a) particulate fouling, b) inorganic fouling, c) bacterial fouling (microbiological fouling), and d) organic fouling

nm–10 μm . Particulate and inorganic fouling are similar, except that they differ in size, and particulate fouling is not necessarily due to an inorganic material. Microbiological fouling (Figure 1c) occurs when a microbiological organism grows to form a viscous layer or a solid layer called a cake layer, which blocks the pores. Organic fouling (Figure 1d) occurs when the particles dissolve and collide with the membrane material, with the particles generally 1–100 nm in size, similar to natural organic matter (NOM). Organic fouling, especially from NOM or proteins such as BSA, is common in water treatment systems.

Dissolved organic fouling refers to the formation of organic matter caused by NOM, in which the material existing in drinking water sources is absorbed and held by the membrane structure. Organic fouling can occur in the form of a decrease in the pore diameter due to the deposition of a molecular layer or slime-like layer on the membrane surface, which gradually hinders the flow of water. The water flux decreases with the level of fouling, which is a major challenge for membrane performance. Finally, a significant amount of fouling may completely inhibit the passage of water, and effective management strategies should be implemented throughout the working life of the membrane¹².

Although APS membranes have shown promising separation performance, their resistance to organic fouling remains unclear. Therefore, the objective of this study was to evaluate the fouling behavior of PSS–PEI APS membranes using BSA as a model foulant. This study focuses on the flux decline, cleaning efficiency, and rejection behavior over multiple cycles.

2. EXPERIMENTAL

2.1. Materials and Equipment. The polyelectrolyte PSS (Mw ~1000 kDa in powder form) and PEI (Mw ~750 kDa, 50

wt.% in water) were purchased from Merck. Sodium acetate and lyophilized BSA powder (>96%) were purchased from Merck. Glacial acetic acid (>99.7%) was purchased from Fisher Scientific. Deionized water was produced using a Farad Lab Equipment Factory water purification system.

2.2. Preparing and Casting the Dope Solution. Both polyelectrolytes were diluted with water to obtain 25 wt.% aqueous solutions. For example, 2.5 g of DI water was added to 2.5 g of PEI and mixed for 3 h to obtain a 25 wt.% PEI solution. Similarly, PSS in the powder form was diluted with DI water to obtain a 25 wt.% PSS solution. Subsequently, both solutions were mixed in a monomer mixing ratio of PSS:PEI (1:2) for 6 h to obtain 10 g of homogeneous dope solution. The monomer weights of PSS and PEI used to calculate the ratios were 206 Da and 43.04 Da, respectively.

The polymer solution was cast on a clean glass plate using a casting knife with a 400 μm gap height. The film was immediately immersed in an acidic coagulation bath (pH ~4) and maintained for 24 h to allow membrane formation. After detachment, the membranes were stored in DI water before testing. The acetate buffer bath was prepared using sodium acetate and acetic acid in water.

2.3. Filtration Experiment. The membrane was cut into circular disks with diameters of 5 cm. The membrane was then pressurized with deionized water for 1 h at 1 bar for compaction. The membrane was ready for filtration immediately after compaction. First, the flux was measured using equation (1).

$$J = \frac{V}{A \times t} \quad (1)$$

where (J) represents the flux ($\text{L m}^{-2} \text{h}^{-1}$), A represents the effective membrane area in m^2 , and t represents the time (h).

The filtration cell was then fed with a 1 gL^{-1} aqueous solution of BSA, which was filtered through the membrane for 20 min at 1 bar of pressure. After filtration, the membrane was backwashed with DI water at 1 bar. The volume of the filtrate was measured, and the permeance was calculated using equation 1. Subsequently, the membrane was backwashed with DI water at 1 bar of pressure by flipping the membrane. The membrane was then returned to its original position to measure the flux for 5 min, thus completing the first cycle. The experiment was conducted for three cycles. The rejection (R) of BSA was calculated using equation (2).

$$R = \left(1 - \frac{C_p}{C_f}\right) \times 100, \quad (2)$$

where C_p and C_f are the BSA concentrations in the permeate and feed, respectively. The BSA concentration was measured using a UV-vis spectrophotometer (Agilent Cary 60, Agilent Technologies). The maximum absorption peak for BSA was observed at 275–280 nm. A straight-line calibration curve was constructed by measuring the UV absorbance of BSA at known concentrations.

2.4. Fouling and the Flux Recovery Ratio (FRR). The FRR was determined using equation (3).

$$FRR = \frac{J_2}{J_0} \quad (3)$$

where J_0 is the initial water flux of the membrane before fouling (measured after compaction and before introduction of the foulant). J_2 is the water flux measured after fouling occurred (after running the feed solution). Flux ratios were obtained to determine the amount of fouling that occurred on the membrane. This indicates the amount of the original flux recovered after cleaning. A value close to one indicates excellent recovery. The reversible fouling ratio (RFR) was determined using equation (4).

$$RFR = \frac{J_2 - J_1}{J_0}, \quad (4)$$

where J_1 is the flux after 5 min of BSA filtration. This represents fouling that can be removed by cleaning, and a value close to one indicates excellent recovery from the backwash.

The irreversible fouling ratio (IFR), which indicates the fouling that remained even after cleaning (irreversible fouling), was

Table 1. Fouling behavior of the PSS–PEI membrane

Fouling	1 st cycle	2 nd cycle	3 rd cycle
FRR	0.31	0.2	0.19
RFR	0.15	0.07	0.06
IRF	0.69	0.8	0.81
TF	0.84	0.87	0.87

calculated using equation (5).

$$FR = \frac{J_0 - J_2}{J_0} \quad (5)$$

Therefore, the total fouling (TF) was calculated as the sum of the RFR and IFR.

3. RESULTS AND DISCUSSION

This experiment was designed to investigate the impact of organic fouling on PSS–PEI APS membranes. Table 1 summarizes the FRR, RFR, IRF, and TF of the complex membranes.

The initial pure water flux (J_0) was $255 \text{ L} \cdot \text{m}^{-2} \cdot \text{h}^{-1}$. As shown in Table 1, the membrane experienced a significant reduction in flux after the first fouling cycle. The flux decreased by 69% compared with the initial value. In the second cycle, the flux was approximately 20% of the original water flux. In the third cycle, the flux was approximately 19.4% of the original water flux. The difference between the second and third cycles was very small, indicating that the fouling behavior became nearly stable after the second cycle.

The RFR represents the portion of fouling that can be removed by cleaning, in this case, by backwashing. A value close to one indicates effective cleaning. In the first cycle, the RFR was approximately 0.15, indicating that only a small amount of fouling was removed. In the second cycle, the RFR was approximately 0.07, and in the third cycle, the RFR was approximately 0.06, indicating very limited cleaning efficiency in both cycles.

The IFRs were approximately 0.69, 0.80, and 0.81 for the first, second, and third cycles, respectively. Values close to one indicate severe irreversible fouling. These results indicate that most of the fouling was irreversible, particularly during the second and third cycles.

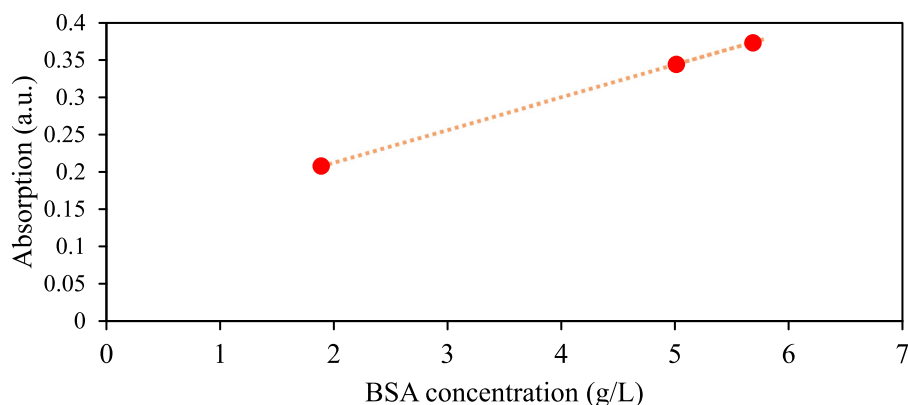


Figure 2. Calibration curve of known concentrations of BSA solution and their absorbance

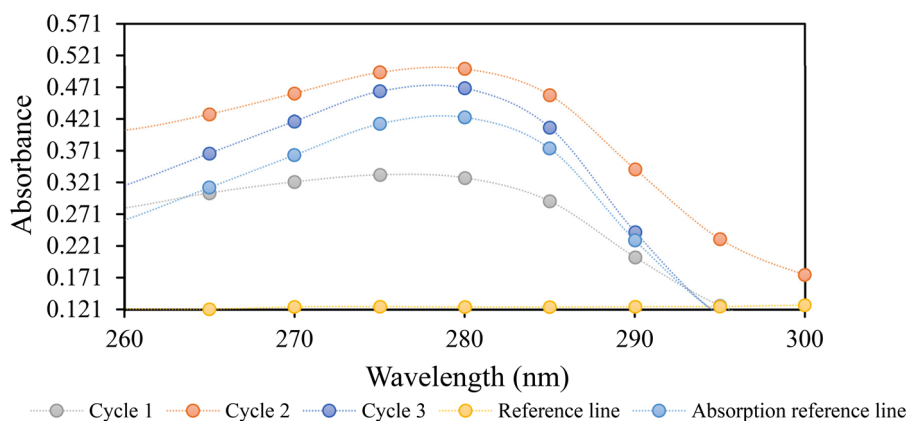


Figure 3. UV-vis spectra of the filtrates after three cycles

The total fouling ratio (TFR), which represents the overall fouling (both reversible and irreversible), was approximately 0.84 in the first cycle and 0.87 in the second and third cycles. These high values confirmed that significant fouling occurred on the membrane surface and inside the pores during all the cycles. These results can be explained by the charged nature of the PSS-PEI membranes. These membranes exhibit a net positive surface charge.⁷ Consequently, the fouling tendency of the membranes is significantly enhanced, resulting in the lower FRRs obtained here.

3.1. Filtration Analysis. The filtrates from the fouling experiments were analyzed using a UV-vis spectrophotometer to measure the BSA concentration. Figure 3 shows the UV spectra of the filtrates before and after three filtration cycles. The feed solution containing 1 gL^{-1} BSA showed maximum absorption in the range of 275–280 (nm) for all trials. The concentration of BSA in the filtrate was significantly lower after the first cycle, and the membrane exhibited a rejection rate of approximately 25% rejection. However, the absorption in the second and third cycles was higher than the feed absorption because of the backwashing step. The elevation is most likely from the first cycle, and the backwash was not sufficient to remove all possible BSA; in more depth, the BSA from first cycle was released in the second cycle, and the BSA from second cycle was released in third cycle, resulting in a higher concentration of BSA in the permeate. Another explanation, assuming that physical cleaning and backwashing were sufficient, is that water cannot remove BSA, and other solvents may be able to dissolve BSA from the membrane into the bulk.

3.2. Comparison with EVOH, PES, PVDF Membranes.

For comparison, commercial membranes fabricated via NIPS were also tested for their fouling propensity. The membrane was pressurized with an aqueous solution of BSA at 0.5 bar following the same steps, that is, three cycles, 20 min of running the foulant, then 1 min of backwash. The first membrane, ethylene vinyl alcohol (EVOH), had a $J_0 = 140 \text{ Lm}^{-2}\text{h}^{-1}$ and showed a FRR of 0.65 with 10% rejection of BSA. The polyether-sulfone (PES) ultrafiltration-type membrane had a $J_0 = 180 \text{ Lm}^{-2}\text{h}^{-1}$ and showed a FRR of 0.6 with 50% to 30% rejection. The polyvinylidene fluoride (PVDF) membrane had a $J_0 =$

$200 \text{ Lm}^{-2}\text{h}^{-1}$ and showed a FRR of 0.4 with 65% to 50% rejection.¹³

4. CONCLUSION

In this study, PSS-PEI membranes were fabricated by aqueous phase separation and tested for organic fouling using BSA. The membranes exhibited a high initial water flux ($255 \text{ Lm}^{-2}\text{h}^{-1}$ at 1 bar). However, after three fouling cycles, the flux decreased to approximately 19% of its original value. FRRs remained low, while IFRs were high (0.69–0.81), indicating dominant irreversible fouling. UV-vis analysis showed unstable rejection behavior, including negative rejection values, in later cycles. This was likely caused by insufficient cleaning and the release of previously adsorbed BSA. Although the fabrication of APS membranes is environmentally friendly, their fouling resistance to protein solutions needs improvement. This study was limited to dead-end filtration and deionized water cleaning. Future work should investigate cross-flow filtration, alternative cleaning methods, and membrane surface modifications to enhance the fouling resistance.

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Enhanced CO₂ Adsorption Performance of Amine-Functionalized MCM-41 Mesoporous Silica

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ABSTRACT

Global carbon dioxide (CO₂) emissions continue to rise, driving an urgent demand for advanced carbon capture technologies. Mesoporous silica—specifically Mobil Composition of Matter No. 41 (MCM-41)—offers considerable potential owing to its ordered pore structure and high surface area. In this study, MCM-41 was synthesized using a sol-gel method and functionalized with two commercial amine-based surface modifiers, Hydrosil 2775 (S1) and Hydrosil 2999 (S2). Structural characterization by Fourier-transform infrared spectroscopy confirmed the successful grafting of amine groups onto the silica framework. Brunauer-Emmett-Teller analysis demonstrated a specific surface area of 334.42 m²/g, confirming the retention of mesoporosity. CO₂ adsorption capacity was evaluated by direct dynamic mass-response measurements. The results demonstrated a marked mass increase, corresponding to a net uptake of approximately 22.8 mg/g. These findings highlight the effectiveness of amine-functionalized MCM-41 as a promising and readily scalable adsorbent for industrial carbon capture applications.

Keywords: MCM-41; CO₂ capture; amine functionalization; mesoporous silica; Hydrosil modifiers; gas adsorption

1. INTRODUCTION

The continuous increase in atmospheric carbon dioxide (CO₂) emissions from industrial activities and fossil fuel combustion has intensified the global need for effective carbon capture technologies. Carbon capture and storage represents a critical strategy to mitigate climate change by trapping emissions at their source. Among various approaches, adsorption onto solid porous materials has gained considerable attention owing to its energy efficiency and ease of regeneration^{1,2}. Mesoporous silica materials, particularly Mobil Composition of Matter No. 41 (MCM-41), are highly promising supports for CO₂ capture owing to their high specific surface area, large pore volume, and well-ordered hexagonal pore structure³. However, pristine silica surfaces exhibit weak physical interactions with CO₂ molecules⁴. To overcome this limitation, chemical modification via amine functionalization is commonly employed. The grafting of amine groups onto the silica framework enhances the chemical affinity for CO₂, leading to markedly improved adsorption capacity and selectivity^{5,6,13}. Previous studies have shown that the performance of amine-functionalized MCM-41 depends heavily on the type of amine used and the loading conditions^{7,8}. In this study, two commercial amine-based modifiers—Hydrosil 2775 and Hydrosil 2999—were used to functionalize synthesized MCM-41. These modifiers offer a scalable and cost-effective approach for developing high-performance adsorbents. The primary objective of this study is to characterize the structural properties of the synthesized materials and evaluate their CO₂ adsorption

performance through dynamic mass-response measurements. By analyzing the interaction between the amine-modified surface and CO₂ gas, this research provides insight into the potential of these materials for industrial-scale carbon capture applications. The structure of the remaining paper is as follows. Section 2 presents the materials and methods used in this study, Section 3 discusses the results and their interpretation, and Section 4 concludes the study.

2. MATERIALS AND METHODS

2.1. Materials and Synthesis Procedure. The synthesis and functionalization of the adsorbents were carried out using high-purity chemical reagents. MCM-41, a mesoporous silica with an ordered hexagonal structure, was used as the primary support framework³. Cetyltrimethylammonium bromide (CTAB, 98%, Sigma-Aldrich) was used as the structure-directing agent, while tetraethyl orthosilicate (TEOS, 99%, Sigma-Aldrich) served as the silica precursor. Sodium hydroxide (NaOH, Sigma-Aldrich) was used to establish the alkaline conditions required for hydrolysis and condensation reactions. MCM-41 was synthesized by dissolving CTAB in deionized water under continuous stirring, followed by the addition of NaOH and dropwise addition of TEOS at 80 °C. The mixture was maintained for 2 h to promote the formation of the silica network. The resulting precipitate was filtered, washed, dried at 60 °C, and calcined at 550 °C for 5 h to remove the surfactant template and obtain



Figure 1. Drying setup with stirring and heating

the ordered mesoporous structure². For surface functionalization, the calcined MCM-41 was dispersed in deionized water, and the pH was adjusted to approximately 10. Hydrosil 2775 (S1) and Hydrosil 2999 (S2) were added separately under continuous stirring at 70 °C and allowed to react overnight to ensure effective grafting of amine groups onto the silica surface⁸. The modified samples were subsequently washed, centrifuged, and dried prior to characterization and CO₂ adsorption testing. The synthesis setup and the final product are illustrated in Figures 1 and 2.

Material properties are summarized in Table 1, highlighting key physical characteristics and functions under identical testing conditions.

2.2. Characterization Techniques. The structural and chemical properties of the samples were analyzed using FTIR spectroscopy and BET analysis. FTIR spectroscopy was used to verify the presence of the silica framework and confirm the successful incorporation of amine groups following functionalization. Characteristic peaks corresponding to Si-O-Si stretching and amine-related bonds were examined. BET analysis was

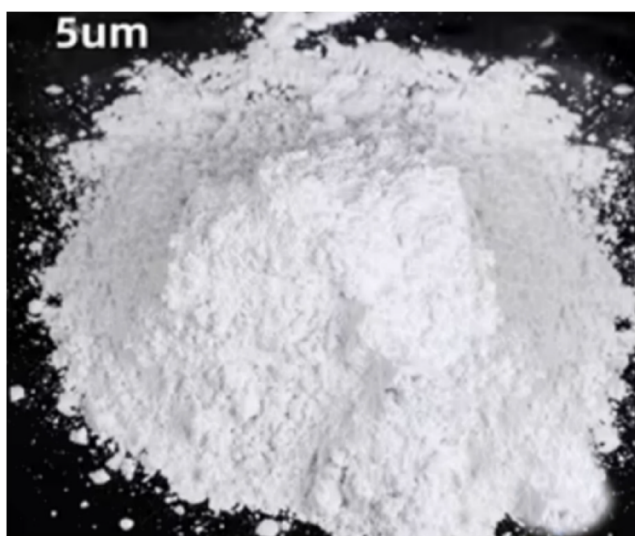


Figure 2. MCM-41 white powder after drying

performed to determine the specific surface area, pore volume, and pore size distribution of the samples. These analyses were conducted under standard conditions to evaluate the effect of functionalization on the structural and adsorption properties of MCM-41.

2.3. Experimental Procedure. CO₂ adsorption experiments were conducted using a high-precision microbalance system to monitor changes in sample mass during gas exposure. Approximately 5–6 mg of each sample was placed on the sample holder inside a sealed chamber connected to a controlled CO₂ supply. Prior to gas introduction, the baseline mass was recorded under ambient conditions to ensure stability. CO₂ was introduced at a constant flow rate, and the mass variation was continuously monitored until equilibrium was reached. Following the adsorption stage, the gas flow was stopped to observe desorption behavior and evaluate the reversibility of the adsorption process. All experiments were conducted under identical environmental and operational conditions to ensure accurate comparison between unmodified and functionalized samples. A summary of the experimental matrix and specimen identifiers is provided in Table 2.

CO₂ adsorption experiments were conducted at a constant flow rate of 50 mL/min under controlled laboratory conditions.

2.3.1. Test setup. The experimental setup consisted of a high-precision analytical microbalance used to monitor mass changes during CO₂ adsorption. Approximately 5–6 mg of each sample was placed in a sealed chamber connected to a controlled CO₂ supply. The initial mass was recorded prior to gas exposure, followed by monitoring until equilibrium was reached. The gas flow was then stopped to observe desorption behavior and evaluate adsorption reversibility. All tests were conducted under identical conditions to ensure reliable comparison.

2.3.2. Instrumentation. The instrumentation used in this study included a high-resolution analytical microbalance (Mettler Toledo) capable of detecting mass variations at the milligram level, enabling real-time recording of adsorption and desorption profiles. Structural and chemical analyses were carried out using an FTIR spectrometer (Thermo Scientific) equipped with an ATR detector to confirm the presence of silica framework peaks and identify amine-related bands following surface modification. BET surface area and pore structure parameters—including specific surface area, pore volume, and average pore diameter—were determined from nitrogen adsorption-desorption isotherms at 77 K using a surface area analyzer (Micromeritics). Instrument calibration was performed according to manufacturer specifications to ensure measurement accuracy and repeatability. The instrumentation used in this study is shown in Figures 3–6.

3. RESULTS AND DISCUSSION

This section presents the key findings obtained from the characterization and CO₂ adsorption testing of MCM-41 before and after surface functionalization. The results demonstrate the impact of incorporating amine-based functional groups on structural properties, chemical composition, and adsorption performance. A combination of FTIR, BET surface analysis, and real-time CO₂ uptake measurements was used to evaluate changes

Table 1. Summary of material characteristics

Sample	Condition	Form	Color	Purpose
MCM-41	Unmodified	Powder	White	CO ₂ adsorption baseline
Hydrosil 2775	Amine modifier	Liquid	Light yellow	Introduces additional active sites
Hydrosil 2999	Ammonium modifier	Liquid	Yellow-brown	Enhances CO ₂ affinity
MCM-41-S1	Functionalized	Powder	Off-white	Evaluates S1 modification effect
MCM-41-S2	Functionalized	Powder	Pale yellow	Evaluates S2 modification effect

Table 2. CO₂ adsorption-desorption test matrix

No.	ID	Sample	Functionalization Type	Mass (mg)	Adsorption/Desorption Time (min)	Temperature
1	A-1	MCM-41 (unmodified)	None	5.70	15/10	25 °C
2	A-2	MCM-41 (unmodified)	None	5.72	15/10	25 °C
3	B-1	MCM-41-S1	S1	5.83	15/10	25 °C
4	B-2	MCM-41-S2	S2	5.80	15/10	25 °C
5	C-1	MCM-41-Mix	S1 + S2	5.85	15/10	25 °C
6	Blank	System baseline check	—	0.00	—	25 °C
7	Rep-1	MCM-41 (unmodified)	None	5.71	15/10	25 °C
8	Stab-A	MCM-41 (unmodified)	None	5.70	Continuous	25 °C
9	Stab-B	MCM-41 (functionalized)	S1 + S2	5.83	Continuous	25 °C
10	Calib	Reference mass (standard)	—	5.00	—	25 °C
11	Final	MCM-41-Mix	S1 + S2	5.85	15 cycles	25 °C

in framework stability, organic loading, textural properties, and adsorption behavior.

3.1. FTIR Characterization. FTIR characterization was conducted to confirm the structural integrity of the mesoporous silica framework before and after functionalization. Figure 7 shows the FTIR spectrum of unmodified MCM-41, where peaks at $\sim 1100\text{ cm}^{-1}$, $\sim 800\text{ cm}^{-1}$, and $\sim 500\text{ cm}^{-1}$ correspond to vibrations of the Si-O-Si network, respectively. The absence of absorption bands in the $2800\text{--}3000\text{ cm}^{-1}$ region confirms

the effective removal of the surfactant template⁷. Following functionalization, new bands at $2850\text{--}2950\text{ cm}^{-1}$ and $\sim 1550\text{--}1650\text{ cm}^{-1}$ are attributed to C-H stretching and N-H bending vibrations, respectively, confirming successful grafting of amine groups onto the silica surface⁸.

Following the FTIR analysis of the unmodified MCM-41 sample, the corresponding spectrum after functionalization is presented in Figure 8.

3.2. BET Surface Area and Pore Structure. BET analysis was conducted to evaluate the surface area and pore structure

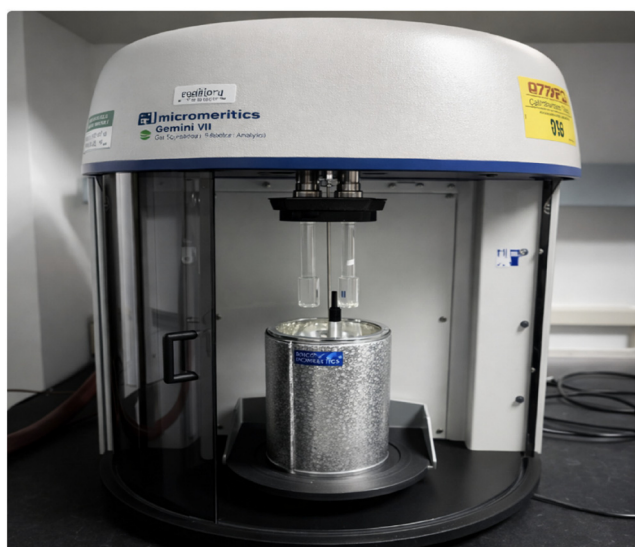
**Figure 3.** BET surface area analyzer used for nitrogen adsorption-desorption measurements**Figure 4.** FTIR spectrometer used for functional group analysis



Figure 5. Vacuum filtration setup used for powder separation and collection

characteristics of the synthesized materials. Unmodified MCM-41 exhibited a specific surface area of $334.42 \text{ m}^2/\text{g}$ and an average pore diameter of 6.53 nm , confirming the formation of a well-defined mesoporous structure. These values fall within the typical range reported for MCM-41 materials in previous studies⁹. As shown in Figure 9, the nitrogen adsorption-desorption isotherm measured at 77 K extends over the complete relative pressure range ($P/P_0 = 0-1.0$). The isotherm exhibits characteristic Type IV behavior with a significant hysteresis loop at high relative pressure, consistent with mesoporous materials. The sharp increase in adsorption at high P/P_0 values is attributed to capillary condensation within the mesopores, further confirming the ordered mesoporous structure of MCM-41. Following surface functionalization, a slight decrease in surface area and pore volume was observed due to partial pore occupation by grafted amine groups, consistent with previous studies on amine-functionalized mesoporous silica systems¹⁰. These results confirm that chemical

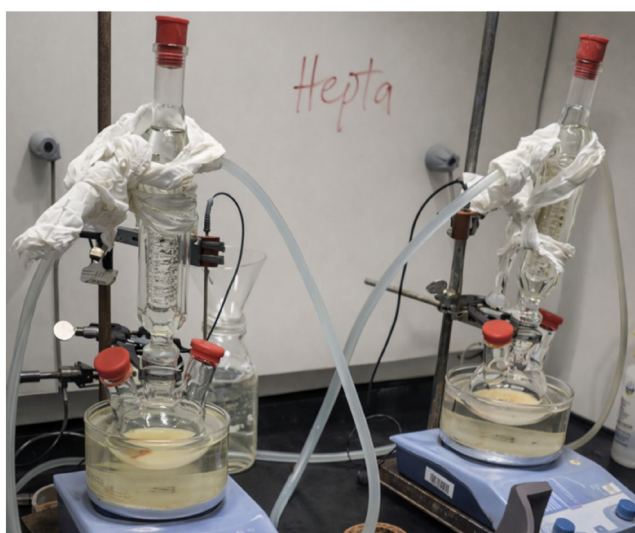


Figure 6. Experimental setup for MCM-41 synthesis under controlled stirring and reflux conditions

modification primarily affected internal surface sites while preserving the overall pore architecture, which is essential for gas adsorption applications.

3.3. CO_2 Adsorption Performance. The CO_2 adsorption-desorption performance of functionalized MCM-41 was evaluated through dynamic mass monitoring under controlled ambient conditions. As shown in Figure 10, the sample mass remained stable at approximately 5.70 mg prior to CO_2 exposure, confirming baseline stability and measurement accuracy. Upon introduction of CO_2 , a rapid increase in mass was observed, indicating fast diffusion of gas molecules into the mesoporous channels and immediate interaction with available adsorption sites. The mass gradually increased until equilibrium was reached at approximately 5.83 mg , corresponding to a net uptake of 0.13 mg (approximately 22.8 mg/g). This enhanced adsorption capacity is attributed to the presence of amine functional groups introduced during surface modification, which provide active sites for interaction with CO_2 molecules¹¹. The adsorption process involves both physisorption and chemisorption mechanisms. The presence of amine groups enables chemical interaction with CO_2 through reversible carbamate formation, while physical adsorption also contributes within the mesoporous structure. This combined mechanism explains the enhanced adsorption performance and the observed reversible behavior. During the desorption phase, initiated by terminating the CO_2 flow, a marked decrease in mass was recorded in Figure 10, indicating that the adsorption process is largely reversible. This behavior suggests that the material can be regenerated under mild conditions, which is advantageous for cyclic carbon capture applications. Similar adsorption-desorption behavior has been reported in previous studies¹².

3.4. Influence of Key Experimental Parameters. This subsection discusses how the selected experimental parameters influenced the CO_2 adsorption performance of the synthesized MCM-41 samples. The main factors considered include material type, surface functionalization treatment, mass variation response, and gas exposure duration. These parameters were selected to assess whether surface functionalization enhances CO_2 capture capacity and whether structural modification influences adsorption kinetics and reversibility.

3.4.1. Effect of material type and surface functionalization. Comparison between unmodified MCM-41 and functionalized samples demonstrated a clear improvement in CO_2 adsorption performance. Unmodified MCM-41 exhibited limited uptake owing to weak interactions between CO_2 molecules and surface silanol groups. Following functionalization with Hydrosil 2775 (S1) and Hydrosil 2999 (S2), a marked increase in adsorption capacity was observed, indicating enhanced affinity toward CO_2 . The mass increased from 5.70 to 5.83 mg , corresponding to a net uptake of 0.13 mg . This improvement is attributed to the amine functional groups introduced by surface modification, which provide active binding sites and promote stronger interactions with CO_2 molecules. These results confirm that surface functionalization substantially enhances the adsorption performance of MCM-41 relative to the unmodified material.

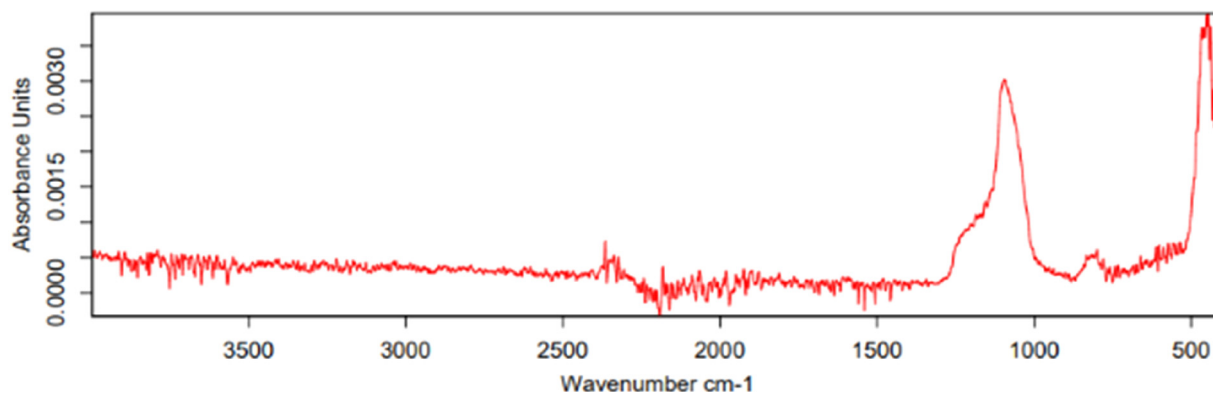


Figure 7. FTIR spectrum of MCM-41 before functionalization, showing characteristic Si-O-Si bands and absence of organic functional groups

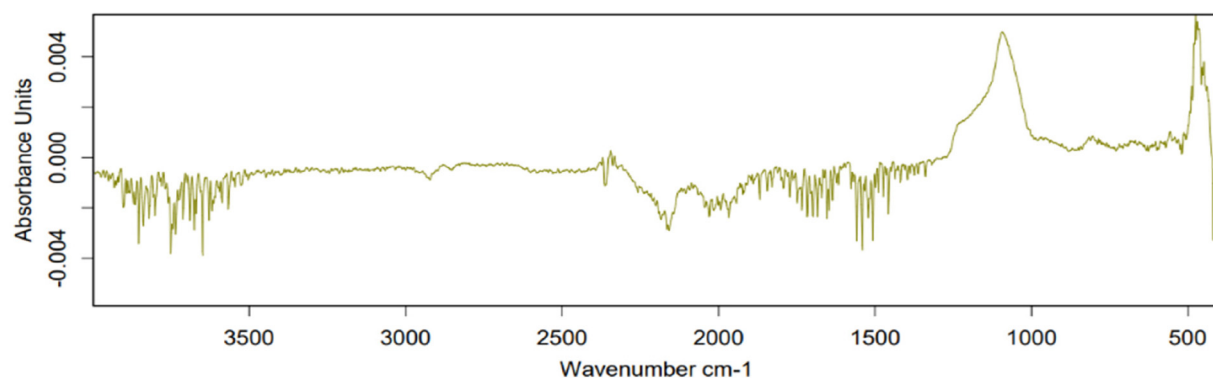


Figure 8. FTIR spectrum after amine functionalization of MCM-41, showing H-N bending and C-H stretching vibrations associated with amine groups. The retention of characteristic Si-O-Si bands confirms that the MCM-41 structural framework was preserved following surface modification

3.4.2. Influence of exposure time and adsorption-desorption behavior. Adsorption time and sample interaction duration play a significant role in the CO₂ uptake process. Both materials exhibited a rapid initial increase in mass, followed by stabilization as equilibrium was reached. After termination

of the gas flow, a decrease in mass was observed, indicating that the adsorption process is largely reversible. The adsorption behavior involves both physisorption and chemisorption mechanisms. While physical adsorption occurs within the mesoporous structure, the presence of amine functional groups

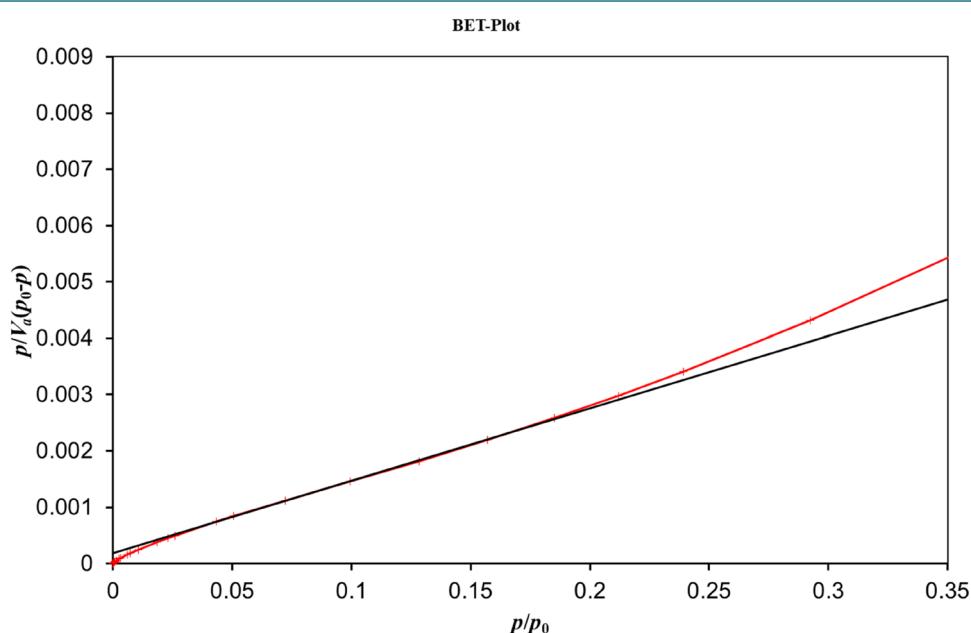


Figure 9. Nitrogen adsorption-desorption isotherm of unmodified MCM-41 at 77 K over the complete relative pressure range ($P/P_0 = 0-1.0$), exhibiting characteristic Type IV behavior with a hysteresis loop indicative of mesoporous materials

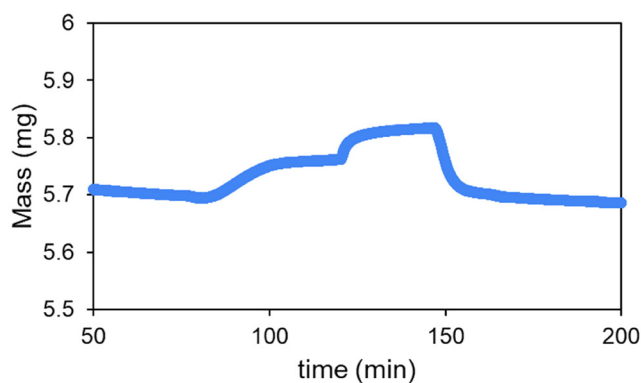


Figure 10. CO₂ adsorption-desorption profile of functionalized MCM-41 showing mass variation as a function of time. The adsorption stage demonstrates rapid CO₂ uptake followed by partial mass recovery during desorption, indicating predominantly reversible adsorption behavior

enables chemical interaction with CO₂ through reversible carbamate formation. The functionalized sample exhibited a slower desorption rate compared to unmodified MCM-41, reflecting stronger amine-CO₂ interaction forces. This behavior highlights the potential for improved capture performance through optimization of amine loading and functionalization conditions.

3.4.3. Interpretation and practical implications. The results demonstrate that functionalization of MCM-41 enhances CO₂ adsorption performance without compromising pore accessibility. Although the improvement is moderate, it confirms the effectiveness of chemical grafting in increasing the density of active adsorption sites. Further optimization—such as increasing amine concentration or adjusting reaction conditions—could significantly enhance performance for real-world carbon capture applications. Overall, the findings highlight the potential of functionalized mesoporous silica as a low-cost, reusable, and efficient solid sorbent for industrial CO₂ separation.

3.4.4. Comparison with previous studies and limitations. The obtained results are consistent with previous studies reporting enhanced CO₂ adsorption performance in amine-functionalized MCM-41 systems due to increased surface reactivity and the presence of active amine sites. The observed improvement in adsorption capacity confirms the effectiveness of surface functionalization in promoting stronger interactions between CO₂ molecules and the adsorbent surface. However, some studies have reported higher adsorption capacities under optimized synthesis and functionalization conditions, indicating that further improvement is achievable. Variations in synthesis parameters, amine loading, and experimental conditions may significantly influence adsorption performance. The present study is subject to certain limitations. The absence of advanced characterization techniques such as scanning electron microscopy (SEM) and elemental analysis (CHN) limits detailed understanding of surface morphology and nitrogen content. Additionally, optimization of functionalization parameters was not extensively explored. Future work should address these limitations and focus

on improving material performance through enhanced characterization and process optimization.

4. CONCLUSIONS

In this study, the synthesis and amine functionalization of MCM-41 were successfully carried out to evaluate its potential for CO₂ capture applications. Structural characterization using FTIR spectroscopy confirmed the effective grafting of amine groups from Hydrosil 2775 and Hydrosil 2999 onto the silica framework, while BET analysis verified a high specific surface area of 334.42 m²/g, confirming the retention of the mesoporous structure following modification. Dynamic CO₂ adsorption tests demonstrated a marked mass response, with the sample mass increasing from 5.70 mg to 5.83 mg, corresponding to a net uptake of approximately 22.8 mg/g. These results indicate that amine-functionalized MCM-41 is a promising and readily scalable adsorbent for CO₂ capture under ambient conditions. From a practical perspective, the developed material offers a cost-effective and efficient approach for industrial CO₂ separation processes. The combination of preserved pore structure and enhanced surface reactivity makes it suitable for repeated adsorption-desorption cycles. Theoretically, this study highlights the importance of surface functionalization in improving gas-solid interactions and optimizing adsorption performance in mesoporous materials. Future work should focus on multicycle stability testing and regeneration energy assessment to further evaluate the feasibility of these materials for large-scale industrial flue gas treatment.

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Enhanced Photocatalytic Performance of Ball-Milled Graphitic Carbon Nitride for Methylene Blue Degradation

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ABSTRACT

This study examines the influence of applying a solvent-free, scalable mechanical ball-milling process on the photocatalytic performance of metal-free graphitic carbon nitride (g-C₃N₄). Structural characterization reveals that optimization of the milling time enables particle size reduction and increases the specific surface area from 5.91 to 9.16 m²g⁻¹ without affecting the inherent crystal phase. Photocatalytic analyses of Methylene Blue degradation demonstrate a pseudo-first-order reaction for the 4 h milled sample, together with a 73.73% degradation efficiency after 45 min under ultraviolet light irradiation. This is equivalent to a four-fold higher rate constant of 0.01937 min⁻¹ compared with those achieved using bulk g-C₃N₄ and numerous noble-metal hybrids reported in recent literature. These findings provide useful and effective guidelines toward establishing high-performance, low-cost, metal-free photocatalysts for the rapid degradation of hazardous dyes in wastewater.

Keywords: g-C₃N₄, ball milling, photocatalysis, methylene blue, organic pollutant degradation

1. INTRODUCTION

Rapid global industrialization and textile production has led to the release of large amounts of synthetic organic dyes into aquatic ecosystems, posing a severe threat to both environmental stability and public health^{1,2}. Among these pollutants, Methylene Blue (MB), which is known for its complex aromatic structure, is unresponsive to traditional biological wastewater treatment strategies³. MB-polluted water is associated with serious health issues, including tissue necrosis, jaundice, and respiratory distress, underscoring the need to develop more sophisticated technologies that ensure complete degradation^{4,5}. Moreover, the presence of such toxins in water bodies is not regulated in many developing countries⁶. According to market report the MB market was valued at approximately \$7.66 billion in 2023 and is projected to grow at an annual rate of 5.2%, reaching around \$10.93 billion by 2030, thereby rendering environmental concerns increasingly significant⁷.

Semiconductor-based heterogeneous photocatalysis has emerged as a key approach for environmental cleanup due to its ability to convert organic toxins into CO₂ and H₂O⁸. Although metal-oxide catalysts have been widely employed for this purpose, their wide bandgaps limit activation to the ultraviolet (UV) range, which contributes <5% of the solar spectrum^{9,10}. Consequently, research has shifted toward the development of low-cost and scalable metal-free photocatalysts¹¹, with graphitic carbon nitride (g-C₃N₄) attracting interest as a sustainable, green

photocatalyst^{12,13}. However, the practical application of bulk g-C₃N₄ is hindered by its small specific surface area and high recombination rate of photogenerated electron-hole pairs¹⁴.

To overcome these bottlenecks, recent studies have explored various modification strategies, including elemental doping¹⁵, heterojunction construction, and morphological engineering to form two-dimensional nanosheets¹⁶. Despite the effectiveness of these methods, they tend to incorporate complex and expensive processes¹⁷. Consequently, there is an urgent need for inexpensive, simple, and chemical-free modification methods to adjust the structural and functional characteristics of g-C₃N₄¹⁸. For instance, mechanical-energy-induced modifications have been demonstrated to tune the morphological features and surface electronic environments of semiconductors¹⁹. However, the effect of ball-milling duration on the photocatalytic activity of metal-free g-C₃N₄ has yet to be clarified²⁰.

The current study aims to fill this gap by investigating a low-cost, scalable, and sustainable top-down mechanical ball-milling strategy to increase catalytic activity without the requirement for chemical additives or complicated surfactants²¹. It was hypothesized that mechanical milling of g-C₃N₄ would increase its surface area and provide more abundant active sites to enhance its photocatalytic efficiency in the degradation of MB. This work aims to establish a scalable and low-cost strategy to enhance metal-free catalyst performance for sustainable environmental applications by correlating milling time, surface area, and degradation kinetics.

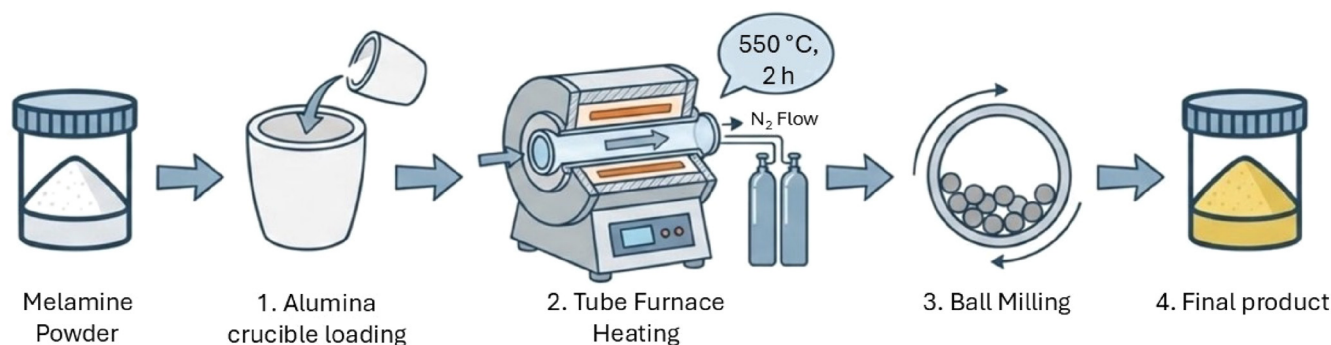


Figure 1. Schematic outline of g-C₃N₄ preparation

2. MATERIALS AND METHODS

2.1. Fabrication of the g-C₃N₄ Photocatalyst. Figure 1 outlines the experimental methodology used to prepare the target g-C₃N₄ powder. Melamine powder (5 g, 99%, Sigma-Aldrich) was placed in an alumina crucible and heated in a tube furnace under a continuous nitrogen flow (Fig. 2a). The furnace was heated to 550 °C at a heating rate of 10 °C min⁻¹, held for 2 h, and allowed to cool naturally to yield g-C₃N₄ as a yellow powder (Fig. 2b). The g-C₃N₄ surface area was modified through mechanical treatment using ball milling (MM5002 mixer mill, Retsch) at 12 Hz (720 rpm) and 23 °C, using a ball/powder mass ratio of 10:1. The samples were milled for 0 h (pristine, no milling), 2 h, or 4 h, and denoted g-C₃N₄-0h, g-C₃N₄-2h, and g-C₃N₄-4h, respectively (Fig. 2c).

2.2. Characterization . X-ray diffractometry (XRD) was used to analyze the crystallinity of the ball-milled g-C₃N₄ samples (Rigaku XRD, Cu K α radiation source, $\lambda = 1.5406 \text{ \AA}$). The XRD patterns were recorded over a 2θ range of 5°–80°. Following sputter-coating with a layer of gold, the morphologies of the g-C₃N₄ samples were analyzed using scanning electron microscopy (SEM, JEOL 5800LV). The microstructural features of the g-C₃N₄ samples were examined using transmission electron microscopy (TEM, JEOL JEM-2100F) at an accelerating voltage of 200 kV. TEM samples were prepared by dispersing g-C₃N₄ powder in ethanol and drop-casting onto a holey carbon-coated copper grid followed by oven drying under air at 80 °C. The surface areas of the g-C₃N₄ samples were measured

using a BELSORP MR1 surface area analyzer (Microtrac MRB). Before analysis, the samples were degassed at 120 °C for 3 h to remove any moisture or adsorbed gases. The specific surface area was determined using the Brunauer–Emmett–Teller (BET) approach to evaluate the effect of ball-milling time. The photocatalytic degradation of MB was monitored using UV–visible (UV-vis) spectroscopy (Agilent Cray-60 UV-vis spectrophotometer) between 700 and 400 nm. Spectra were recorded in absorbance mode with an average collection time of 0.075 s, data interval of 0.5 nm, and scan rate of 400 nm min⁻¹. The reported electronic bandgap for g-C₃N₄ is ~2.7 eV²², which enables absorption in the visible light region and is therefore critical for its photocatalytic activity in the degradation of MB. To compare the intrinsic activities of the ball-milled samples and evaluate the kinetics of MB degradation, a pseudo-first-order model was used to obtain the rate constant based on the Langmuir–Hinshelwood approach (Equation 1):²³

$$-\ln \left(\frac{C}{C_0} \right) = kt \quad (1)$$

A plot of $\ln \left(\frac{C}{C_0} \right)$ vs. time was constructed and each dataset (0, 2, and 4 h) was fitted independently to determine the rate constant k , where the slope of each line represents the degradation rate. To evaluate degradation efficiency, the overall percentage of MB removed from the system was calculated using Equation 2:

$$\text{Degradation (\%)} = \left(\frac{C_0 - C_t}{C_0} \right) \times 100 \quad (2)$$

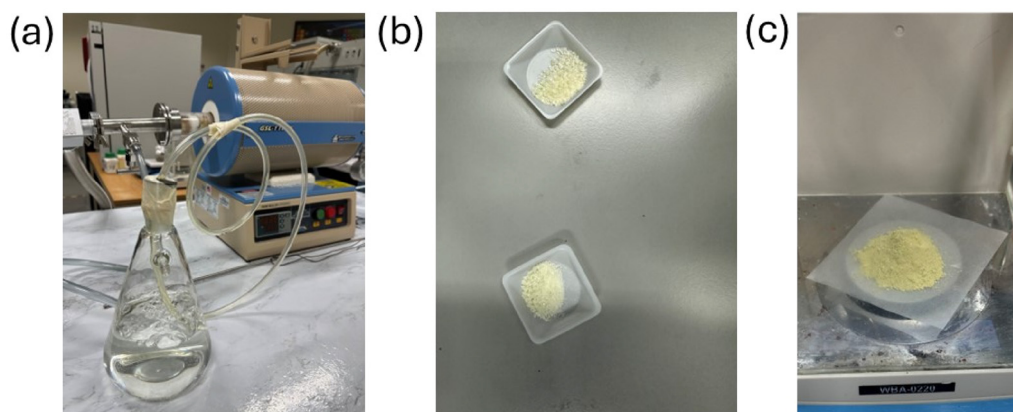


Figure 2. Photographic images of the synthesis procedure. (a) The tubular furnace used for melamine polymerization under a nitrogen atmosphere. (b) The yellow g-C₃N₄ powder obtained from the furnace. (c) The g-C₃N₄ powder after ball milling for 4 h

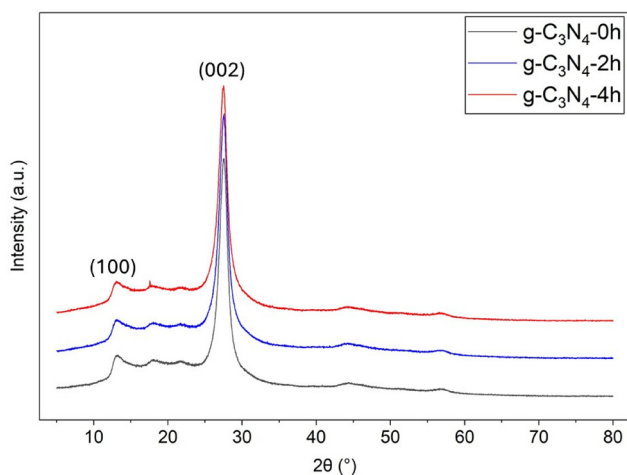


Figure 3. Stacked XRD patterns of the g-C₃N₄ samples prepared using different ball-milling durations (0, 2, and 4 h)

3. EXPERIMENTAL

To evaluate the photocatalytic efficiency of ball-milled g-C₃N₄, MB was used as a model contaminant. For each experiment, a 5 mM MB solution prepared in deionized water (50 mL) was placed in a beaker. Subsequently, the desired g-C₃N₄ photocatalyst (75 mg) was added to the solution and thoroughly dispersed by continuous magnetic stirring at 500 rpm for 30 min. The beaker was wrapped in aluminum foil to maintain dark conditions and prevent photodegradation, allowing the system to reach equilibrium and establish a baseline MB concentration for UV-vis characterization. After 30 min, the suspension was divided into two parts. One part was irradiated with a 60 W UV lamp while the other was maintained in the dark to account for any degradation originating from non-photocatalytic pathways. All experiments were repeated in triplicate for each photocatalyst variant. Aliquots were collected at fixed 15-min intervals under both irradiation conditions and analyzed using UV-vis spectrophotometry.

4. RESULTS AND DISCUSSION

4.1. XRD Analysis. The XRD patterns of the g-C₃N₄ specimens subjected to ball milling for 0, 2, and 4 h are presented in Fig. 3. All samples displayed two characteristic reflections corresponding to g-C₃N₄: a weak signal at ~13°(100), which was assigned to the in-plane structural packing of the tri-s-triazine units, and a strong peak at ~27°(002), corresponding to the inter-layer stacking of conjugated aromatic layers, consistent with the standard hexagonal phase (JCPDS 87-1526)²⁴. The detection of both peaks in all three samples confirms that ball milling did not alter the crystalline phase of g-C₃N₄.

However, a gradual reduction in peak intensity accompanied by slight broadening of the (002) reflection was observed with increasing milling time, suggesting decreased long-range stacking order and reduced crystallite size²⁵. This is consistent with the partial exfoliation of the bulk material into thinner nanosheets, which can enhance the photocatalytic activity by increasing

the number of exposed active sites and shortening the charge-transport pathways without altering the semiconducting phase of the material.

4.2. SEM Morphological Analysis . The SEM images presented in Fig. 4 clearly show a gradual decrease in particle size and reduced aggregation with increasing ball-milling time. Specifically, g-C₃N₄-0h consists of large, densely packed flakes with strong agglomeration. After 2 h of milling, the particles become noticeably smaller and the agglomerates begin to break apart, indicating partial exfoliation. The sample subjected to ball milling for 4 h exhibits the most significant decrease in particle size, with dispersed individual particles and reduced aggregation. This confirms that ball milling effectively reduced the particle size and by breaking large clusters into smaller fragments.

4.3. TEM Analysis. TEM was performed on the g-C₃N₄-4h sample to further investigate its morphology and microstructural features. The micrographs shown in Fig. 5 reveal the characteristic sheet-like morphology of g-C₃N₄, as expected after prolonged ball milling. Specifically, this nanosheet morphology indicated a greater abundance of active sites and increased light absorption capability. The absence of large agglomerates was consistent with the SEM and BET results, which revealed the largest surface area (9.16 m² g⁻¹) and lowest degree of aggregation among the investigated samples. These large wrinkled nanosheet clusters, which are characteristic of layered g-C₃N₄, are shown in Fig. 5a, while Fig. 5b reveals thinner, semi-transparent regions, indicating partial exfoliation. Additionally, Fig. 5c shows fragmented sheets of g-C₃N₄ with reduced stacking and increased edge exposure, whereas the high-magnification image in Fig. 5d confirms the presence of porous g-C₃N₄ nanostructures.

4.4. BET Surface Area Analysis. The specific surface areas of the unmilled and ball-milled g-C₃N₄ samples were determined using a multipoint BET method. An apparent increase in surface area was observed with increasing ball-milling duration. Specifically, the unmilled powder exhibited a BET surface area of 5.91 m² g⁻¹, while the 2 and 4 h ball-milled samples exhibited increased areas of 8.99 and 9.16 m² g⁻¹, respectively, as shown in Fig. 6. These findings can be accounted for by considering that the mechanical energy imparted by prolonged ball milling continuously shears and fractures the large, bulk g-C₃N₄ flakes into thinner exfoliated nanosheets and smaller fragments, greatly increasing the external surface area available for nitrogen adsorption. Notably, an increased surface area correlates strongly with enhanced photocatalytic activity since it facilitates interfacial contact between the catalyst and the dye, thereby promoting adsorption and enhancing reaction rates. The g-C₃N₄-0h sample exhibited the lowest adsorbed volume across all relative pressures, while the g-C₃N₄-2h and g-C₃N₄-4h samples showed higher uptake, consistent with their increased surface areas.

4.5. UV-vis Analysis. To evaluate the adsorption behavior and photocatalytic activity of the synthesized photocatalysts, the degradation of MB was monitored under UV irradiation and compared with that of the MB solution stored in the dark for >75 min. UV light was used as an irradiation source to ensure

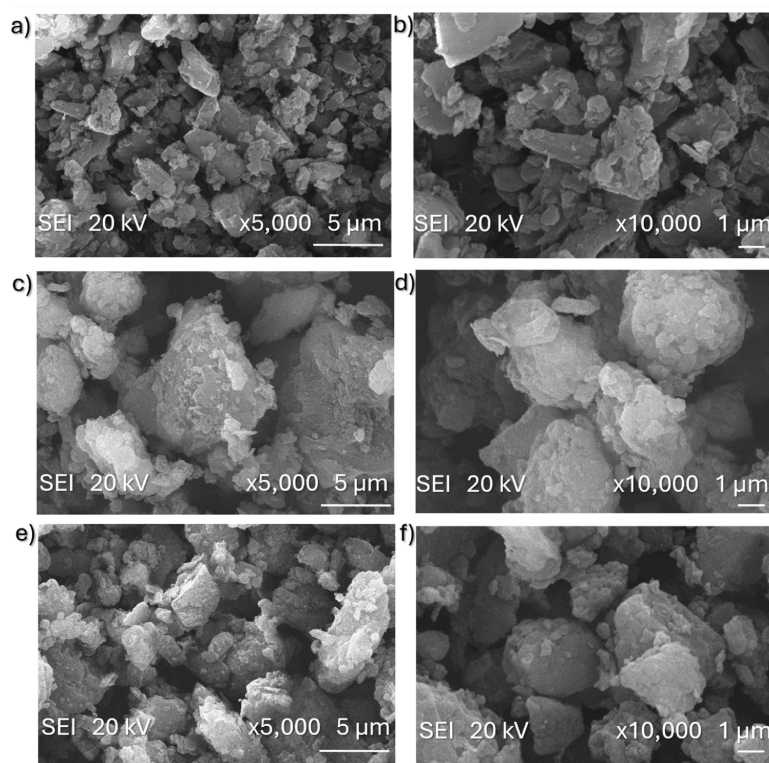


Figure 4. SEM images of the g-C₃N₄ specimens subjected to ball milling for (a, b) 0 h, (c, d) 2 h, and (e, f) 4 h. Panels (a, c, e) represent low magnification images showing the general morphology, while panels (b, d, f) are higher magnification images showing the surface texture and increased structural refinement induced by ball milling

stable and controlled photocatalytic conditions. Specifically, preliminary experiments conducted under visible solar light showed significant intermittency owing to fluctuations in light intensity, ultimately leading to solution heating and evaporation. These effects complicated data interpretation and reproducibility.

In contrast, UV irradiation provided a constant and controllable light intensity, eliminating variability associated with solar light and minimizing evaporation effects. This allowed reliable comparison of photocatalytic performance among the ball-milled g-C₃N₄ samples under identical conditions. Therefore, UV light

was chosen to ensure experimental consistency, reproducibility, and fair performance evaluation.

MB exhibits a maximum characteristic absorption signal at ~664 nm; thus, the decrease in absorbance at this wavelength was tracked to assess the degree of dye degradation. Among the investigated catalysts, the samples maintained in the dark exhibited minimal reductions in MB absorbance peak intensity (Fig. 7b, 7d, and 7f), with the smallest reduction being observed for the g-C₃N₄-0h sample (Fig. 7b). The slightly enhanced reductions observed for the g-C₃N₄-2h and g-C₃N₄-4h samples (Fig. 7d

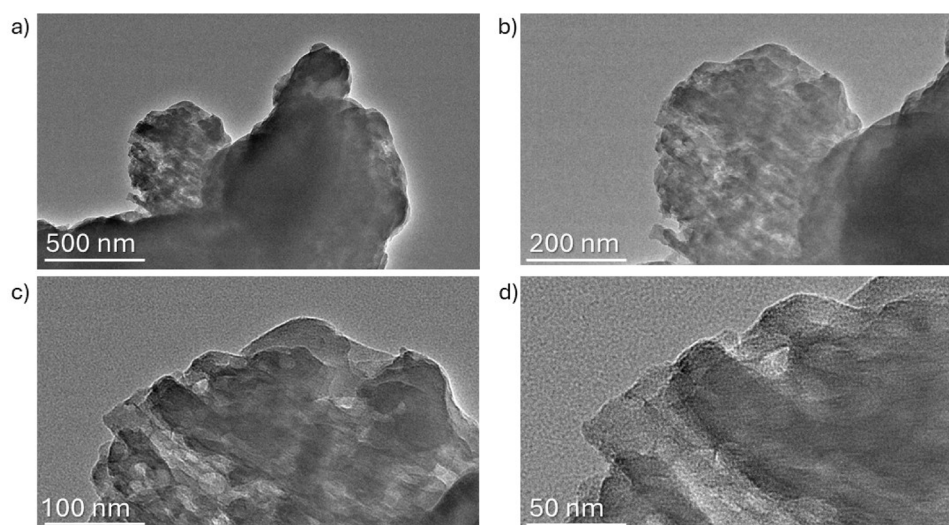


Figure 5. TEM micrographs of the g-C₃N₄-4h sample at different magnifications, with scale bars of (a) 500 nm, (b) 200 nm, (c) 100 nm, and (d) 50 nm

and 7f, respectively) were likely due to their larger surface areas. In contrast, rapid degradation was observed during UV-assisted photocatalysis, particularly for the g-C₃N₄-2h and g-C₃N₄-4h samples (Fig. 7c and 7e). The signature peak of the MB dye at ~664 nm decreased progressively with increasing UV irradiation time, confirming enhanced MB degradation via photocatalytic pathways. This reflects the role of ball milling in increasing the number of active surface sites and promoting contact between the dye and the catalyst.

A pseudo-first-order model was used to evaluate the reaction kinetics of MB degradation according to Equation 3:

$$\ln\left(\frac{C_0}{C_t}\right) = kt. \quad (3)$$

Fig. 7 shows full, unfitted kinetic plots for all samples exposed to UV irradiation for 75 min. Although all photocatalysts produced an initial linear decay region, an apparent non-linear deviation appeared after 45 min for the g-C₃N₄-4h sample. This deviation is common in photocatalytic dye degradation and is attributed to mass-transfer limitations²⁶. In the early stages of the reaction, the MB concentration was high, and abundant active sites were available, facilitating adsorption kinetics and accounting for the observed linear behavior. However, after 45 min, the dye concentration decreased significantly in the g-C₃N₄-4h system (Fig. 7e) and the solution became more transparent. Beyond this point, the reaction was limited by the low dye concentration and reduced number of active sites. This behavior has been widely reported for MB, as the kinetics of the later stages become diffusion- and adsorption-controlled rather than purely photocatalytic, owing to reduced UV absorbance²⁷. All samples were subjected to pseudo-first-order kinetic fitting using the Langmuir–Hinshelwood model (Fig. 8b). To ensure consistent and mathematically rigorous comparison across all photocatalysts, fitting was performed over the initial 45 min of the reaction to avoid the non-linear deviation observed for the g-C₃N₄-4h sample. The observed "bending" in the $\ln(C/C_0)$ curve violates the Langmuir–Hinshelwood model assumptions and is attributed to rapid initial removal of MB. As the dye concentration decreases significantly, the reaction transitions from being surface-controlled to being limited by mass transfer and diffusion of the remaining dye molecules to the active sites. The

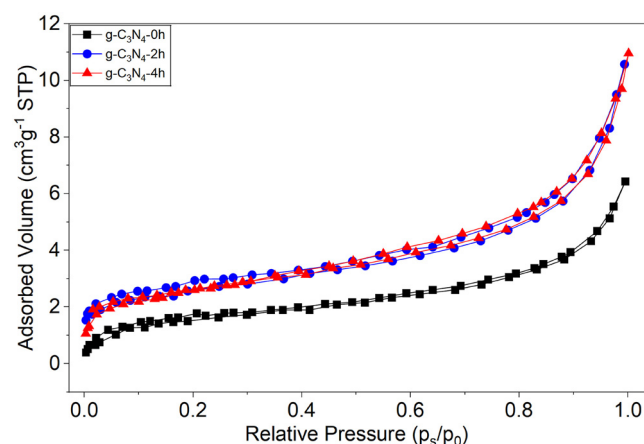


Figure 6. Nitrogen adsorption–desorption isotherms of the g-C₃N₄ samples before milling and after 2 and 4 h of milling

Table 1. C_0 and C_t represent the maximum absorbance intensities at $t = 0$ and 45 min, respectively. Efficiency was calculated using Equation 2

C_0 (arb.units)	C_{45} (arb.unis)	Efficiency (%)
0.47213	0.22276	51.80
0.62247	0.28246	54.62
0.56407	0.14819	73.73

obtained findings reveal that while the 0 h and 2 h samples maintain linear progressions for longer durations, the structural modifications and increased surface area induced by ball milling directly enhance the intrinsic early stage kinetics. Moreover, the extracted pseudo-first-order rate constants revealed distinct photocatalytic behavior among the three g-C₃N₄ samples. The g-C₃N₄-4h sample exhibited the highest initial rate constant ($k = 0.01937 \text{ min}^{-1}$) followed by the g-C₃N₄-2h ball-milled sample ($k = 0.01615 \text{ min}^{-1}$), and finally the g-C₃N₄-0h sample ($k = 0.01584 \text{ min}^{-1}$). This standardized approach ensures consistency by evaluating all catalysts during their primary linear degradation phase before physical constraints, such as mass-transfer limitations and depletion of available adsorption sites, begin to dominate the reaction. By truncating the fitting window to 45 min, we account for the non-linear "bending" observed in the g-C₃N₄-4h sample's curve at later stages, which would otherwise violate the Langmuir–Hinshelwood model assumptions. This flattening after 45 min is attributed to a significant drop in MB concentration and fewer available active sites, making the reaction diffusion-controlled rather than purely photocatalytic. While the 0 h and 2 h samples maintain linear progressions for longer durations, this 45-min comparison confirms that the structural modifications and increased surface area induced by ball milling directly enhance the intrinsic early-stage kinetics.

The photocatalytic performance of the samples was subsequently evaluated by comparing the MB dye degradation efficiency after 45 min of UV light irradiation. As presented in Table 1, the absorbance intensities (C_0 and C_t) were used to determine the percentage removal, according to Equation 2.

A clear improvement trend was observed with increasing UV treatment time. Specifically, the g-C₃N₄-0h sample exhibited a baseline efficiency of 51.80%. This value increased to 54.62% for the g-C₃N₄-2h sample, while the g-C₃N₄-4h exhibited the highest photocatalytic efficiency of 73.73%. This substantial decrease in absorbance intensity indicates that ball milling for 4 h greatly increases the active surface area and promotes charge-carrier separation within the catalyst.

4.6. Comparative Study of MB Degradation Over Various g-C₃N₄ Catalysts. A comparison was subsequently performed between the g-C₃N₄-4h sample and other reported g-C₃N₄ catalysts subjected to complex chemical and noble-metal modifications. As summarized in Table 2, the 73.73% degradation efficiency for the current metal free g-C₃N₄-4h catalyst over a period of 45 min corresponded to a rate constant of 0.01937 min^{-1} . This kinetic performance is superior to that of the Ag/g-C₃N₄ nanocomposite described by Naga-jyothi et al. (0.01576 min^{-1}), which requires costly noble metals and a long irradiation period of 100 min²⁸. Moreover, compared with the Sm₂O₃/sulfur-doped graphitic carbon nitride (CNS) heterojunction synthesized by Jourshabani et al. (0.0146

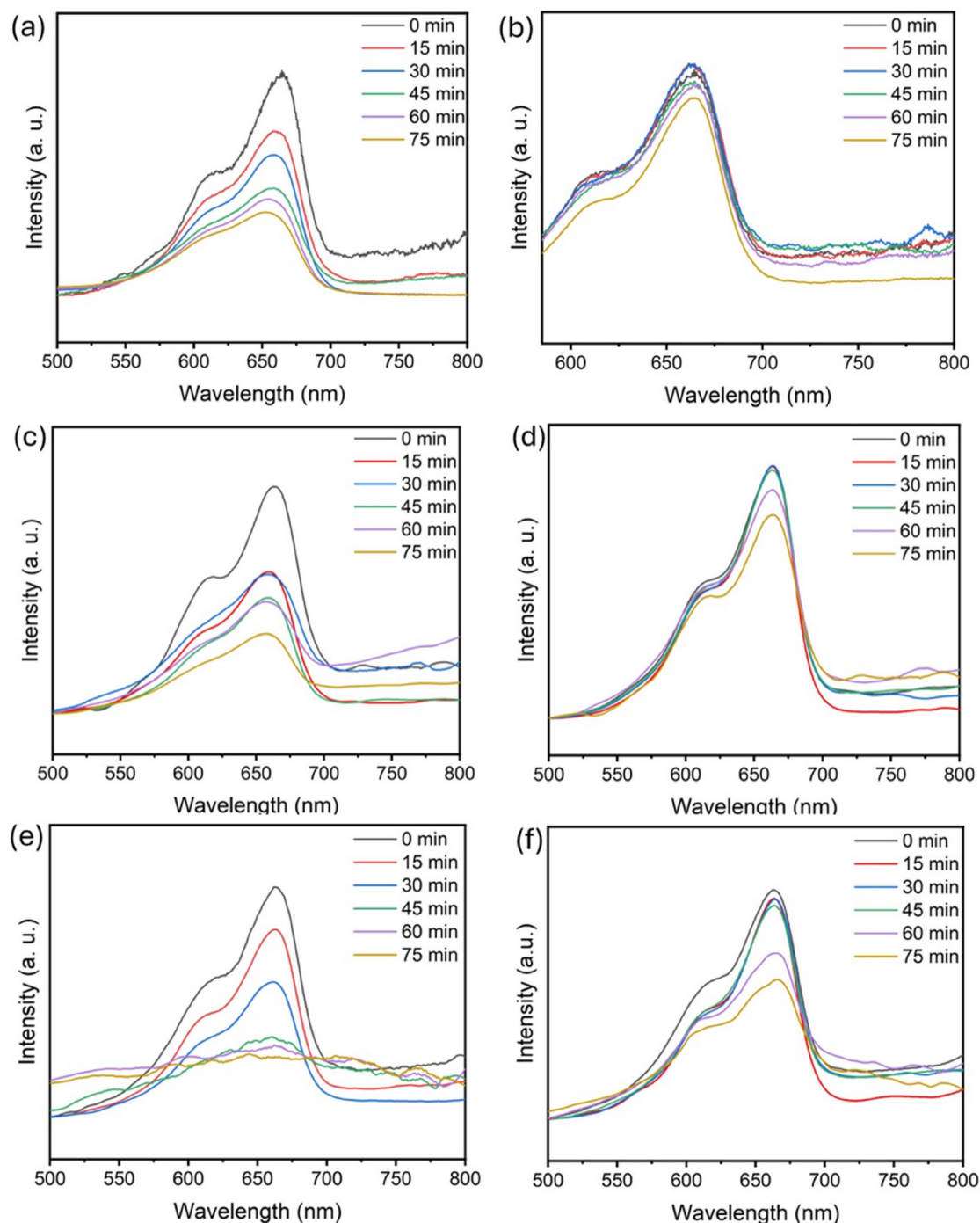


Figure 7. UV-vis plots showing the photocatalytic degradation of MB dye at different time intervals (a) g-C₃N₄-0h under UV irradiation; (b) g-C₃N₄-0h under dark conditions; (c) g-C₃N₄-2h under UV irradiation; (d) g-C₃N₄-2h under dark conditions; (e) g-C₃N₄-4h under UV irradiation; and (f) g-C₃N₄-4h under dark conditions

min⁻¹)²⁹, the present ball milling approach was more time-efficient. The substantial performance enhancement observed for g-C₃N₄-4h can be attributed to mechanical reduction of the crystallite size and increase of the BET surface area (i.e., from 5.91 to 9.16 m²g⁻¹), which effectively increased the active site density without the requirement for hazardous chemical precursors or costly dopants. Consequently, this work confirms that solvent-free mechanical milling represents a vigorous and potentially competitive approach to prepare photocatalysts for wastewater treatment, yielding comparable perfor-

mance to more sophisticated multicomponent photocatalytic systems.

5. CONCLUSIONS

This study demonstrates that mechanical ball milling is an effective strategy for tuning the photocatalytic behavior of g-C₃N₄ without altering its intrinsic crystal phase. The 4 h milling process successfully increased the BET surface area from 5.91 to 9.16

Table 2. Comparison of the MB photocatalytic degradation performance and pseudo-first-order rate constants (k) between the optimized ball-milled g-C₃N₄-4h sample and various modified g-C₃N₄ materials reported in the literature

Photocatalyst type	Modification method	Time (min)	Efficiency (%)	Rate constant k (min ⁻¹)	Reference
Ball milled g-C ₃ N ₄	Ball milling (4 h)	45	73.73	0.01937	This work
g-C ₃ N ₄ -S ₁₀	Co-pyrolysis (NaNO ₃)	120	70	0.01	Chang et al. ³⁰
Pure g-C ₃ N ₄	Thermal	120	40	0.0042	Chang et al. ³⁰
CNS (S-doped)	Chemical doping	150	54	0.044	Jourshabani et al. ²⁹
Pristine g-C ₃ N ₄	Thermal	100	48	0.00626	Nagajyothi et al. ²⁸

m²g⁻¹, thereby increasing the active site density. Consequently, the g-C₃N₄-4h sample exhibited the highest pseudo-first-order rate constant of 0.01937 min⁻¹, significantly outperforming the g-C₃N₄-0h (0.01584 min⁻¹) and g-C₃N₄-2h (0.01615 min⁻¹) samples, achieving 73.73% MB degradation over a 45 min period. Comparison with the literature further confirmed that this simple mechanical approach rivals the kinetics of complex noble metal hybrids such as Ag/g-C₃N₄ (0.01576 min⁻¹) and Sm₂O₃/CNS (0.0146 min⁻¹). Overall, these results demonstrate a low-cost and scalable approach for maximizing the photocatalytic efficiency of metal-free photocatalysts for the removal of hazardous organic dyes from wastewater. Future efforts should focus on the incorporation of these large-surface-area nanostructures into

flow-through systems to overcome mass-transfer constraints at later reaction stages.

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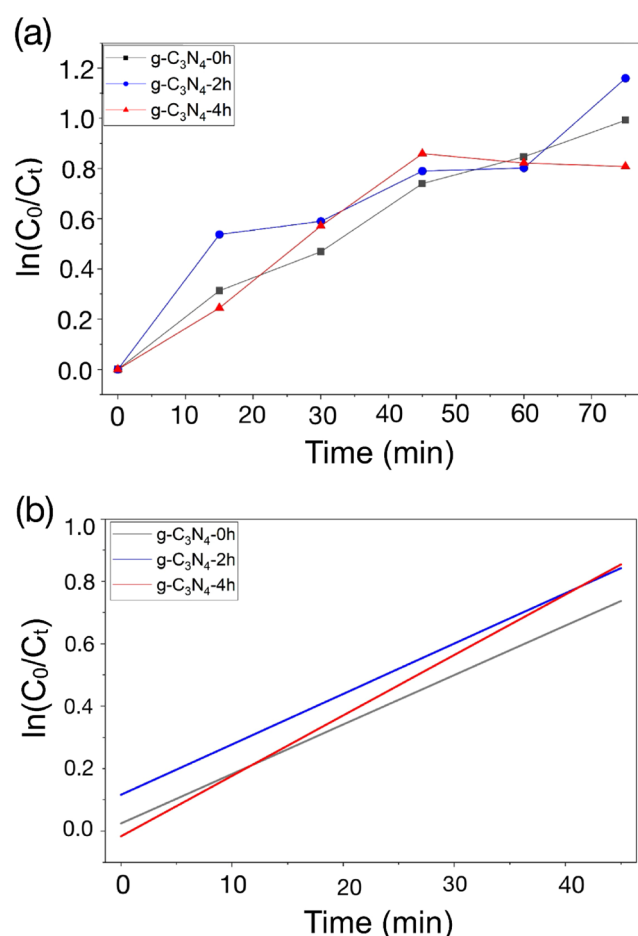


Figure 8. (a) Full kinetic plots for all samples (0, 2, and 4 h) under UV irradiation for 75 min. (b) Pseudo-first-order kinetic fitting for all samples standardized to a 45 min

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Sputtered $\text{TiO}_2/\text{Al}_2\text{O}_3$ Multilayer Coatings as Transparent Anti-Soiling Solutions for Solar Photovoltaics in Humid-Arid Regions

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ABSTRACT

Under the backdrop of Saudi Vision 2030, the Kingdom of Saudi Arabia is expanding its solar energy sector. However, soiling and high humidity in coastal arid regions such as Dhahran considerably reduce photovoltaic (PV) module efficiency. This study was aimed at investigating the deposition and optimization of multilayer anti-soiling coatings fabricated using reactive DC magnetron sputtering to mitigate dust accumulation on solar panel surfaces. Three thin-film configurations were deposited on glass substrates: a TiO_2 monolayer, a $\text{TiO}_2/\text{Al}_2\text{O}_3$ bilayer, and a $\text{TiO}_2/\text{Al}_2\text{O}_3/\text{TiO}_2$ sandwich structure. The samples were annealed at temperatures ranging from 100 to 400 °C and characterized in terms of optical transmittance, surface wettability, and field durability. The results demonstrate that the layer configuration considerably influences the coating performance. The bilayer film annealed at 200 °C exhibits the optimal light transmission and higher water contact angle of 66°. Overall, this study presents a transparent and durable coating solution to mitigate soiling losses in humid and arid climates.

Keywords: anti-soiling, coatings, solar panels, TiO_2 , hydrophobicity, sputtering

1. INTRODUCTION

In recent years, the Kingdom of Saudi Arabia (KSA) has focused on diversifying its energy sector to integrate and expand clean energy sources. Under the backdrop of Saudi Vision 2030, the country aims to reduce the long-term dependence on hydrocarbons and increase investment in sustainable energy¹. Saudi Arabia receives among the highest solar irradiance worldwide (approximately 5,644 Wh/m² per day) and experiences long average sunlight durations (approximately 8.9 h per day)². Under these conditions, photovoltaic (PV) solar energy represents one of the most effective technologies for electricity generation. Notably, Saudi Vision 2030 seeks to increase renewable energy production to 60 GW, with 66.67% generated from solar and the remainder from wind³. Moreover, the national target is to produce half of all electricity from renewable energy sources by 2030⁴. In this context, PV technology is favored owing to its cost-effectiveness, scalability, and robustness. The cost of rooftop PV systems has decreased considerably, by nearly 80%, to approximately 3.75 SAR per watt⁵. Additionally, this technology is highly scalable, with a rooftop PV system covering an industrial building of approximately 29,000 m² in Abqaiq City, Saudi Arabia, and demonstrating high performance ratios (approaching 94.2%)⁶.

Despite these advantages, PV deployment in Saudi Arabia faces major environmental challenges. Soiling is a primary problem arising from the arid climate, where dust and sand particles accumulate on solar panels, blocking sunlight and ultimately reducing energy efficiency. A study conducted in Dhahran, Saudi

Arabia, indicates that PV modules left uncleaned for six months can lead to a 50% reduction in power output⁷. Another notable problem is high humidity, especially in coastal regions such as Dhahran. Humidity levels can reach as high as 73%⁸, resulting in increased light scattering and reflection, which can degrade PV performance⁹. Studies have reported a 40% power drop at 76.32% humidity, with efficiency decreasing from 12.04% to 9.7% as humidity rises from 48% to 60%¹⁰. Additionally, humidity promotes the adhesion of dust to PV systems via the formation of mud layers through capillary forces between condensed vapor and dust particles; these deposits are challenging to remove. Humidity also increases particulate adhesion, creating a localized environment that can promote long-term corrosion and delamination within PV modules¹¹. Considering these aspects, effective cleaning strategies for PV solar panels are crucial to ensure performance in arid regions. Existing cleaning approaches can be classified into natural, mechanical/electromechanical, electrostatic, and surface-coating-based methods. Natural cleaning relies on rainfall and wind. Although water washing represents an effective cleaning method, this resource is limited in arid areas¹². Mechanical methods such as robotic wipers and vibration systems are effective and can restore up to 99.9% of the original performance. Nevertheless, they are cost-intensive and require continuous maintenance¹³. Electrostatic methods, including electrodynamic screens, use electric fields to repel dust with over 90% efficiency. Although this solution is water-free and suitable for arid regions, it requires an external power source¹⁴.

Among coatings, hydrophobic layers can repel water and promote particle removal; hydrophilic coatings facilitate wetting and dirt repellence; and anti-static coatings reduce dust adhesion. In arid regions, coatings are particularly promising because they maintain non-wetting properties under humid conditions, preventing dust adhesion. Moreover, coatings enable self-cleaning with minimal moisture, addressing the challenge of water scarcity.

To synthesize these coatings, TiO_2 is widely used owing to its unique properties and multifunctional photocatalytic activity. However, to improve the conductivity of TiO_2 for photovoltaic applications¹⁵, it remains crucial to enhance the separation and mobility of electron-hole pairs while reducing their recombination to extend carrier lifetime.

Overall, an ideal anti-soiling coating for conditions prevalent in the KSA must meet several requirements: First, it should exhibit high optical transparency to maximize solar transmission to PV cells. Second, it must be mechanically strong and durable to survive the harsh environmental conditions, such as high temperatures, intense ultraviolet (UV) radiation, and sandstorms. Lastly, the coating must be scalable and easy to apply over large areas. Among thin-film synthesis techniques, physical vapor deposition (PVD), specifically, magnetron sputtering, is a promising approach¹⁶. Sputtering offers precise control over film thickness, composition, and adhesion, which are critical for tuning optical, mechanical, and anti-soiling performance.

Considering these aspects, this study aimed to fabricate a novel anti-soiling coating via reactive DC sputtering. A $\text{TiO}_2/\text{Al}_2\text{O}_3/\text{TiO}_2$ multilayer structure was selected because TiO_2 provides excellent self-cleaning properties, while Al_2O_3 acts as a barrier, thereby reducing charge recombination and improving durability¹⁷. The sputtering process was optimized to achieve a balance among transparency, durability, and dust-repellent properties for deployment in humid and arid regions.

2. METHODOLOGY

2.1. Substrate Preparation. Glass substrates were cleaned via ultrasonication (Branson 3510 Ultrasonic Cleaner, USA) for 10 min in each of the following solutions: Hellmanex cleaning solution, deionized water, acetone, and isopropyl alcohol. Before deposition, the samples were placed in a UV-ozone cleaner (Ossila, K) to remove contaminants and improve surface wettability. Half of the selected samples were covered to create reference areas for comparison between coated and uncoated surfaces.

2.2. Thin-Film Deposition. Coatings were deposited using an NCS-3000 magnetron sputtering system (NANO-MASTER, Inc., USA). The structure consisted of TiO_2 and Al_2O_3 arranged in a $\text{TiO}_2/\text{Al}_2\text{O}_3/\text{TiO}_2$ sequence. High-purity ceramic targets were used. Samples were rotated during deposition and placed 16 cm from the target. The base pressure was 4.38×10^{-5} Torr, and the working pressure was maintained at 7.95×10^{-3} Torr using argon gas. Radio frequency power of 100 W was found to be excessive, whereas 10 W led to insufficient film formation. Therefore, a power of 50 W was selected for all deposition steps. Argon flow rates were 55 sccm for TiO_2 and 12 sccm for Al_2O_3 . All depositions were performed at 25–30 °C temperature for a total duration of 1 h. After deposition, the samples were annealed at 100, 200, 300, and 400 °C to evaluate the effect of temperature on film properties. Annealing was performed in ambient air, and the samples were then allowed to cool to room temperature.

2.3. Characterization. The optical transmittance and absorbance of the coated glass were determined using a V-670 JASCO UV-Vis/near-infrared (NIR) spectrophotometer (Japan). Surface wettability was measured using a KRÜSS DSA25 drop-shape analyzer (Germany) to determine hydrophobic or hydrophilic behavior. Field testing was performed by

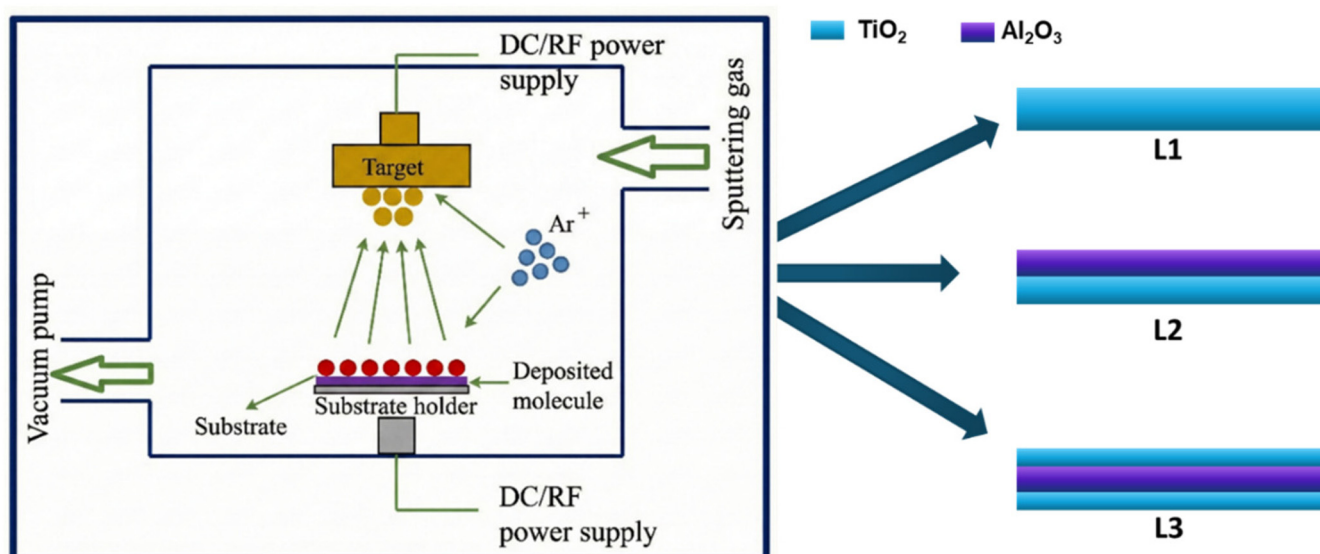


Figure 1. Schematic illustration of the magnetron sputtering deposition setup used for the fabrication of anti-soiling coatings on glass substrates. The diagram shows the sputtering target, plasma generation, and substrate positioning during deposition. This process enables the formation of uniform thin films that modify the surface properties of the glass, improving resistance to dust adhesion and enhancing anti-soiling performance

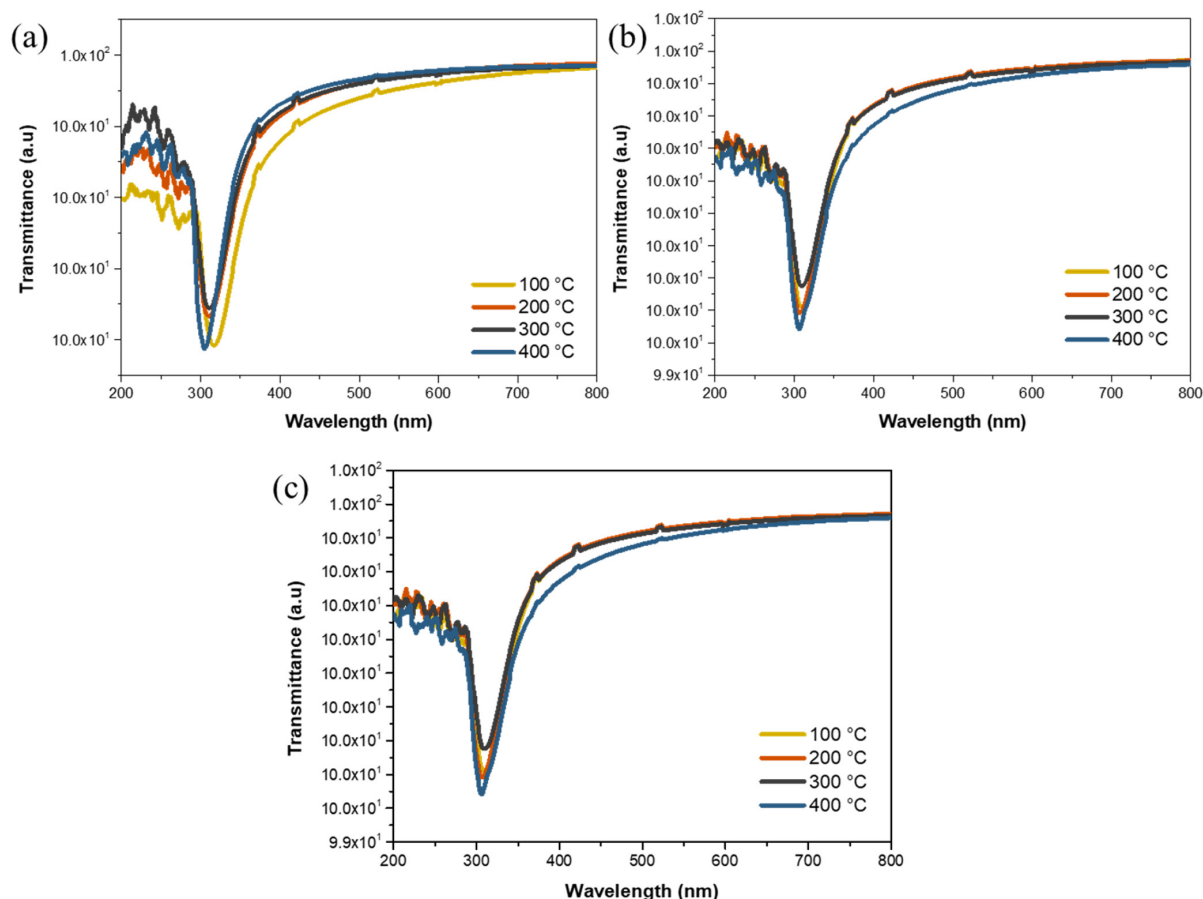


Figure 2. Optical transmittance spectra of (a) TiO_2 layer (L1), (b) $\text{TiO}_2/\text{Al}_2\text{O}_3$ bilayer (L2), and (c) $\text{TiO}_2/\text{Al}_2\text{O}_3/\text{TiO}_2$ layer (L3) thin films annealed at different temperatures, showing high transparency in the visible region with annealing-dependent variations in optical transmittance

exposing samples to outdoor conditions for 10 days. Three samples annealed at 200 °C were half-covered to enable a direct comparison between the coated and uncoated sides after dirt exposure. The samples were imaged using an Olympus DSX1000 digital microscope (Japan).

3. RESULTS AND DISCUSSION

Magnetron sputtering enabled uniform thin-film deposition for the anti-soiling coating (Fig. 1). A TiO_2 monolayer (L1) served as the control film. This structure was then modified by introducing Al_2O_3 in two configurations: a $\text{TiO}_2/\text{Al}_2\text{O}_3$ bilayer (L2) and a $\text{TiO}_2/\text{Al}_2\text{O}_3/\text{TiO}_2$ sandwich structure (L3). The deposited thin films were annealed at different temperatures for phase development and further characterization.

3.1. Optical Properties. Optical transparency represents a critical performance parameter for anti-soiling coatings on PV modules. PV operation is based on the conversion of incident photons into electron-hole pairs within the semiconductor. Therefore, a reduction in surface transparency decreases the photon flux reaching the active solar cell and device efficiency¹⁸. High transmittance in the visible and NIR spectrum (350–800 nm) and high absorbance in the UV region (~300 nm) are desirable. The transmission of 350–800 nm spectra enables

the light to reach the PV module beneath it, thereby generating power output efficiently. The high-energy UV radiation, which is unsuitable for PV devices, is absorbed by the anti-soiling layer, preventing it from reaching the PV module. This reduces the device's overheating and can enhance its durability^{18,19}. To evaluate transparency, the annealed samples were subjected to UV-Vis absorption spectroscopy (Fig. 2). For L1, annealing at 400 °C resulted in the highest transmittance across the visible region. The sample annealed at the lowest temperature (100 °C) resulted in the highest absorption in the UV region. Samples annealed at 200 and 300 °C showed intermediate transmittance and UV absorption. For L2, visible transmittance decreased after annealing at 400 °C, while samples annealed between 100 and 300 °C maintained higher transmittance across the visible spectrum. Samples annealed at 400 and 100 °C exhibited similar UV absorption. Given its better visible transmittance, the sample annealed at 100 °C was deemed superior to the 400 °C sample. The enhanced optical parameters at lower temperatures are attributable to the bilayer configuration. The L3 sandwich structure displayed similar trends. Lower annealing temperatures led to enhanced transmittance in the visible range and UV absorbance comparable to that of the 400 °C annealed film. The results indicate that the incorporation of the Al_2O_3 layer likely led to enhanced performance at lower annealing temperatures.

3.2. Surface Wettability. Surface wettability determines the interaction between water droplets and the coating surface and is typically evaluated through contact angle measurements. In arid environments such as Saudi Arabia, controlling wettability is essential to minimize the capillary forces induced during humid periods, which encourage dust adhesion onto the panel surface¹⁷. The contact angle depends on the surface energy and roughness, which are influenced by the annealing temperature¹⁸. As shown in Fig. 3, for L1, samples annealed at 100, 200, and 400 °C showed contact angles of 41.6°, 38.4°, and 23.6°, respectively, indicating reduced hydrophobicity with increasing temperature. For L2, the contact angles were 62.3°, 65.8°, and 59.8° for 100, 200, and 400 °C annealing, respectively, indicating stable contact values even at higher annealing temperatures. For L3, values of 50.6°, 46.5°, and 41.4° were noted for 100, 200, and 400 °C annealing. While this sample also showed a gradual reduction in hydrophobicity with increasing temperature, it was less notable compared with that for L1. Overall, the annealing temperature of the sputter-coated film influences both optical properties and wettability. Increasing the annealing temperature leads to reduced hydrophobic behavior.

3.3. Performance Comparison. A comparative assessment of L1, L2, and L3 revealed that the annealing temperature plays a crucial role in the optical and surface properties. Based on visible-light transmittance, UV absorption, and surface wettability, the optimal annealing temperature was 200 °C for L1, L2, and L3. Although L1 annealed at 400 °C exhibited the highest visible light transmittance, the contact angle was extremely low. By contrast, L1 annealed at 200 °C demonstrated comparable visible transmittance and UV absorption values along with a higher contact angle of 40.4°, indicating reduced hydrophilicity compared with the sample annealed at 400 °C. Similarly, for L2 and L3, the most favorable combination of visible transmittance and UV absorption was observed for films annealed at 200 °C. Figure 4 (a) compares the transmittance spectra of control L1 with the

best-performing L2 and L3 layers. L3 demonstrated higher transmittance in the NIR region but reduced transmittance in part of the visible region, whereas L1 and L2 recorded similar but slightly lower transmittance in the visible region. Notably, L2 displayed more pronounced UV absorption than L1 and L3. Figure 4 (b) compares the contact angle values for the best-performing samples of L1, L2, and L3. The water contact angle increased from 42° for L1 to 66° and 46° for L2 and L3, respectively. Although all surfaces remained within the weakly hydrophilic range (contact angle <90°), moderate hydrophilicity is beneficial for anti-soiling in arid regions because it prevents strong chemical bonding between dust particles and the surface. This makes it easier for wind or rain to remove dust compared with highly hydrophilic surfaces, which may promote mud-layer formation in a humid atmosphere. The increased contact angle (66°) for L2 relative to L1 (pure TiO₂) is consistent with the surface-passivation effects of Al₂O₃,¹⁷ which reduces surface energy and promotes self-cleaning, while preserving the photocatalytic activity. In summary, the L2 layer, with a thin Al₂O₃ layer on TiO₂, demonstrates the most balanced combination of visible-light transmittance, UV absorption, and wettability, indicating its superior performance as an anti-soiling coating for high-efficiency and durable PV applications.

3.4. Field Performance Test. While laboratory characterization clarifies intrinsic properties of the coatings, the actual anti-soiling performance must be tested under real-world environments. A 10-day field test was conducted by exposing half-coated samples to outdoor conditions. After exposure, the samples were washed with water without using any brush. As shown in Fig. 5, the uncoated portion exhibited notable accumulation of fine dust particulates, whereas the coated regions appeared visibly cleaner. This indicates that the Al₂O₃ layer mitigated the electrostatic attraction of surface charge.

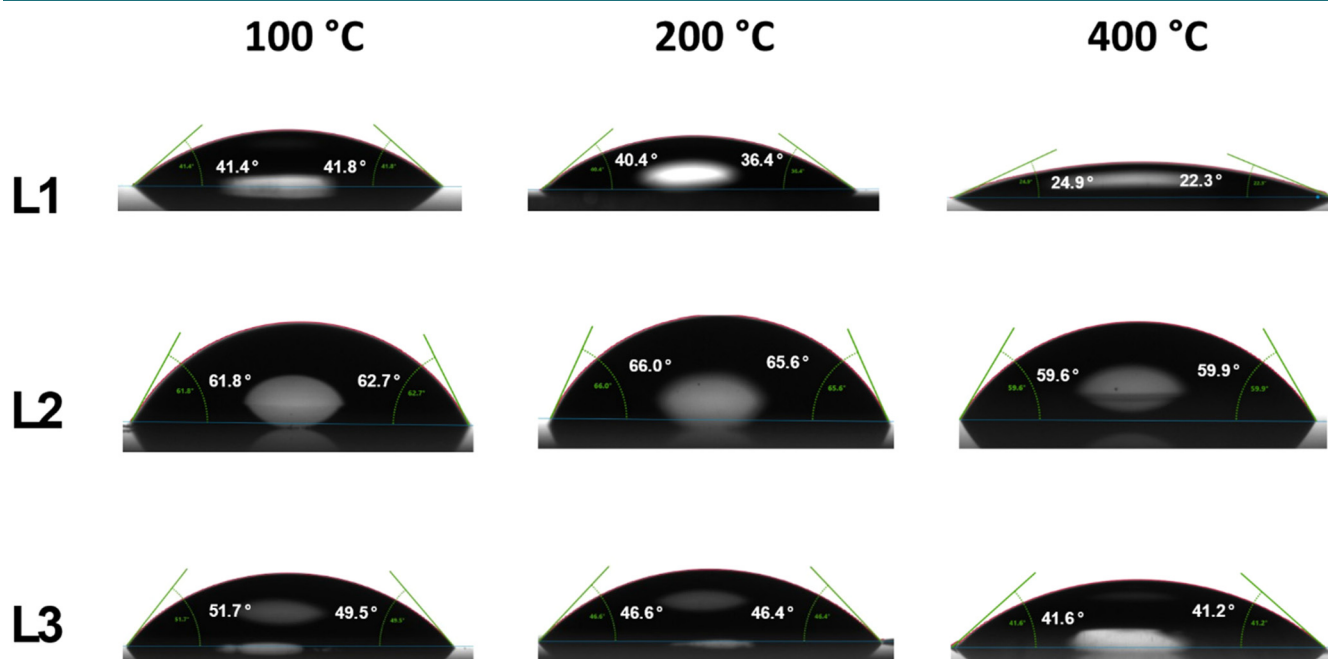


Figure 3. Contact angle measurements for L1, L2, and L3 annealed at 100, 200, and 400 °C

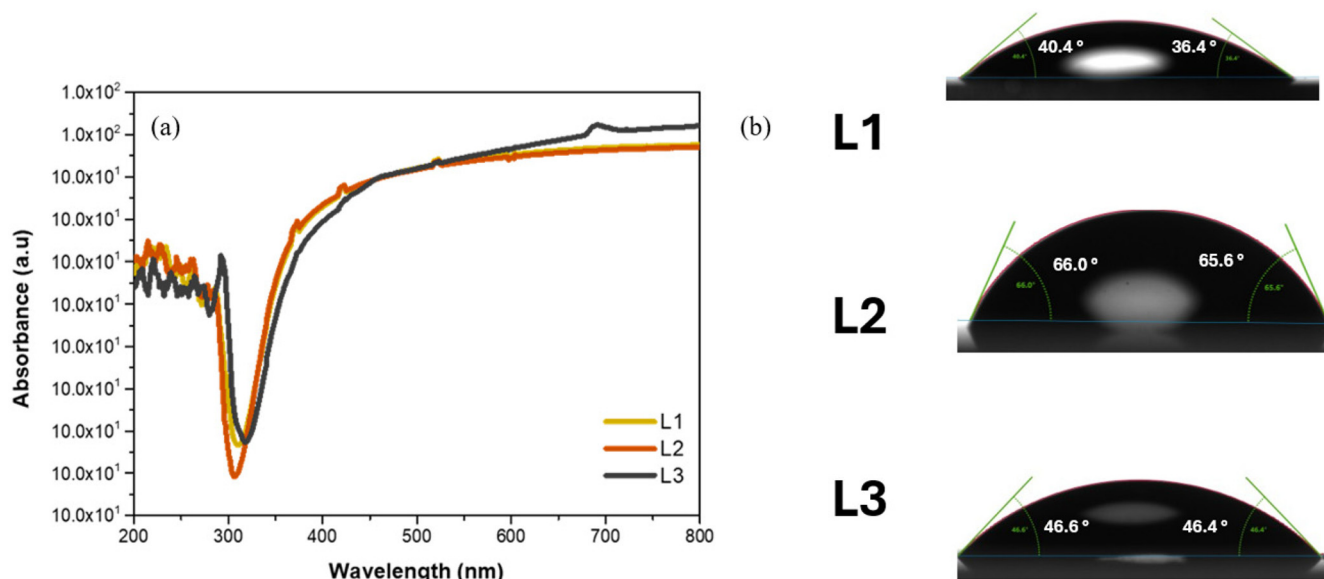


Figure 4. Water contact angle measurements for L1, L2, and L3 thin films annealed at 200 ° C

3.5. Discussion and Limitations. The findings highlight that $\text{TiO}_2/\text{Al}_2\text{O}_3$ multilayer coatings can mitigate performance degradation in PV modules operating under humid-arid conditions. The bilayer annealed at 200 ° C demonstrated the optimal balance of transparency and durability. However, several limitations remain to be addressed: First, while the reactive DC magnetron sputtering method provides precise control over thin film parameters, testing in this study was conducted on small-

scale glass substrates. Future research can evaluate the uniformity and cost-effectiveness of this coating for large-scale PV modules. Additionally, field durability was assessed over a short period; long-term studies are necessary to determine how these multilayers behave over time. Lastly, while the 50 W power and 100–400 ° C annealing range enabled clear optimization, a broader range of deposition powers and temperatures can be explored in future work.

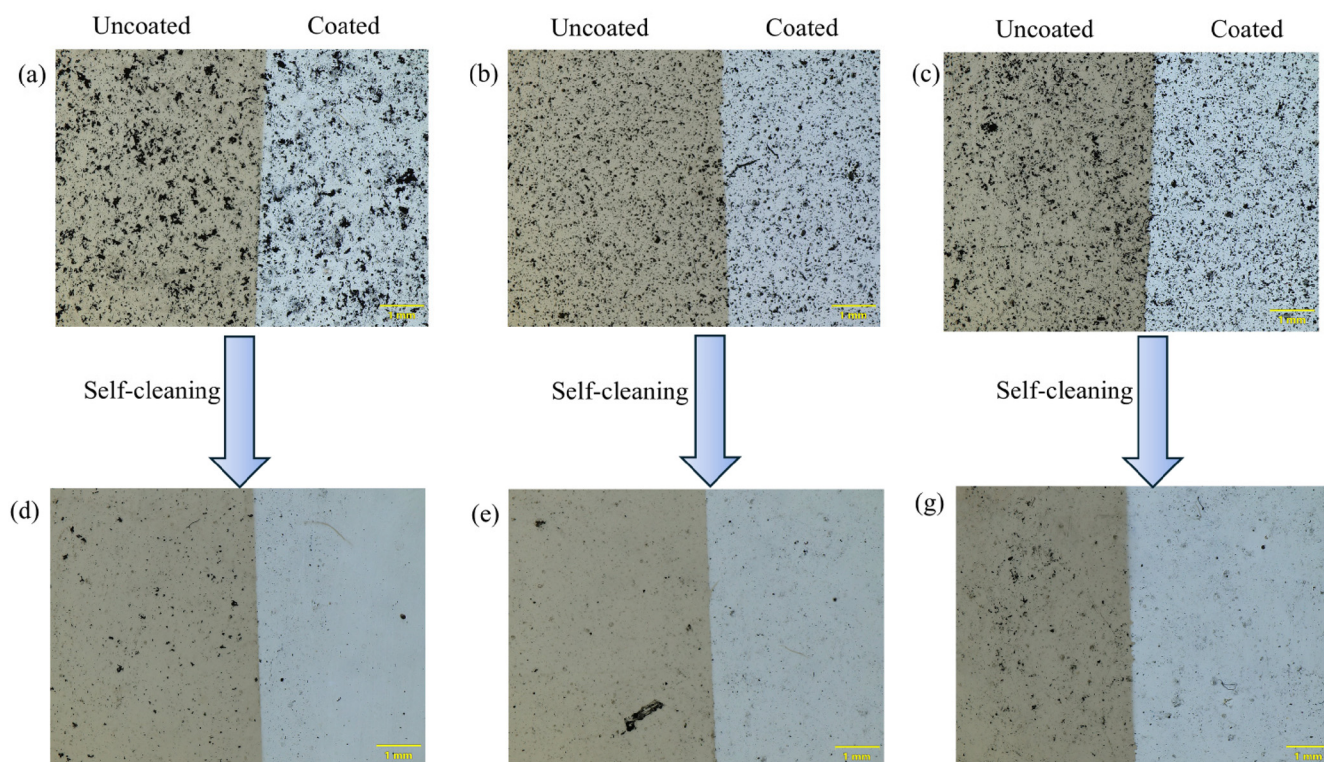


Figure 5. Optical microscopy images of (a,d) L1, (b,e) L2, and (c,g) L3 samples annealed at 200 ° C. (a-c) dust deposition before rinsing and (d, e, g) surfaces after self-cleaning. Each image compares the uncoated region (left) with the coated region (right)

4. CONCLUSION

This study addressed key environmental challenges affecting PV modules in Saudi Arabia, i.e., dust accumulation and humidity, by developing multilayer anti-soiling coatings using magnetron sputtering. The control TiO_2 coating was modified through the addition of an Al_2O_3 passivation layer and a $\text{TiO}_2/\text{Al}_2\text{O}_3/\text{TiO}_2$ sandwich structure. Among the three film configurations, L2 and L3 outperformed the control TiO_2 layer in terms of enhanced visible-light transmittance, UV absorption, and water contact angle. The L2 configuration also exhibited high transparency and could mitigate dust adhesion in field tests. Consequently, the proposed coating strategy offers an efficient solution for increasing the output of solar panels, supporting the KSA's goal to achieve 50% renewable-energy generation by 2030.

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Impact of Cation Dissolution on Kinetics of CO₂ Mineralization in Carbonate Rocks

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ABSTRACT

There is a growing need for technologies that mitigate emissions associated with the continued use of fossil fuels. Carbon capture and storage is a promising large-scale CO₂ mitigation approach. However, the kinetics of mineral dissolution and its impact on solution chemistry and subsequent mineralization potential during early reaction stages remain poorly constrained. This study examines the dissolution kinetics of carbonate rocks under high-pressure brine and brine–CO₂ conditions in the context of geological carbon dioxide (CO₂) storage and mineralization. The primary aim of the study is to quantify the lithology-dependent chemical responses and early-time dissolution behavior under controlled subsurface-like conditions. Experiments were conducted using limestone and dolomite core plugs placed in sealed reaction cells at 2000 psi and 75 °C, with time-resolved measurements of pH and dissolved cation concentrations. Early-time calcium release rates were quantified using concentration–time slopes and were normalized by the geometric surface area to enable direct kinetic comparisons across systems. The results showed systematic differences between lithologies and fluid conditions. Dolomite systems exhibit stronger buffering capacity and higher effective dissolution rates than limestone under brine-only conditions, whereas the presence of CO₂ lowers the initial pH and alters early-time calcium mobilization in a lithology-dependent manner. These trends suggest that the early reaction stages are governed by the kinetics before the onset of progressive pH buffering. Overall, the findings provide quantitative insights into the carbonate dissolution behavior under CO₂-rich conditions and support an improved understanding of mineral–fluid interactions relevant to subsurface CO₂ storage and mineralization strategies.

Keywords: carbonate dissolution, CO₂–brine systems, dissolution kinetics, fluid–rock interactions, geological CO₂ storage

1. INTRODUCTION

There is an increased global interest in reducing carbon emissions owing to the increasing impact of greenhouse gas emissions and projections of worsening climate effects without effective mitigation strategies^{1,2}. Although international efforts have increasingly emphasized emission reduction and carbon removal strategies, fossil fuels are expected to remain a major component of the global energy mix for decades^{3,4}. This highlights the need for technologies that mitigate emissions associated with the continued use of fossil fuels.

Carbon capture and storage (CCS) in deep geological formations is widely recognized as a promising large-scale CO₂ mitigation approach owing to their substantial storage capacity⁵. Several trapping mechanisms contribute to long-term CO₂ retention in subsurface environments, among which solubility trapping and mineralization are considered the most significant⁶. Mineralization is often regarded as the most secure mechanism because it permanently converts CO₂ into stable carbonate minerals^{7,8}. Solubility trapping involves the dissolution of injected CO₂ into the formation brines, a process that is strongly influenced by pressure, temperature, salinity, and brine pH⁹. Dissolved CO₂ lowers

the brine pH, generating mildly acidic conditions that can promote mineral dissolution, particularly in carbonate reservoirs¹⁰. This dissolution is an important precursor to mineralization because it releases dissolved divalent cations such as Ca²⁺ and Mg²⁺ into the solution. These cations may contribute to carbonate precipitation and mineral trapping as the system evolves. Moreover, mineral trapping depends on the availability of divalent cations such as Ca²⁺ and Mg²⁺, supplied either by the brine or released from the reservoir rocks through dissolution⁸. Therefore, in practice, solubility trapping, carbonate dissolution, and mineralization are dynamically coupled processes governed by mineralogy, fluid composition, and reaction kinetics^{6,8}.

Previous studies have reviewed the trapping mechanisms and mineralization pathways in geological CO₂ storage systems^{5–8}, investigated pore-scale evolution and geochemical alterations in carbonate reservoirs during CO₂–brine interaction^{10–12}, and quantified the dissolution kinetics of carbonate minerals under different CO₂ conditions^{13–15}. These studies have shown that the carbonate dissolution behavior is strongly influenced by mineralogy, fluid composition, saturation state, and reaction conditions, and that dissolved cation release plays an important role in controlling fluid chemistry and the subsequent mineralization

Table 1. Summary of related studies and gaps addressed in this work

Reference	System / Scale	Main focus	Key relevance	Remaining gap
5–8	Reviews / geological CO ₂ storage systems	Trapping mechanisms, mineralization pathways, and CO ₂ storage processes	Establishes the importance of solubility trapping and mineralization	Broad reviews; no direct early-time limestone–dolomite comparison
10	Carbonate and sandstone reservoirs / pore scale	CO ₂ –brine interaction and pore-scale evolution	Shows geochemical alteration during CO ₂ –brine–rock interaction	Pore-scale focus rather than controlled core-scale comparison
11	Carbonate rocks / experimental system	Rock response to CO ₂ -related interaction	Supports experimental study of carbonate response to CO ₂	Focuses on rock-property response rather than kinetic lithology comparison
12	Carbonates / pore scale or fundamental properties	Carbonate behavior under reactive conditions	Provides background on carbonate behavior in reactive systems	Foundational background, not a direct comparative reactive study
13,14	Carbonate minerals and carbonate rocks / kinetic and experimental studies	Dissolution kinetics and CO ₂ -related carbonate reactivity	Provides kinetic background for carbonate dissolution under CO ₂ conditions	Focus on mineral-scale or process-specific behavior
15	Carbonate rocks / microstructure	Localized versus distributed dissolution and role of microstructure	Highlights the role of rock structure in dissolution behavior	Emphasizes microstructure rather than bulk lithology response
This study	Limestone and dolomite core plugs / core scale	Early-time dissolution kinetics under brine-only and brine–CO ₂ conditions	Direct comparison of pH evolution, cation release, and early-time Ca dissolution	Addresses the lack of direct core-scale limestone–dolomite comparison

behavior^{10,12,13,15}. Collectively, these studies provide important insights into carbonate dissolution, CO₂–brine interactions, and mineral–fluid behavior relevant to geological CO₂ storage.

However, the available literature mostly focuses on general trapping mechanisms, equilibrium behavior, long-term geochemical evolution, and mineral- and pore-scale processes^{5,6,8,10,12}. Quantitative experimental data on early-time cation dissolution kinetics remain limited, particularly at the core scale and for direct comparisons between limestone and dolomite under the same controlled brine-only and brine–CO₂ conditions. In particular, variations in previous studies in terms of scale, lithology, and experimental focus have obscured the specific research gap. Although the thermodynamic behavior of CO₂–brine systems is relatively well established, the kinetics of mineral dissolution and its impact on solution chemistry and subsequent mineralization potential during early reaction stages remain poorly understood. This is important because early-stage kinetics determine how rapidly the brine approaches saturation and the consequent initiation of mineralization processes, which may also affect the near-wellbore chemical conditions. Table 1 summarizes selected studies on carbonate dissolution and CO₂–brine interactions and highlights the research gaps addressed in the present study.

The primary aim of the study is to quantify lithology-dependent chemical responses and early-time dissolution behavior under controlled subsurface-like conditions. Thus, this study investigated the dissolution kinetics of carbonate rocks under high-pressure brine and brine–CO₂ conditions relevant to geological CO₂ storage. Controlled static experiments were conducted on limestone and dolomite core plugs to quantify pH evolution, cation release, and early time calcium dissolution rates, providing a direct kinetic comparison across lithologies

and fluid conditions. This enables direct assessment of lithology-dependent early reaction behavior under matched experimental conditions. The findings of this study improve our understanding of the geochemical processes that influence subsequent mineralization.

2. MATERIALS AND METHODOLOGY

2.1. Materials. Carbonate rocks are cation-rich, making them a preferred choice for studying the cation dissolution behavior in brine systems relevant to CO₂ mineralization and dissolution processes⁸. Accordingly, two Indiana Limestone and two Maquoketa Dolomite core plugs with nearly identical geometries were selected for this study (Figure 1). The mineralogical differences between the limestone and dolomite samples were confirmed using X-ray diffraction (XRD) and X-ray fluorescence (XRF) analyses¹⁶. The XRD patterns of the limestone samples showed dominant peaks corresponding to calcite, whereas the dolomite samples exhibited characteristic peaks matching the dolomite reference patterns, confirming the dominant mineral phases in each rock. This interpretation was further supported by the XRF elemental composition (Table 2), which indicates that the limestone samples contain very high Ca content (≈ 97 wt%) with negligible Mg, whereas the dolomite samples contain significant Mg (≈ 19 wt%) alongside Ca, consistent with the CaMg(CO₃)₂ mineral structure. Together, the XRD and XRF results confirmed the mineralogical differences between the two carbonate lithologies.

The brines were prepared using ACS reagent-grade salts containing NaCl, CaCl₂, MgCl₂, NaHCO₃, and Na₂SO₄. The synthetic brine composition was selected to mimic the major ionic

Table 2. Elemental composition of the carbonate samples determined by XRF

Rock type	Ca (wt.%)	Mg (wt.%)	Cl (wt.%)	Al (wt.%)	Fe (wt.%)
Indiana Limestone	97.36	0.2281	0.7899	0.3293	0.3154
Maquoketa Dolomite	78.05	19.41	0.7485	0.3166	1.009

composition of Arabian Gulf seawater and to provide a representative saline environment for investigating carbonate dissolution under CO₂-brine conditions. The composition of the synthetic brine is summarized in Table 3. Prior to the experiments, the synthetic brine had an initial pH of 7.52, establishing the chemical baseline before rock-fluid interaction.

This study used CO₂ gas supplied by Air Liquide, Saudi Arabia, with brine prepared using deionized water.

2.2. Methodology.

2.2.1. Petrophysical properties. The petrophysical properties of the core plugs were measured using a helium porosimeter (HEP-E, VINCI Technologies, Nanterre, France) and a liquid permeameter (LP-100A, Porous Materials Inc., Ithaca, NY, USA) to determine the porosity, grain density, and permeability. The helium porosimeter operates by gas expansion and Boyle's law, and the liquid permeameter measures steady-state single-phase liquid flow through plug-sized core samples. Distilled water was used as the permeating fluid for the liquid permeability measurements, while helium gas was used as the expansion gas for porosity and grain-density determination. The core plugs were used under dry conditions for the porosity measurements and under fully brine-saturated conditions for the permeability measurements¹⁷. Table 4 summarizes the geometric and petrophysical properties of the limestone and dolomite core samples used in this study.

To perform the liquid permeability measurements, a brine solution (Table 3) was required. The brine was loaded into an accumulator and connected to a permeability pump to prevent corrosion within the pump. Permeability measurements were conducted at flow rates of 1, 2, and 3 cc/min until pressure stabilization was achieved. The pressure drops recorded at each flow rate were used to calculate the permeability, as listed in Table 4.

2.2.2. Test prototypes and experimental parameters.

The experimental program consisted of four sealed reaction cells (Figure 5) used to investigate the carbonate dissolution kinetics under controlled brine-only and brine-CO₂ conditions. Each reaction cell contained a single cylindrical carbonate core plug,

resulting in four test specimens: two dolomite samples (DL-1 and DL-2) and two limestone samples (LS-1 and LS-2). Two reaction cell geometries were employed: three cells with identical external geometries (Type A) and one cell with a different external shape (Type B). Despite the differences in external geometry, both cell types were designed with identical internal capacities (1000 mL) to ensure consistent fluid volumes and comparable boundary conditions across all experiments.

After the core samples were lowered into the reaction cells, they were filled with a fixed brine volume of 725 mL. In selected experiments, 200 mL of CO₂ was introduced into the reaction cell while maintaining a system pressure of 2000 psi. Under these high-pressure conditions, a significant portion of the injected CO₂ dissolved in the brine, resulting in elevated dissolved CO₂ concentrations. The dissolved CO₂ reacted with water to form carbonic acid (H₂CO₃), which lowered the solution pH and established CO₂-brine conditions representative of subsurface CO₂ storage environments. All the experiments were conducted under static chemical loading with no imposed fluid flow, mechanical loading, or cyclic stress applied to the specimens. Static conditions were selected to isolate the intrinsic chemical kinetics of carbonate dissolution under controlled pressure and temperature conditions. By eliminating fluid flow, transport effects such as advection and dispersion were minimized; thus, the observed changes in pH and dissolved cation concentrations primarily reflected rock-fluid reaction processes. The operating pressure and temperature were maintained at constant values of 2000 psi and 75 °C, respectively, to simulate the subsurface reservoir conditions. A summary of the experimental configurations, including the specimen identifiers, fluid volumes, and operating conditions, is presented in Table 5.

All reaction cells were connected to a high-pressure pumping system to maintain the operating pressure at 2000 psi throughout the experimental period. Following pressurization, the cells

Table 3. Properties of the synthetic brine

Ions	Composition (ppm)
Na ⁺	18,300
Ca ²⁺	650
Mg ²⁺	2,110
SO ₄ ²⁻	4,290
Cl ⁻	32,200
HCO ₃ ⁻	120
TDS	57,670
pH value	7.52

**Figure 1.** Geometry of core plugs used in this study

Table 4. Geometric and petrophysical properties of the core plugs

Sample	Length (mm)	Diameter (mm)	Porosity (%)	Permeability (mD)	Grain Density (g/cc)
LS-1	69.37	38.16	17.75	88	2.692
LS-2	69.3	38.18	17.99	89	2.694
DL-1	70.4	38.25	17.01	75	2.85
DL-2	70.12	38.24	17.04	74	2.827

Table 5. Summary of experimental conditions for all tests

Cylinder	Rock ID	Lithology	Brine Volume (ml)	CO ₂ Volume (ml)	Pressure (psi)	Temperature (°C)	Cell Geometry
1	DL-1	Dolomite	725	0	2000	75	Type A
2	DL-2	Dolomite	725	200	2000	75	Type A
3	LS-1	Limestone	725	0	2000	75	Type A
4	LS-2	Limestone	725	200	2000	75	Type B

were placed inside a temperature-controlled oven and maintained at 75 °C. Once thermal equilibrium was established, the experiments were initiated and allowed to proceed under static conditions with no imposed fluid flow, mechanical loading, or cyclic stress applied to the specimens. Figure 3 illustrates the experimental setup, with the arrangement of the reaction cells within the temperature-controlled oven and their connection to a common high-pressure manifold for uniform pressure control.

The dissolution behavior was monitored through periodic brine sampling during the experimental runs. At weekly intervals, aliquots of approximately 5–10 mL were withdrawn from each reaction cell and filtered to remove the suspended particulates. pH measurements were performed immediately after sampling to track the temporal evolution of solution chemistry. The pH was measured using a glass-electrode pH probe, with a typical measurement uncertainty of approximately ± 0.01 to ± 0.05 pH units depending on calibration and probe condition. The filtered samples were subsequently analyzed by ion chromatography (IC) to quantify the dissolved cation concentrations as a function of the reaction time¹⁸. For the IC measurements, the analytical precision was estimated using a relative standard deviation (RSD) of approximately 1%.

Sampling resulted in a minor pressure loss within the reaction cells; thus, to maintain constant experimental conditions, the system pressure was restored following each sampling event using a high-pressure pump. Distilled water was used for pressure

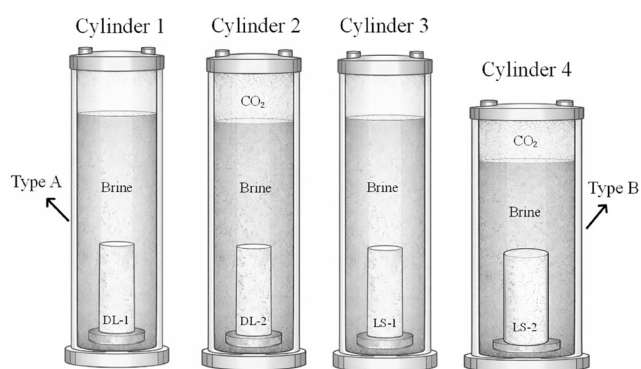
compensation owing to the incompatibility of saline fluids with the pumping system. The injected volumes required for pressure restoration were equal to the withdrawn sample volumes (≈ 5 –10 mL/event), which corresponded to $<1.4\%$ of the total brine volume (725 mL). Therefore, the effect of dilution on the system was minimal and did not significantly influence the measured pH or dissolved cation concentration. This procedure ensured that stable pressure was maintained throughout the experimental period.

3. RESULTS AND DISCUSSION

The chemical evolution of carbonate rocks under high-pressure brine and brine–CO₂ conditions reflects the combined effects of CO₂-induced acidification, mineral dissolution kinetics, and progressive buffering under static conditions. Brine-only systems evolve without externally imposed acidity, with their behavior primarily governed by mineral buffering and progression towards chemical equilibrium. By contrast, brine–CO₂ systems exhibit an initial acid-driven response due to carbonic acid formation, followed by gradual neutralization as carbonate dissolution consumes acidity. The mineralogical differences between limestone and dolomite further modulate these responses¹¹.

3.1. Cation Evolution. Dissolved cation concentrations provide direct evidence of carbonate–fluid interactions, capturing both early-time dissolution kinetics and subsequent chemical equilibration behavior under static conditions¹². Limestone dissolution is dominated by calcite and typically equilibrates rapidly, whereas dolomite dissolution involves coupled Ca²⁺ and Mg²⁺ release and proceeds more slowly owing to mineral-specific reaction kinetics. Under CO₂-bearing conditions, increased solution acidity enhances the chemical driving force for early-stage dissolution, while progressive neutralization and approach toward saturation limit sustain cation release over time¹³.

3.1.1. Dolomite systems. In dolomite-bearing systems under brine-only conditions (Figure 4a), the Ca and Mg concentrations do not follow a simple monotonic trend, indicating that the fluid chemistry evolves progressively during the reaction¹⁴. As dissolution proceeds, the brine composition changes and the system moves closer to carbonate equilibrium; therefore,

**Figure 2.** Schematic of the reaction cells and experimental configurations

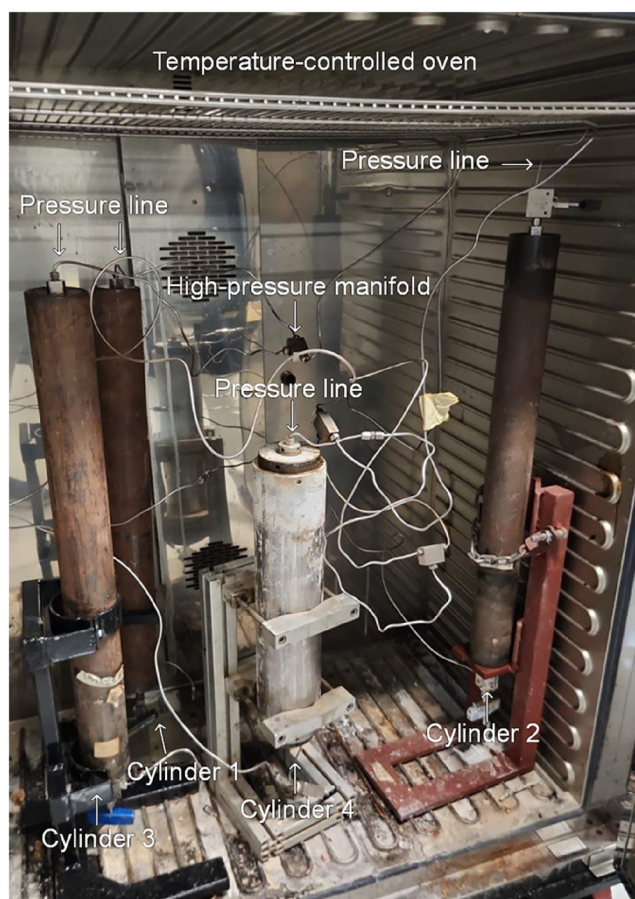


Figure 3. High-pressure, temperature-controlled experimental setup used for dissolution experiments

the measured cation concentrations reflect not only ongoing mineral dissolution but also changing saturation conditions and acid-neutralization effects that can modify the net Ca and Mg response. The observed non-monotonic Ca and Mg behavior may also reflect the evolving saturation conditions and possible carbonate precipitation processes reported in CO₂-reactive carbonate systems^{11,19}. Ca starts at very high levels (4.2×10^3 ppm) and drops sharply within the first week (to 1.5×10^3 ppm), whereas Mg rises from a few 10^2 ppm to $\sim 10^3$ ppm. This early behavior is consistent with rapid release of Ca²⁺ from the most reactive carbonate surfaces (freshly exposed dolomite faces and/or minor Ca-rich phases such as calcite impurities), followed by rapid removal of Ca²⁺ from the solution as the fluid becomes less undersaturated and secondary Ca-bearing solids begin to form.

The mid-test rebound in Ca (around day 14), alongside relatively steady Mg, suggests episodic re-exposure of the reactive surface area combined with intermittent precipitation control of Ca²⁺.

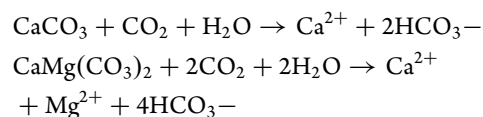
The late stage is characterized by extremely low Ca (near a few 10^2 ppm), whereas Mg peaks ($\sim 1.9 \times 10^3$ ppm) before collapsing by the final sampling point. This pattern is consistent with an incongruent carbonate reaction, where Ca is preferentially removed from the solution (most commonly by calcite or Ca-rich carbonate precipitation), whereas Mg accumulates until Mg-bearing carbonates begin to limit Mg²⁺, driving the terminal Mg drop²⁰.

Under brine-CO₂ conditions (Figure 4b), the process is more chemically directed. Ca decreases steadily from 2.3×10^3 ppm to $3\text{--}4 \times 10^2$ ppm, whereas Mg increases from 6×10^2 ppm to 1.6×10^3 ppm. The dissolved CO₂ forms carbonic acid, which lowers the pH and sustains carbonate dissolution. Under these conditions, the system experiences stronger dissolution kinetics and a larger reactive zone than CO₂-free brine at the same pressure and temperature. The continued decline in Ca, despite acid-driven dissolution, implies the efficient removal of Ca by secondary sinks during the reaction. In contrast, Mg²⁺ is less rapidly scavenged and accumulates in the solution, leading to an increased Mg/Ca ratio in the final stage. Mechanistically, this behavior reflects a CO₂-driven dissolution front accompanied by near-surface precipitation, which suppresses Ca in the bulk brine while allowing Mg to track the ongoing dolomite reaction more directly.

3.1.2. Limestone systems. In limestone-brine systems (Figure 5a), Ca starts at relatively high level (~ 2000 ppm) and trends downward overall, with a small mid-term rebound (dropping to ~ 1600 ppm after approximately one week, rising to ~ 1800 ppm at approximately two weeks, then declining to a few hundred ppm by ~ 35 days). Mg increases to a peak ($\sim 1200\text{--}1300$ ppm at $\sim$ two weeks), remains stable through $\sim$ three to four weeks ($\sim 1100\text{--}1200$ ppm), and then drops sharply near the end. This behavior reflects a transition from early net ion release to late-stage removal from the solution, with Ca decreasing sooner and more strongly than Mg.

In the presence of CO₂ (Figure 5b), the system exhibited stronger transients. Ca concentration started at ~ 2200 ppm, decreased rapidly (~ 1000 ppm by ~ 10 days), rebounded (~ 1800 ppm by ~ 17 days), and declined to $\sim 500\text{--}600$ ppm by ~ 38 days. Mg mirrored this dip-rebound-decline pattern. Compared with brine-only conditions, CO₂ produced larger excursions and faster early changes. This is consistent with CO₂-driven acidification enhancing early carbonate reactivity, followed by progressive stabilization, where both Ca and Mg decrease simultaneously. The late convergence of Ca and Mg suggests that long-term control involves coupled processes that affect both cations rather than simple calcite dissolution alone.

3.2. pH Evolution. Under CO₂-rich conditions, the dissolved CO₂ reacts with water to form carbonic acid, which promotes carbonate dissolution and contributes to acid neutralization. The primary dissolution reactions can be represented as follows:



These reactions illustrate how calcite and dolomite dissolution consume acidity while releasing dissolved cations into the solution. Accordingly, the pH evolution reflects the balance between CO₂-derived acidity and carbonate buffering. Brine-only systems are expected to exhibit a stable or increasing pH as carbonate dissolution consumes protons, whereas brine-CO₂ systems initially exhibit suppressed pH, followed by recovery as acid-neutralization reactions dominate. Owing to the distinct buffering capacity between limestone and dolomite, pH trends must be interpreted across all systems and within individual

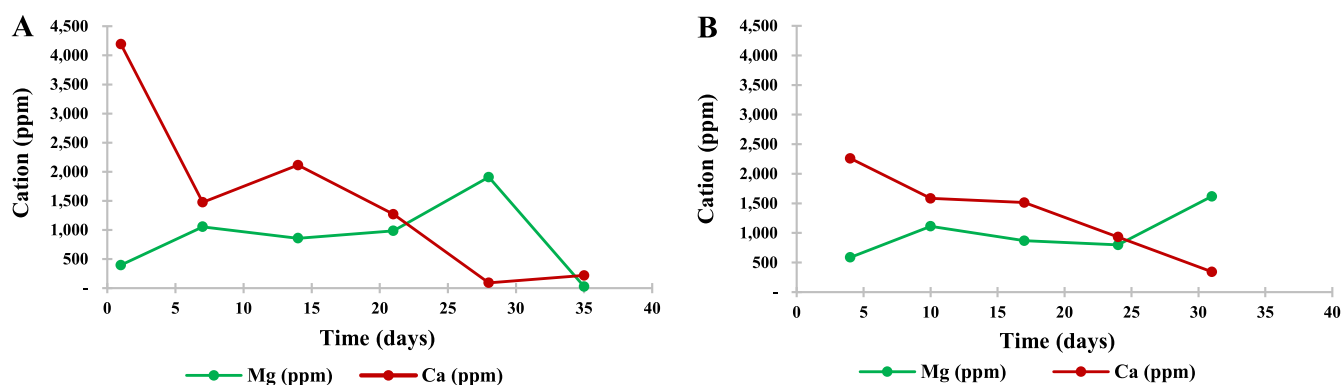


Figure 4. Ca^{2+} and Mg^{2+} in dolomite systems under (a) brine-only and (b) brine- CO_2 conditions

lithologies. Although a fixed CO_2 volume (200 mL) was introduced into the reaction cell, solution acidity is primarily governed by the resulting CO_2 partial pressure (pCO_2) under the maintained system pressure of 2000 psi. The injected CO_2 volume mainly establishes CO_2 -rich conditions, whereas the chemical behavior of the system is governed by the elevated pCO_2 and the resulting formation of carbonic acid.

For dolomite (Figure 6a), a strong time-dependent neutralization trend was observed. In brine-only, pH was initially ≈ 5.2 at ~ 7 days and rose steadily to near-neutral/weakly alkaline values (≈ 7.0 by ~ 21 days and ≈ 7.3 by ~ 35 days), consistent with progressive dolomite buffering. In the brine- CO_2 condition, the measured pH was already higher at the first sampling point (≈ 6.35 at ~ 10 days) and then climbed to ~ 7.2 – 7.3 by ~ 24 – 31 days, implying faster early acid neutralization in the presence of CO_2 , followed by a plateau as the system approached carbonate equilibrium.

In contrast, the limestone systems (Figure 6b) exhibited considerably greater pH stability. In brine-only, pH remained at approximately 6.6–6.8 from ~ 7 to ~ 35 days, indicating rapid establishment of a near-steady carbonate equilibrium. In brine- CO_2 , only a modest mid-term acidification was observed (≈ 6.5 at ~ 24 days), followed by recovery toward ~ 6.9 – 7.0 by ~ 31 – 38 days, consistent with temporary CO_2 -driven acidification and subsequent buffering by calcite dissolution.

Overall, the key distinction lies in both amplitude and kinetics. Dolomite exhibits a large pH swing over weeks, signaling slower but stronger cumulative buffering, whereas limestone remains

near neutral throughout, showing rapid buffering and early stabilization with only small CO_2 -driven perturbations. At the end, both systems become nearly neutral, but dolomite maintains a slightly higher pH (7.2–7.3) than limestone (6.9–7.0).

3.3. Quantitative Evaluation of Dissolution Kinetics.

To compare the carbonate dissolution kinetics across lithologies and fluid compositions quantitatively, early-time Ca^{2+} release rates were derived from the measured concentration–time data. Calcium was selected as the primary kinetic tracer because of its direct stoichiometric association with carbonate mineral dissolution in both the limestone and dolomite systems.

3.3.1. Early-time Ca^{2+} release rates. The initial dissolution behavior was quantified using the early-time slope of the Ca^{2+} concentration–time curve, defined in Eq. (1).

$$R_{\text{Ca},0} = \frac{\Delta C_{\text{Ca}}}{\Delta t} \quad (1)$$

where C_{Ca} is the dissolved calcium concentration (ppm) and t is the time (days). The slopes were calculated using the first two sampling points to capture the initial kinetic responses of the system. Later, progressive acid neutralization, chemical equilibration, and potential secondary precipitation processes began to influence the measured cation concentrations, implying that the system no longer reflected the initial dissolution behavior purely. Therefore, the first concentration interval provided the most representative estimate of the initial dissolution

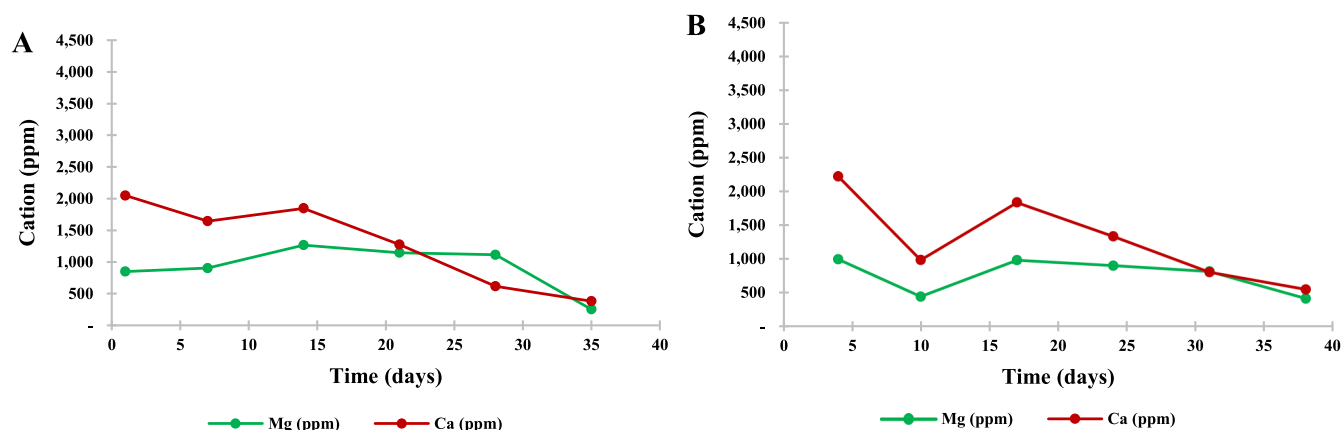


Figure 5. Ca^{2+} and Mg^{2+} in limestone systems under (a) brine-only and (b) brine- CO_2 conditions

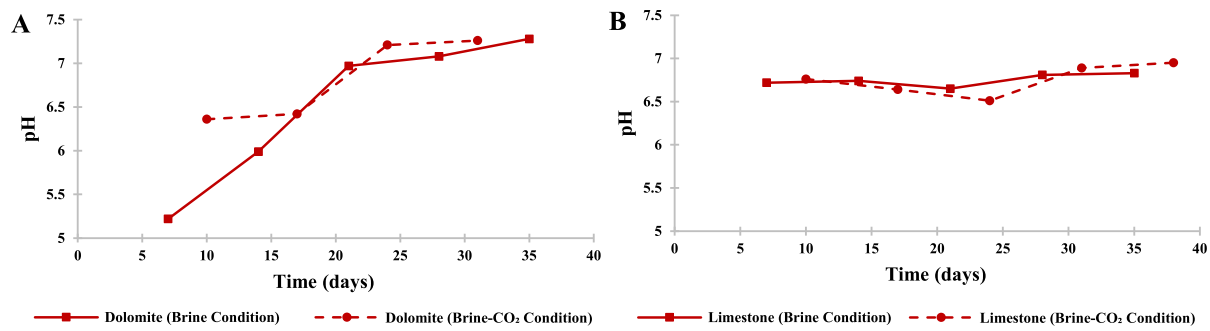


Figure 6. pH evolution for dolomite (a) and limestone (b) samples under brine-only and brine-CO₂ conditions

Table 6. Early-time Ca²⁺ dissolution slopes and surface-area normalized dissolution rates

Cylinder	Lithology	Condition	Early-time slope (ppm · day ⁻¹)	r _{Ca,0} (mol · m ⁻² · day ⁻¹)
1	Dolomite	Brine	-452.9	-0.773
2	Dolomite	Brine-CO ₂	-112.6	-0.192
3	Limestone	Brine	-67.4	-0.115
4	Limestone	Brine-CO ₂	-205.0	-0.350

rate before the secondary processes affected the chemical evolution of the system. The calculated early-time slopes (Table 6) show clear lithology- and CO₂-dependent contrasts. The negative sign of the slope indicates a net decrease in the dissolved Ca²⁺ concentration over time, reflecting rapid early-stage chemical adjustment, followed by progressive solution neutralization and secondary-process control. Moreover, the dolomite brine-only system exhibited the largest slope, indicating the most rapid initial chemical adjustment. The limestone systems displayed smaller early-time slopes, consistent with faster equilibration and a weaker pH buffering capacity relative to dolomite. Notably, the presence of CO₂ suppressed the magnitude of the early-time Ca²⁺ decline in dolomite, while substantially increasing early calcium mobilization in limestone.

3.3.2. Surface-area normalized dissolution rates. To enable a direct comparison of dissolution kinetics independent of specimen size, Ca²⁺ release rates were normalized to the exposed geometric surface area of each core plug, according to Eq. (2).

$$r_{Ca,0} = \frac{1}{A} \frac{dn_{Ca}}{dt} \quad (2)$$

where n_{Ca} is the number of moles of dissolved calcium calculated from the measured concentrations and fixed brine volume (0.725 L), and A is the geometric surface area of the cylindrical core plug determined from the measured dimensions (Table 4). The geometric surface area was used as a consistent normalization basis for all specimens, recognizing that the effective reactive surface area may differ owing to pore-scale roughness and mineral heterogeneity.

The resulting surface-area normalized dissolution rates (Table 6) confirmed that dolomite exhibited higher effective dissolution rates than limestone under brine-only conditions. CO₂ modified the dissolution kinetics in a lithology-dependent manner, reducing the apparent initial dissolution rate in dolomite and enhancing early calcium release in limestone¹⁵. These contrasts indicate that the early reaction stage is kinetically controlled and strongly

influenced by the mineralogy and fluid composition¹⁹. Collectively, these findings demonstrate that the early-stage cation release plays a critical role in regulating both CO₂ solubility enhancement and the initiation of mineral trapping in carbonate reservoirs. From a CCS perspective, the results emphasize that short-term dissolution kinetics can strongly influence the timing and extent of mineralization, particularly in systems where Ca²⁺ and Mg²⁺ availabilities limit carbonate formation. These results are consistent with previous studies showing that carbonate dissolution behavior depends strongly on mineralogy and CO₂-related reaction conditions, while the present work extends this understanding through a direct early-time core-scale comparison between limestone and dolomite under controlled brine-only and brine-CO₂ conditions. Therefore, incorporating early-time kinetic behavior into reactive transport and reservoir-scale models is essential for improving the prediction of long-term CO₂ storage security. Future work should extend this framework to flowing systems and longer reaction times to better represent field-scale conditions and mineralization potential.

4. CONCLUSIONS

This study examined the dissolution kinetics of carbonate rocks under high-pressure brine and brine-CO₂ conditions relevant to geological CO₂ storage and mineralization. Through controlled core-scale experiments and time-resolved measurements of pH and dissolved cation concentrations, this work provides quantitative insights into the early-stage mineral-fluid interactions that govern CO₂ trapping behavior in carbonate reservoirs.

The following conclusions were drawn:

1. The experimental systems exhibited systematic and reproducible pH and cation evolution, demonstrating that the applied pressure-temperature conditions and static experimental design are well-suited for isolating the early-time dissolution behavior.
2. Carbonate lithology strongly controlled the chemical response, with dolomite displaying a greater buffering capacity and more sustained cation release than limestone. This reflects

the fundamental differences in mineral composition and dissolution kinetics.

3. The presence of CO₂ significantly modified the early-stage dissolution behavior by lowering the initial pH and altering the calcium release in a lithology-dependent manner, thereby directly influencing the short-term availability of divalent cations for mineralization.

4. Quantified early-time Ca²⁺ dissolution rates indicate that the initial CO₂–brine–rock interactions are predominantly kinetics-controlled, preceding progressive acid neutralization and partial chemical equilibration.

The present results suggest that early-time lithology-dependent dissolution and cation release may influence CO₂ buffering, the onset of mineral trapping, and geochemical evolution in carbonate storage systems. However, several limitations should be acknowledged: The experiments were conducted on a limited number of four core-scale samples (~70 mm in length). Furthermore, the experiments were performed under static conditions with no imposed fluid flow and over a limited duration of approximately 35–38 days.

In natural reservoirs, additional processes, such as fluid flow, larger spatial heterogeneity, and much longer reaction times (years to decades), may influence rock–fluid interactions. Therefore, the results represent laboratory-scale observations of early dissolution kinetics and provide insight into processes relevant to CO₂ storage, whereas direct extrapolation to reservoir-scale behavior requires further investigation.

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Methanol Slug Sizing as a Mobility Control Strategy for Viscous Fingering Supersession in Miscible scCO₂ EOR: A CMG-GEM Simulation Study

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ABSTRACT

This study examined how methanol (MeOH) can improve the sweep efficiency of miscible CO₂ flooding in enhanced oil recovery (EOR) applications—a process characterized by efficient miscible oil displacement but poor areal sweep efficiency, in which the viscosity contrast between the injected and resident fluids causes CO₂ to channel through preferential paths. Vertical core flooding simulations were conducted using CMG-GEM software to evaluate the effect of MeOH slug size on displacement behavior and oil recovery at one pore volume (1 PV) injected. The analysis showed that small MeOH fractions primarily increased the supercritical CO₂ (scCO₂)–oil miscibility, density, and viscosity, producing only minor improvements in macroscopic sweep efficiency. By contrast, larger fractions sufficiently increased the scCO₂ viscosity, shifting the mobility contrast (M) to stabilize the advancing front, delay breakthrough (BT), and consolidate the scCO₂ channels. At sufficiently high MeOH volumes, the displacement transitioned into a near-piston-like advance with complete suppression of fingering and near-complete sweep of the core. These shifts in flow behavior increased recovery factors (RF) from approximately 73% for pure scCO₂ injection to nearly 99% when MeOH occupied half or more of the injected PV. Overall, the findings demonstrate that MeOH acts as both a microscopic efficiency modifier and a hydrodynamic stabilizer, with its effectiveness strongly dependent on the injected proportion. This work suggests that MeOH-assisted scCO₂ flooding may offer a practical pathway to improving sweep efficiency in miscible EOR processes and motivates future laboratory validation and evaluation of hybrid strategies such as water-alternating-gas (WAG) with MeOH buffering.

Keywords: CO₂ flooding, enhanced oil recovery (EOR), viscous fingering, mobility contrast, alcohol buffers, front stabilization

1. INTRODUCTION

EOR techniques are commonly required after primary and secondary mechanisms become insufficient, typically recovering only ~10% of the original oil in place (OOIP)¹ EOR strategies span thermal, chemical, and gas-injection methods, each selected based on reservoir conditions, oil properties, and operational feasibility. Among these techniques, miscible CO₂ flooding has been widely applied owing to its ability to achieve multicontact miscibility (MCM), swell the oil phase, reduce viscosity, and enhance displacement efficiency² When the injection pressure exceeds the minimum miscibility pressure (MMP), CO₂ diffuses rapidly into the crude oil, enriching the gas phase and lowering the interfacial tension (IFT), thereby enabling favorable flow behavior.

In miscible CO₂ flooding, viscous fingering arises owing to the injection of low-viscosity CO₂ into a considerably more viscous oil³ When the IFT is nearly eliminated under miscible conditions, no capillary barrier exists to dampen interfacial disturbances, and any microscopic fluctuation at the CO₂–oil interface amplifies freely⁴ The injected CO₂, continually driven by the pressure gradient, seeks paths of least resistance and

penetrates the oil through narrow advancing channels rather than displacing it uniformly. This behavior minimizes the energy required to displace the highly viscous phase⁵ As miscibility and decreasing pressure toward the outlet further reduce local resistance ahead of the front, these channels accelerate, elongate, and branch, forming the classic unstable displacement geometry known as viscous fingering⁶ Extensive efforts have been made to address this challenge. Enick *et al.*⁷ provided a comprehensive 40-year review of CO₂ thickeners, detailing various mobility and conformance control techniques, including WAG, surfactant-alternating-gas (SAG), foam-assisted-water-alternating-gas (FAWAG), and CO₂ flooding profile improvement. Although these methods have demonstrated efficacy in mitigating viscous fingering, the associated economic and practical constraints limit their field scale implementation. Rudyk *et al.*⁸ investigated the feasibility of ethanol and MeOH as CO₂ cosolvents to enhance its molecular weight and consequently increase displacement efficiency, reporting a 19.4% increase in liquid-phase oil recovery over a pressure range of 20–60 MPa. Fang *et al.*⁹ employed molecular dynamics simulations to analyze the atomic-level behavior of CO₂/N₂ flooding slugs, finding

that CO₂ injected as the front slug markedly improves oil recovery owing to its high miscibility with crude oil and the propelling effect of N₂. Djabbarah¹⁰ demonstrated that CO₂-alcohol mixtures modify MMP while increasing CO₂ density and viscosity, proposing two injection strategies: (1) premixing the chemicals before injection and (1) injecting alternating slugs of CO₂ and alcohol. Al-Azani *et al.*¹¹ investigated organic additives as CO₂ co-injection agents to mitigate gravity override and mobility instability during gas flooding; their experimental study on blending CO₂ with triethyl citrate demonstrated that the additive increased CO₂ viscosity and density, leading to improved sweep efficiency and reduced segregation. However, this approach has practical limitations, including the need for precise compositional control, potential phase separation under reservoir conditions, and uncertainties regarding chemical retention. Li *et al.*¹² developed a poly(vinyl acetate)-styrene (PVAc-S) polymer thickening system with ethanol as a cosolvent, reporting a 24-fold increase in CO₂ viscosity under reservoir conditions; dual-core experiments demonstrated improved mobility control, while NMR imaging confirmed a stabilized displacement front and enhanced micropore fluid mobilization. However, polymer-based thickeners may suffer from injectivity, retention, and economic limitations at the field scale.

While CO₂ EOR has been extensively studied, the use of MeOH as a discrete buffering slug in Berea sandstone has not been explored; previous studies have focused on alternative chemicals or on continuous MeOH co-injection with CO₂. MeOH is miscible with both crude oil and CO₂.⁸ Furthermore, its intermediate density—falling between that of oil and scCO₂ (570.1 < 744 < 877 kg/m³)—yields density and viscosity values more compatible with oil than CO₂, thereby supporting a stable displacement front. The increased viscosity and density of the CO₂-MeOH mixture are attributed to strong intermolecular interactions between the hydrogen-bonding groups in MeOH and the induced dipoles in CO₂. These interactions are stronger than the dispersion forces in pure CO₂, leading to (1) restricted molecular motion, which increases viscosity, and (2) stronger molecular attraction, which reduces intermolecular distance and increases mixture density.¹³ This study investigated how MeOH slugs with varying PV fractions influenced BT, CO₂ mobility, displacement stability, and oil RF in vertical miscible scCO₂ core floods. Using a CMG-GEM simulation framework with slug fractions ranging from 1% to 90% PV, this study identified a transition from primarily improving scCO₂-oil miscibility to thickening the mixture, shifting M toward hydrodynamic front stabilization at higher fractions.⁴

2. METHODOLOGY

2.1. Experimental Description. Vertical upward core flooding was simulated by injecting a MeOH pre-slug followed by scCO₂ for a total injection of 1 PV (Figure 1). The primary variable was the MeOH-to-CO₂ injection ratio (Table 1), evaluated in terms of CO₂ mass production behavior and RF trends. All tests were conducted under identical operating conditions.

The core model corresponded to a 30.5 cm Berea sandstone plug with a diameter of 3.78 cm; the core properties are summarized in Table 2. Berea sandstone was simulated by setting typical

values for rock properties and relative permeability, as shown in Figure 2, and was selected because it is among the most common reservoir analogs in Saudi Arabia.¹⁴ The displaced oil was Saudi Arabian light crude, and all fluid properties used in the simulations are listed in Table 3.

2.2. Simulation of Core Flooding. Core flood simulations were conducted using the CMG-GEM compositional simulator, with the model configuration illustrated in Figure 3. Fluid injection and production were imposed at a fixed rate of 0.25 cm³/min at both the inlet and outlet to maintain steady displacement conditions. The back-pressure regulator was set to 24.132 MPa—sufficiently above the CO₂ MMP (17.24 MPa at 99 °C)¹¹—to ensure single-phase miscible CO₂ flow. A confining pressure of 27.579 MPa was applied to maintain mechanical integrity and enforce upward displacement. Under these conditions, the total injection duration was 4.4 h, corresponding to 1 PV of injected fluids. These pressure and temperature conditions ensured the supercritical state of CO₂, as verified by NIST.¹⁵

All binary interaction coefficients were assigned a value of zero, and water saturation (*S_w*) was initialized at its irreducible value (*S_w* = 0.20).

3. RESULTS AND DISCUSSION

3.1. General Overview of Outcomes. The results presented in Figure 4 reveal a consistent delay in scCO₂ BT with increasing MeOH fraction, ultimately achieving no BT conditions at high MeOH PV fractions. This behavior reflects improvement in M, primarily through viscous thickening of the displacement front and subsequent suppression of viscous fingering.⁴ In parallel, the plateau in scCO₂ mass production gradually diminished with increasing slug size, indicating a more uniform advancement of the displacement front.²

Regarding RF, Figure 5 illustrates that the RF recorded at the end of injection follows a polynomial increase with MeOH slug size before plateauing at 0.5 PV. At this plateau, RF reaches 98.95%, a marked improvement over the 73.48% recorded for the pure scCO₂ baseline. Collectively, these results demonstrate that MeOH buffers stabilize the displacement front, mitigate early BT, and substantially enhance the mobilization and recovery of previously trapped oil.

3.2. Initial Observations: Base scCO₂ Injection. The baseline simulation represented the upward injection of 1 PV of pure scCO₂ into a Berea sandstone core to establish a quantitative reference for subsequent co-injection runs. The scCO₂ mass production rate, and RF were extracted from the simulation outputs and plotted in Figures 6 and 7, respectively. These results establish a benchmark for subsequent comparisons involving MeOH-augmented floods.

As shown in Figure 6, CO₂ BT occurred at 27% PV of injected gas. The scCO₂ mass rate curve exhibited an exponential increase before stabilizing beyond the deviation point at 0.49 PV, where the inlet and outlet volumetric rates equilibrated at 0.25 cm³/min. The transient growth in mass rate followed the empirical relationship developed by fitting the simulation output:

$$\dot{m}_{\text{CO}_2} = 658.46 \text{PV}^{11.886} \quad (1)$$

Table 1. Sizes of MeOH slugs tested

Case	Base Case	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8	Case 9	Case 10	Case 11
Injection (MeOH %PV)	0%	1%	5%	10%	20%	30%	40%	50%	60%	70%	80%	90%

Table 2. Properties of the Berea core sample

Diameter (cm)	Length (cm)	PV (cc)	Porosity (%)	Permeability (mD)
3.79	30.48	65.33	19	260

where $\dot{m}_{CO_2}$ denotes the mass production rate of scCO₂ and PV indicates pore volume of injected scCO₂.

The excellent fit of this relationship ($R^2 = 0.95$) highlights the exponential propagation of the gas front during the growth. The sharp rise near BT indicates the onset of viscous fingering, caused by the unfavorable M between the low viscosity CO₂ and the displaced oil. In this regime, localized gas intrusions penetrate the oil phase through preferential pore pathways, allowing a fraction of scCO₂ to reach the outlet prematurely while the remaining injected gas continued to mobilize oil within the core⁵. This behavior reflects a hydrodynamically unstable yet thermodynamically consistent displacement, in which early gas arrival does not necessarily imply poor miscible sweep but rather an unstable front.

The corresponding recovery trend in Figure 7 shows an oil RF of 28.88% at BT, followed by a gradual increase to 73.48% RF at 1 PV injected. The inflection point at 0.49 PV in Figure 7 aligns with the scCO₂ mass rate deviation in Figure 6; both signal a shift in the governing mobility regime. Before BT, the displacement was relatively stable and dominated by limited gas mobility. After BT, continued scCO₂ injection increased its saturation (S_{CO_2}) and relative permeability (k_{r,CO_2}), thereby amplifying M and promoting fingering extension. Despite the observed instability, the front advanced uniformly with no evidence of gravity

override. The consistent distribution of scCO₂ across the core and the absence of CO₂ accumulation at the top layer (Figure 8) confirm this behavior, attributed to the small vertical dimensions of the core and the water-wet rock characteristics.

The evolution of M before and after BT can be expressed as follows:

$$M = \frac{K_{rCO_2} @ S_{avg,CO_2BT} \mu_o}{K_{ro} @ S_{wi} \mu_{CO_2}}, \text{ Before BT} \quad (2)$$

$$M = \frac{K_{rCO_2} @ S_{CO_2,2} \mu_o}{K_{ro} @ S_{wi} \mu_{CO_2}}, \text{ After BT} \quad (3)$$

where M denotes the mobility ratio, S_{avg,CO_2BT} denotes the scCO₂ average saturation at BT, K_{ro} denotes the oil relative permeability, and μ_{CO_2} denotes the scCO₂ viscosity.

The increase in M after BT marks the hydrodynamic shift from a frontal displacement regime to a fingered flow regime. The overall displacement efficiency continued to rise but at a diminishing rate as scCO₂ occupied the most conductive pore channels, leaving residual oil in less accessible regions.

This baseline behavior forms a reference framework for evaluating MeOH-assisted injections. In this context, MeOH acted as an intermediate cosolvent that temporarily bridges the scCO₂

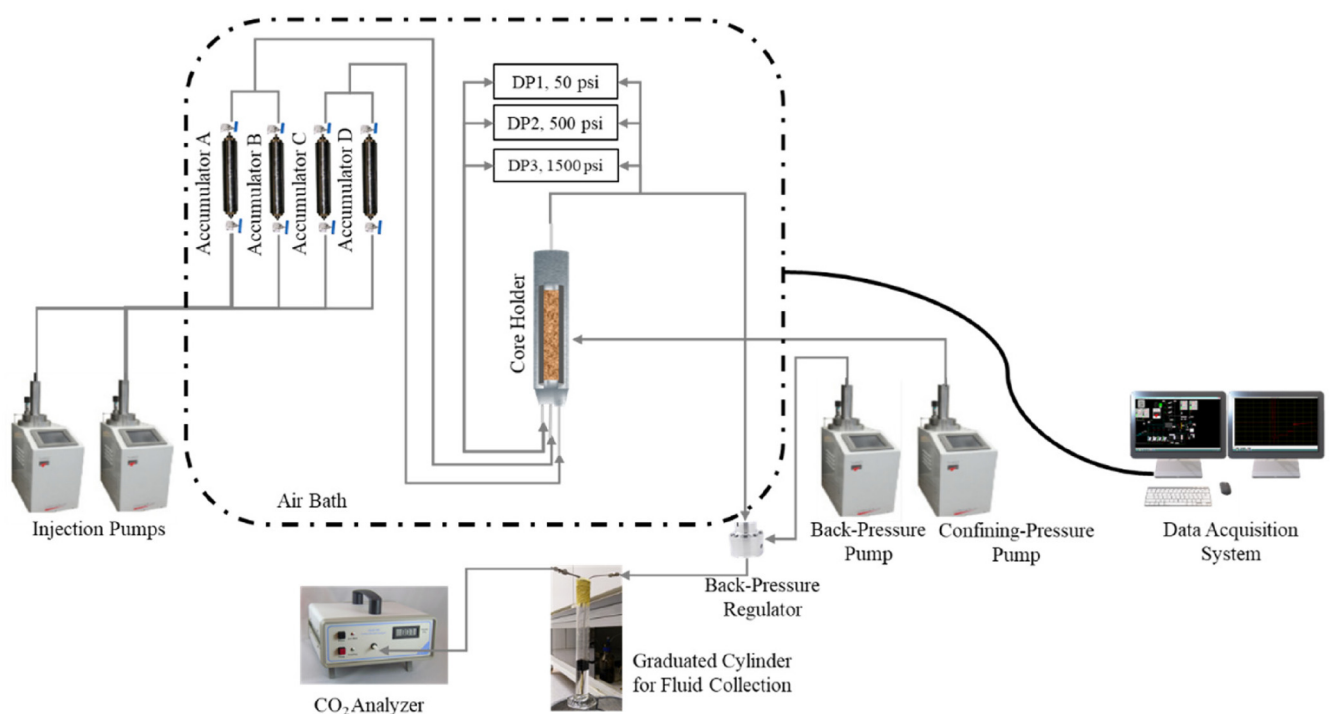
Figure 1. Schematic of experimental setup¹¹

Table 3. Properties of the fluids used in the simulation

Fluid/Property	Critical Pressure (MPa)	Critical Temperature (K)	Density (kg/m ³)	Normal Boiling Point (K)
MeOH	8.01	512.5	744	337.8
Crude oil	1.3	960	877	810.9
scCO ₂	7.40	300	570.1	255.4

and oil phases, introducing both thermodynamic and hydrodynamic benefits. Initially, MeOH created a transition zone that reduced the interfacial tension and increased solubility, while thickening the front through higher viscosity and density⁴. As the injection progressed, scCO₂ dissolved into the MeOH-rich region, gradually shortening its stabilizing window and diluting the buffer. This displacement reflected the transient coupling of miscibility enhancement and CO₂ thickening. Once M reached a favorable range, hydrodynamic stabilization of the front geometry occurred, delaying BT, improving sweep, and increasing RF compared to pure scCO₂.

3.3. Parametric Analysis of MeOH Buffer Sizes.

3.3.1. scCO₂ mass production rate. The scCO₂ mass production behavior for all MeOH-buffered scenarios can be interpreted using Darcy's law, expressed as follows:

$$\dot{m}_{CO_2} = \rho \frac{k A k_{rCO_2}}{L \mu_{CO_2}} \Delta P \quad (4)$$

where k_{rCO_2} denotes the relative permeability of scCO₂, A denotes the cross-sectional area of the core, L denotes the core length, ΔP denotes the differential pressure. As k , A , L , and ΔP remain constant across all cases, the trend in Figure 4 ultimately reduces to the outlet mobility term:

$$\dot{m}_{CO_2} \propto \frac{k_{rCO_2}}{\mu_{CO_2}} \quad (5)$$

The expected trend is consistent with intermolecular force (IMF) theory: the IMFs of the front strengthen as MeOH content increases, driven by enhanced dipole-induced dipole interactions. These interactions reduce intermolecular spacing and increase resistance to flow, thereby raising mixture viscosity and density. As the density increases, the dispersion forces responsible for improved microscopic efficiency and solubility with oil

increases. Viscosity is also expected to increase throughout; however, its impact on unifying the front geometry will become apparent only after a favorable viscosity ratio between phases is achieved.^{4,13} This threshold is the factor that gives IFT dominance in controlling flow geometry at low MeOH fractions, before M assumes its role in consolidating channels through sufficient thickening at higher fractions⁴.

As shown in Figure 4 and quantified in Table 4, the BT timing for the low-slug cases (1%, 5%, 10%, and 20% MeOH) remained unchanged relative to the 100% scCO₂ base case, with BT values confined to the narrow range of 0.264–0.276 PV. This minimal deviation confirmed that low MeOH fractions provided negligible hydrodynamic stabilization to the advancing front. To achieve effective stabilization, the cumulative viscosity of the displacing fluid must be at least 30% of the oil viscosity⁴. The slight smoothing observed in the CO₂ mass rate curves for these cases in Figure 4 therefore originates from thermodynamic effects—namely the modest increase in scCO₂ viscosity and its enhanced dissolution capacity—rather than from improved sweep control. In practical terms, 1–20% MeOH slugs alter fluid properties but not flow geometry, leaving BT essentially governed by viscous instability rather than buffer-driven mobility control. The final

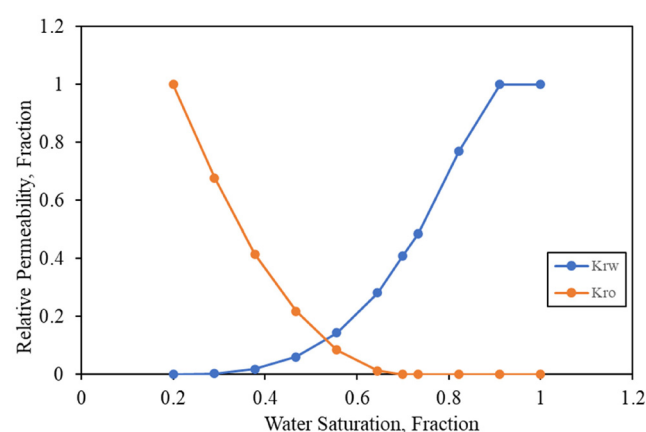


Figure 2. Relative permeability of the simulated system with water as the base permeability

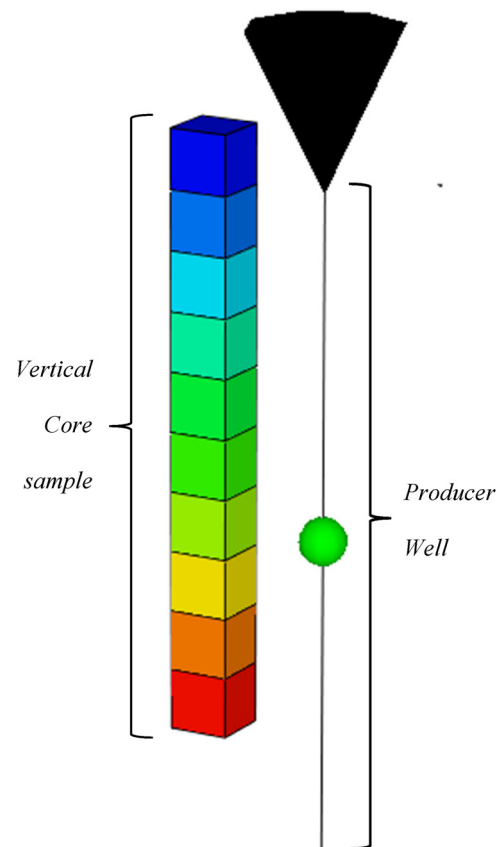


Figure 3. Simulated core flooding setup

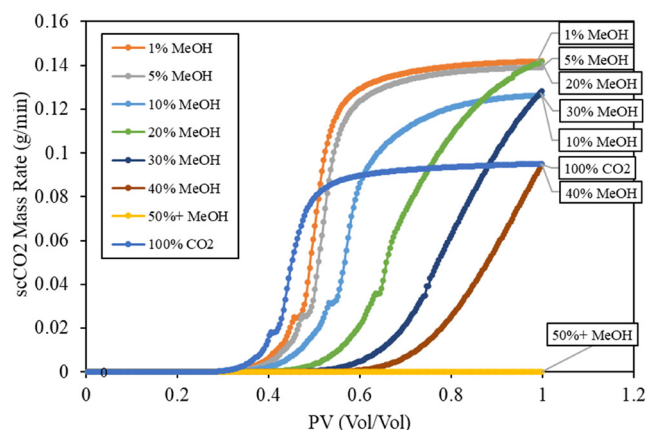


Figure 4. scCO₂ mass production rate over time, as simulated by CMG-GEM

CO₂ mass production rate decreased progressively with increasing MeOH proportion (0.141–0.126 g/min), further confirming the dominance of viscosity increase in Eq. (4). The trend begins to shift at the 0.2 PV MeOH slug, where the final CO₂ mass rate recovers to 0.142 g/min, indicating the first hydrodynamic contribution of MeOH. At this slug size, MeOH begins to partially stabilize the displacement front, consolidating CO₂ flow into thicker and better-connected pathways, which increases the

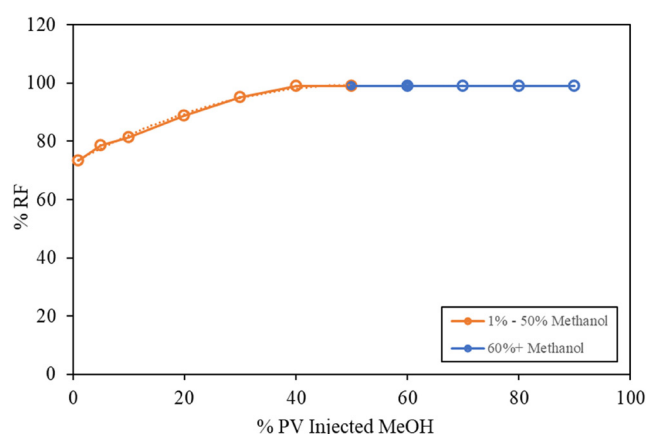


Figure 5. Final RF trend with different MeOH PV fractions

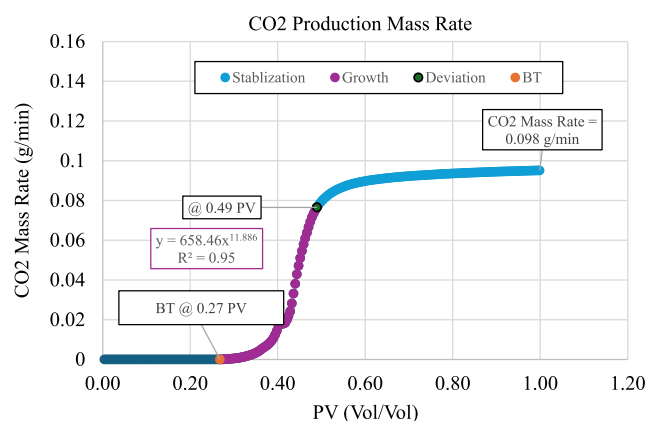


Figure 6. scCO₂ mass production rate behavior for 1 PV scCO₂ injection

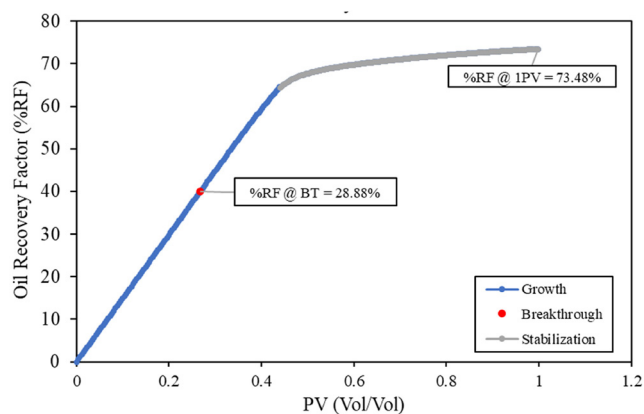


Figure 7. RF for 1 PV scCO₂ injection

effective gas relative permeability at the outlet and enhances the produced CO₂ mass.

A closer inspection of the final CO₂ mass production rates in Table 4 reveals an important nuance within the low-slug regime. Although the BT timing remains unchanged, the final mass rates for 1%, 5%, and 10% MeOH (0.141, 0.139, and 0.127 g/min, respectively) are all higher than the 100% CO₂ base case (0.0951 g/min). This confirms that even trace additions of MeOH sufficiently increased CO₂ viscosity and solvency, as predicted from IMF behavior¹³. These enhancements raised the CO₂ mobility ($k_{r,CO_2}/\mu_{CO_2}$) at the outlet without altering the flow geometry, as evidenced by the negligible variation in BT values (0.2640 to 0.2755 PV). The subsequent decline in the final scCO₂ mass rate from 5% to 10% MeOH reflects the growing thickening effect—scCO₂ viscosity increases more rapidly than relative permeability rises, causing the mobility term to weaken.

The first deviation from this thermodynamic pattern appears at 20% MeOH, where the final CO₂ mass rate climbs again to 0.142 g/min. This rebound signals the earliest onset of hydrodynamic influence: MeOH is now sufficiently voluminous to begin linking and consolidating the CO₂ micro-fingers into thicker, more coherent flow channels, increasing k_{r,CO_2} at the outlet. Although this hydrodynamic contribution is still weak and insufficient to delay BT, it is strong enough to counterbalance the viscosity increase and raise the final mass rate—an effect that later evolves into the smoother curves and delayed BT observed

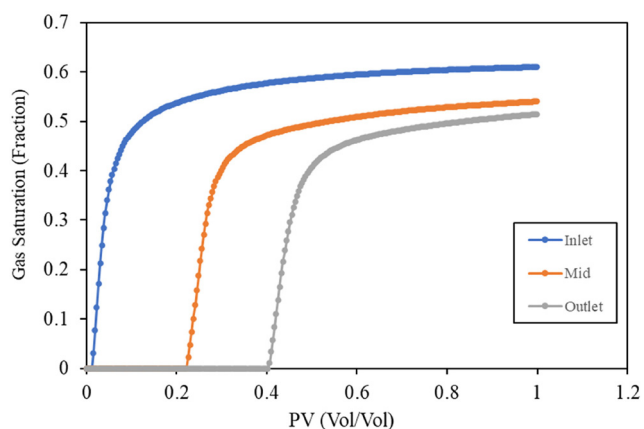


Figure 8. scCO₂ saturation distribution across the core sample during 1 PV flooding

Table 4. Mass production rate and BT values for cases

Case	Base Case	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 9	Case 10	Case 11
BT (PV)	0.268	0.272	0.276	0.264	0.264	0.279	0.364	0.448	NA	NA	NA
$\dot{m}_{\text{CO}_2}$ @ BT (g/min)	1.01×10^{-5}	5.04×10^{-6}	6.61×10^{-7}	2.16×10^{-6}	1.05×10^{-8}	1.17×10^{-15}	1.40×10^{-14}	3.59×10^{-14}	NA	NA	NA
$\dot{m}_{\text{CO}_2}$ @ 1 PV (g/min)	0.095	0.141	0.139	0.127	0.142	0.129	0.098	0.066	NA	NA	NA

for the 30%–50% cases. Beyond this point, the dual mechanism emerges: thermodynamic thickening reduces scCO₂ mobility, while hydrodynamic stabilization unifies the gas front, producing the characteristic declining final mass rates and increasingly piston-like displacement observed at higher slug fractions.

The influence of hydrodynamic stabilization is also reflected in the final CO₂ mass production rates, which decrease consistently with increasing MeOH proportion, dropping from 0.129 g/min (30% PV) to 0.098 g/min (40% PV) and 0.066 g/min (50% PV). Although the buffer delays BT, it simultaneously reduces the volume of pore space immediately accessible to free CO₂, as a larger portion of the core is occupied by the MeOH-rich zone. Combined with the suppression of channeling, this leads to lower gas saturation at the outlet within 1 PV, thereby reducing $k_{r\text{CO}_2}$ in accordance with Eq. (4). Consequently, despite the enhanced sweep efficiency, the reduction in the effective gas mobility leads to a more rapid decline in the mass production rate as slug size increases.

Collectively, the 30%–50% PV range constitutes the first regime in which MeOH exerts a dominant hydrodynamic role. In this range, the increased hydrogen-bonding density drives the viscosity and M toward a stable sweep, and the displacement front is effectively stabilized, resulting in delayed BT at the outlet. This region marks the transition from a fingering-controlled displacement to a buffered, mobility-regulated front, which becomes increasingly piston-like as the MeOH fraction increases.

The trends observed in the moderate-slug regime (30%–50% PV) continue and become fully pronounced, as the MeOH fraction increases into the 70%–90% PV range. All cases exceeding 50% PV MeOH exhibited no CO₂ BT within 1 PV of injection, signaling a complete transformation in the displacement regime. At this point, the MeOH buffer was sufficiently large to fully suppress the formation and propagation of CO₂ fingers, forcing the displacing phase to advance through a single, unified, piston-like front. This complete elimination of BT is the clearest indicator that hydrodynamic stabilization has overtaken IFT reduction, which typically amplifies fingering and now dominates sweep behavior^{4,5}

Consistently, the CO₂ mass production rates for 70%–90% PV slugs diminished further, approaching zero within 1 PV. This continued decline originates from the same dual mechanism observed at 30%–50% PV, but amplified by the much larger buffer volume: (1) most of the core pore space was occupied by the MeOH-rich zone, leaving minimal volume available for free CO₂ to mobilize to the outlet, and (2) the strong suppression of channeling markedly reduced S_{CO_2} , lowering k_{CO_2} in accordance with Eq. (5). Even though the front advanced more uniformly, the MeOH barrier blocked scCO₂ from reaching the outlet within 1 PV, causing the mass rate to collapse toward zero.

Overall, the 50%–90% MeOH regime represents the fully developed buffered-displacement state: the CO₂ front became entirely stabilized, BT was eliminated, channeling was fully suppressed, and outlet gas mobility dropped to negligible values. This marks the ultimate stage of MeOH-driven mobility control, where thermodynamic thickening of the gas phase and hydrodynamic front stabilization combine to produce a near-perfect piston-like sweep.

3.3.2. Oil recovery factor. The impact of MeOH on oil RF can be interpreted alongside the front-stability framework by examining Figure 9 and Table 5. All RF curves were identical up to 100% scCO₂ BT, where differences initially emerged through modifications in solubility, followed by changes in the local mobility regime and sweep efficiency once the cumulative mixing and compositional changes reached a threshold.

For the low-slug cases (1%, 5%, and 10% MeOH), BT, PV and RF at BT remained nearly unchanged (~40%) relative to the 100% CO₂ base case, confirming that these small slugs did not yet stabilize the front hydrodynamically. However, the final RF values at 1 PV were consistently higher than those of the base case. The base scCO₂ flood recovered by approximately 73.5%, whereas the 1%–10% MeOH floods yielded increasing RF values from 78.1% to 81.4%. This recovery increase occurred because MeOH mixed with CO₂ and enhanced miscibility throughout the core by strengthening the molecular attraction between the injection fluid and the oil, thereby increasing the solvency of the CO₂–MeOH phase and enabling extraction of additional oil after BT, even though the front geometry remained fingering-dominated.

At 20% MeOH, the behavior began to transition. BT PV remained close to the earlier cases; however, the RF curve in Figure 9 departed earlier from the base case after BT and climbed more steeply, reaching 88% recovery. At this stage, MeOH both

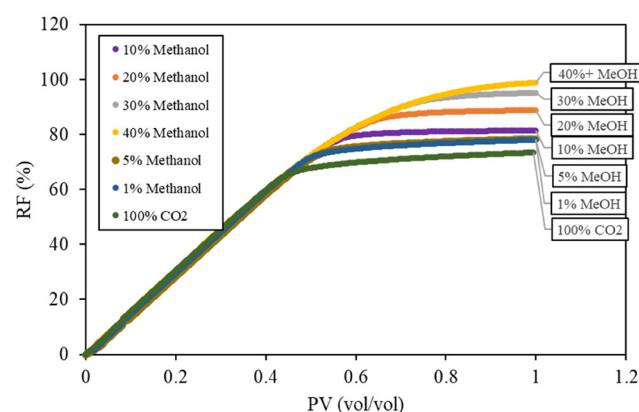
**Figure 9.** Oil RF curves for MeOH slugs at 1 PV

Table 5. Oil RF values for all simulated MeOH slug cases

Case	Base Case	1% MeOH	5% MeOH	10% MeOH	20% MeOH	30% MeOH	40% MeOH	50% MeOH	70% MeOH	80% MeOH	90% MeOH
%RF@ BT (%)	40.0263	40.7478	41.3138	39.6178	39.6699	41.9805	54.3789	65.9451	NA	NA	NA
%RF@ 1 PV (%)	73.4826	78.1448	78.4799	81.4392	88.8100	95.1744	98.9100	98.9762	98.9762	98.9762	98.9762

enhanced miscibility and increased molecular association within the mixture¹³. The longer buffer slightly reduced the effective M and encouraged scCO₂ to flow through more continuous, better-connected pathways, increasing the post-BT recovery slope.

For intermediate slugs (30%, 40%, and 50% MeOH), the hydrodynamic contribution became much more evident. In addition to the shift of BT to a higher PV, the RF curves diverged into increasingly steeper recovery profiles after BT. The longer MeOH buffers maintained separation between the oil-MeOH and scCO₂-MeOH regions for longer, enhancing the properties of scCO₂ discussed above and increasing the contact period of the thicker MeOH layer with oil, further suppressing fingering¹⁶. Final RF rose markedly into the mid-90% range, with the 50% slug reaching approximately 98.9%. In this regime, MeOH acted through a clear dual mechanism: enhancing miscibility while simultaneously stabilizing the front hydrodynamically, improving volumetric sweep and late-time recovery.

For the largest slugs (70%, 80%, and 90% MeOH), the behavior approached a fully stabilized limit. There was effectively no scCO₂ BT within 1 PV, and the RF curves approached a plateau close to the maximum RF (~99%). The MeOH zone was now sufficiently long to enforce a nearly piston-like advance while achieving maximum miscibility enhancement.

3.3.3. Interpreting MeOH-scCO₂ front behavior through kinematic theory. To verify the proposed evolution of flow behavior across the MeOH-CO₂ injection scenarios, the results were examined through the theoretical framework established by Bischofberger *et al.*⁴ They performed controlled miscible displacements in a Hele-Shaw geometry, injecting a low-viscosity fluid into a higher viscosity one under conditions of vanishing interfacial tension. By systematically varying the viscosity ratio while maintaining IFT near zero, they directly visualized the evolution of finger morphologies—from highly ramified, rapidly branching structures at unfavorable M, to slowed, uniform, non-branching behavior characteristic of proportionate growth as M approached unity.

Their findings demonstrated that miscible viscous fingering evolves through three distinct regimes: (1) a fingering-dominated regime, (2) a proportionate growth transition regime, and (3) a fully stabilized regime, in which the interface advances as a coherent front. The initial stage is governed by the characteristic wavelength (λ) of the most unstable mode—the physical spacing between the adjacent advancing fingers—until the M value reaches a threshold that allows the front to begin stabilizing. This description mirrors the transition observed when MeOH sufficiently altered scCO₂ viscosity to initiate the hydrodynamic effect.

According to classical Saffman-Taylor theory, λ decreases as M becomes increasingly unfavorable, and in the limit of vanishing

IFT, the dispersion relationship predicts:

$$\lambda \propto \sqrt{\frac{\sigma}{\mu_o - \mu_{CO_2}}} \quad (6)$$

where σ denotes the IFT, μ_o and μ_{CO_2} denote the viscosities of oil and scCO₂, respectively. This suggests a continued reduction in λ value when a low-viscosity fluid invades a higher viscosity one ($\mu_{CO_2} \ll \mu_o$) under miscible conditions, deteriorating displacement stability as the system produces increasingly finer and more branching fingers. This behavior is consistent with the base case scCO₂ flood and the small MeOH slugs (1%–10%), where thin channels dominate owing to increased miscibility and thus reduced IFT, while a favorable mobility contrast has not yet been achieved. This explains the occurrence of slightly earlier BT (0.2641 PV at 20% MeOH < 0.2679 PV for the base case, Table 4) and the exponential growth characteristics of the mass rate curves.

Bischofberger *et al.*⁴ further demonstrated that IFT suppression alone does not determine stability. Even at IFT approaching zero, miscible flows underwent a sharp transition once the viscosity ratio μ_{CO_2}/μ_o fell within the range 0.69–1.0. In this range, the displacement entered proportionate growth: a mode in which fingers thickened, ceased branching, and advanced at comparable velocities, so that channels no longer multiply but instead grew uniformly. This theoretical shift explains the behavior observed once MeOH reached ~0.2 PV, as the viscosity of the scCO₂-rich phase increased sufficiently to shift M toward the proportionate growth domain. As a result, the reduction in the $(\mu_o - \mu_{CO_2})$ term began to dominate over the IFT contribution to λ , signaling the onset of increased spacing between adjacent fingers and hence more consolidated channel flow. In parallel, the final scCO₂ mass rate rebounded to 0.142 g/min, reinforcing the onset of channel thickening and increased connectivity—precisely the behavior predicted by the Bischofberger *et al.* framework at the onset of proportionate growth.

When MeOH reached 30%–50% PV, M improvement became dominant, and the system entered the proportionate growth transition regime. scCO₂ channels consolidated into fewer, wider structures, delaying BT substantially and producing the smoother, less branched mass rate trends characteristic of proportionate growth.

Finally, at 70%–90% MeOH, the system entered the fully stabilized regime: λ became large, fingers merged into a single coherent structure, and the displacement approached piston-like behavior. The simulation results—no BT, negligible scCO₂ mass at 1 PV, and nearly uniform oil sweep (~99% RF)—mirror the theoretical kinematic predictions with striking fidelity.

This study thus verified the transitions and microscopic physical mechanisms underlying the macroscopic behavior observed

in the simulations: the system progressed from Saffman–Taylor-dominated fingering to piston-like flooding, adhering to the kinematic theory framework.

4. CONCLUSIONS

This study quantified how MeOH–CO₂ slug sizing governs displacement stability, scCO₂ mobility, and ultimate RF in vertical miscible core flooding. The results showed a clear progression from fingering-dominated flow to a fully stabilized piston-like advance as the MeOH fraction increased. The effect of MeOH addition on increasing scCO₂ density, viscosity, and miscibility with oil aligns with the expected increase in IMFs, while the behavioral transition in front geometry can be accurately described through the Saffman–Taylor kinematic framework. The following key conclusions were drawn.

- For low MeOH slugs (1%–20% PV), BT remained unchanged (0.264–0.276 PV vs. 0.268 PV base case), confirming the absence of hydrodynamic stabilization. The scCO₂ mass rate at 1 PV increased slightly (0.127–0.142 g/min vs. 0.095 g/min) owing to reduced IFT and subsequently enhanced k_{rCO_2} rather than a change in flow geometry. RF improved only marginally (73%–78%), indicating that miscibility increased but sweep efficiency did not.
- The 30%–50% PV range marked the onset of hydrodynamic influence: BT shifted to 0.28–0.44 PV, reflecting partial suppression of fingering and the formation of thicker, more coherent scCO₂ pathways. The final scCO₂ mass rate decreased considerably (0.129 → 0.098 → 0.066 g/min), reflecting lower outlet gas saturation as sweep improved. RF increased sharply, rising from ~88% at 20% PV to ~98%–99% at 50% PV, demonstrating a transition toward piston-like advance.
- For high MeOH slugs (≥70% PV), no scCO₂ BT occurred within 1 PV, indicating full front stabilization and complete suppression of channeling. The mass production approached zero because most of the PV was occupied by MeOH, leaving minimal free gas near the outlet. RF plateaued at ~99%, confirming that the sweep was essentially complete and that MeOH fractions beyond 50% PV did not contribute meaningful incremental recovery.

Overall, MeOH is an effective mobility control agent whose stabilizing ability scales with injected volume. Low-range slugs influence fluid properties only, mid-range slugs begin reshaping flow geometry, and high-range slugs impose full hydrodynamic control, with ultimate RF corresponding directly to these regime shifts. Laboratory core flooding experiments are recommended to validate the alignment of the simulated trends with scCO₂–MeOH flooding behavior. The assumptions of zero binary interaction coefficients and the neglect of capillary effects in the pores restrict the reliability of upscaling the results, further emphasizing the need for laboratory validation of results. Additionally, hybrid buffering strategies—such as MeOH-assisted WAG—should be explored to mitigate fingering at low MeOH fractions and improve sweep without requiring large solvent volumes. To extend these findings to reservoir-scale applications, the environmental and economic feasibility of MeOH-assisted scCO₂ flooding should be evaluated.

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