

CURRENT TREND AND STUDIES IN **ENGINEERING**



All Sciences Academy

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Editor

Asst. Prof. Dr. Umut ÖZKAYA





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Weirs: Among the Oldest Hydraulic Structures

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ABSTRACT

Weirs are among the oldest hydraulic structures constructed for various purposes, such as flood control, discharge measurement, reduction of channel discharge, lowering of water levels, and regulation of free-surface flows. Weirs can be classified in various ways based on different characteristics. These classifications may be made according to the position of the weir axis relative to the main flow direction, the intended use, the ratio of crest length to upstream head, the weir geometry, the plan geometry, and the flow conditions over the weir. Weirs classified according to these different characteristics significantly influence the hydraulic behavior of the flow and give rise to distinct flow characteristics. Consequently, variations in weir geometry and flow conditions can increase the complexity of the hydraulic problems under study and necessitate different solution approaches for each weir type. Various methods are employed in the design of these structures and the determination of discharge coefficients. Among these, open-channel experiments and computational fluid dynamics software are frequently preferred methods. The objective of studies employing these methods is to understand the behavior of the flow passing over weirs and to determine discharge coefficients for discharge calculation. In these studies, the parameters investigated regarding their effects on discharge capacity are weir geometry, main channel flow conditions, Froude number, weir height and length, inlet geometry, channel geometry, and downstream conditions.

Keywords – computational fluid dynamics, hydraulic structures, open channel experiments, water resources, weirs

INTRODUCTION

Water, an indispensable substance for humanity, has played a pivotal role in the development of civilizations from ancient times to the present day. Throughout history, many civilizations were established near water basins and flourished on lands enlivened by water; proximity to these basins significantly influenced the historical significance of these civilizations. Human beings have an enduring need for water. It is utilized for a multitude of purposes, such as drinking, irrigation, energy production, and industrial processes, making it impossible to conceive of life on Earth without it. Despite its vital importance, however, water resources which are finite to begin with are dwindling due to inefficient use. Consequently, it is essential to determine and protect the quantity and quality of water resources within a comprehensive planning framework (Yüksel, 2023:1; Öbek, 2024:1).

Various scientific disciplines are actively working to prevent the depletion of water resources, enhance their utilization efficiency, and ensure that usage meets needs in an optimal manner. One such discipline is hydraulics, a sub-field of civil engineering. This field encompasses the design and construction of hydraulic structures such as dams, weirs, hydroelectric power plants, and weirs.

This section focuses on weirs, one of the significant hydraulic structures mentioned above. Weirs are among the oldest hydraulic structures built for purposes such as flood control, discharge measurement, reducing channel discharge, lowering water levels, or regulating free-surface flows. These structures are classified according to various characteristics. Hydraulic behavior varies across different types, a factor that must be carefully considered during the design process; indeed, weirs can be classified in various ways based on different criteria. First, weirs can be classified based on the orientation of the weirs axis relative to the direction of the main flow: frontal-intake weirs and side-intake weirs (Ulucan, 2017:1). A weir is termed a frontal-intake weirs when positioned approximately perpendicular to the flow direction, and a side-intake weir when placed parallel to the flow direction. Regarding their intended use, weirs employed particularly at dams and reservoirs to safely convey excess water downstream are referred to as overflow spillways. Weirs can also be classified based on the ratio of the crest length to the upstream head (H_0/L_w). According to this classification, weirs with a ratio in the 0–0.1 range are classified as long-crested; those in the 0.1–0.4 range as broad-crested; those in the 0.4–1.5 range as short-crested; and those exceeding 1.5 as sharp-crested (Hargreaves et al., 2014: 136; Jiang et al., 2018:1; Imanian et al., 2021:1). Furthermore, weirs can be classified according to their plan geometry. In this context, in addition to weirs with linear geometry, there are labyrinth weirs developed to achieve a greater crest length within the same width and piano-key weirs, which represent an advanced geometric form of labyrinth weirs. Weirs may also be classified based on flow conditions as free-flow or submerged-flow weirs. These various classifications demonstrate the influence of weirs geometry and layout on the hydraulic characteristics of the flow passing over the weir.

As previously mentioned, weirs with finite crest lengths can be divided into four main groups. Broad-crested weirs, which are frequently the subject of studies in the literature, stand out in this context. As previously

mentioned, the H_0/L_w ratio for broad-crested weirs ranges from 0.1 to 0.4. In their research on this type of weir, Hager and Schwalt (1994: 24) stated that it could serve as a discharge measurement structure, provided it has a standard shape. However, they also established requirements specifying a minimum width of 0.30 m or greater and a minimum weir body height of 0.15 m, with vertical upstream and downstream faces (Öbek, 2024: 4).

Side weirs are hydraulic structures constructed in various forms such as rectangular, triangular, trapezoidal, labyrinth, circular, or piano-key shapes designed to discharge excess water via side channels to prevent flooding within the main channels. They may also be constructed to divert a specific portion of the channel flow elsewhere or to regulate water levels and discharges. To fulfill these functions, they are positioned either parallel to the main channel or at specific angles to it. Side weirs have a wide range of applications, including irrigation, flood control, sanitation, and various other water resource and environmental projects (Kartal, 2022:24).

Solutions vary depending on the specific hydraulic characteristics of the weirs. Consequently, the literature contains numerous studies focused on understanding the behavior of flow over weirs, determining discharge coefficients to calculate discharges, and optimizing weir designs. Key factors influencing weir performance include weir length, the water level above the crest, and most notably the discharge coefficient, which varies according to the weir's shape. Many researchers have conducted studies on various weir geometries to enhance performance. Overall, research in this field tends to focus on the effects of weir geometry, main channel flow conditions, Froude number, weir height and length, inlet geometry, channel geometry, and downstream conditions on discharge capacity.

Hydraulic Solution Methods for Weir Problem

The flow characteristics of weirs are significantly influenced by these classifications. The hydraulic behavior of these structures varies depending on the classification, and the complexity of solving the associated problems increases accordingly. Consequently, various methods are employed to address these problems. These methods include open-channel experiments, numerical methods, analytical and semi-analytical approaches, regression models, and artificial neural networks. Among the methods mentioned,

open-channel experiments and numerical methods are described in detail in this study.

Open Channel Experiments

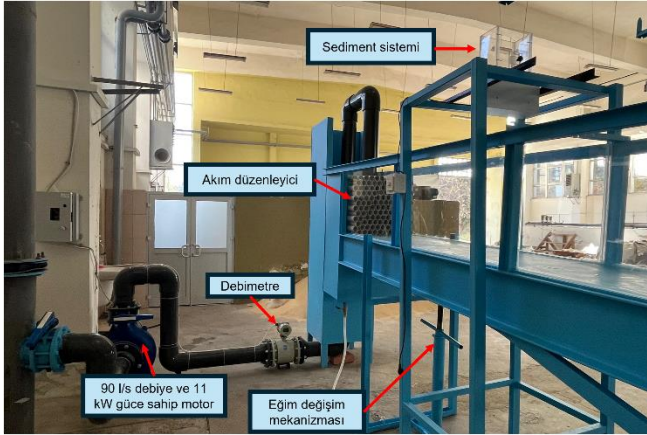
Open-channel experiments are extensively conducted to analyze complex flow conditions and accurately characterize flow properties in weir-related problems. Experimental studies carried out in open-channel systems under varying geometric and hydraulic conditions are crucial for weir design and the reliable estimation of discharge capacity. Figure 1 illustrates an example of a broad-crested weir experiment conducted in an open-channel test setup. This experiment was performed in an open-channel system at the Karadeniz Technical University Hydraulics Laboratory; images of this channel are presented in Figure 2. In these experiments, the dimensions of the open-channel system are critical, as they are directly related to scaling effects. Scaling is a powerful tool in the design of physical models and can be used to ensure that analysis results are like those of a prototype (Zhou et al., 2020:1508; Yuan et al., 2019:5766). The Froude number is widely used to characterize dynamic similarity in hydraulics (Heller, 2011:295). Depending on the specific problem, a length scale is first determined, which subsequently dictates the scales for discharge, time, and velocity. Slope is another key factor influencing the solution; therefore, the channel slope must be adjusted to match the slope of the basin being modeled. Measurement systems constitute a vital component of these experiments. Various types of flow meters are used to measure and control the discharge supplied to the channel, with electromagnetic flow meters being the most preferred option. Water depth is another parameter continuously monitored during experiments, with ultrasonic depth gauges frequently chosen for this purpose. Velocity measurement devices can be quite expensive; although acoustic doppler devices are among the preferred options for velocity measurement, their high cost may sometimes preclude their use. Micro-propeller current meters are used as an alternative in experimental setups. Additionally, measuring velocity using a Pitot tube remains one of the traditional methods. The accuracy and precision of the instruments used are the most critical factors regarding measurement.



Figure 1. An image from an experiment with broad-crested weir



(a)



(b)

Figure 2. Open channel experiment system in Karadeniz Technical University Hydraulic Laboratory (a) general view (Günay et al., 2026:1), (b) significant sections of channel in the upstream side

Computational Fluid Dynamics Software

In addition to open-channel experiments, commercial computational fluid dynamics (CFD) software is frequently used to solve hydraulic problems, thanks to advancing technology. Although various commercial software packages may be employed, the standard strategy involves first

validating the numerical model against experimental data; consequently, many studies rely on experimental results for this purpose. Determining the appropriate solution model is the initial step in numerical analysis. While different software packages may use varying terminology for solution options, the fundamental process involves dividing the established model into finite volumes using a defined mesh and solving the equations for mass, energy, and momentum within each volume. This section focuses on ANSYS Fluent, a prominent CFD software application. The solution process begins by launching Fluent from the suite of programs available within the Workbench interface. Initially, the model is constructed using DesignModeler, SpaceClaim, or Discovery, with all boundaries being named during this stage (Sayıl et al., 2025:6). Subsequently, the meshing phase begins; the software offers various methods for generating the mesh system, with the objective of optimizing mesh quality. To achieve this, mesh sensitivity analyses are conducted, typically involving the creation of at least three different mesh levels to select the optimal system, thereby ensuring the results are independent of the specific mesh structure used. Following this, the setup phase commences; this is the stage where solution methods are selected, boundary conditions are defined, and the solution process is initiated. Here, the solver can be configured as pressure-based or density-based, the velocity formulation (absolute or relative) is determined, and the magnitude and direction of gravitational acceleration are specified. Next, the physical model is selected, followed by the choice of the turbulence model, a critical component in many such studies (Günay et al., 2026:2). In CFD studies concerning weir problems, significant effort has been directed toward selecting an appropriate turbulence model. Once the materials and boundary conditions for the model have been defined, the solution process can begin. The choice of time step is a critical factor here; an excessively large time step should be avoided, as it can lead to erroneous results and significantly increase the Courant number. After these parameters are established, the solution is executed. Figure 3 shows the modelling of a weir and its mesh system. Figure 4 displays an image from an analysis performed using Fluent, showing the water surface profile of the flow over the spillway.

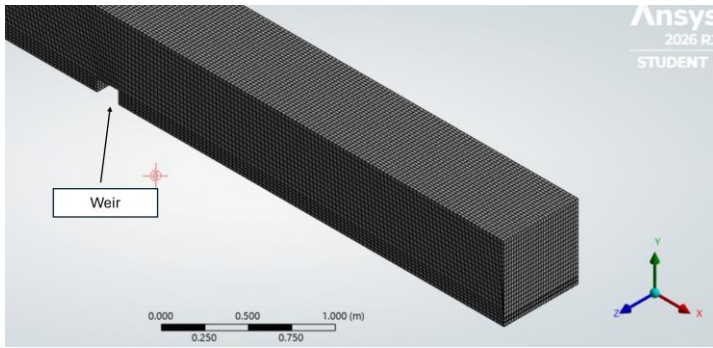


Figure 3. Modelling of a weir and structured mesh system in ANSYS Fluent

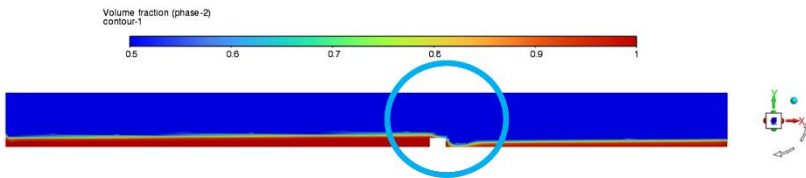


Figure 4. A results image from ANSYS Fluent analysis

Literature Review

There are numerous studies in the literature concerning weirs. As mentioned above, there are many different types of weirs, which means different hydraulic behaviors that need to be considered during the design phase. This is because these different types significantly alter the characteristics of the flow. Consequently, many experimental, theoretical, and numerical studies have been conducted to investigate parameters such as discharge capacity, the discharge coefficient, the resulting water surface profile, and flow characteristics.

Aghayari et al. (2009:246) conducted experiments on rectangular side weirs under subcritical flow conditions and proposed a mathematical model to estimate the discharge coefficient. Emiroğlu et al. (2010:37) investigated the effect of labyrinth geometry on discharge capacity through experiments on triangular labyrinth-type side weirs. The results indicated that the discharge coefficient of labyrinth side weirs could be higher than that of conventional rectangular side weirs. Bal et al. (2011:33), Şimşek et al. (2011:47), and Soydan et al. (2012:47) examined flow velocity profiles over broad-crested weirs with rectangular, curved, and trapezoidal cross-sections, respectively, using both experimental measurements and CFD analyses. In

these studies, they tested multiple turbulence closure models. Regarding the results, Bal et al. (2011:33) demonstrated that the SST turbulence model yielded more successful results, whereas Şimşek et al. (2011:47) found that the RNG k- ϵ model performed better for curved weirs. On the other hand, Soydan et al. (2012:47) determined that the standard k- ϵ model was more suitable for trapezoidal weirs. Emiroğlu et al. (2011:319) conducted laboratory experiments to determine the discharge capacity of sharp-crested side weirs with rectangular cross-sections. Based on the experimental results, they developed a discharge coefficient equation that accounts for various dimensions of the weir geometry. Haun et al. (2011:397) numerically investigated water flow over a broad-crested weir with a trapezoidal cross-section using CFD. The results obtained in the study were compared with measurements from experiments conducted at various flow rates. Dursun et al. (2012:55) investigated the discharge capacity of semi-elliptical labyrinth-type side weirs and developed an ANFIS model using the obtained data. The model's performance was compared with various regression methods, demonstrating that the ANFIS approach could be utilized to predict the discharge coefficient. Vatankhah (2012:76) developed an analytical approach to determine the water surface profile along a side weir; this approach offered a solution specifically for evaluating side weir flow in triangular channels. Hargreaves et al. (2007:136) compared CFD results regarding free-surface flow over a broad-crested weir with existing experimental data. The results highlighted the success of CFD in calculating free-surface profiles, pressure and velocity distributions, and discharge rates over the weir. Říha and Zachoval (2014:1) experimentally investigated side weirs with varying inclination angles under low Froude number conditions, establishing relationships between the weir inclination angle and the upstream and downstream Froude numbers. Aydin (2016:1) proposed a semi-analytical equation to determine the discharge capacity of rectangular side weirs. Maranzoni et al. (2017:1) investigated the discharge capacity of short-crested side weirs in a channel and identified the Froude number and weir height as significant parameters. Jiang et al., (2018:1) numerically analyzed various turbulence models for trapezoidal broad-crested weirs. The study's results generally demonstrated that an increase in the upstream angle has a negative effect on the discharge coefficient. Wang et al., (2018:83) used Flow-3D to investigate the effects of side weirs with different crest

angles on Froude number distribution, water surface and velocity profiles, and the discharge coefficient. A comparison of the numerically obtained depth results with experimental measurements revealed error rates of less than 5.63%. In their study, Muhsun et al., (2020:1067) experimentally and numerically examined the flow over curved Crump weirs under varying channel slopes and flow conditions; ANSYS Fluent was employed for the CFD analysis. The experimental and numerical results were evaluated using statistical analysis, which revealed no significant difference between the water surface profiles. Daneshfaraz et al. (2021:88) numerically evaluated the impact of openings located at different positions on a trapezoidal broad-crested weir. They compared these numerical results with data obtained from a published experimental study and concluded that the openings in the broad-crested weir increased the discharge coefficient. Imanian et al. (2021:1) investigated the discharge coefficient and separation zones of a rectangular broad-crested weir using both experimental and numerical methods. They determined that, among the turbulence models employed, the $k-\omega$ SST and LRR models yielded the most successful results. Nourani et al. (2021:1) examined the hydraulic characteristics of flow over broad-crested weirs using ANSYS Fluent and validated their findings against experimental data. The results revealed that adding upstream and downstream ramps to the weirs, as well as sloping the crest surface, improved water flow performance compared to standard horizontal-crested weirs. Furthermore, the study demonstrated that a steeper slope at the weir crest resulted in a higher water flow coefficient. Kartal and Emiroğlu (2022:1) experimentally investigated combined side weir-gate systems, in which a side weir and a gate are used together. The results indicated that a higher discharge could be passed through the combined side weir-gate system than through a side weir or a gate used in isolation. In a subsequent study, Kartal and Emiroğlu (2024:1) numerically validated the experimental results obtained from this same type of combined side weir structure. The findings showed that the geometry of the weir and gate significantly influenced the discharge capacity of the combined system. Wang et al. (2024:1), on the other hand, conducted experimental studies on rectangular side weirs of varying widths and heights and demonstrated that the discharge coefficient is influenced by the Froude number and the ratios of weir height and width to flow depth.

RESULTS AND DISCUSSION

This study focuses on spillways, presenting their general definitions, classifications, design methodologies, and a review of the relevant literature. The scope of this study can be outlined as follows:

Weirs are among the oldest hydraulic structures, constructed for various purposes such as flood control, discharge measurement, reduction of channel flow velocity, lowering of water levels, and regulation of free-surface flows.

Weirs can be classified based on the orientation of the weir axis relative to the main flow direction specifically, as frontal-intake or side-intake weirs. Regarding their intended use, weirs designed to safely convey excess water from dams and reservoirs to the downstream area are termed “spillways”. Furthermore, they can be categorized into four classes (long-crested, broad-crested, short-crested, and sharp-crested) based on the ratio of the upstream water head to the crest length.

Numerous studies have been conducted to enhance weir performance. These studies employ open-channel experiments, computational fluid dynamics software, artificial neural networks, and analytical methods.

The parameters examined in these studies regarding their impact on discharge capacity include weir geometry, main channel flow conditions, Froude number, weir height and length, inlet geometry, channel geometry, and downstream conditions.

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Investigation of the Effects of Longitudinal Keel's Heel Part Modification on the Resistance and Sailing Performance of Bodrum Gulets*

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ABSTRACT

Bodrum Gulets are a distinctive class of sailing yachts characterized by their elliptical or rounded stern, pronounced sheer line, concave bow, and longitudinal keel. Originally used for military, cargo, fishing, and sponge diving purposes, they have evolved into modern yachts under the influence of Türkiye's Blue Voyage tourism. Despite this evolution, the design of their longitudinal keels has remained largely unchanged. This study investigates the effects of changing the longitudinal keel's aft part geometry on the resistance and sailing performance of Bodrum Gulets. A Bodrum Gulet with a length overall (L_{OA}) of 33.8 m is selected as the reference model, and three alternative designs—SKG-01, SKG-02 and SKG-03—are developed by changing the geometry of the longitudinal keel's aft part. Total resistance values at speeds between 5 and 12 knots are determined using the Holtrop–Mennen method, while sailing performance is evaluated through Velocity Prediction Program (VPP) analysis. The results show that the proposed keel modifications can reduce total resistance by up to 3.05%. From the sailing performance perspective, the SKG-02 design achieves the highest hull speed, with an increase of 0.12–0.15 knots compared with the reference model under the investigated wind conditions. These findings demonstrate the potential of modest longitudinal keel modifications to improve the performance of Bodrum Gulets.

Keywords – Bodrum Gulet, Yacht Design, Sailing Yacht, Longitudinal Keel, VPP

INTRODUCTION

Achieving an optimal balance between minimizing resistance and maximizing stability for efficient sailing is seen as the key challenge in sailing yacht design (Marchaj, 1982). In this context, achieving low-emission targets requires both an efficient propulsion system and a hull form optimized for minimal hydrodynamic resistance (Seo et al., 2012). For sailing yachts, keel design is a critical aspect of hull form optimization and overall yacht design. In this context, identifying the appropriate keel type and optimizing its geometric parameters are essential for improving hull form characteristics and reducing resistance.

With distinctive characteristics of round stern form (Gür, 2020; Köyağasıoğlu, 2014; Kükner, 2007; B. İ. Turan, 2021) and violin-shaped fore form (Köyağasıoğlu, 2014; Kükner, 2009; B. İ. Turan & Özcan, 2018), Bodrum Gulets are listed among specific figures of maritime heritage. In addition to their broad hull forms and spacious interiors, Bodrum Gulets are renowned for their satisfactory sailing performance and seaworthiness (Gammon et al., 2005). Although gulet has historically been used to refer to schooner-type sailing vessels (Fossati & Diana, 2004; Kademoğlu, 2000;

Köyağasioğlu, 2014) and their Mediterranean adaptations (Özen, 2017), the term has increasingly been used to describe a distinctive hull form that can be combined with different rigging configurations (B. İ. Turan, 2023a; B. İ. Turan & Akman, 2021, 2025; B. İ. Turan & Özcan, 2018). Generally, these yachts feature a longitudinal keel with an inclination angle ranging from 2° to 3° (Kükner et al., 2009). Figure 1 illustrates the general arrangement plan and the profile view of a Bodrum Gulet.

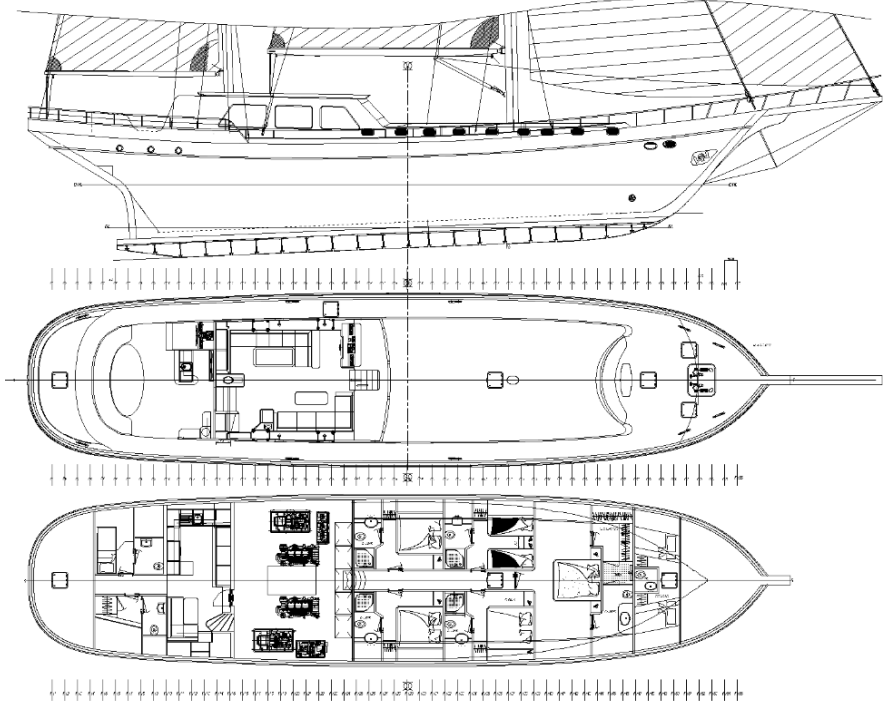


Figure 1. General arrangement plan and the profile view of a Bodrum Gulet

Various studies have investigated the effects of keel geometry and configuration through experimental and numerical approaches to improve hydrodynamic efficiency under various operational conditions. These studies encompass a wide range of methods and applications demonstrating the impact of keel modifications on drag reduction, maneuverability, and overall sailing performance. Helvacioğlu et al. (2018) analyzed how different keel types influence a sailing yacht's resistance, motion and acceleration. Hao et al. (2025) investigated the hydrodynamic performance of unmanned sailboats by structurally optimizing the keel and rudder configurations, using CFD analysis and MAXSURF simulations. The optimized h-type keel achieved a 32% reduction in resistance at 5 knots and significantly improved initial stability, thereby enhancing overall maneuverability and energy efficiency. Sfakianaki et al. (2013) experimentally evaluate the effect of a keel bulb on a $\frac{1}{4}$ scale model of a 50-ft sailing yacht in calm water, focusing on drag, side force, trim, and wave formation for various speeds and leeway angles. Results

indicate that in leeway angles of 3.5° to 7° , the keel bulb significantly improved side force and reduced drag, with observable benefits also in wave pattern formation at higher speeds. Castegnaro et al. (2021) propose an engineering method based on a Velocity Prediction Program (VPP) and XFLR5 simulations to optimize daggerboard and rudder planforms for small racing yachts. Applied to a 4.6 m skiff, the method revealed that increasing daggerboard draft from 0.9 to 1.3 m reduced racing time by 21.5 seconds, with an optimum aspect ratio shift enhancing both upwind and downwind performance.

Scientific research on gulets can be traced back to the 1960s, with Nutku and Küçük (1963) conducting one of the earliest systematic technical investigations through model-scale resistance tests. A 1/8-scale model of a gulet was tested under different loading conditions at speeds ranging from 10 to 20 m/s and following the initial tests, the hull form was modified by extending the waterlines toward the stern, which led to a 44.5% reduction in resistance compared with the original configuration. Kükner et al. (2009) conducted a TÜBİTAK-supported study on Turkish-type gulets, commonly known as Bodrum Gulets, to characterize their principal hull form features and investigate their hydrodynamic performance. The study incorporated model-scale experiments and hull form optimization analyses, providing a systematic assessment of the design and performance characteristics of this distinctive vessel type. In another study (Gammon et al., 2005), hydrostatic and hydrodynamic characteristics of Turkish-type gulets were investigated and optimization studies were conducted using a multi-objective genetic algorithm. Kükner and Kınacı proposed A method based on artificial neural networks to estimate the form factor of Turkish-type Bodrum Gulets was developed by Kükner and Kınacı (2009). In another study (Kınacı, 2009), a software tool using the 1- C_p method was developed for serial hull form generation. In the study of Turan and Akman (2021) the effects of two different stern form on Bodrum Gulets were investigated In terms of hydrostatic parameters and resistance values for cruising speed. Turan et al. (2021), compared the hull forms of Bodrum Gulets with Tirhandil type boats from design, hydrostatic and resistance-based perspectives. In another research, (B. İ. Turan, 2021) gulets used for fishing purposes with Bodrum Gulets used for marine tourism were compared to investigate the influence of intended use on hull form design. Turan and Özcan (2023), Bodrum Gulets developed a usage intensity map based on operational activity on board during Blue Voyage. Turan (2023a) analyzed the impact of ketch and schooner rig types on the sailing performance of Bodrum Gulets using Velocity Prediction Program (VPP) and proposed a design framework. Additionally, Turan (2023b) examined the effect of engine number in Bodrum Gulets from the engineering and layout implications' perspectives. More recently, Turan and Akman (2025) investigated the effect of longitudinal keel angel on sailing performance of Bodrum Gulets. In another study, (B. İ. Turan et al., 2026),

two-loop generative design process was applied to generate various longitudinal keel alternatives and selected alternatives' hydrodynamic characteristics were compared using CFD. While previous research has predominantly focused on hydromechanical analyses, hull form optimization, and design frameworks, no study has yet examined the impact of potential modifications to the longitudinal keel—a critical component of the underwater profile—on sailing performance. This study aims to explore how the geometry of the heel part, which is located in the aft part of the longitudinal keel, affects the resistance and sailing performance characteristics of Bodrum Gulets.

METHODOLOGY

A Bodrum Gulet with an overall length (L_{OA}) of 33.85 m, a breadth (B) of 7.80 m is selected as the reference model (Figure 2). The keel angle of the reference model is 2.53° . The hull model is created using the lines plan of the Bodrum Gulet in Rhino software (2020).

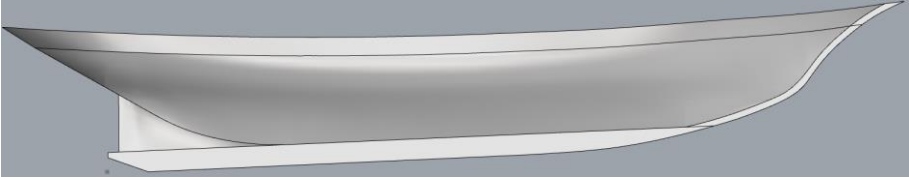


Figure 2. Reference model

Three alternative designs with different geometries in the heel region of the longitudinal keel of the reference Bodrum Gulet were developed to investigate their effects on the hydrostatic, hydrodynamic, and sailing performance characteristics of the vessel. In the first design, designated SKG-01 (Figure 3), the additional section extending aft of the sternpost, which was retained as a support for the rudder stock, was removed. In the design alternative designated SKG-02 (Figure 4), the corners of the model developed for SKG-01 were removed to provide the aft region of the longitudinal keel with a more organic geometry. In the third design alternative developed for the heel region of the keel, designated SKG-03 (Figure 5), the protrusion similar to that of the reference model was retained; instead, the corners of this region were rounded to obtain a more organic geometry. To enable a consistent comparison of the alternative designs, the portion of the vessel above the waterline is intended to remain unchanged from the reference design. In addition, maintaining a constant vessel displacement is defined as another design constraint. Accordingly, for all alternative models, the differences between the waterline length (L_{WL}), waterline breadth (B_{WL}), and displacement (Δ) and the corresponding values of the reference model are constrained to less than 1%.

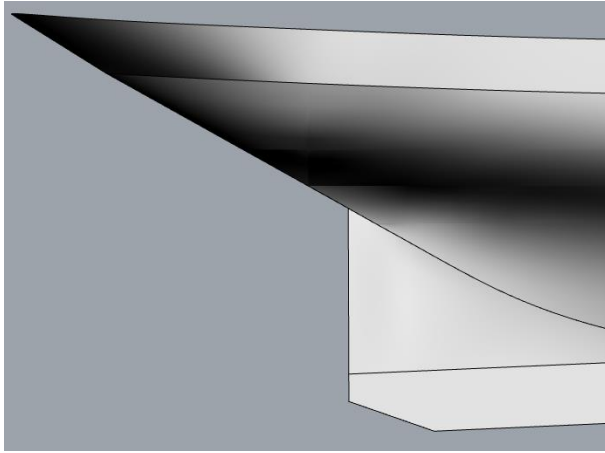


Figure 3. SKG-01

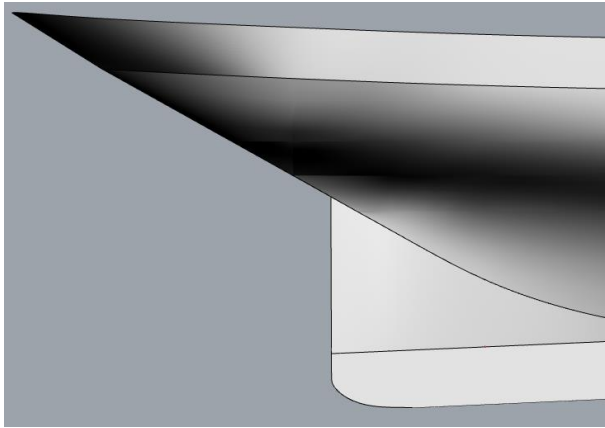


Figure 4. SKG-02

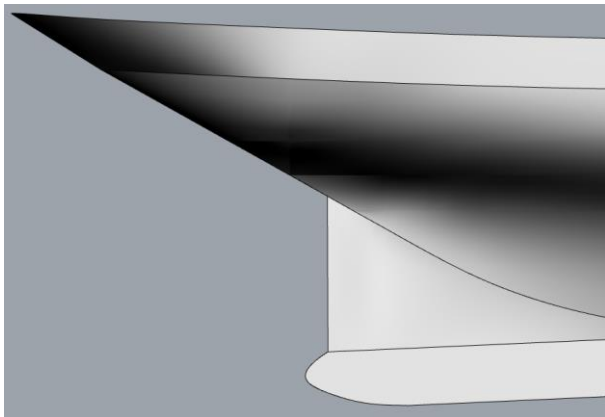


Figure 5. SKG-03

The Holtrop–Mennen method is initially employed for the resistance prediction process. Based on regression analyses of experimental data obtained from model tests conducted at different scales, the Holtrop–Mennen method provides an effective approach for predicting the resistance of displacement-type hulls (Birk, 2019; A. E. Turan, 2009). In the study conducted by A. E. Turan (2009), the Holtrop–Mennen method was reported to provide the closest agreement with the experimental model-test results for a gulet hull form. Furthermore, this method has previously been employed to predict the resistance and power characteristics of Bodrum Gulets (Akman & Turan, 2023; B. İ. Turan et al., 2021; B. İ. Turan & Akman, 2021). Accordingly, the Holtrop–Mennen method was selected in the present study for the resistance prediction of Bodrum Gulet hulls. In Holtrop–Mennen method (Elkafas et al., 2019; Holtrop & Mennen, 1982), The total resistance of a vessel, (R_T), is obtained as the sum of the viscous resistance component, (R_V), and the wave resistance component, (R_W). The viscous resistance is calculated using the following equation:

$$R_V = (1 + k)R_F \quad (1)$$

Where R_F represents frictional resistance. Form factor; k can be calculated as the function of parameters below (Elkafas et al., 2019):

$$k = f\left(\frac{B}{L}, \frac{T}{L}, \frac{L}{L_R}, \frac{L^3}{\nabla}, C_P, c\right) \quad (2)$$

Here, L_R denotes the run length calculated using a statistically derived formulation, whereas c represents a coefficient based on the stern form coefficient, which varies depending on the hull form type. The wave resistance; R_W is calculated as:

$$R_W = c_1 c_2 c_3 \nabla \rho g e^{(m_1 F_n^d + m_2 \cos(\lambda F_n^{-2}))} \quad (3)$$

Here, c_1, c_2, c_3, m_1, m_2 ve λ represent coefficients related to the hull form of the vessel (Holtrop & Mennen, 1982).

In the sail performance evaluation process, VPP Module of Maxurf™ (2023) software is employed. Velocity Prediction Programs (VPPs) are widely used tools for predicting the performance of sailing yachts (Levin & Larsson, 2017). The Kerwin Model, introduced by J. E. Kerwin in 1978, is widely recognized as the first Velocity Prediction Program (VPP) developed specifically for sailing yachts (Böhm, 2014). VPPs are computational tools used to predict sailing performance by integrating the geometric characteristics of a vessel with the prevailing environmental conditions. The VPP employs an iterative procedure to determine the maximum boat speed at which the resistance is balanced by the component of the aerodynamic force parallel to the sailing direction, the hydrodynamic side force is balanced by the component of the aerodynamic force perpendicular to the sailing direction, and the hydromechanical righting moment is balanced by the aerodynamic

heeling moment (Cairoli, 2002). The output of a VPP is commonly presented in the form of polar performance diagrams, which enable the assessment of the optimal boat speed under different sailing conditions (Zannotti, 2020). Figure 6 illustrates the parameters used in the VPP analysis with their corresponding values for sailing performance analysis process of the research as well as the modelled version of the reference model with sail and rigging.

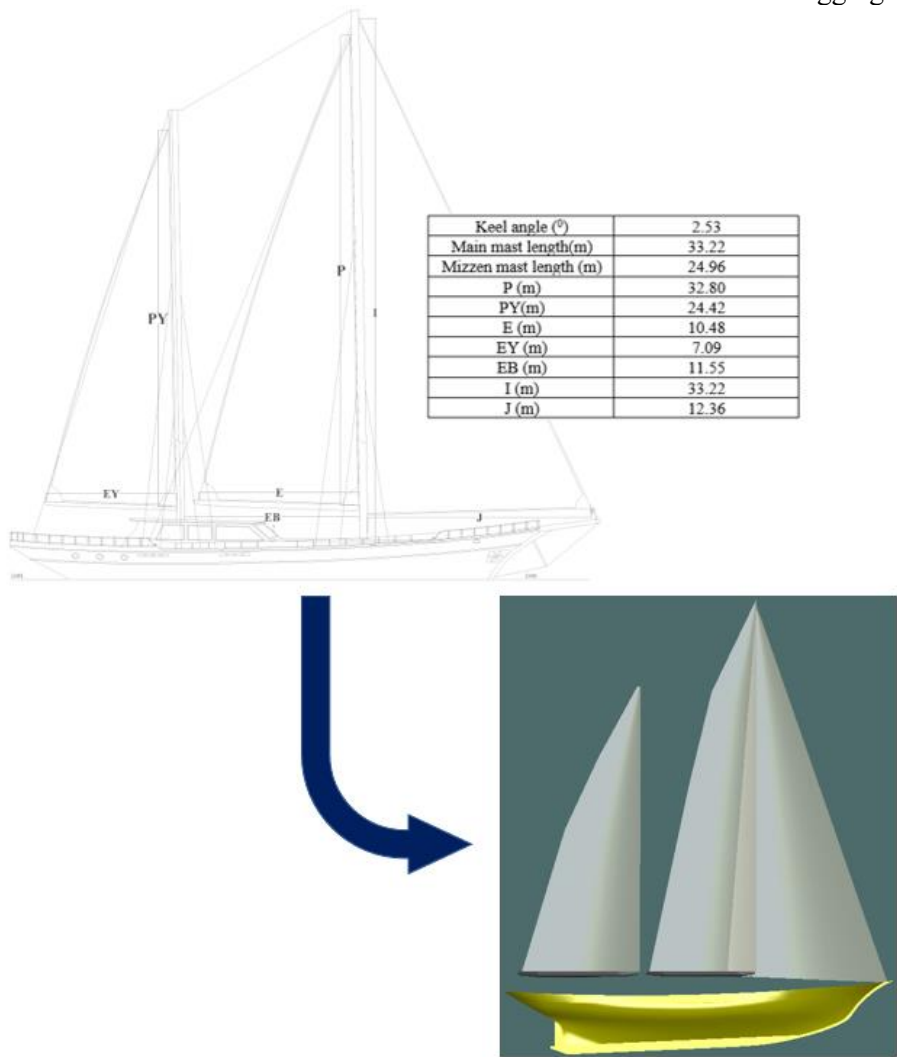


Figure 6. Reference model with sail and rigging

RESULTS AND DISCUSSION

Hydrostatics of the hull forms

The hydrostatic values of the modified Bodrum Gulet hulls are presented in Table 1. As expected, there is no remarkable changes occur between the reference model and the alternative designs.

Table 1. Hydrostatic values of the reference model and the created designs

Parameters	Reference Model	Alternative Models		
		SKG-01	SKG-01	SKG-01
Δ (ton)	124.7	124.600	124.900	124.700
Displ. volume (m³)	121.63	121.598	121.815	121.646
T (m)	3.240	3.247	3.247	3.247
LWL	26.36	26.367	26.367	26.367
B_{WL}	6.930	6.930	6.930	6.930
WSA (m²)	205.44	205.005	205.287	205.047
A_M (m²)	7.199	7.199	7.199	7.199
Waterplane. area (m²)	132.65	132.658	132.658	132.658
C_P	0.562	0.562	0.563	0.562
C_B	0.205	0.205	0.205	0.205
C_M	0.365	0.365	0.365	0.365
C_{WP}	0.726	0.726	0.726	0.726
LCB (m)	11.97	11.979	11.961	11.975
LCF (m)	12.17	12.173	12.173	12.173
LCB (% L_{WL})	45.41	45.431	45.362	45.415
LCF (% L_{WL})	46.16	46.168	46.168	46.168
Immersion (TPc)	1.360	1.360	1.360	1.360

Resistance calculations

According to the resistance calculations performed using the Holtrop–Mennen method over the speed range of 5–12 knots, reducing the frontal area of the longitudinal keel of the Bodrum Gulet hull results in a reduction in resistance. Examination of the resistance values of the three alternative designs (SKG-01, SKG-02 and SKG-03) shows that all three alternatives exhibit lower resistance than the reference model, while the differences in resistance among the alternatives become particularly pronounced at speeds of 10 knots and above. For the cruising speed of 10 knots, the difference in resistance values of the reference model and the alternative models vary between 0.40 kN and 0.50 kN. The resistance values obtained for the three

alternative designs, together with those of the reference model, are presented in Table 2.

Table 2. Resistance values

Speed (knots)	Resistance Values (kN)			
	Reference Model	SKG-01	SKG-02	SKG-03
5.00	3.10	2.90	2.90	2.90
5.25	3.40	3.20	3.20	3.20
5.50	3.70	3.50	3.50	3.50
5.75	4.00	3.80	3.80	3.80
6.00	4.40	4.20	4.20	4.20
6.25	4.80	4.50	4.60	4.60
6.50	5.20	5.00	5.00	5.00
6.75	5.70	5.40	5.40	5.40
7.00	6.20	5.90	5.90	5.90
7.25	6.80	6.50	6.50	6.50
7.50	7.40	7.10	7.10	7.10
7.75	8.10	7.80	7.80	7.80
8.00	8.90	8.50	8.50	8.60
8.25	9.80	9.40	9.40	9.40
8.50	10.90	10.50	10.50	10.50
8.75	12.20	11.70	11.70	11.80
9.00	13.70	13.20	13.20	13.20
9.25	15.30	14.80	14.80	14.80
9.50	17.00	16.50	16.50	16.50
9.75	18.60	18.10	18.20	18.20
10.00	20.20	19.70	19.80	19.70
10.25	21.70	21.20	21.30	21.30
10.50	23.30	22.70	22.80	22.80
10.75	25.00	24.40	24.50	24.40
11.00	26.90	26.20	26.30	26.30
11.25	29.20	28.40	28.50	28.50
11.50	32.00	31.10	31.20	31.20
11.75	35.30	34.30	34.40	34.40
12.00	39.40	38.20	38.30	38.30

Sail performance calculations

An examination of the polar performance diagram (Figure 8) of the Bodrum Gulet selected as the reference model in the present study shows that, as expected, the maximum hull speed is achieved at a wind angle in the range of 80–90°. Furthermore, the maximum hull speed values presented in Table 4 indicate that modifications in the longitudinal keel’s heel part results in an

increase in hull speed in terms of sailing performance. Among the alternative designs, SKG-02 achieves higher hull speeds than both the other alternatives and the reference model. The difference in maximum hull speed between the reference model and SKG-01 is 0.12 knots at a wind speed of 6 knots, increasing to 0.15 knots at a wind speed of 18 knots. Polar diagrams for the alternatives (SKG-01, SKG-02 and SKG-03) are presented in Figure 9.

Table 3. Maximum hull speeds

Wind Speed (knots)		Reference Model	SKG-01	SKG-02	SKG-03
6	Maximum hull speed (knot)	7.67	7.73	7.79	7.73
	Wind angle at maximum hull speed	84.39	84.17	88.84	84.07
8	Maximum hull speed (knot)	9.52	9.60	9.71	9.60
	Wind angle at maximum hull speed	86.22	84.69	85.25	84.27
10	Maximum hull speed (knot)	10.99	11.04	11.10	11.04
	Wind angle at maximum hull speed	85.41	84.14	84.12	84.03
12	Maximum hull speed (knot)	11.67	11.73	11.78	11.74
	Wind angle at maximum hull speed	92.52	86.54	86.44	83.74
14	Maximum hull speed (knot)	12.18	12.23	12.27	12.23
	Wind angle at maximum hull speed	88.60	89.15	89.07	89.44
16	Maximum hull speed (knot)	12.58	12.63	12.67	12.68
	Wind angle at maximum hull speed	91.54	91.26	91.26	91.12
18	Maximum hull speed (knot)	12.87	12.98	13.02	12.99
	Wind angle at maximum hull speed	93.36	89.44	93.36	93.36

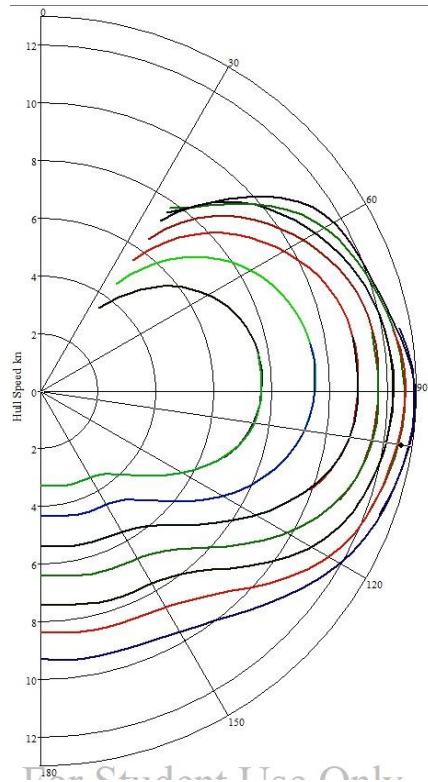


Figure 7. VPP Results of the reference model

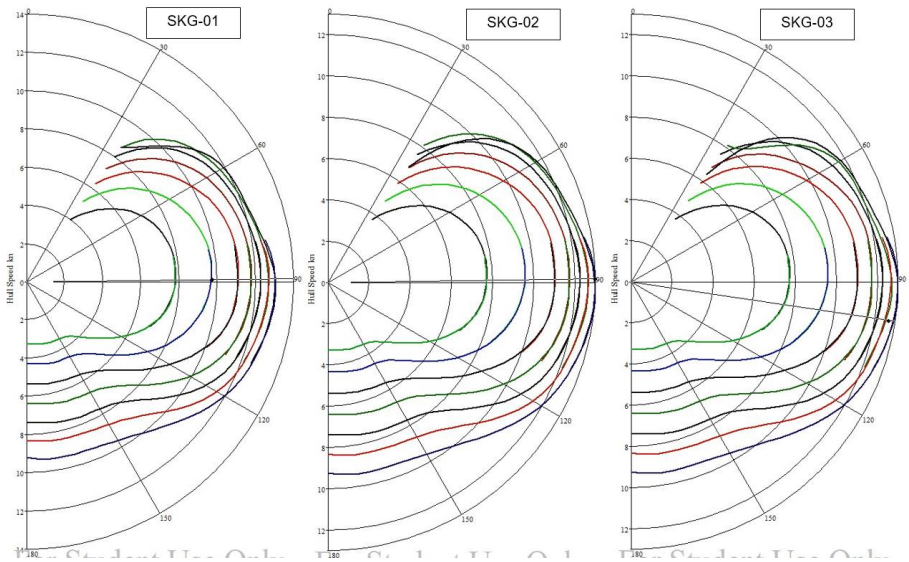


Figure 8. VPP Results of alternative designs

CONCLUSION

This study investigates the impact of longitudinal keel design—a distinctive feature of Bodrum Gulets—on hydrostatics, resistance and sailing performance characteristics. To evaluate such impacts, three alternative designs were developed by the heel part geometry of the longitudinal keel. These alternative designs are compared with the reference model in terms of hydrostatics, resistance and sail performance. According to the results, the following key findings are obtained:

- A consistent reduction in total resistance was observed as aft part geometry of the longitudinal keel, primarily due to a decline in the pressure resistance component. Compared to the reference model, the SKG-01 and SKG-03 alternatives exhibits a 2.48 % reduction in total resistance at a cruising speed of 10 knots. For speed of 12 knots, SKG-01 represents the lowest resistance value, which corresponds to 3.05% decrease compared to the reference model.
- The comparison between the alternative designs and the reference model reveals that the differences in hydrostatic values are minimal. Accordingly, it is inferred that modifications to the keel heel part geometry may be applicable not only to newly designed vessels but also to the longitudinal keel configurations Bodrum Gulets in service.
- It is observed that changing the aft part geometry of the longitudinal keel positively affects the sailing performance of Bodrum Gulet-type vessels, partly as a consequence of the reduction in resistance discussed in the preceding sections.

The results of this research confirm that even minor geometric modifications to the longitudinal keel can significantly influence the resistance values and consequently environmental impact of Bodrum Gulets. Future research is encouraged to explore alternative keel types beyond the traditional longitudinal design with the aim of further enhancing hydrodynamic efficiency and promoting sustainable maritime operations.

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Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflict of Interest

Authors confirm that there are no relevant financial or non-financial competing interests to report for this research.

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Reynolds and Stefan Number Effects on the Steady-State Performance of a PCM Double-Pipe Heat Exchanger: Closed-Form Correlations and Gaussian-Process Modeling

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ABSTRACT

Most data-driven studies of phase change material (PCM) heat exchangers target transient melting behavior and rely on large datasets, while the steady-state performance of continuously operated units has received little attention. This study develops a dimensionless, data-driven framework for the steady-state heat transfer of a double-pipe heat exchanger with a PCM layer in the annulus between counter-flowing hot and cold streams. Using sixteen CFD operating points for two organic (RT31, RT50) and two inorganic (SP31, SP50) PCMs over Reynolds numbers of 500–2000, the performance is expressed through the Nusselt number and the effectiveness as functions of the Reynolds and Stefan numbers. The two outputs prove to be governed by distinct mechanisms: the Nusselt number is predominantly flow-driven and, once normalized by the PCM conductivity, nearly material-independent, whereas the effectiveness separates into two material-dependent bands, with the inorganic PCMs (0.94–0.97) outperforming the organic ones (0.81–0.83). Each output is therefore matched to a suitable model—a closed-form correlation for the Nusselt number ($R^2 = 0.869$) and an uncertainty-aware Gaussian-process surrogate for the effectiveness (leave-one-out $R^2 = 0.998$)—while a Sobol analysis confirms the complementary roles of the two groups. The framework yields transferable correlations and reliable predictions from a strictly limited dataset.

Keywords – Phase change material; double-pipe heat exchanger; dimensionless correlation; Stefan number; Gaussian-process regression; data-driven modeling

INTRODUCTION

Growing global energy demand, the depletion of fossil resources, and the need to integrate intermittent renewable sources have intensified the search for efficient energy-storage solutions. Thermal energy storage (TES) plays a central role in this effort by decoupling energy supply from demand, and among the available approaches, latent-heat storage based on phase change materials (PCMs) has attracted particular attention owing to its high energy-storage density per unit volume, near-isothermal operation, and chemical stability [1,2]. By absorbing and releasing large amounts of latent heat during melting and solidification, PCMs enable peak-load shifting, waste-heat recovery, and improved efficiency across building, industrial, and renewable-energy applications. However, the widespread deployment of PCM-based systems is constrained by a well-known limitation: the intrinsically low thermal conductivity of most PCMs restricts the rate at which heat can be stored and recovered, making the design of the surrounding heat exchanger decisive for overall performance [3].

Consequently, a substantial body of experimental and numerical work has examined how heat-exchanger geometry, PCM type, and operating conditions govern the thermal performance of PCM heat exchangers. Zhang et al. [4] investigated a purpose-built finned-tube PCM heat exchanger using air as the heat transfer fluid (HTF) and organic PCM A27 packed within the tubes, combining charging and discharging experiments with a validated CFD model across varying HTF velocities, temperatures, and PCM thermal conductivities; they reported that a higher HTF flow rate substantially shortens the phase-change completion time, while enhancing PCM thermal conductivity yielded up to 46% and 35% reductions in melting and solidification times, respectively. Adopting a comparative perspective, Dongellini et al. [5] experimentally contrasted a finned-tube latent thermal energy storage (LTES) unit immersed in two commercial paraffinic PCMs against an equivalent sensible storage using water, varying the exchanger geometry, HTF mass flow rate, and inlet temperature; although the latent configuration increased heat-storing capacity by up to 200%, the average HTF–PCM heat transfer rate dropped by up to 40% for Reynolds numbers above 2000, a penalty that could be limited to 5–10% through a 1-row exchanger and low flow rates. Extending this line of inquiry toward generalizable design guidance, Herbinger and Groulx [6] experimentally characterized a modular vertical finned tube-and-shell PCM heat exchanger with a variable number of finned tubes (4, 8, and 12), proposing mean power and normalized power as comparative metrics and framing them as a first step toward the design rules that the latent-heat storage community still lacks.

Because the conduction-limited heat transfer within the PCM remains the principal bottleneck, a large number of studies have focused on passive enhancement techniques—most notably extended surfaces and fin geometries—to accelerate the phase-change process. Marzouk et al. [7] numerically studied paraffin-wax melting in a helical-coil heat exchanger with water as the HTF, comparing a plain tube against longitudinal and constructed-fin configurations in ANSYS Fluent; constructed fins raised the liquid fraction by 65% and shortened melting time by 50% by enlarging the heat transfer surface area. Building on the idea that PCM arrangement is itself a design variable, Kareem et al. [8] optimized the size and configuration of an air-to-multiple-PCM heat exchanger using a 2D ANSYS Fluent model supported by experiments, employing PCMs of different melting temperatures (RT25HC and RT21HC) arranged in series; they demonstrated that the series arrangement strongly affects phase-change behavior, with complete melting of both PCMs occurring in under 4 hours while solidification of RT21HC required more than 12 hours. Collectively, these studies confirm that geometry and material selection can markedly improve phase-change rates, yet they also reveal that mapping the full design

space through repeated high-fidelity simulations is computationally demanding.

This computational burden has, more recently, motivated the use of machine-learning (ML) models as fast surrogates for predicting PCM thermal behavior. Amudhalapalli and Devanuri [9] used ML algorithms to predict the transient melt fraction of a shell-and-tube PCM heat exchanger enhanced with a hybrid metal-foam and graphene-nanoplatelet combination, generating training data from numerical simulations across porosities, nanoparticle volume fractions, and exchanger orientations, and found that linear regression predicted the time-dependent melt fraction most accurately among the models tested. Focusing on real-time state estimation, Anooj et al. [10] proposed a recurrent-neural-network (RNN) technique to infer the liquid fraction of a PCM-based thermal management system from surface-temperature history, training the model on 345 numerically generated samples and reproducing the temporal liquid fraction with a correlation up to 0.99 and RMSE below 0.015 at a fraction of the computational cost. Addressing the influence of dataset construction itself, Yang et al. [11] evaluated several RNN architectures for predicting the thermal performance of cylindrical PCM-filled earth-air heat exchangers, reporting that weakly correlated inputs degraded accuracy, that a mid-sized 1024-group dataset best balanced training cost and accuracy, and that the gated-recurrent-unit model performed best overall ($R^2 = 0.997$). Taken together, these works establish ML as an effective predictive tool for PCM systems, but they consistently rely on large, simulation-generated datasets and treat the model as a purely predictive instrument.

Beyond prediction alone, several studies have coupled ML with CFD and optimization algorithms to actively guide the design of PCM-based TES units. Darzi et al. [12] combined CFD with a feed-forward back-propagation neural network and genetic-algorithm optimization to design a finned TES unit, building the design matrix through response surface methodology; their network predicted complete melting time with under 2.98% error, and the optimization identified fin configurations that dramatically reduced melting time relative to a finless enclosure. Similarly, Khalid et al. [13] integrated CFD with a Levenberg–Marquardt-trained feed-forward ANN to model the melting dynamics of nanoparticle-enhanced PCM combined with novel fractal H-shaped fins in a molten-salt system, where the hybrid configurations improved total melting time by up to 60% while the ANN accurately captured the temperature distribution and melting behavior. Al Arni et al. [14] likewise investigated dynamic melting of RT35 in the annulus of a shell-and-tube heat exchanger with openings in a 3D model, using a neural-network analysis to reveal that a slot diameter near 5.5 mm maximized the early-stage melting volume fraction while raising inlet pressure cut melting time by 43.8%. These hybrid AI–CFD frameworks demonstrate the value of data-driven methods for reducing design cost, yet

the learned models remain black-box mappings tied to a specific geometry rather than transferable physical relations.

In parallel, physics-informed and system-level modeling approaches have sought to embed governing physics or long-term operation directly into the predictive framework. Priyadarshi et al. [15] developed a physics-informed neural network (PINN) to predict the outlet parameters of a desiccant-coated energy exchanger, solving multiple physics-based partial differential equations on a single domain with a maximum discrepancy of $\pm 7.8\%$ and—crucially for the present context—achieving good agreement for both steady-state and transient cases, before extending the work to assess storage effectiveness across five PCMs. At the system scale, Zhang et al. [16] developed and validated a Modelica-based model of an integrated latent-heat storage system coupling a PCM-to-air heat exchanger with an air-conditioning unit, optimizing PCM slab thickness and airflow rate over full cooling-season simulations for five European climates and identifying RT25 as the best-performing PCM, with energy-saving ratios ranging from 16% to 44.7%. These approaches point toward more physically grounded and application-oriented modeling, reinforcing the notion that embedding physical structure into data-driven models is both feasible and beneficial.

Despite this considerable progress, three gaps emerge from the reviewed literature. First, virtually all ML-assisted PCM studies target transient quantities—melt fraction, complete melting time, or the temporal evolution of the phase front—whereas the steady-state heat-transfer performance of a continuously operated PCM heat exchanger has received little attention, even though many regenerative systems operate under sustained, quasi-steady conditions. Second, the existing data-driven models are trained on large datasets comprising hundreds to thousands of samples generated from extensive additional simulations, leaving open the question of how to build a reliable and physically consistent model when only a limited dataset is available. Third, and most importantly, these studies employ ML predominantly as a black-box predictor and do not distill the underlying physics into a generalizable dimensionless correlation; closed-form relations expressing the heat-transfer performance in terms of governing dimensionless groups such as the Reynolds and Stefan numbers are notably absent. Moreover, the double-pipe regenerative configuration, in which the PCM occupies the annulus between counter-flowing hot and cold streams, remains comparatively unexplored relative to the widely studied shell-and-tube and finned-tube arrangements.

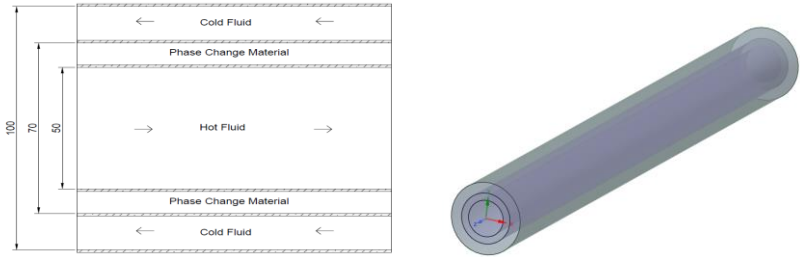
To address these gaps, the present study investigates the steady-state heat-transfer performance of a regenerative double-pipe heat exchanger with organic (RT31, RT50) and inorganic (SP31, SP50) PCMs placed in the annular region, using numerical data obtained for Reynolds numbers of 500–2000 under laminar, counter-flow conditions. Rather than treating the four PCMs as discrete categorical cases, their thermophysical properties are

recast into dimensionless groups—principally the Stefan number—so that the heat-transfer performance can be expressed through dimensionless outputs, namely the Nusselt number and the effectiveness. A data-driven framework is then developed to (i) derive interpretable closed-form dimensionless correlations of the form $Nu, \epsilon = f(Re, Ste)$ via symbolic regression, (ii) construct an uncertainty-aware Gaussian-process surrogate that reports predictive confidence bounds without requiring additional CFD runs, and (iii) validate the models under the small-data constraint using leave-one-out cross-validation together with a sensitivity analysis of the governing parameters. In this way, the study reframes a conventional parametric PCM comparison as a physically consistent, dimensionless, and data-efficient modeling methodology, providing both generalizable correlations and a transparent workflow for building reliable surrogate models from limited thermal-engineering datasets.

MATERIALS AND METHODS

Numerical Model

A numerical model of a double-pipe heat exchanger incorporating an intermediate PCM storage layer was developed in ANSYS Fluent. The configuration consists of three concentric tubes with inner-to-outer diameters of 50, 70, and 100 mm and a common length of 1000 mm. Hot pure water flows through the innermost tube and cold pure water through the outermost tube in a counter-flow arrangement, while the phase change material occupies the annular gap between them. The problem is solved under steady-state, laminar conditions, and the phase change is treated using the enthalpy–porosity approach. The 2D and 3D representations of the model are presented in Figure 1.



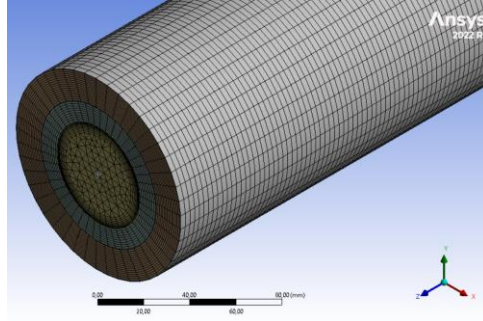


Figure 1: Geometry of double pipe heat exchanger

To ensure that the numerical solution was independent of spatial discretization, a grid-independence study was performed by generating five successively refined meshes, with local refinement applied at the solid–liquid interface where the thermal gradients are steepest. The mean temperature of the hot fluid was monitored as the convergence indicator. As shown in Figure 2, this quantity decreased with increasing cell count and levelled off beyond approximately 8×10^5 cells, where further refinement produced no appreciable change. The mesh containing 800,000 cells was therefore adopted for all subsequent computations, offering a reliable balance between numerical accuracy and computational cost.

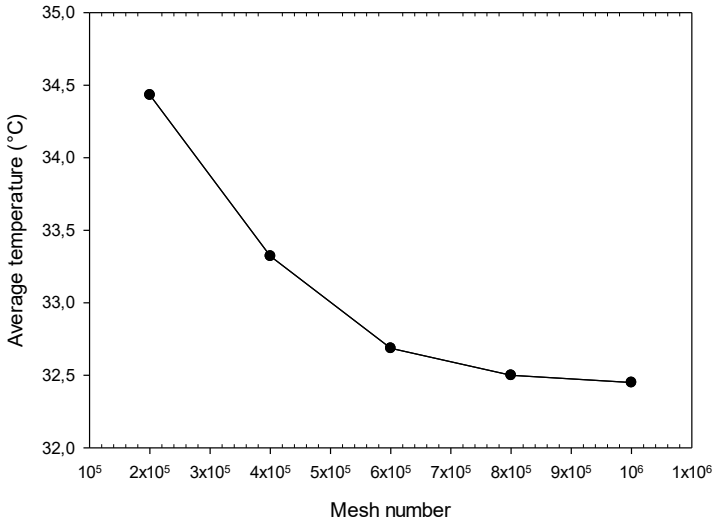


Figure 2: Variation of the average temperature with increasing mesh number

The reliability of the numerical model was assessed by comparing its predictions against the experimental measurements. As presented in Figure 3, the computed average temperatures follow the experimental trend closely across the examined range, with the deviation remaining within 11% at the

worst point. This level of agreement confirms that the adopted model captures the governing heat-transfer behavior with acceptable accuracy and provides a trustworthy basis for the dimensionless analysis developed in the following sections.

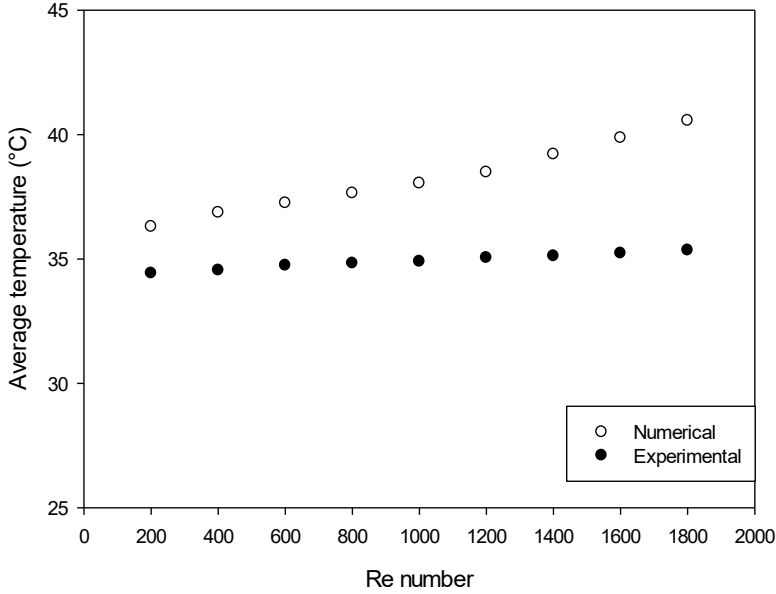


Figure 3: Validation graph for the study

Under the steady-state, laminar, and incompressible assumptions adopted in this study, the time-dependent terms vanish and the flow and thermal fields are governed by the following conservation equations. For the water streams, continuity and momentum conservation are expressed as:

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \rho \mathbf{g} \quad (2)$$

where $\mathbf{u}$, p , ρ , and μ denote the velocity vector, pressure, density, and dynamic viscosity, respectively, and $\rho \mathbf{g}$ accounts for buoyancy effects within the melting region. Energy conservation across the fluid and PCM domains is written as:

$$\nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (k \nabla T) \quad (3)$$

with h the specific enthalpy, k the thermal conductivity, and T the temperature.

The melting and solidification of the PCM within the annular region are modeled using the enthalpy–porosity technique, in which the liquid–solid interface is not tracked explicitly. Instead, the total enthalpy is decomposed into a sensible part and a latent contribution,

$$h = h_{ref} + \int c_p dT + \beta L(4)$$

where L is the latent heat of fusion and β is the liquid fraction, varying between 0 in the fully solid state and 1 in the fully liquid state within the melting range. The mushy region is treated as a porous zone whose permeability decreases as the material solidifies, progressively suppressing the local velocity to zero in the solid phase.

Since the aim is to characterize the sustained heat-transfer behavior rather than the transient melting process, the equations are solved in steady-state form. This reflects the operation of a continuously running unit, in which both streams flow simultaneously and the PCM reaches a stationary thermal state with a non-migrating phase interface. Time-dependent metrics such as melting time or liquid-fraction growth therefore fall outside the present scope; the PCM is treated as a thermally active medium governing the steady exchange between the streams.

Velocity-inlet conditions were imposed at the hot- and cold-fluid inlets, with the hot stream entering at 31 °C for the RT31/SP31 cases and 50 °C for the RT50/SP50 cases, while the cold stream was fixed at 20 °C in all runs. The inlet velocity of the hot fluid was set according to the target Reynolds number ($Re = 500, 1000, 1500, 2000$), and a counter-flow arrangement was established between the two streams. Pressure-outlet conditions were applied at both outlets, and no-slip was enforced at all solid walls. The Reynolds number was varied through the hot-fluid inlet velocity to isolate its effect on the steady heat-transfer performance.

The governing equations were solved with the finite-volume-based ANSYS Fluent solver using the SIMPLE algorithm for pressure–velocity coupling. Second-order upwind schemes were adopted for the momentum and energy equations to ensure spatial accuracy, and convergence at each step was judged by residual thresholds of 10^{-3} for continuity and momentum and 10^{-6} for the energy equation.

Phase Change Materials

Two organic (RT31, RT50) and two inorganic (SP31, SP50) commercial phase change materials were considered, selected such that each melting-temperature level (~31 °C and ~50 °C) is represented by one organic and one inorganic material, allowing a paired comparison between the two PCM families. Their thermophysical properties, compiled from the manufacturer datasheets, are listed in Table 1. Compared with the organic RT grades, the inorganic SP grades offer higher thermal conductivity, greater density, and larger heat-storage capacity, while exhibiting a mild thermal hysteresis of roughly 2 K between their melting and congealing peaks; the RT grades, by contrast, show no appreciable supercooling.

Table 1: Thermophysical properties of the phase change materials.

Property	RT31	SP31	RT50	SP50	Unit
Type	organic	inorganic	organic	inorganic	—
Melting range	29–34	31–33	45–51	50–51	°C
Main melting peak	31	32	49	50	°C
Main congealing peak	31	30	50	48	°C
Heat storage capacity *	165	210	160	220	kJ/kg
Specific heat capacity	2	2	2	2	kJ/kg·K
Density (solid / liquid)	0.88 / 0.76	1.35 / 1.25	0.88 / 0.76	1.5 / 1.4	kg/L
Thermal conductivity	0.2	0.5	0.2	0.6	W/m·K
Volume expansion	12.5	5	12.5	8	%
Max. operating temp.	50	50	70	80	°C

*Combined latent and sensible heat over the datasheet measurement window; the latent component used in the analysis is extracted separately.

Dimensionless Formulation

To generalize the results beyond the four specific materials and to express the heat-transfer behavior in a transferable form, the governing operating and material parameters were recast into dimensionless groups. The flow condition is represented by the Reynolds number, the phase-change characteristics of the PCM by the Stefan number, and the resulting thermal performance by the Nusselt number and the effectiveness.

The flow regime of the hot stream is characterized by the Reynolds number,

$$Re = \frac{\rho u D_h}{\mu}$$

where ρ and μ denote the density and dynamic viscosity of the working fluid, u the mean inlet velocity, and D_h the hydraulic diameter of the hot-fluid tube.

Phase-change heat transfer belongs to the classical class of moving-boundary (Stefan) problems, whose governing dimensionless group is the Stefan number. It represents the ratio of sensible to latent heat:

$$Ste = \frac{c_p \Delta T}{L}$$

where c_p and L are the specific heat and latent heat of fusion of the PCM, and ΔT the driving temperature difference. A small Ste indicates latent-dominated storage, while a larger value reflects a greater sensible contribution.

The choice of the driving temperature difference requires attention in this configuration. Defining it as the difference between the hot-fluid inlet and the PCM melting temperature is unsuitable here, since the hot-fluid inlet

was deliberately set close to each PCM's melting point, giving a vanishing or negative value. As the PCM annulus is bounded by the hot stream on one side and the cold stream on the other, the physically meaningful driving potential is the difference between the two streams:

$$\Delta T = T_{h,in} - T_{c,in}$$

This is consistent with the maximum temperature difference used in the effectiveness definition and gives $\Delta T = 11$ K for the 31 °C cases and 30 K for the 50 °C cases.

Since the storage capacity reported in the datasheets combines latent and sensible contributions over a finite measurement window ΔT_w , the latent heat of fusion was obtained by subtracting the sensible part:

$$L = Q_{cap} - c_p \Delta T_w$$

With $\Delta T_w \approx 15$ K for all four materials, this gives the latent-heat values and corresponding Stefan numbers listed in Table 2.

Table 2: Derived latent heat and Stefan numbers of the PCMs.

PCM	Qcap (kJ/kg)	ΔT_w (K)	L (kJ/kg)	ΔT (K)	Ste
RT31	165	15	135	11	0.163
SP31	210	15	180	11	0.122
RT50	160	15	130	30	0.462
SP50	220	15	190	30	0.316

The heat-transfer performance is expressed through the Nusselt number, defined on the PCM side so that the dimensionless output reflects the behavior of the phase-change medium rather than the working fluid:

$$Nu = \frac{U D_h}{k_{pcm}}$$

where U is the overall heat transfer coefficient obtained from the simulations and k_{pcm} the thermal conductivity of the PCM. Normalizing with k_{pcm} distinguishes materials that share a similar U but differ in conductivity.

The overall performance is additionally quantified by the effectiveness, defined through the ε -NTU framework as the ratio of the actual to the maximum attainable heat transfer rate:

$$\varepsilon = \frac{\dot{Q}_{act}}{\dot{Q}_{max}}$$

where C_{min} is the smaller of the two stream heat-capacity rates.

Combining the four Reynolds numbers with the four PCMs yields sixteen steady-state operating points, forming a 4×4 grid in the (Re, Ste) plane. Each point is associated with two dimensionless outputs, Nu and ε , which constitute the dataset for the data-driven correlations developed in the following section.

It should be noted that, across the four materials, the Stefan number and the PCM-to-fluid thermal-conductivity ratio vary in a correlated manner, since moving from organic to inorganic PCMs raises both the latent heat and the conductivity. Their independent effects therefore cannot be fully separated within this dataset. Accordingly, (Re, Ste) is adopted as the primary governing pair, and the conductivity ratio is discussed separately rather than used as an independent regression input.

Data-Driven Methodology

Building on the dimensionless dataset, a data-driven framework was employed to derive interpretable correlations and to model the heat-transfer performance under the limited-data constraint. The framework combines three complementary elements: symbolic regression to obtain closed-form correlations, a Gaussian-process surrogate to provide predictions with quantified uncertainty, and a leave-one-out validation procedure supported by a sensitivity analysis. In all cases the Reynolds and Stefan numbers served as inputs, and the Nusselt number and effectiveness as the modeled outputs.

Symbolic regression was used to obtain closed-form correlations directly from the data, without assuming a fixed functional form in advance. Unlike conventional black-box models, this approach searches over combinations of variables and mathematical operators to yield explicit expressions relating Nu and ϵ to Re and Ste. Given the small dataset, the search was constrained to low-complexity expressions, which reduces the risk of overfitting and produces correlations consistent with the power-law relations commonly used in heat-transfer analysis.

To complement the explicit correlations, a Gaussian-process regression (GPR) surrogate was constructed. GPR models the output as a Gaussian process and provides, at each input, both a predicted mean and an associated variance:

$$y(x) = \mu(x) \pm \sigma(x)$$

The mean $\mu(x)$ gives the prediction, while the standard deviation $\sigma(x)$ defines a confidence bound around it. This allows estimates at intermediate Reynolds and Stefan numbers—not directly covered by the sixteen CFD points—to be reported together with their reliability rather than as single deterministic values, which is particularly valuable here since no additional simulations were performed.

Given the limited size of the dataset, model performance was assessed using leave-one-out cross-validation, the most suitable strategy when data are scarce. Each of the sixteen points is withheld in turn while the model is trained on the remaining fifteen and tested on the excluded one. Since every point serves for both training and testing without reserving a fixed test set,

this provides an honest performance estimate under the small-data constraint.

To identify which input governs the heat-transfer response, a variance-based (Sobol) sensitivity analysis was carried out on the fitted model. This approach decomposes the total variance of the output and attributes it among the inputs, quantifying how much of the variation in performance is explained by the Reynolds number and by the Stefan number. It thereby reveals the relative influence of flow and phase-change effects on the predicted results.

The predictive accuracy of the models was quantified using three standard metrics: the coefficient of determination (R^2), the root-mean-square error (RMSE), and the mean absolute error (MAE),

$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_i (y_i - \hat{y}_i)^2}$$

$$\text{MAE} = \frac{1}{N} \sum_i |y_i - \hat{y}_i|$$

where y_i , $\hat{y}_i$, and $\bar{y}$ denote the actual, predicted, and mean values, respectively. Together these provide complementary measures of correlation and absolute error for both the symbolic and Gaussian-process models.

RESULTS AND DISCUSSION

The steady-state results are recast into the dimensionless framework and summarized in Table 3. The study covers four Reynolds numbers ($\text{Re} = 500\text{--}2000$) under laminar counter-flow conditions and four PCMs—two organic (RT31, RT50) and two inorganic (SP31, SP50)—spanning a Stefan-number range of 0.122–0.462 across two melting-temperature levels ($\sim 31^\circ\text{C}$ and $\sim 50^\circ\text{C}$). The sixteen resulting points, listed with their Nusselt number and effectiveness, form the basis for the analysis. As shown below, Nu reflects mainly the flow condition, whereas ϵ responds more strongly to the material's phase-change characteristics.

Table 3: Dimensionless dataset of the sixteen steady-state operating points.

PCM	Re	Ste	Nu	ϵ
RT31	500	0.163	23.99	0.806
RT31	1000	0.163	32.64	0.817
RT31	1500	0.163	38.57	0.823
RT31	2000	0.163	43.09	0.826
SP31	500	0.122	20.33	0.943
SP31	1000	0.122	28.27	0.952
SP31	1500	0.122	33.68	0.956
SP31	2000	0.122	37.89	0.958
RT50	500	0.462	23.98	0.806
RT50	1000	0.462	32.64	0.818
RT50	1500	0.462	38.53	0.823
RT50	2000	0.462	43.05	0.826
SP50	500	0.316	19.25	0.956
SP50	1000	0.316	26.88	0.964
SP50	1500	0.316	32.15	0.968
SP50	2000	0.316	36.25	0.970

Nu evaluated on the PCM side with the annular hydraulic diameter ($Dh = 0.02$ m).

Effect of Reynolds and Stefan Numbers

Figure 4 shows the variation of the Nusselt number with the Reynolds number for the four PCMs. For every material Nu increases monotonically with Re , rising by about 80% from $Re = 500$ to 2000 as the stronger convective transport in the hot stream intensifies the heat exchange across the PCM annulus; the increase is steepest at low Re and gradually flattens. A key feature is that the four materials collapse into two closely spaced groups rather than four distinct curves. Because Nu is normalized by the PCM thermal conductivity, the higher conductivity of the inorganic SP grades is largely absorbed into the normalization, leaving the Reynolds number as the dominant factor. Thus, in dimensionless form, the Nusselt number reflects primarily the flow condition rather than the material identity.

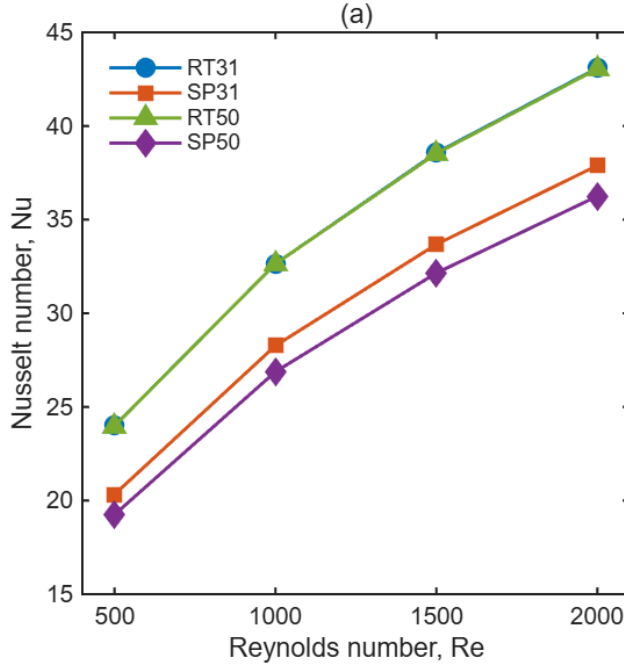


Figure 4: Variation of the Nusselt number with the hot fluid Reynolds number for the four phase change materials.

Figure 5 shows the variation of the effectiveness with the Reynolds number. In contrast to the Nusselt number, ϵ separates the four materials into two well-defined bands: the inorganic SP31 and SP50 reach high values of 0.94–0.97, while the organic RT31 and RT50 remain markedly lower at 0.81–0.83. The effectiveness also rises with Re , but only slightly, so that the gap between the two families far exceeds the variation caused by the flow rate. This clear grouping originates from the higher thermal conductivity and larger latent-heat storage of the inorganic PCMs, which enable the exchanger to approach its maximum attainable heat transfer more closely. Hence, whereas the Nusselt number is governed mainly by the flow condition, the effectiveness is dictated primarily by the phase-change characteristics of the material, as captured by the Stefan number.

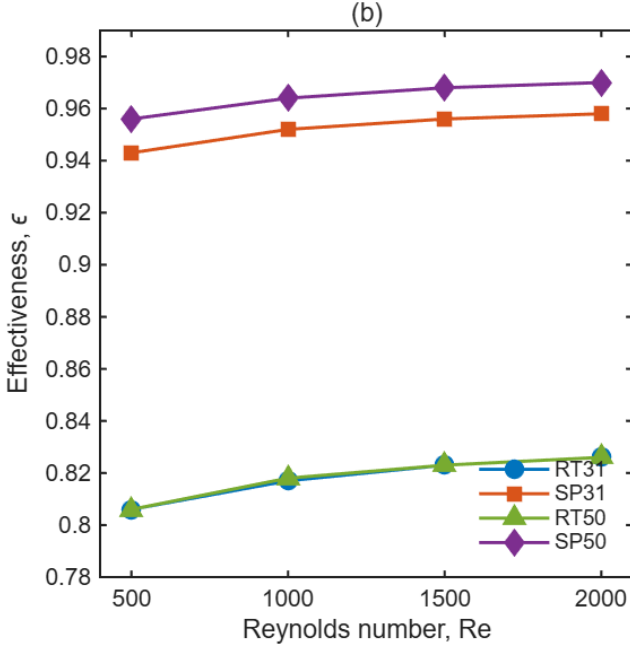


Figure 5: Variation of the effectiveness with the hot-fluid Reynolds number for the four phase change materials.

Data-Driven Correlations

A closed-form correlation for the Nusselt number was obtained by log-linear regression:

$$Nu = 1.49 \cdot Re^{0.439} \cdot Ste^{0.029}$$

The fit reproduces the CFD data well, achieving a coefficient of determination of $R^2 = 0.869$, with the predicted values lying almost entirely within $\pm 10\%$ of the simulated ones, as shown in the parity plot of Figure 6. The exponent of the Reynolds number (0.439) is close to the value expected for developing laminar internal flow, confirming that the flow condition governs the Nusselt response. In contrast, the Stefan-number exponent is very small (0.029), so that removing Ste from the correlation reduces R^2 only marginally, from 0.869 to 0.864. This negligible dependence provides quantitative confirmation that, in dimensionless form, the Nusselt number is essentially controlled by the Reynolds number and is nearly insensitive to the phase-change properties of the material.

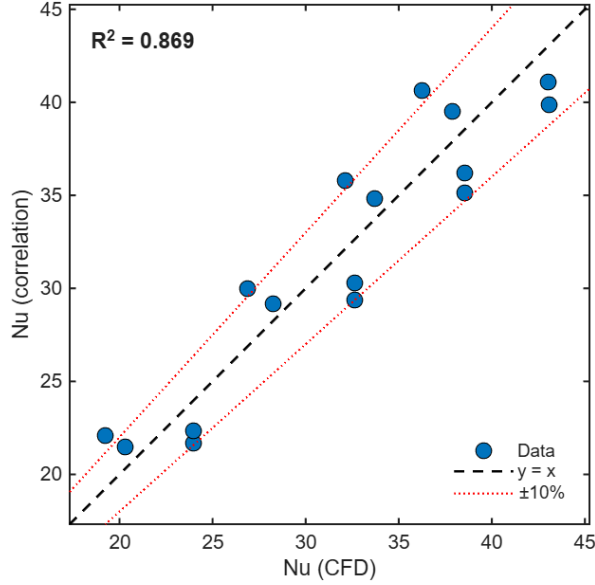


Figure 6: Parity plot comparing the CFD Nusselt numbers with those predicted by the closed-form correlation; dashed line denotes perfect agreement and dotted lines the $\pm 10\%$ band.

Unlike the Nusselt number, the effectiveness could not be captured by a power-law correlation. Because ε varies only weakly with Re and instead separates into two discrete, material-dependent bands, a continuous power-law form fails to represent it: a linear regression in Re and Ste yields a leave-one-out R^2 of -0.29 , indicating no predictive capability. The effectiveness was therefore modeled with a Gaussian-process regression (GPR) surrogate, which accommodates the nonlinear, grouped structure of the data.

The GPR model, trained with an ARD squared-exponential kernel, reproduces the effectiveness with high accuracy. Under leave-one-out cross-validation—the appropriate test given the limited dataset—it attains $R^2 = 0.998$, $RMSE = 0.0035$, and $MAE = 0.0029$, with all predictions lying within ± 0.02 of the CFD values, as shown in the parity plot of Figure 7.

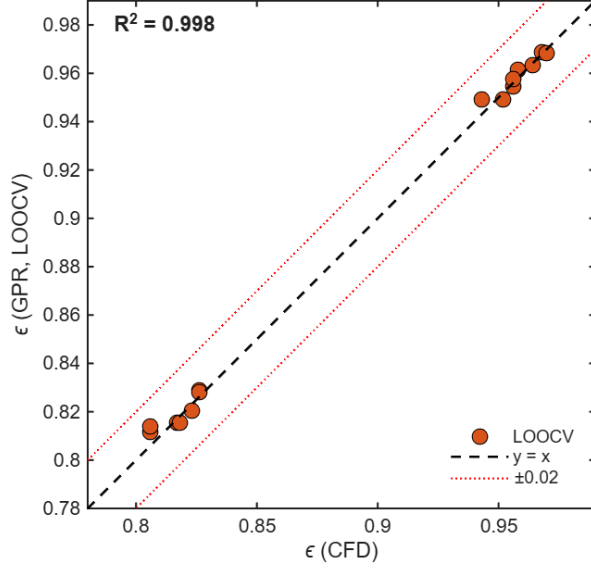


Figure 7: Parity plot of the GPR-predicted effectiveness against the CFD values under leave-one-out cross-validation; dashed line denotes perfect agreement and dotted lines the ± 0.02 band.

The stark contrast between the GPR (LOOCV $R^2 = 0.998$) and the linear model ($R^2 = -0.29$) confirms that the discrete, phase-change-driven behavior of the effectiveness is well described by a flexible probabilistic surrogate but not by a fixed closed-form expression. In addition, the GPR provides a predictive variance at each point, allowing effectiveness estimates at intermediate Reynolds and Stefan numbers to be reported together with confidence bounds without further simulation.

Sensitivity Analysis

To quantify the relative influence of the two governing groups, a variance-based (Sobol) sensitivity analysis was performed on the fitted surrogates, sampling Re and Ste over their full ranges. The resulting first-order indices, shown in Figure 8, confirm the complementary roles of the two inputs in a striking manner.

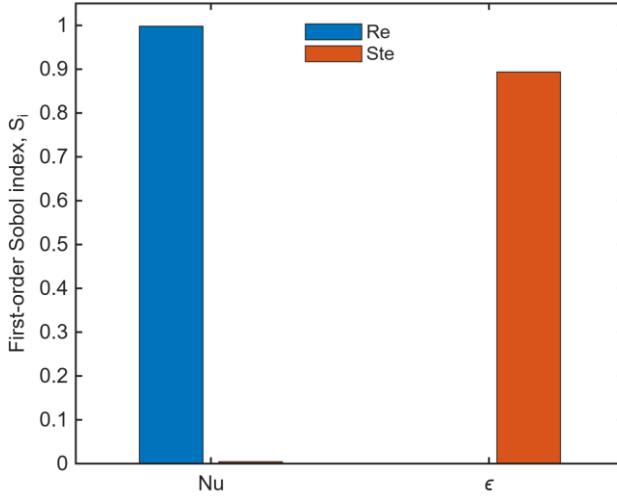


Figure 8: First-order Sobol sensitivity indices of the Reynolds and Stefan numbers for the Nusselt number and the effectiveness.

For the Nusselt number, almost the entire output variance is attributable to the Reynolds number ($S_{Re} = 0.998$), with a negligible Stefan-number contribution ($S_{Ste} \approx 0$). The effectiveness exhibits the opposite pattern: its variance is governed almost entirely by the Stefan number ($S_{Ste} = 0.894$), while the Reynolds number is practically inactive ($S_{Re} \approx 0$). These indices provide a quantitative and independent confirmation of the trends observed earlier: the Nusselt number is a flow-driven quantity controlled by Re, whereas the effectiveness is a material-driven quantity governed by the phase-change characteristics encapsulated in Ste. The near-orthogonal sensitivity of the two outputs also indicates that Re and Ste act as complementary, non-redundant descriptors of the system's steady-state thermal performance.

Taken together, the results give a consistent and physically coherent picture. The two outputs are governed by distinct mechanisms and therefore call for different tools: the Nusselt number, controlled almost entirely by Re, is captured by a compact closed-form correlation ($R^2 = 0.869$), while the effectiveness, dictated by the phase-change characteristics through Ste, follows a discrete material-dependent pattern better represented by an uncertainty-aware Gaussian-process surrogate (LOOCV $R^2 = 0.998$); the Sobol analysis confirms this separation quantitatively. Beyond the specific findings, matching each output to the most appropriate model yields accurate, interpretable relations even under a strictly limited dataset, providing transferable correlations and an uncertainty-aware predictive capability for PCM-based double-pipe heat exchangers without further high-fidelity simulations.

CONCLUSION

This study revisited a steady-state CFD dataset of a double-pipe heat exchanger with an intermediate PCM layer and reframed it as a dimensionless, data-driven modeling problem. Two organic (RT31, RT50) and two inorganic (SP31, SP50) phase change materials were examined over a Reynolds-number range of 500–2000, with their performance expressed through the Nusselt number and the effectiveness as functions of the Reynolds and Stefan numbers. The main findings are as follows:

- The Nusselt number increases monotonically with the Reynolds number and, once normalized by the PCM conductivity, becomes nearly insensitive to the material, making it a predominantly flow-driven quantity.
- The effectiveness separates into two distinct material-dependent bands, with the inorganic PCMs ($\varepsilon = 0.94\text{--}0.97$) markedly outperforming the organic ones ($\varepsilon = 0.81\text{--}0.83$), being governed primarily by the Stefan number.
- A compact closed-form correlation, $Nu = 1.49 \cdot Re^{0.439} \cdot Ste^{0.029}$ ($R^2 = 0.869$), accurately represents the Nusselt number, whereas the effectiveness—unsuited to a fixed power law—was modeled by a Gaussian-process surrogate achieving a leave-one-out R^2 of 0.998.
- A variance-based Sobol analysis confirmed the complementary roles of the two groups, attributing the Nusselt variance almost entirely to Re ($S_{Re} = 0.998$) and the effectiveness variance to Ste ($S_{Ste} = 0.894$).

Overall, the study demonstrates a transferable methodology for building accurate, interpretable models from a strictly limited dataset by matching each output to the most suitable data-driven tool, delivering closed-form correlations and an uncertainty-aware predictive capability without additional simulations. Its main limitation is that the sixteen-point dataset does not allow the correlated Stefan number and conductivity ratio to be fully decoupled; future work could enrich the dataset with more PCMs and operating conditions, extend the approach to transient behavior, and incorporate enhancement techniques such as fins, porous inserts, or nanoparticles.

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An Effectiveness-NTU Analysis of a Plate Heat Exchanger under Different Flow and Thermal Conditions

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ABSTRACT

The thermal performance of a counter-flow plate heat exchanger was investigated experimentally through the effectiveness-NTU framework, with the number of transfer units and the capacity ratio evaluated as primary results rather than as intermediate quantities. Pure water was used on both sides of a fixed transfer area, and the hot-side Reynolds number varied from 6000 to 18000 at hot-side inlet temperatures of 25, 35, 45 and 55 °C, with the cold-side inlet temperature held constant at 20 °C. Since the transfer area is fixed, the number of transfer units reflects the overall heat transfer coefficient alone, and its increase with the Reynolds number was found to depend strongly on the inlet temperature: the increase is essentially complete by $Re = 12000$ at 25 °C, whereas at 55 °C it continues throughout the tested range and reaches 39.2%. A separation of the effectiveness increase into its two contributions showed that the dominant mechanism changes with temperature, the reduction in the capacity ratio accounting for 59% of the increase at 25 °C and the rise in NTU accounting for 72% at 55 °C. The classical counter-flow relation agreed with the measurements to within 3% at 25 °C, while the deviation increased to about 15% at 55 °C, indicating that the number of transfer units is underestimated at higher inlet temperatures under the constant-property assumption. Three dimensionless correlations were developed for effectiveness, NTU and the capacity ratio in terms of the Reynolds number and the inlet temperature ratio, with coefficients of determination of 0.943, 0.873 and 0.984 respectively, and all predicted values within $\pm 10\%$ of the measurements.

Keywords – Plate heat exchanger, effectiveness-NTU method, thermal performance, dimensionless correlation, Reynolds number.

INTRODUCTION

Plate heat exchangers (PHEs) accommodate a large heat-transfer surface within a small volume, which has made them a preferred choice for compact thermal duties across chemical processing, food production, energy systems and HVAC installations [1-4]. Their gasketed, modular construction allows the transfer area to be resized by adding or removing plates, and maintenance is considerably simpler than in shell-and-tube units. These advantages have sustained a broad research effort spanning plate geometry, flow structure, working-fluid modification, fouling, material selection and, more recently, data-driven performance prediction [5]. Compact and regenerative exchangers have been investigated along the same lines, ranging from the experimental characterization of operating parameters and the application of machine-learning methods to design criteria to the use of organic and inorganic phase-change media in regenerative units, the

insertion of turbulators in double-pipe geometries and the parametric assessment of phase-change behavior under varying operating conditions [6,7].

The corrugation pressed into each plate constitutes the strongest geometric influence on performance. Martin [8] developed a theoretical framework relating chevron geometry to both thermal and hydraulic behavior, while Kanaris et al. [9] demonstrated that undulated surfaces can be tuned to balance heat transfer against pressure loss. The chevron angle governs how vigorously the channel flow is disturbed, and therefore affects heat-transfer rate, pressure drop and pumping cost. Numerical studies have extended this understanding: Dvořák and Vít [10] used CFD to reproduce the thermal and flow fields in recuperative plate units and reported that plate pitch and wall thickness influence both the transfer coefficient and the pressure penalty. At the lower end of the flow range, Močnik et al. [11] visualized dimpled channels between $Re = 70$ and 469 and identified distinct stagnant and active regions whose relative proportions change with flow rate, with fully turbulent conditions emerging only above $Re = 469$.

A second line of research modifies the working fluid rather than the surface. Javadi et al. [12] measured clear gains in transfer rate when nanoparticles were dispersed in the base fluid, but also recorded an accompanying rise in pressure loss, so that the net benefit depends on how the two effects are weighed against each other. Zheng et al. [13] reached a comparable conclusion for several nanofluids in solar-driven PHEs, and Ahmadi et al. [14] attributed the underlying conductivity enhancement to temperature, particle shape and concentration. Rios-Irribé et al. [15] moved outside Newtonian behavior altogether, employing CFD to show how fluid rheology reshapes the thermal-hydraulic response of the channel.

Structural enhancement forms a third group. Yang et al. [16] examined water flowing over strip fins in eighteen geometric variants and related performance to the ratio between the leading-tip area of an individual cell and the square of the fin thickness. Song et al. [17] condensed offset-strip-fin behavior into a combined heat-transfer and friction correlation, while Jiang et al. [18] characterized the same fin family under cryogenic liquid-helium conditions. More recent studies have coupled geometry to formal optimization: Wang et al. [19] applied topology optimization with a moving-asymptote scheme to generate a new channel layout, and He et al. [20] combined a neural network with a multi-objective genetic algorithm to tune a continuous dimple-plate design, reporting a substantial performance gain over a conventional baseline.

A smaller body of work evaluates PHEs through the effectiveness-NTU framework rather than through local transfer coefficients, which places effectiveness, NTU and the capacity ratio at the center of the analysis. Jouhara et al. [21] conducted both experimental and theoretical investigations on multi-pass heat-pipe-based exchangers, varying the

Reynolds number and the number of flow passes; they found the two to be strongly correlated with the transfer rate, with system effectiveness improving as passes were added. Sundar and Mouli [22] measured the effectiveness and number of transfer units of a plate unit operating with $\text{Fe}_3\text{O}_4\text{-SiO}_2/\text{water}$ hybrid nanofluids under laminar conditions, focusing on particle loading and mass flow rate. They reported that raising the volume concentration and Reynolds number enhanced both effectiveness and NTU, reaching improvements of 13.23% and 24.51% respectively at 1.0% volume fraction and $\text{Re} \approx 572$ relative to water, and proposed a generalized correlation for the two parameters. Studies of this kind remain the exception: the majority of experimental PHE investigations report effectiveness alone and treat NTU and the capacity ratio as intermediate quantities rather than as reported results.

Data-driven modelling has grown rapidly as an alternative to classical correlations. Selbaş et al. [23] trained a neural network to predict the heat-transfer rate and effectiveness of plate exchangers from experimental data, achieving correlation coefficients of 0.9994 and 0.9976 respectively, and then distilled the trained weights into a simplified analytical expression to support thermal design. Turk et al. [24] and Aradağ et al. [25] compared network estimates directly against conventional Nusselt-number and friction correlations for gasketed units, treating the network as an alternative to classical correlations rather than a supplement to them. Dheenamma et al. [26] searched systematically for the best network configuration in corrugated PHEs, using Reynolds number, Prandtl number and concentration as inputs for CMC and XG solutions, and reported that specific architectures yielded very low prediction errors. Longo et al. validated networks against large refrigerant databases for condensation [27] and boiling [28] inside brazed plate exchangers, incorporating plate geometry, operating conditions and refrigerant properties and reaching mean absolute percentage errors of 3.6% and 4.8% respectively. Hybrid schemes have followed: Khan et al. [29] replaced the genetic algorithm inside an optimization loop with a network to cut computation time while retaining comparable thermal performance, Sun et al. [30] chained CFD, NSGA-II, a neural network and TOPSIS into a single design system, and Jin et al. [31] applied the same route to optimize intermittent spray cooling of plate-fin surfaces.

Two gaps emerge from this body of work. First, effectiveness is almost invariably reported on its own, even though it is fully determined by the number of transfer units and the capacity ratio; separating these two influences reveals which physical mechanism produces a given performance gain, information that is lost when effectiveness alone is tabulated. Second, the classical counter-flow effectiveness-NTU relation is routinely invoked as a qualitative consistency check but is seldom tested quantitatively against measured triplets of effectiveness, NTU and capacity ratio. The present study addresses both. A set of operating points obtained from a counter-flow

plate heat exchanger is analyzed as a complete dimensionless set: the variation of NTU with flow and thermal conditions is mapped, the measured effectiveness gain is decomposed into its NTU and capacity-ratio contributions, the deviation from the classical relation is quantified across the full test matrix, and dimensionless correlations are developed for all three quantities in terms of the Reynolds number and the inlet temperature ratio.

MATERIALS AND METHODS

Experimental System and Data Reduction

The measurements analyzed in this study were obtained on a gasketed counter-flow plate heat exchanger with a fixed heat-transfer area, operated with pure water on both the hot and cold sides. Because the unit remained unchanged throughout the test programme, every variation reported in the following sections originates in the flow and thermal conditions rather than in geometry. The physical specification of the exchanger is given in Table 1.

Table 1: Physical specification of the plate heat exchanger.

Property	Value
Plate material	AISI 304 stainless steel
Unit designation	SD-005
Number of plates	12 (six passes)
Heat-transfer area, A_s	480 cm ²
Overall dimensions	450 × 250 × 100 mm
Maximum working pressure	10 bar
Maximum working temperature	100 °C

Stainless steel was selected for its corrosion resistance and dimensional stability across the temperature range examined. The plates were assembled so that the hot and cold streams flow in opposite directions, a counter-flow arrangement that yields the highest attainable effectiveness for a given transfer area and capacity ratio and therefore provides the natural reference against which the measurements are later compared.

The experimental programme follows a full factorial arrangement of five hot-side Reynolds numbers and four hot-side inlet temperatures, as summarized in Table 2. The cold stream was held constant throughout, in both inlet temperature and flow rate, so that the hot side alone was varied.

Table 2: Operating conditions for the experiments

Parameter	Values
Hot-side Reynolds number, Re	6000, 9000, 12000, 15000, 18000
Hot-side inlet temperature, $T_{h,in}$	25, 35, 45, 55 °C
Cold-side inlet temperature, $T_{c,in}$	20 °C (constant)
Cold-side Reynolds number	constant
Working fluid	pure water, both streams
Flow arrangement	counter-flow

The Reynolds number characterizes the flow regime within the channels and is evaluated from the channel hydraulic diameter:

$$Re = (\rho V D_h) / \mu$$

The heat capacity rate of each stream is the product of its mass flow rate and specific heat, and the capacity ratio is formed from the smaller and larger of the two:

$$C_c = \dot{m}_c c_{pc}$$

$$C_h = \dot{m}_c c_{ph}$$

$$c = C_{min} / C_{max}$$

The maximum thermal driving potential is fixed by the inlet temperature difference, from which the maximum transferable heat follows:

$$\Delta T_{max} = T_{h,in} - T_{c,in}$$

$$\dot{Q}_{max} = C_{min} \Delta T_{max}$$

Effectiveness is defined as the ratio of the heat actually exchanged to this ideal limit:

$$\varepsilon = \dot{Q}_{act} / \dot{Q}_{max}$$

The number of transfer units is obtained from the overall heat transfer coefficient and the transfer area:

$$NTU = (UA_s) / C_{min}$$

The form of this last definition warrants emphasis, because NTU is frequently interpreted as a proxy for exchanger size. In a comparison across units of different capacity that reading is valid, since a larger A_s raises NTU directly. Here it does not apply: the transfer area is fixed at 480 cm² for every operating point, so NTU cannot register a geometric effect and instead tracks the group U/C_{min} alone. Any change in NTU reported in the following sections is therefore a change in the thermal conductance of the system relative to the limiting capacity rate, which is precisely what renders the quantity informative in a single-unit study.

A final dimensionless group is introduced for the correlations developed later, in which the two inlet temperatures are combined into a temperature ratio evaluated on the absolute scale:

$$\theta = T_{h,in} / T_{c,in}$$

Expressing the thermal condition in this form, rather than as a temperature in degrees Celsius, keeps the correlations dimensionally consistent and, as shown later, also improves their agreement with the measured data.

The accuracy of the developed correlations is evaluated using three statistical measures. The coefficient of determination (R^2) quantifies the overall agreement between the predicted and measured values:

$$R^2 = 1 - \frac{\sum (y_{exp} - y_{pred})^2}{\sum (y_{exp} - \bar{y}_{exp})^2}$$

The mean absolute percentage error (MAPE) gives the average relative deviation between the predicted and measured values:

$$MAPE = \frac{100}{N} \sum \left| \frac{y_{exp} - y_{pred}}{y_{exp}} \right|$$

The maximum deviation is the largest absolute relative deviation among all data points:

$$Max\ deviation = \max \left(\left| \frac{y_{exp} - y_{pred}}{y_{exp}} \right| \right) \times 100$$

RESULTS AND DISCUSSION

Variation of NTU with Flow and Thermal Conditions

The number of transfer units increases with both the Reynolds number and the hot-side inlet temperature, but the two variables do not act independently: the Reynolds number ceases to be effective at low inlet temperatures while continuing to raise NTU at high ones. This behavior is shown in Figure 1.

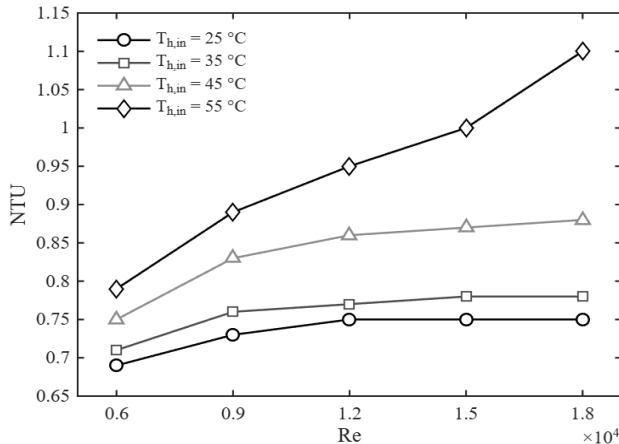


Figure 1: Variation of the number of transfer units with Reynolds number at the four hot-side inlet temperatures.

Over the whole Reynolds range the total gain in NTU rises steeply with inlet temperature, amounting to 8.7% at 25 °C, 9.9% at 35 °C, 17.3% at 45 °C and 39.2% at 55 °C. The more revealing measure, however, is where within that range the gain is realized. At 25 °C the entire increase is complete by $Re = 12000$, and the final two points coincide at 0.75; at 35 °C only 1.3 percentage points of the total remain above $Re = 12000$, and at 45 °C only 2.3. At 55 °C the behavior is qualitatively different: 15.8 percentage points of growth still occur between $Re = 12000$ and $Re = 18000$, so that roughly half of the total gain is delivered in the upper half of the Reynolds range and no plateau is reached anywhere within the tested window.

This behavior has a practical consequence. Since pumping power increases more rapidly with flow rate than the transfer rate does, raising the Reynolds number beyond the point at which NTU becomes constant provides no benefit. In the present exchanger this point lies near $Re = 12000$ for inlet temperatures up to 35 °C, whereas above 45 °C the flow rate can be increased throughout the tested range with a continuing improvement. The recommended operating Reynolds number therefore depends on the thermal condition and cannot be stated as a single value.

At 55 °C this transition occurs beyond the tested range. At this temperature the dynamic viscosity of the hot water is approximately half of its value at 25 °C, and its thermal conductivity is higher. As a result, the heat transfer on the hot side is stronger at every Reynolds number and continues to improve with increasing velocity over a wider range. Therefore, increasing the flow rate remains effective in raising NTU at high inlet temperatures, whereas it produces little further improvement at low inlet temperatures.

The distinction between the two temperature regimes is also relevant to the selection of the operating Reynolds number. When the inlet temperature is at or below 35 °C, NTU becomes nearly constant above $Re = 12000$, so operating at a higher Reynolds number does not improve thermal performance. When the inlet temperature is 45 °C or higher, NTU continues to increase across the entire tested range, and a higher Reynolds number remains beneficial. The most suitable operating Reynolds number therefore depends on the inlet temperature and cannot be expressed as a single value for the exchanger.

Effect of the Capacity Ratio on Thermal Performance

The improvement in effectiveness with increasing Reynolds number results from two separate effects whose relative importance changes across the temperature range. The capacity ratio decreases with both the Reynolds number and the inlet temperature, and in a counter-flow arrangement a lower capacity ratio corresponds to a higher effectiveness at a fixed NTU.

Effectiveness is therefore improved both by the increase in NTU and by the reduction in the capacity ratio.

The decrease in the capacity ratio with the Reynolds number is a direct result of the experimental arrangement, in which the cold stream is held constant. At $Re = 6000$ the two streams carry comparable capacity rates, and the ratio lies between 0.75 and 0.85. As the hot-side flow rate is increased while the cold side remains fixed, the hot stream attains the larger capacity rate and the ratio decreases towards 0.40. An increase in the inlet temperature produces the same trend at every Reynolds number, the ratio decreasing by approximately 0.10 between 25 °C and 55 °C.

The contribution of each effect can be examined separately using the counter-flow effectiveness relation, in which effectiveness is expressed as a function of NTU and the capacity ratio:

$$\varepsilon = (1 - \exp[-NTU(1 - c)]) / (1 - c \exp[-NTU(1 - c)])$$

The state at $Re = 6000$ is denoted by (NTU_1, c_1) and that at $Re = 18000$ by (NTU_2, c_2) . The separate effect of each variable is obtained by changing that variable alone while keeping the other fixed. Evaluating this over the full Reynolds range at each inlet temperature and expressing the result as the percentage of the total effectiveness increase produced by each effect, gives the distribution shown in Figure 2.

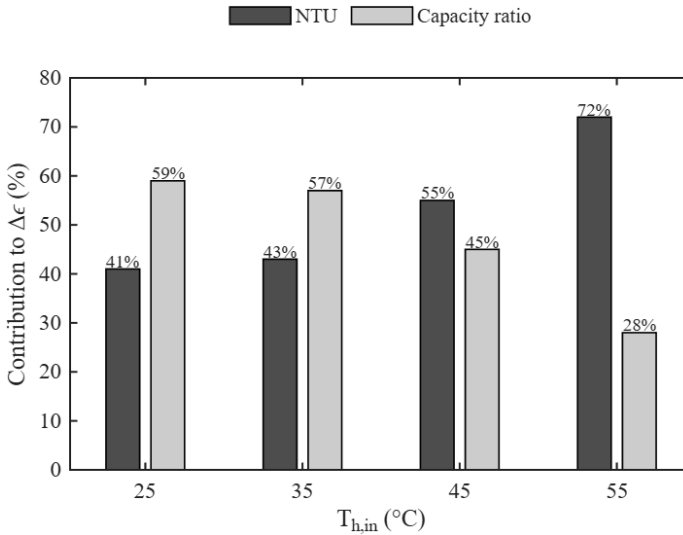


Figure 2: Percentage contributions of the NTU increase and the capacity-ratio reduction to the total effectiveness increase between $Re = 6000$ and $Re = 18000$, at the four hot-side inlet temperatures.

The dominant effect changes with the inlet temperature. At 25 °C the larger part of the increase in effectiveness, 59%, results from the reduction in the capacity ratio rather than the improvement in heat transfer. At 55 °C the

situation is reversed, and 72% of the increase results from the rise in NTU. The reason for this change becomes clear when the two effects are considered in absolute terms rather than as percentages. The effect of the capacity ratio remains almost constant across the four temperatures, whereas the effect of NTU increases by a factor of more than four between 25 °C and 55 °C. The change is therefore caused by the increasing effect of NTU, which is consistent with its stronger increase at higher inlet temperatures.

This result refines an earlier conclusion reported for the same exchanger [32], in which the inlet temperature was found to affect performance mainly through the capacity ratio. The present analysis shows that this holds at lower inlet temperatures but changes above approximately 45 °C. It should be noted that the separation is a first-order one, as the interaction between the two variables is not fully accounted for, so the values represent the relative weights of the two effects rather than an exact balance.

Comparison with the Classical Effectiveness-NTU Relation

Since the effectiveness, NTU and capacity ratio are known at every operating point, the classical counter-flow relation can be tested quantitatively rather than used only as a qualitative check. Each measured pair of NTU and capacity ratio was substituted into the counter-flow relation, and the resulting effectiveness was compared with the measured value. The deviation, defined as the predicted value minus the measured value expressed as a percentage of the measured value, is shown in Figure 3.

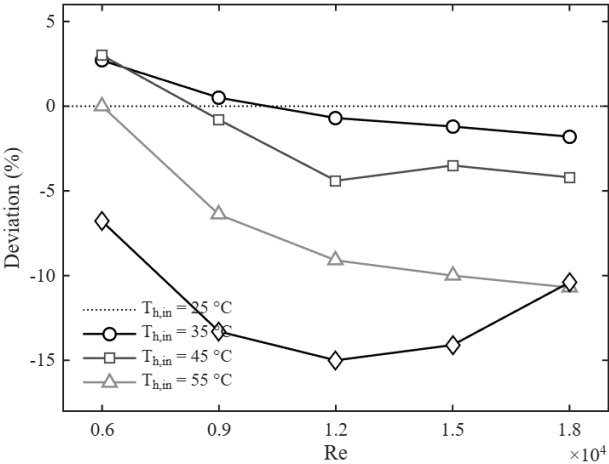


Figure 3: Deviation of the classical counter-flow relation from the measured effectiveness as a function of Reynolds number, at the four hot-side inlet temperatures.

The relation agrees closely with the measurements at the lower inlet temperatures and departs from them as the temperature increases. At 25 °C the agreement is within 3% of every Reynolds number, and at 35 °C within

about 4%. This level of agreement is comparable to the combined uncertainty of the temperature and flow measurements and supports both the data reduction procedure and the assumed counter-flow arrangement. As the inlet temperature increases, the deviation grows, reaching about 11% at 45 °C and 15% at 55 °C.

The sign of the deviation is also informative. At the higher inlet temperatures the predicted effectiveness is consistently lower than the measured value. Since the counter-flow arrangement gives the highest effectiveness attainable for a given NTU and capacity ratio, this indicates that NTU has been underestimated at these temperatures rather than that the exchanger exceeds the theoretical limit. The most likely reason is the constant-property assumption used in evaluating the overall heat transfer coefficient, since the dynamic viscosity of water decreases by about half between 25 °C and 55 °C, so that properties taken at the inlet temperature understate the true heat transfer at higher temperatures. The maximum deviation of about 15% nevertheless remains within an acceptable range for engineering heat transfer analysis, and the classical relation therefore provides a reliable estimate at low and moderate inlet temperatures. This limitation motivates the correlations developed in the following section, which are obtained directly from the measurements and thus include the temperature dependence without relying on the constant-property assumption.

Development of Dimensionless Correlations

Dimensionless correlations were developed for the three quantities examined in this study, each expressed as a power-law function of the Reynolds number and the inlet temperature ratio θ . A power-law form was selected because its exponents indicate directly how strongly each variable influences the predicted quantity. The correlations obtained are:

$$\varepsilon = 0.0521Re^{0.224}\theta^{3.349}$$

$$NTU = 0.1504Re^{0.161}\theta^{2.832}$$

$$c = 121.24Re^{(-0.565)}\theta^{(-1.885)}$$

The correlations are valid over the range covered by the experiments and should not be extrapolated beyond it. This range extends from a Reynolds number of 6000 to 18000 and a hot-side inlet temperature of 25 °C to 55 °C, with the cold-side inlet temperature held constant at 20 °C. The corresponding capacity ratio varies from 0.40 to 0.85 and NTU from 0.69 to 1.10, with pure water as the working fluid on both sides. The accuracy of each correlation is summarized in Table 3.

Table 3: Accuracy of the developed correlations.

Predicted quantity	R^2	Mean deviation	Maximum deviation
Effectiveness, ϵ	0.943	3.1%	6.8%
NTU	0.873	3.4%	8.7%
Capacity ratio, c	0.984	2.6%	8.0%

The three correlations differ in accuracy in a way that reflects the nature of each quantity. The capacity ratio is represented most closely, with $R^2 = 0.984$, because it is determined almost entirely by the mass flow rates and fluid properties and does not involve the heat transfer process itself. The effectiveness follows, with $R^2 = 0.943$. The NTU correlation gives the lowest value, $R^2 = 0.873$, and the reason is structural rather than numerical: a single power-law function increases continuously with the Reynolds number and therefore cannot reproduce the levelling-off of NTU at the lower inlet temperatures. As a result, the correlation overestimates NTU at high Reynolds numbers for 25 °C and underestimates it at 55 °C. A functional form that allows this levelling-off would improve the fit, but at the expense of the simple interpretability that the power-law form provides.

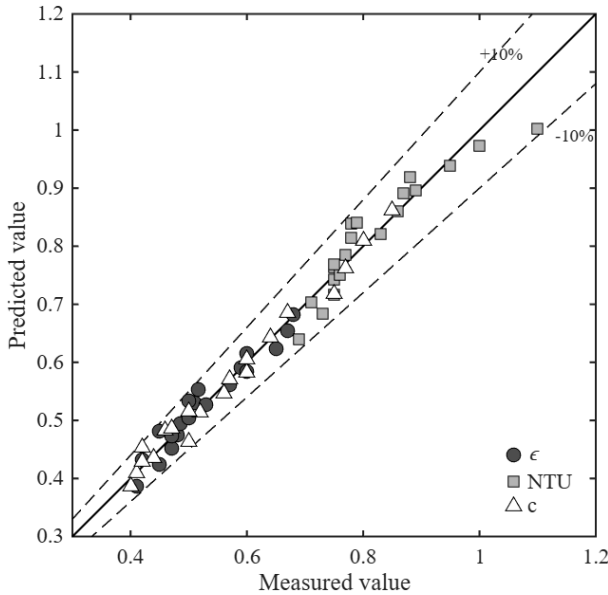


Figure 4: Comparison of the values predicted by the three correlations with the measured values of effectiveness, NTU and capacity ratio.

Figure 4 compares the values predicted by the three correlations with the corresponding measured values. All predicted values lie within $\pm 10\%$ of the measurements, and the points are distributed closely around the line of

perfect agreement, confirming that the correlations represent the experimental data reliably across the tested range.

CONCLUSION

The thermal performance of a counter-flow plate heat exchanger was examined through the effectiveness-NTU framework, with the number of transfer units and the capacity ratio treated as primary results rather than as intermediate quantities. The main findings are as follows.

1. The increase in NTU with the Reynolds number depends strongly on the inlet temperature. At 25 °C the increase is essentially complete by $Re = 12000$, whereas at 55 °C NTU continues to rise throughout the tested range, with a total increase of 39.2%. Because the transfer area is fixed and the cold stream is held constant, this behavior reflects the overall heat transfer coefficient alone: once the hot-side resistance becomes much smaller than the fixed cold-side resistance, a further increase in velocity has little effect.

2. The mechanism that improves effectiveness changes with the inlet temperature. At 25 °C, 59% of the increase in effectiveness results from the reduction in the capacity ratio and 41% from the rise in NTU, whereas at 55 °C these proportions are reversed to 28% and 72%. This reversal is caused by the increasing effect of NTU at higher inlet temperatures, while the effect of the capacity ratio remains almost constant.

3. The classical counter-flow relation agrees with the measurements to within 3% at 25 °C, but the deviation increases with the inlet temperature and reaches about 15% at 55 °C. The sign of the deviation indicates that NTU is underestimated at the higher inlet temperatures, most likely because of the constant-property assumption used in evaluating the overall heat transfer coefficient. This deviation nevertheless remains within an acceptable range for engineering analysis.

4. Three dimensionless correlations were developed for effectiveness, NTU and the capacity ratio in terms of the Reynolds number and the inlet temperature ratio, with coefficients of determination of 0.943, 0.873 and 0.984 respectively. All predicted values lie within $\pm 10\%$ of the measured values. The correlations are valid for Reynolds numbers from 6000 to 18000 and hot-side inlet temperatures from 25 °C to 55 °C, with a constant cold-side inlet temperature of 20 °C.

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Adsorption in Metal-Organic Framework (MOF)-Based Nanocomposite Materials:

Part A: Mechanisms

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ABSTRACT

Metal–organic frameworks (MOFs) and MOF-based nanocomposites offer exceptionally high specific surface areas, tunable pore structures, and extensive functionalization potential for adsorption. This Part A focuses on the fundamental structure and chemistry of MOFs and on the mechanisms governing adsorption in MOF-based nanocomposites, including pore filling and molecular sieving, coordination at open metal sites, electrostatic interaction and ion exchange, Lewis acid–base interaction and surface complexation, hydrogen bonding, π – π /hydrophobic interactions, and adsorption–detoxification coupling in redox-active MOFs. It also examines adsorption isotherms, kinetic models, thermodynamic parameters, MOF-specific pore-filling models, and operational parameters affecting adsorption performance.

Keywords – Metal-organic framework (MOF); nanocomposite; adsorption mechanisms; pore filling; open metal sites; electrostatic interaction; adsorption isotherms; adsorption kinetics; thermodynamics.

INTRODUCTION

Rapid industrialization, urbanization, agricultural intensification, and population growth have released a wide range of contaminants-including heavy metals, synthetic dyes, antibiotics, per- and polyfluoroalkyl substances (PFAS), radionuclides, and various anionic species-into surface and groundwater. These contaminants are commonly characterized by resistance to biodegradation, potential toxicity or endocrine-disrupting effects even at low concentrations, and the ability to bioaccumulate in food chains (Bai et al., 2017; Meena et al., 2025).

PFAS compounds, in particular, are commonly referred to as “forever chemicals” because of their environmental persistence and bioaccumulation potential, and they are reported to be exceptionally resistant to environmental degradation (Cousins et al., 2020).

In April 2024, the U.S. Environmental Protection Agency (EPA) issued the National Primary Drinking Water Regulation (NPDWR) for PFAS, establishing individual maximum contaminant levels and a hazard index for specified PFAS mixtures (U.S. Environmental Protection Agency, EPA, 2024).

Although conventional methods such as precipitation, ion exchange, membrane filtration, electrochemical treatment, and biological treatment can

be effective to a certain extent, they present several limitations, including high operating costs, secondary waste/sludge generation, limited selectivity, and inadequate performance at low contaminant concentrations. Adsorption is widely used in water and wastewater treatment because of its operational simplicity, relatively low energy demand, high removal efficiency, and the possibility of adsorbent regeneration under appropriate conditions (Crini & Lichtfouse, 2019; Wang & Peng, 2010).

However, the limitations of activated carbon, zeolites, clays, and conventional biomass-based adsorbents in terms of adsorption capacity, selectivity, control over pore structure, and surface functionalization have directed researchers toward advanced porous materials with higher surface areas, tunable pore architectures, and functional groups tailored to target contaminants (Ghosh et al., 2019).

In this context, metal-organic frameworks (MOFs) emerged in the early 1990s as a product of developments in coordination chemistry and crystal engineering and have become one of the most prominent classes of materials in adsorption science over the past two decades. MOFs consist of secondary building units (SBUs), composed of metal ions or metal-ion clusters, connected by organic linkers to form ordered porous networks (Furukawa et al., 2013). The ability of some MOFs to achieve Langmuir surface areas exceeding 7000 m²/g, the nearly unlimited combinations of metal nodes and organic linkers, and the molecular-level tunability of pore size and chemistry are among the key features that distinguish MOFs from conventional porous adsorbents (Mahreni et al., 2020).

Nevertheless, practical limitations of pristine MOFs—including difficulties associated with handling them as powders, limited water/moisture stability, low mechanical strength, and performance losses upon reuse—have encouraged their integration with magnetic nanoparticles, graphene/graphene oxide, biochar, polymer matrices, and secondary metal/MOF phases to form nanocomposites. Such MOF-based nanocomposites combine the high porosity of the MOF with the mechanical strength, magnetic separability, or additional functional groups of the supporting/secondary component, thereby providing synergistic performance enhancement (Zamel et al., 2025).

Adsorption-based separation is governed not only by the accessible surface area of an adsorbent but also by the chemical nature, spatial distribution, and energetic heterogeneity of its adsorption sites. Metal-organic

frameworks (MOFs) provide an unusually versatile platform for examining these relationships because their metal nodes, organic linkers, pore dimensions, topology, and surface functionality can be tuned at the molecular level. When MOFs are integrated with secondary phases to form nanocomposites, the resulting interfaces introduce additional binding environments and transport pathways, making adsorption behavior inherently multimechanistic (Easun et al., 2017).

Accordingly, a mechanistic interpretation of adsorption in MOF-based nanocomposites requires consideration of both framework structure and adsorbate properties. Pore filling and molecular sieving are controlled by pore dimensions and connectivity, whereas coordinatively unsaturated metal centers can promote direct Lewis acid-base coordination. Surface charge and solution chemistry govern electrostatic attraction and ion exchange, while hydrogen bonding, π - π interactions, hydrophobic interactions, and surface complexation may become dominant for specific organic molecules or ionic contaminants. In redox-active frameworks, adsorption may additionally be coupled with chemical transformation or detoxification of the captured species (Easun et al., 2017; Maia et al., 2021).

Quantitative interpretation is equally important for distinguishing these contributions. Equilibrium isotherms provide information on adsorption capacity and surface heterogeneity, kinetic models describe the rate and possible transport limitations of uptake, and thermodynamic parameters indicate the energetic feasibility and temperature dependence of the process. MOF-specific pore-filling and molecular-simulation approaches further extend conventional adsorption models for highly porous frameworks. Operational variables such as pH, adsorbent dosage, contact time, temperature, ionic strength, competing ions, and relative humidity can alter both the dominant mechanism and the observed adsorption performance (Essalmi et al., 2024; Maia et al., 2021).

Part A therefore focuses specifically on the mechanistic foundations of adsorption in MOFs and MOF-based nanocomposites. After outlining the structural and chemical features that determine adsorption-site accessibility, it critically examines the principal adsorption mechanisms, isotherm and kinetic descriptions, thermodynamic interpretation, pore-filling models, and operating parameters that control adsorption performance. This mechanistic framework provides the conceptual basis for understanding why different

MOF architectures and nanocomposite interfaces exhibit distinct adsorption behaviors.

FUNDAMENTAL STRUCTURE AND CHEMISTRY OF MOFs

Secondary Building Units and Organic Linkers

The building blocks of MOFs consist of two principal components: (i) secondary building units (SBUs), composed of metal ions or multinuclear metal–oxo clusters, and (ii) long-chain organic linkers containing functional groups such as carboxylate, imidazolate, and pyrazolate that connect these units. The geometry of the SBUs (e.g., octahedral, trigonal-prismatic, or square-planar) and the length and angle of the linker largely determine the topology, pore size, and pore geometry of the resulting MOF. In some MOF families (e.g., HKUST-1 and MOF-74), coordination sites on the SBU are initially occupied by solvent molecules and become vacant after activation; these sites, known as open metal sites (OMS), provide strong binding sites for adsorption (Furukawa et al., 2013).

Porosity, Surface Area, and Topological Diversity

One of the most distinctive characteristics of MOFs is the presence of ordered, interconnected micro- and mesopores within the crystal structure. These pores provide accessible internal surface area for gas storage, molecular sieving, and adsorption applications. Within the concept of reticular synthesis, MOF series with the same topology but different pore dimensions can be obtained by using organic linkers of different lengths; such isorecticular MOFs (e.g., the IRMOF family) allow systematic tuning of pore size (Furukawa et al., 2013). Some MOFs reported in the literature, including NU-1000, MOF-808, and PCN-224, exhibit hierarchical structures containing both micro- and mesopores, which can facilitate the diffusion of relatively large molecules such as PFAS and antibiotics (Li et al., 2021).

Major MOF Families

Although tens of thousands of different MOF structures have been reported, only a limited number of MOF families are frequently used in adsorption applications and preferred as supporting or primary components in nanocomposite production. These include zinc–imidazolate zeolitic

imidazolate frameworks (ZIFs; e.g., ZIF-8 and ZIF-67), zirconium–carboxylate UiO series (UiO-66 and UiO-67), copper–trimesate HKUST-1, aluminum/chromium/iron–terephthalate MIL series (MIL-53, MIL-100, and MIL-101), zinc–terephthalate MOF-5 family, magnesium/nickel–dihydroxyterephthalate MOF-74 family, and zirconium–porphyrin PCN series (PCN-222, PCN-224, PCN-999, and PCN-250). Table 1 comparatively summarizes the metal centers, typical BET surface areas, pore characteristics, water stability, and major application areas of representative MOF families. Figure 1 provides a schematic representation of the MOF structure.

Table 1. Comparative characteristics of major MOF families frequently used in adsorption applications

MOF Family	Typical Metal / Linker	BET Surface Area (m ² /g)	Water Stability	Key Application	References
ZIF-8	Zn ²⁺ / 2-methylimidazolate	~1300–1900	High	Gas separation, DAC, membranes	Singh et al., 2025
UiO-66 / UiO-67	Zr ₆ O ₄ (OH) ₄ / terephthalate, biphenyldicarboxylate	~1000–3000	High	PFAS, heavy metals, gas adsorption	Ilić et al., 2025
HKUST-1 (Cu-BTC)	Cu ²⁺ / trimesate (open-metal site)	~1500–1850	Moderate–Low	CO ₂ /gas adsorption, Hg ⁰ removal	Wang et al., 2025
MIL-53 / MIL-100 / MIL-101	Al ³⁺ , Cr ³⁺ , Fe ³⁺ / terephthalate, trimesate	~1500–4500	Moderate–High (MIL-101 Cr)	Heavy metal, dye, antibiotic removal	Rani et al., 2020
MOF-5 / MOF-74	Zn ²⁺ , Mg ²⁺ , Ni ²⁺ / terephthalate, dihydroxyterephthalate	~800–3800	Low–Moderate	Gas storage, decarbonization	Choi et al., 2008
PCN-222/224/999	Zr ₆ cluster/porphyrin linker	~2000–2600	High	PFAS removal, photocatalysis	Zhang et al., 2024
MOF-808 / CALF-20	Zr ₆ cluster; Zn ²⁺ -oxalate/triazolate	~1500–2000 / ~500–600	High	PFAS (MOF-808), industrial CO ₂ capture (CALF-20)	Oktavian et al., 2024

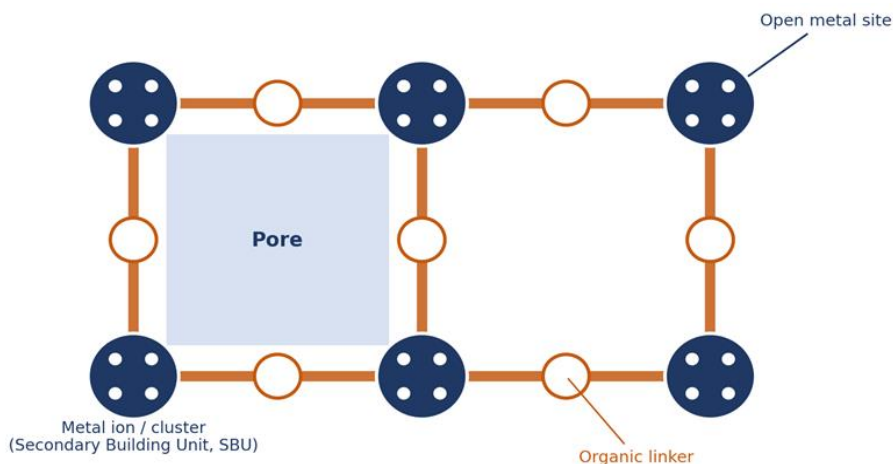


Figure 1. Schematic representation of a metal-organic framework (MOF): metal nodes (SBUs), organic linkers, and micro/mesoporous voids.

ADSORPTION MECHANISMS IN MOFs AND MOF-BASED NANOCOMPOSITES

Adsorption in MOF-based nanocomposites does not generally proceed through a single mechanism; rather, multiple mechanisms often operate simultaneously. Their relative contributions depend on the Lewis acidity of the MOF metal center, the functional groups of the linker, pore size and geometry, the surface chemistry of the support/secondary component, and the molecular structure of the target contaminant. Figure 2 summarizes the principal mechanisms operating simultaneously in MOF-based nanocomposite adsorbents.

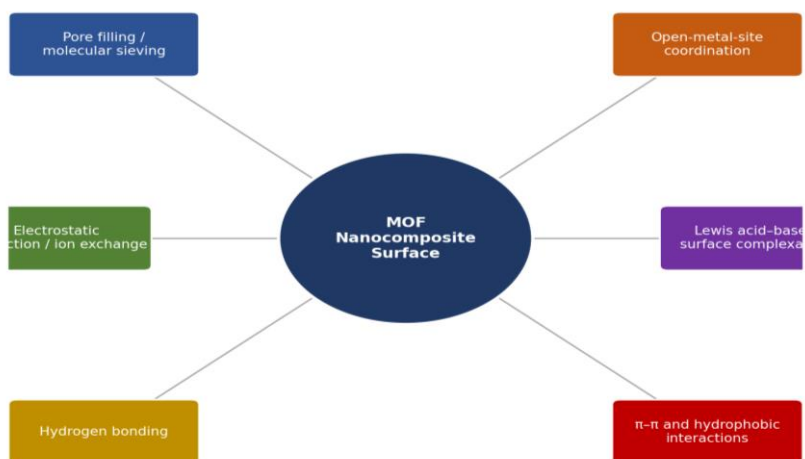


Figure 2. Principal adsorption mechanisms operating simultaneously in MOF-based nanocomposite adsorbents.

Pore Filling and Molecular Sieving

The ordered micro/mesoporous structure of MOFs provides a selective molecular-sieving effect depending on the size and shape of adsorbate molecules. The narrow pore aperture of ZIF-8, approximately 0.34 nm, permits selective adsorption of small gas molecules such as CO₂ while restricting the entry of larger molecules (Kadhom & Deng, 2018). In contrast, hierarchical micro–mesoporous MOFs such as NU-1000, MOF-808, and PCN-999 facilitate diffusion of relatively large and amphiphilic molecules such as PFAS into the pores and can reach equilibrium on the order of seconds (Li et al., 2021).

Open Metal Sites Coordination

In MOFs containing coordinatively unsaturated sites, such as HKUST-1, MOF-74, and some MIL structures, metal centers exposed after activation act as strong Lewis-acid sites and can form direct coordination bonds with electron-donating molecules such as CO₂, H₂S, and NO (Keshavarz et al., 2026). Compared with physisorption, this mechanism provides higher binding energies and high selectivity even at low partial pressures; however, the strong affinity of open metal sites for water molecules can lead to competitive adsorption between CO₂ and water under humid conditions (Camarere et al., 2025).

Electrostatic Interaction and Ion Exchange

The net charge arising from functional groups on the MOF surface or on the support component (GO, biochar) generates electrostatic attraction with oppositely charged ions in solution. The direction and magnitude of this interaction depend on solution pH; for anionic contaminants such as PFAS, positively charged MOFs containing cationic metal centers or protonated amino groups have been reported to exhibit higher adsorption efficiency (Li et al., 2021). For heavy-metal cations, ion exchange involving the replacement of exchangeable protons or alkali-metal ions on the MOF surface by target metal ions is frequently reported (Ghumman et al., 2025).

Lewis Acid–Base Interaction and Surface Complexation

MOF metal centers can act as electron-pair acceptors (Lewis acids) and form inner-sphere complexes with contaminants bearing electron-donating (Lewis-base) groups such as hydroxyl, carboxyl, or amino groups. This mechanism plays a dominant role particularly in the removal of heavy-metal oxyanions (arsenate, chromate, selenite) and anionic species such as fluoride and phosphate; in the Al@Fe-MOF nanocomposite, Se(IV) adsorption capacity and free adsorption energy were reported to increase markedly relative to pristine Fe-MOF (Zamel et al., 2025).

Hydrogen Bonding

Hydrogen bonds formed between carbonyl, hydroxyl, and amino groups in MOF linkers and electronegative atoms in antibiotic, dye, or PFAS molecules make an important contribution to adsorption. Hydrogen bonding and van der Waals interactions have been reported as key driving mechanisms in antibiotic adsorption, while the size, geometry, and functional groups of the antibiotic directly affect adsorption behavior. Hydrogen bonding, ligand interactions, and amidation reactions have also been shown to act together in tetracycline removal (Islam et al., 2025).

π - π and Hydrophobic Interactions

π - π stacking and hydrophobic interactions may occur between aromatic-ring-containing MOF linkers (terephthalate, trimesate, and porphyrin derivatives) and aromatic/hydrophobic groups in dyes, antibiotics, or PFAS molecules. For PFOS removal by PCN-224, a very high maximum

capacity of 963 mg/g has been attributed to multiple adsorption sites arising from the combined action of orthogonal cationic channel pores, hydrophobic porphyrin units, and acidic Zr_6 clusters (Zhang et al., 2024).

Adsorption–Detoxification Coupling in Redox-Active MOFs

Some MOFs can not only physically or chemically adsorb contaminants but also reduce the toxicity of the adsorbed species through redox activity. In the redox-active Co/Ni/Cu-HHTP MOF series, framework architecture and the metal coordination environment determine adsorption capacity as well as redox activity and sensing performance, enabling simultaneous capture, in situ detoxification, and real-time monitoring of heavy-metal cations on a single material platform (Damacet et al., 2026).

ISOTHERM, KINETIC, AND THERMODYNAMIC PARAMETERS

Adsorption Isotherms

Adsorption isotherms describe the relationship between the amount of adsorbate at equilibrium and its equilibrium concentration in solution at a constant temperature and provide information on the surface properties of MOF/nanocomposite adsorbents. The Langmuir isotherm assumes monolayer adsorption on a homogeneous surface and provides the maximum adsorption capacity (q_{max}) and Langmuir constant (K_L), whereas the Freundlich isotherm is an empirical model describing multilayer adsorption on heterogeneous surfaces. The Temkin isotherm assumes a linear decrease in the heat of adsorption with increasing adsorbate–adsorbent interactions. The Dubinin–Radushkevich (D–R) isotherm provides an average free-energy parameter useful for distinguishing physical from chemical adsorption. The Sips isotherm (combined Langmuir–Freundlich isotherm) is a three-parameter adsorption equation combining characteristics of the Langmuir and Freundlich models. It therefore combines the theoretical basis of Langmuir with the empirical nature of Freundlich: at low concentrations it behaves similarly to the Freundlich model, whereas at high concentrations it approaches a saturation limit analogous to the Langmuir model (De Vargas Brião et al., 2023).

Reported isotherm fits for MOF-based adsorbents vary with both material family and contaminant type. Adsorption of Congo red and methylene blue by $\text{MnFe}_2\text{O}_4@\text{MOF}-5$ was found to fit the Langmuir isotherm well (Akinbola et al., 2025), while methylene-blue adsorption by the $\text{UiO}-66/\text{MIL}-101(\text{Fe})-\text{GOCOOH}$ composite also followed the Langmuir model ($q_{\text{max}} = 448.71 \text{ mg/g}$) (Eltaweil et al., 2020). For tetracycline adsorption, experimental data for MOF-5 were reported to be well described by the Freundlich and Sips isotherms (Islam et al., 2025). This variation indicates that adsorbent surface chemistry—whether characterized by homogeneous open metal sites or heterogeneous distributions of functional groups—directly shapes isotherm behavior. Figure 3 presents the maximum adsorption capacities (q_{max} , mg/g) of selected MOF-based (nano)composite adsorbents for different contaminant groups, compiled from the literature.

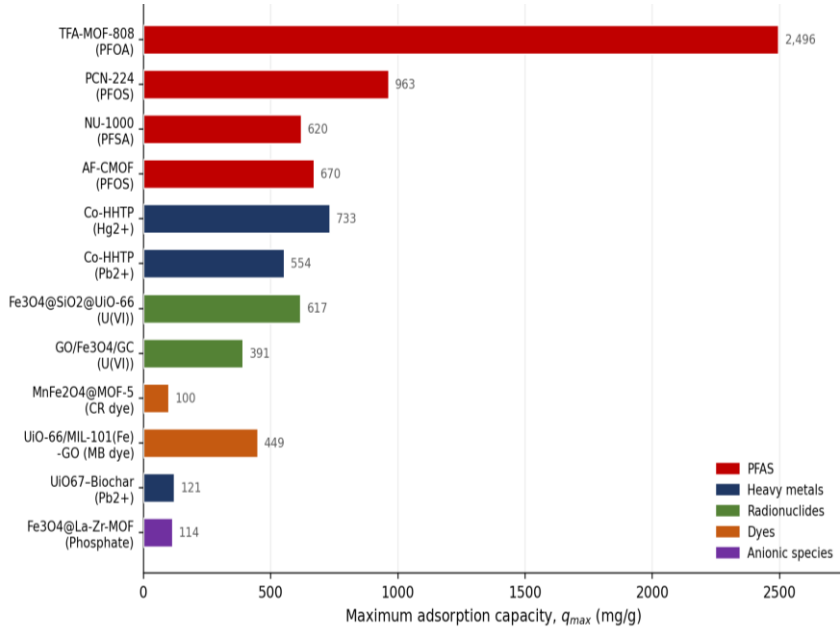


Figure 3. Maximum adsorption capacities (q_{max} , mg/g) of selected MOF-based (nano)composite adsorbents for different contaminant groups, compiled from the literature.

Adsorption Kinetics

Kinetic models describe the adsorption rate and the approach of the process toward equilibrium. The pseudo-first-order (Lagergren) model generally describes systems dominated by physisorption, whereas the pseudo-

second-order model more appropriately describes systems in which chemisorption is the rate-determining step (Ho et al., 1999). The intraparticle-diffusion (Weber-Morris) model is used to analyze multistage diffusion processes (Weber et al., 1963). U(VI) adsorption kinetics in the GO/Fe₃O₄/GC magnetic composite followed the pseudo-second-order model (Yang et al., 2021), and the same kinetic behavior was observed for both Congo red and methylene blue in MnFe₂O₄@MOF-5 (Akinbola et al., 2025). In the UiO-66/MIL-101(Fe)-GOCOOH composite, fitting to the intraparticle-diffusion model indicated that adsorption proceeded through three stages (Eltaweil et al., 2020). Table 2 presents the isotherm and kinetic models frequently used in MOF-based adsorption studies.

Table 2. Isotherm and kinetic models frequently used in MOF-based adsorption studies.

Model	General Equation (simplified)	Physical Meaning
Langmuir	$q_e = q_{\max} \cdot K_L \cdot C_e / (1 + K_L \cdot C_e)$	Homogeneous surface, monolayer adsorption
Freundlich	$q_e = K_F \cdot C_e^{(1/n)}$	Heterogeneous surface, multilayer adsorption
Temkin	$q_e = (RT/b) \cdot \ln(A_T \cdot C_e)$	Linearly decreasing heat of adsorption
Dubinin–Radushkevich	$q_e = q_s \cdot \exp(-K_{ad} \cdot \epsilon^2)$	Distinction between physical/chemical adsorption, average free energy
Pseudo-first-order	$dq_t/dt = k_1(q_e - q_t)$	Rate expression dominated by physisorption
Pseudo-second-order	$dq_t/dt = k_2(q_e - q_t)^2$	Rate expression dominated by chemisorption
Intraparticle diffusion	$q_t = k_{id} \cdot t^{0.5} + C$	Multistage diffusion process

Thermodynamic Parameters

Thermodynamic analyses use parameters such as the standard Gibbs free-energy change (ΔG°), enthalpy change (ΔH°), and entropy change (ΔS°) to determine whether adsorption is spontaneous and whether it is exothermic or endothermic. U(VI) adsorption on GO/Fe₃O₄/GC was reported to be endothermic but spontaneous, with $\Delta H^\circ = 11.57$ kJ/mol and $\Delta G^\circ < 0$. In contrast, methylene-blue adsorption on the UiO-66/MIL-101(Fe)-GOCOOH composite was shown to be endothermic and spontaneous, with both physisorption and chemisorption characteristics (Eltaweil et al., 2020).

MOF-Specific Pore-Filling Models

For describing gas and vapor adsorption in highly porous MOFs, the Dubinin-Astakhov (D-A) pore-filling model and molecular-simulation-based

grand canonical Monte Carlo (GCMC) approaches are frequently used in addition to conventional Langmuir/Freundlich models. In modeling water-vapor adsorption–desorption cycles, experimental isotherms can be interpreted using density functional theory (DFT); in the case of CALF-20, framework flexibility and water–framework interactions have been shown to directly affect adsorption behavior (Oktavian et al., 2024).

PARAMETERS AFFECTING ADSORPTION PERFORMANCE

The performance of MOF-based nanocomposite adsorbents is affected by numerous operational parameters, including solution pH, adsorbent dosage, contact time, initial contaminant concentration, temperature, ionic strength, and coexisting competing ions.

- pH: pH directly affects the direction and magnitude of electrostatic interactions by determining both the surface charge of the MOF/nanocomposite and the ionization state of the contaminant. In the MnFe₂O₄@MOF-5 composite, 100% removal of Congo red was achieved at neutral pH, whereas increasing the adsorbent dosage had no pronounced effect on the sorption process (Akinbola et al., 2025). The optimum pH for PFOS removal was reported to be around 3, and protonated surface groups at low pH increased electrostatic attraction toward anionic PFAS (Loughran et al., 2023).
- Adsorbent dosage and contact time: In general, removal efficiency increases with increasing adsorbent dosage and contact time, but equilibrium is reached after a certain saturation point; in hierarchical porous MOFs such as NU-1000, equilibrium can be reached in less than one minute (Liu et al., 2026).
- Temperature: Depending on whether adsorption is exothermic or endothermic, increasing temperature may increase or decrease capacity; in GO/Fe₃O₄/GC, capacity increased with temperature because U(VI) adsorption was endothermic (Yang et al., 2021).
- Ionic strength and competing ions: Competition between other ions in solution (Na⁺, K⁺, Mg²⁺, Ca²⁺, Al³⁺, Cl[−], SO₄^{2−}, etc.) and the target contaminant for adsorption sites can reduce selectivity and overall capacity; however, coexisting anions and humic acid were reported to

have a negligible effect on PFOS adsorption by PCN-224 (Amari et al., 2024).

- Relative humidity (gas/vapor adsorption): In CO₂ capture applications, high relative humidity may reduce capacity through competition from water for open metal sites; therefore, development of water-stable, humidity-tolerant MOFs such as CALF-20 and MIL-120 is critical for industrial applicability (Loughran et al., 2023).

Table 3 summarizes representative adsorption performance of MOF-based nanocomposite adsorbents for different contaminant classes together with the corresponding isotherm and kinetic models.

Table 3. Representative adsorption performance of MOF-based nanocomposite adsorbents for different contaminant classes, together with appropriate isotherm and kinetic models.

Adsorbent	Target Contaminant	q _{max} (mg/g)	Isotherm	Kinetics	References
Co-HHTP MOF	Hg ²⁺	733	-	-	Damacet et al., 2026
Co-HHTP MOF	Pb ²⁺	554	-	-	Damacet et al., 2026
Co-HHTP MOF	Cd ²⁺	169	-	-	Damacet et al., 2026
UiO-67-biochar (MBC)	Pb(II)	121.1	-	Pseudo-second-order	Ghaedi et al., 2025
UiO-67-biochar (MBC)	Cd(II)	59.7	-	Pseudo-second-order	Ghaedi et al., 2025
Fe ₃ O ₄ @SiO ₂ @UiO-66	U(VI)	616.5	Langmuir	-	Zamel et al., 2025
GO/Fe ₃ O ₄ /GC	U(VI)	390.7	Langmuir	Pseudo-second-order	Zhang et al., 2025
Fe ₃ O ₄ @La-Zr-MOF	Phosphate	113.6	Langmuir	Pseudo-second-order	Yang et al., 2021
MnFe ₂ O ₄ @MOF-5	Methylene blue	88.9	Langmuir	Pseudo-second-order	Akinbola et al., 2025
MnFe ₂ O ₄ @MOF-5	Congo red	100	Langmuir	Pseudo-second-order	Akinbola et al., 2025
UiO-66/MIL-101(Fe)-GOCOOH	Methylene blue	448.71	Langmuir	Pseudo-first-/second-order	Eltaweil et al., 2020
C/NiFe-LDH composite	Methyl orange	323.6	Langmuir	Pseudo-second-order	Murtaza et al., 2024
C/NiFe-LDH composite	Congo red	448.4	Langmuir	Pseudo-second-order	Murtaza et al., 2024
Fe ₃ O ₄ @MIL-53(Al)	Congo red	234.4	-	-	Zhang et al., 2021
Fe ₃ O ₄ @MIL-53(Al)	Bisphenol A	160.9	-	-	Zhang et al., 2021
TFA-MOF-808	PFOA	2496	-	-	Zhang et al., 2024

PCN-224	PFOS	963	-	-	Zhang et al., 2024
PCN-224	PFHxS	517	-	-	Zhang et al., 2024
NU-1000	PFSA (general)	400–620	-	Rapid (<1 min)	Liu et al., 2026
AF-CMOF (Cu-MOF/SiO ₂)	PFOS	670	-	-	Amari et al., 2024
Al-PMOF (Co-doped)	CO ₂	3.32 mmol/g	-	-	Shang et al., 2022
Cu-NH ₂ @MOF-303	Water vapor (AWH)	+38% (relative to reference)	-	Instantaneous (~0.1 min)	Singh et al., 2025

CONCLUSION

Part A demonstrates that adsorption in MOF-based nanocomposites is best understood as the combined outcome of pore architecture, metal-node chemistry, linker functionality, interfacial properties, and adsorbate characteristics rather than as a single universal mechanism. Pore filling and molecular sieving govern access to internal adsorption space, while open metal sites can provide strong coordination interactions. Electrostatic attraction and ion exchange are strongly dependent on solution chemistry, whereas Lewis acid-base interactions, surface complexation, hydrogen bonding, π - π stacking, and hydrophobic interactions provide additional selectivity toward specific ionic and organic adsorbates. Redox-active frameworks further broaden this mechanistic landscape by coupling adsorption with chemical transformation.

The review of equilibrium, kinetic, and thermodynamic descriptions also shows that model selection must be linked to the physicochemical characteristics of the adsorbent-adsorbate system. Langmuir-, Freundlich-, Sips-, Temkin-, and Dubinin-type approaches describe different aspects of surface heterogeneity and pore filling, while pseudo-first-order, pseudo-second-order, and intraparticle-diffusion models provide complementary information on uptake rates and transport limitations. Thermodynamic parameters and MOF-specific pore-filling or molecular-simulation approaches are valuable for interpreting energetic effects that cannot be captured by capacity data alone.

Overall, the mechanistic performance of MOF-based nanocomposites is highly sensitive to pH, contact time, adsorbent dosage, temperature, ionic strength, competing species, and humidity. Future mechanistic studies should

therefore integrate structural characterization with equilibrium, kinetic, thermodynamic, and transport analyses under realistic multicomponent conditions. Such an integrated approach is essential for establishing reliable structure-property-mechanism relationships and for guiding the rational design of MOF-based nanocomposites with predictable adsorption selectivity, capacity, and rate.

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Adsorption in Metal-Organic Framework (MOF)-Based Nanocomposite Materials: Part B: Synthesis Strategies and Applications

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ABSTRACT

Metal-organic frameworks (MOFs) and MOF-based nanocomposites are attractive adsorbents because of their high porosity, tunable pore chemistry, and capacity for integration with functional secondary phases. This Part B focuses on MOF synthesis strategies and the principal classes of MOF-based nanocomposite adsorbents, including magnetic MOFs, graphene/graphene oxide-MOF composites, biochar-MOF composites, mixed-matrix systems, bimetallic/multivariate MOFs, and core-shell hybrids. Applications in heavy-metal, dye, antibiotic, PFAS, radionuclide, and anionic-species removal, as well as CO₂ capture and atmospheric water harvesting, are examined together with water stability, regeneration, reusability, scalability, cost, environmental sustainability, current challenges, and future perspectives.

Keywords – Metal-organic framework (MOF); nanocomposite; synthesis strategies; magnetic MOF; graphene oxide-MOF; biochar-MOF; PFAS; heavy-metal removal; CO₂ capture; atmospheric water harvesting.

INTRODUCTION

The practical value of metal-organic frameworks (MOFs) as adsorbents depends not only on their intrinsic porosity and surface chemistry but also on how they are synthesized, processed, combined with secondary phases, and deployed under realistic operating conditions. Crystal size, phase purity, pore accessibility, defect density, morphology, and surface functionality can all be altered by the synthesis route. Consequently, the transition from a pristine MOF powder to an application-oriented nanocomposite requires deliberate control of both framework formation and composite architecture (Li et al., 2021; Mourdikoudis, 2025).

Solvothermal and hydrothermal routes remain central to MOF production, while microwave-assisted, sonochemical, electrochemical, and mechanochemical methods offer opportunities to reduce synthesis time, modify particle characteristics, or decrease solvent and energy requirements. Post-synthetic modification and exchange provide additional routes for introducing target-specific binding sites without completely reconstructing the parent framework. At the same time, integration with magnetic nanoparticles, graphene or graphene oxide, biochar, polymers, secondary metals, or other MOF phases can address limitations associated with powder handling, separation, mechanical robustness, water stability, and regeneration (Li et al., 2021; Mourdikoudis, 2025).

These synthesis and composite-design strategies have enabled MOF-based adsorbents to be applied across a wide spectrum of separation problems. Representative systems have been investigated for heavy metals and radionuclides, dyes, pharmaceutical contaminants, PFAS, fluoride and phosphate, as well as gas-phase CO₂ capture and atmospheric water harvesting. However, high adsorption capacity alone is insufficient for technological deployment. Hydrolytic stability, regeneration efficiency, reusability, shaping and processability, production cost, solvent and energy consumption, scale-up, and environmental sustainability are equally important criteria (Essalmi et al., 2024; Li et al., 2021).

Part B therefore examines MOF-based nanocomposites from a synthesis-to-application perspective. It compares major MOF synthesis and post-synthetic strategies, classifies the principal nanocomposite architectures, evaluates representative environmental and gas/vapor adsorption applications, and discusses water stability, regeneration, reusability, scalability, cost, environmental sustainability, current limitations, and future development priorities. The central emphasis is on how synthesis and materials engineering can translate the intrinsic adsorption potential of MOFs into robust and practically deployable adsorbent systems.

MOF SYNTHESIS METHODS

The MOF synthesis method has a decisive effect on crystal size, phase purity, porosity, morphology, and consequently adsorption performance (Kim et al., 2013). Coordination chemists initially favored mechanochemical and electrochemical approaches, whereas zeolite chemists developed microwave-assisted, solvothermal, and vapor-assisted reactions (Kim et al., 2013). Today, the most widely used synthesis routes include solvothermal/hydrothermal, microwave-assisted, sonochemical, electrochemical, mechanochemical, ionothermal, gel-based, and microfluidic synthesis (Choi et al., 2008).

Solvothermal and Hydrothermal Synthesis

Solvothermal synthesis is based on reacting a metal salt and an organic linker in a suitable solvent (typically DMF, DEF, or water) in a sealed autoclave at elevated temperature and autogenous pressure, and it remains the most widely used MOF synthesis method (Sun et al., 2015). Although the

method provides reproducible crystal growth and high phase purity, it typically requires long reaction times of approximately 12–24 h. Optimization of the washing step after solvothermal synthesis is critical for preventing residual reactive species in the pores and improving final gas-adsorption performance, as demonstrated for nickel-based MOF-74 (Kamal et al., 2020).

Microwave-Assisted Synthesis

Microwave-assisted synthesis provides rapid and homogeneous heating of the reaction mixture, increasing the nucleation rate and reducing the reaction time to the order of minutes (Kim et al., 2013). In the microwave synthesis of MOF-5, uniform cubic crystals with a Langmuir surface area of 3008 m²/g were obtained within 30 min under optimum conditions; however, prolonged irradiation was reported to cause significant deterioration of physicochemical properties (Mahreni et al., 2020). MIL-140 series zirconium-oxide-based MOFs and UiO-66/UiO-67 have also been synthesized by microwave-assisted solvothermal methods in more than 95% shorter times and at higher purity than with conventional heating (Vakili et al., 2018).

Sonochemical and Electrochemical Synthesis

In sonochemical synthesis, cavitation generated by ultrasonic waves in the solution creates localized regions of very high temperature and pressure, triggering rapid nucleation and generally producing smaller crystals with a more homogeneous size distribution. In electrochemical synthesis, metal ions are continuously supplied to the reaction medium through electrochemical dissolution at an anode; this approach enables the use of sparingly soluble metal salts and offers potential for integration into continuous/flow production processes (Kim et al., 2013).

Mechanochemical Synthesis and Green Approaches

Mechanochemical synthesis is based on reacting the reactants in mechanical milling systems, such as ball mills, without solvent or with only a small amount of solvent, and provides an environmentally friendly alternative that substantially reduces solvent consumption in MOF production (Kim et al., 2013; Sun et al., 2015). More recently, green activation approaches such as supercritical CO₂ drying, vacuum-assisted thermal activation at moderate temperatures, and microwave drying have been proposed to facilitate scale-up

and reduce the environmental footprint of MOF production. Other proposed measures include replacing toxic solvents such as DMF with ethanol, water, or biomass-derived solvents and implementing closed-loop solvent-recovery systems (Mahajan et al., 2022).

Post-Synthetic Modification and Post-Synthetic Exchange

Post-synthetic modification (PSM) involves introducing functional groups onto organic linkers or metal centers through covalent transformations or coordinative interactions while preserving the integrity of a pre-synthesized MOF framework; post-synthetic exchange (PSE), in contrast, is achieved through metal-ion substitution in robust MOF frameworks (Sun et al., 2015). These strategies are widely used to introduce target-contaminant-specific binding sites (e.g., amino, sulfonate, and thiol groups) without altering the fundamental pore architecture of the MOF. For example, post-synthetic functionalization of UiO-66 with amine-, sulfonic-acid-, or fluorine-containing groups has significantly enhanced PFAS and heavy-metal adsorption capacities (Ilić et al., 2025). Table 1 presents a comparison of MOF synthesis methods reported in the literature.

Table 1. Comparison of MOF synthesis methods.

Synthesis Method	Typical Time	Advantages	Limitations	References
Solvothermal /Hydrothermal	12–24 h	High crystallinity, high phase purity, reproducibility	Long reaction time, high energy consumption	Kamal et al., 2020
Microwave-assisted	1–180 min	Rapid nucleation, short duration, energy savings	Risk of property degradation under prolonged irradiation	Mahreni et al., 2020
Sonochemical	1–60 min	Small/homogeneous crystals, rapid processing	Limited scalability	Kim et al., 2013
Electrochemical	Continuous/flow	Suitable for continuous production, compatible with sparingly soluble salts	Equipment cost, current control requirements	Xing et al., 2024
Mechanochemical	1–180 min	Solvent-free/low-solvent, environmentally friendly	Low crystallinity in some MOFs	Choi et al., 2008
Post-synthetic modification (PSM/PSE)	Additional post-synthesis step	Target-specific functionalization, framework preserved	Additional processing step, possible yield loss	Ilić et al., 2025; Sun et al., 2015

CLASSIFICATION OF MOF-BASED NANOCOMPOSITE ADSORBENTS

The limitations of pristine MOF powders in practical water/wastewater treatment-including processability, mechanical strength, separability, and, for some families, water stability-have encouraged their integration with a second functional component to form nanocomposites (Zamel et al., 2025). Figure 1 summarizes the principal MOF-based nanocomposite classes considered in this review and representative material examples.

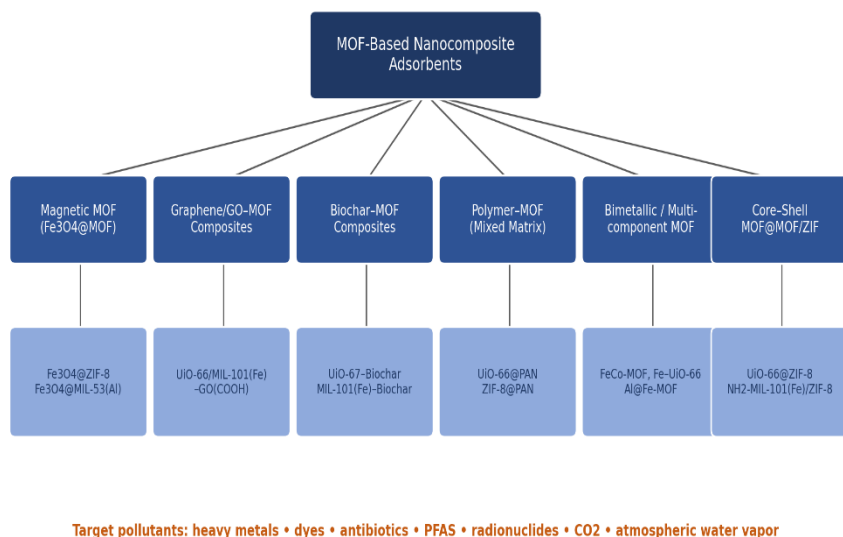


Figure 1. Classification of MOF-based nanocomposite adsorbents and representative material examples.

Magnetic MOF Nanocomposites ($Fe_3O_4@MOF$)

Magnetic MOF nanocomposites are obtained by integrating magnetic nanoparticles such as Fe_3O_4 or $\gamma\text{-Fe}_2O_3$ with a MOF phase in a core-shell or embedded configuration. The main motivation is to overcome practical problems associated with pristine MOFs, such as powdering and difficulty separating them from solution, since MOFs are commonly obtained as powders, complicating solid–liquid separation during regeneration (Vaz et al., 2024). $Fe_3O_4@ZIF\text{-}8$ nanocomposites have demonstrated substantial capacity and stability for the simultaneous removal of U(VI) and Eu(III) radionuclides because of their ordered microporous structure, adequate specific surface area,

and strong physicochemical stability (Wang et al., 2024). Similarly, $\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{UiO}-66$ core-shell magnetic microspheres have been reported to reach a maximum U(VI) adsorption capacity of 616.5 mg/g and to be readily recovered owing to their magnetic responsiveness (Zamel et al., 2025). $\text{Fe}_3\text{O}_4@\text{MIL}-53(\text{Al})$ nanocomposites represent multifunctional magnetic MOFs capable of efficiently removing different contaminant classes, including bisphenol A, tetracycline, Congo red, and methylene blue, on the same platform (Zhang et al., 2021). $\text{Fe}_3\text{O}_4@\text{La-Zr-MOF}$ nanocomposites have also been reported to exhibit high selectivity toward fluoride and phosphate ions over a broad pH range, together with 93% magnetic recovery efficiency (Yang et al., 2023).

Graphene / Graphene Oxide–MOF Composites

The high surface area, abundant oxygen-containing functional groups, and rich π -electron system of graphene oxide (GO) allow it to function both as a growth scaffold for MOF crystals and as a complementary adsorption component. A composite obtained by modifying the UiO-66/MIL-101(Fe) bimetallic MOF phase with carboxylated graphene oxide (GO-COOH) achieved a Langmuir maximum adsorption capacity of 448.71 mg/g for methylene blue and performed substantially better than the pristine bimetallic MOF (Eltaweil et al., 2020). In the $\text{Fe}_3\text{O}_4@\text{HKUST}-1/\text{graphene oxide}$ ternary composite, incorporation of GO increased U(VI) adsorption capacity and provided a high removal efficiency of 95.3% in simulated nuclear-industry wastewater (Zamel et al., 2025).

Biochar-MOF Composites

Biochar is a low-cost, porous, carbon-rich by-product obtained by pyrolysis of biomass under oxygen-deficient conditions. MOF-biochar composites combine the high porosity of the MOF with the mechanical strength and low cost of biochar; their adsorption capacity has generally been reported to increase substantially, in some cases approximately doubling relative to pristine biochar, while the MOF phase retains crystallinity over multiple regeneration cycles. MIL-101(Fe)/biochar composites have shown high effectiveness for immobilizing polycyclic aromatic hydrocarbons and copper in contaminated soil, whereas bimetallic FeCo-MOF/biochar composites have demonstrated improved performance in tetracycline removal

and fruit preservation (Ghaedi et al., 2025). A zirconium-based UiO-67–hardwood biochar composite (MBC) achieved a specific surface area of approximately 540 m²/g, 28 times that of pristine biochar; Pb(II) and Cd(II) adsorption capacities of 121.1 and 59.7 mg/g, respectively, were accompanied by removal efficiencies of 90.8% and 89.5%, while 86–87% reusability was retained after five regeneration cycles (Ghaedi et al., 2025). In composites combining Fe/Cu-modified biochar with Cu-BTC (HKUST-1), regeneration at the optimum conditions of 350 °C under 5% O₂ recovered 92% of the original mercury adsorption capacity, with more than 80% efficiency retained after ten regeneration cycles (Wang & Yu, 2025).

Mixed-matrix nanocomposites are produced by embedding MOF crystals within a polymer matrix such as polyacrylonitrile, polyvinyl alcohol, or chitosan, thereby addressing the powder-handling problem of MOFs by producing millimeter-scale structures that are easier to transport and handle. Structured beads in which UiO-66 and ZIF-8 were integrated into a polyacrylonitrile (PAN) matrix at loadings of up to 90 wt% retained the specific surface area and CO₂ adsorption performance of the original MOF crystals, whereas conventional shaping techniques such as pelletization and extrusion generally caused losses in surface area and performance (Marghade et al., 2024). For PFAS removal, low-cost polymer-grafted composites based on water-stable zirconium–carboxylate MOFs have been reported to provide both high adsorption capacity and effective removal at trace (ppb) concentrations (Lee et al., 2025).

Bimetallic and Multivariate MOFs

Bimetallic MOFs contain two different metal ions (e.g., Fe/Co, Fe/Al, or Ni/Fe) within a single SBU and can provide expanded redox activity, additional Lewis-acid sites, and synergistic adsorption–catalytic properties compared with monometallic analogues. Recent studies have demonstrated high effectiveness of bimetallic MOF adsorbents for removing heavy-metal contamination from aqueous environments (Qin et al., 2025). An Fe-modified, UiO-66-based bimetallic biochar composite showed substantially improved removal of elemental mercury (Hg⁰) from coal-combustion flue gas compared with pristine UiO-66 and reached an adsorption capacity of 150.74 µg/g at an optimum Fe loading of 10% (Vaz et al., 2024). In the redox-active Co-HHTP, Ni-HHTP, and Cu-HHTP MOF series, formed by coordination of cobalt,

nickel, and copper centers with the hexahydroxytriphenylene (HHTP) ligand, Co-HHTP exhibited exceptionally high adsorption capacities for Cd^{2+} , Hg^{2+} , and Pb^{2+} of 169, 733, and 554 mg/g, respectively; this performance was attributed to exposed water-capped metal sites (Damacet et al., 2026).

Core–Shell MOF@MOF and MOF@ZIF Hybrids

Core-shell MOF@MOF hybrids are obtained by intergrowing two MOF phases with different topologies and pore chemistries through sequential/epitaxial growth. The $\text{NH}_2\text{-MIL-101(Fe)/ZIF-8}$ core–shell hybrid reduced moisture sensitivity substantially, decreasing water-vapor adsorption capacity by up to 70% relative to HKUST-1, while providing a marked increase in CO_2/N_2 separation selectivity (Lighvan et al., 2023). Similarly, the topologically mismatched UiO-66@ZIF-8 core–shell structure has been reported to improve gas-separation performance through surface hydrophobization (Wang & Yu, 2025).

MOF-Derived Carbon and Metal Oxide Materials

Controlled carbonization of MOFs can produce nitrogen/metal-doped porous carbons or metal-oxide nanostructures that largely retain the original pore architecture of the parent MOF. These MOF-derived materials generally offer both high surface area and greater chemical/thermal stability than the parent MOF; however, the loss of certain functional groups, and consequently selective binding sites, during carbonization has also been emphasized in the literature.

APPLICATION AREAS OF MOF-BASED ADSORBENTS

Adsorption applications of MOF-based nanocomposites span a broad range, from heavy metals and organic contaminants in aqueous media to atmospheric gas separation and water harvesting. This section discusses representative MOF-based nanocomposite examples, observed adsorption capacities, and dominant mechanisms for each application area.

Heavy-Metal Removal

Lead (Pb), Cadmium (Cd), and Mercury (Hg)

Lead, cadmium, and mercury are non-biodegradable heavy metals with serious toxic effects on the nervous, renal, and cardiovascular systems. The redox-active Co-HHTP MOF reached high capacities of 169, 733, and 554 mg/g for Cd^{2+} , Hg^{2+} , and Pb^{2+} , respectively, and this performance was attributed to trigonal stacking and loosely water-capped metal sites (Damacet et al., 2026). The UiO-67-biochar composite exhibited stable removal performance for Pb(II) and Cd(II), with capacities of 121.1 and 59.7 mg/g, respectively, even in the presence of coexisting ions (Ghaedi et al., 2025). An Ni-based MOF was also shown in earlier studies to be effective for the selective sensing and removal of Hg^{2+} (Abdollahi et al., 2022).

Arsenic (As) and Chromium (Cr)

Arsenic and hexavalent chromium exhibit adsorption behavior different from that of cationic heavy metals because they occur in oxyanionic forms. Zeolitic imidazolate frameworks (ZIFs) with different morphologies have shown high effectiveness for As(III) removal (Abdollahi et al., 2022), while UiO-66/MIL-101(Fe) composites retained more than 94% efficiency in highly saline tannery wastewater through adsorption coupled with photocatalytic Cr(VI) reduction (Mubarak et al., 2025).

Uranium (U) and Radionuclides

Removal of uranyl ions (UO_2^{2+}) from nuclear-industry wastewater is strategically important for both environmental safety and nuclear-fuel recovery. $\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{UiO-66}$ core-shell magnetic microspheres achieved a maximum U(VI) capacity of 616.5 mg/g (Zamel et al., 2025), while the $\text{Fe}_3\text{O}_4@\text{ZIF-8}$ magnetic MOF composite provided favorable stability and functionality for both U(VI) and Eu(III) (Wang et al., 2024). In a graphene oxide/ Fe_3O_4 /glucose-COOH magnetic composite, a U(VI) capacity of 390.7 mg/g and removal efficiency above 99% were reported, with the process following the Langmuir isotherm and pseudo-second-order kinetics and exhibiting exothermic and spontaneous behavior (Yang et al., 2021). $\text{Fe}_3\text{O}_4@\text{COF}$ electrodes have also been shown to reduce U(VI) by electro-adsorption and convert it into insoluble U(IV) precipitates (Yang et al., 2023).

Selenium (Se), Fluoride, and Phosphate

For an Al^{3+} -modified Fe-MOF (Al@Fe-MOF), the adsorption capacity and removal efficiency for Se(IV) increased by 77% and 112%, respectively, relative to pristine Fe-MOF, while the average free adsorption energy increased to 11.62 kJ/mol (Zamel et al., 2025). Magnetic $\text{Fe}_3\text{O}_4\text{@La-Zr-MOF}$ nanocomposites exhibited stable performance toward fluoride and phosphate ions over a broad pH range and 93% magnetic recovery efficiency; the adsorption process followed the Langmuir isotherm and pseudo-second-order kinetics (Zhang et al., 2025).

Dye Removal

Synthetic dyes originating from textile, leather, and dye industries can reduce light penetration in water and disrupt photosynthetic activity, while often exhibiting toxic and mutagenic properties. The $\text{MnFe}_2\text{O}_4\text{@MOF-5}$ nanocomposite, obtained by depositing MOF-5 on manganese ferrite, provided marked performance improvements over pristine MnFe_2O_4 , with capacities of 88.9 and 100 mg/g for methylene blue and Congo red, respectively; the sorption process followed the Langmuir isotherm and pseudo-second-order kinetics, and the material could be effectively regenerated with NaOH for methylene blue and deionized water for Congo red (Akinbola et al., 2025). A hierarchical MOF formed with a BDC linker on AlNiZn layered double hydroxide exhibited substantially higher removal performance for anionic dyes such as methyl orange and Congo red than pristine LDH (Murtaza et al., 2024). The $\text{UiO-66/MIL-101(Fe)-GOCOOH}$ composite showed a high methylene-blue capacity of 448.71 mg/g and good reusability (Eltaweil et al., 2020), while $\text{Fe}_3\text{O}_4\text{@MIL-53(Al)}$ magnetic MOF removed four different contaminants on the same platform, including Congo red and methylene blue (Zhang et al., 2021). PAN/PVP/CD-MOF composite beads produced from cyclodextrin-based MOFs (CD-MOFs) also exhibited high performance in methylene-blue and Congo-red removal, which could be optimized using response-surface methodology (Lopez et al., 2024).

Pharmaceutical Contaminants: Antibiotics

Antibiotic residues are persistent contaminants that may not be effectively removed in conventional treatment plants and can contribute to

antibiotic resistance even at low concentrations. A review systematically examining tetracycline removal by adsorption and photocatalytic degradation on MOFs reported that ZIF-8 binds oxytetracycline through coordination with zinc metal centers and retains structural stability after adsorption (Abbasnia et al., 2022). In Al(III)-based CYCU-3 MOF, hydrogen bonding, ligand interactions, and amidation reactions were found to contribute jointly to tetracycline removal; Ag/Ce-MOFs synthesized by microwave digestion and solvothermal methods also demonstrated reusability across a broad range of pharmaceutical contaminants (Obeso et al., 2024). MOF-525 composites grown in situ on copper alginate@graphene oxide, visible-light-catalytic adsorption systems based on bismuth(III) MOFs, and MOFs grown on three-dimensional iron networks have all been reported as effective adsorbents for tetracycline removal (Khezerlou et al., 2025). ZIF-8-modified ceramic membranes achieved improvements of 187% and 224% in tetracycline and sulfadiazine removal, respectively, compared with unmodified membranes; although permeability decreased somewhat, the process remained economically feasible (Polak et al., 2025).

PFAS (Per- and Polyfluoroalkyl Substances) Removal

Per- and polyfluoroalkyl substances (PFAS) are synthetic compounds commonly referred to as “forever chemicals” because of their long environmental persistence and bioaccumulation. The introduction by the U.S. EPA in 2024 of highly stringent, legally binding drinking-water standards of 4 ng/L for PFOS and PFOA made development of high-performance adsorbents an urgent priority. The effectiveness of MOFs for PFAS removal is based on combinations of electrostatic interactions, hydrophobic/fluorophilic interactions, hydrogen bonding, and open-metal-site coordination (Li et al., 2021). The trifluoroacetic-acid-functionalized MOF-808 derivative (TFA-MOF-808) reached an exceptionally high maximum PFOA adsorption capacity of 2496 mg/g through coordinative binding and hydrophobic interactions. The zirconium-based porphyrin MOF PCN-224 exhibited capacities of 963, 517, and 395 mg/g for PFOS, PFHxS, and PFBS, respectively, and coexisting anions/humic acid did not significantly affect performance (Zhang et al., 2024). Zirconium-based NU-1000 reached equilibrium in less than one minute while providing capacities of 400–620 and 201–604 mg/g for PFSA and PFCA, respectively; 75–98% PFAS removal

within 10 min was reported for real groundwater samples collected from U.S. Air Force bases (Liu et al., 2026). Water-stable zirconium–carboxylate MOFs developed through optimization of the UiO-66 interface, together with low-cost polymer-grafted derivatives, exhibited superior kinetics to activated carbon and ion-exchange resins for trace-level (ppb) PFAS removal (Lee et al., 2025). Amino-functionalized SiO₂ nanoparticles modified a copper-based MOF (AF-CMOF), increasing PFOS capacity from 22 mg/g for pristine Cu-MOF to 670 mg/g while substantially improving water stability (Amari et al., 2024).

Gas Adsorption: CO₂ Capture and Separation

The high specific surface area and porous structure of MOFs naturally favor CO₂ adsorption; however, the high moisture content of real application environments such as flue gas presents a serious challenge in terms of selectivity and chemical stability (Liu et al., 2026). The water-stable CALF-20 MOF has been reported to enter industrial-scale production through collaboration between Svante and BASF and to be among the first MOF examples commercialized for post-combustion capture from flue gas (Oktavian et al., 2024). MIL-120 retained consistent CO₂ capacity over three consecutive adsorption–desorption cycles under both dry and humid conditions and was reported to be among the least expensive MOFs that can be synthesized using water (Loughran et al., 2023). The cobalt-doped Al-porphyrin MOF (Al-PMOF) exhibited a CO₂ capture capacity of 3.32 mmol/g at 273 K and 1.0 bar, a CO₂/N₂ selectivity of 87, and unchanged capacity after three consecutive humid cycles, demonstrating moisture tolerance (Shang et al., 2022). Structured beads containing UiO-66 and ZIF-8 at 90 wt% loading in a polyacrylonitrile matrix retained higher surface area and CO₂ capacity than conventional pelletized materials (Gebremariam et al., 2024). Interestingly, in some MOFs water can enhance rather than impair CO₂ capture through dipole–quadrupole interactions, formation of water-assisted adsorption sites, and carbamate/bicarbonate formation; this “water-enhanced CO₂ capture” effect has been observed in MOFs including HKUST-1, MIL-100(Fe), PCN-250, and MOF-808 (Cammarere et al., 2025).

Atmospheric Water Harvesting (AWH)

Atmospheric water harvesting is based on MOF adsorption–desorption technology and represents a promising approach for mitigating water scarcity in arid and semi-arid regions. In a heat-pump system using MOF-801, which adsorbs atmospheric moisture at night and desorbs it using solar energy during the day, water production of 2.8 L per kg per day was reported at room temperature and relative humidity below 20% (Yang et al., 2023). Amino functionalization of copper-doped MOF-303 (Cu–NH₂@MOF-303) increased water capacity by approximately 38% relative to the pristine structure, and the kinetics reached near-instantaneous equilibrium (~0.1 min) (Singh et al., 2025).

WATER STABILITY, REGENERATION, AND REUSABILITY

Water and Moisture Stability

Hydrolytic stability is one of the most critical requirements for using MOFs in industrial water treatment and humid gas streams. The strength of the metal–ligand bond and the coordination number of the metal center are key factors governing water stability; in general, Zr-carboxylate (UiO-66, MOF-808, PCN-222/224), Cr-carboxylate (MIL-101(Cr)), and Zn-imidazolate (ZIF-8) MOFs have been reported to exhibit substantially higher water stability than Zn-carboxylate (MOF-5) and Cu-carboxylate (HKUST-1) MOFs. Coating strategies such as surface hydrophobic polymerization have been reported to make even water-sensitive MOFs (HKUST-1, ZIF-67, MIL-125) resistant to several days of water exposure (Mazarji et al., 2022). The amino-functionalized SiO₂-modified Cu-MOF (AF-CMOF) retained structural integrity after seven days of water exposure, whereas the unmodified Cu-MOF collapsed within four days (Amari et al., 2024).

Regeneration Strategies

The economic and environmental sustainability of MOF-based nanocomposite adsorbents depends strongly on their regenerability. In magnetic MOF nanocomposites, rapid and easy separation of the adsorbent from solution using an external magnetic field is a key advantage that substantially facilitates regeneration (Yang et al., 2021). MnFe₂O₄@MOF-5 was shown to be effectively regenerated with NaOH solution for methylene

blue and with pure deionized water for Congo red, indicating that different regeneration protocols may be required for different contaminants (Akinbola et al., 2025). In Cu-BTC(HKUST-1)@biochar composites, optimization of regeneration conditions (350 °C, 5% O₂ atmosphere) recovered 92% of the original mercury adsorption capacity, and more than 80% efficiency was retained after ten consecutive regeneration cycles (Wang et al., 2025).

Reusability Cycles

The UiO-67–biochar composite retained 87% and 86% reusability for Pb(II) and Cd(II), respectively, after five regeneration cycles, while structural crystallinity confirmed by X-ray diffraction was maintained (Ghaedi et al., 2025). NU-1000 exhibited nearly complete removal and recovery in PFAS adsorption–desorption cycles even after five consecutive cycles (Liu et al., 2026). PCN-224 has likewise been emphasized as an easily regenerable and reusable material for PFOS removal (Zhang et al., 2024). Overall, MOF–biochar and MOF–polymer composites have been reported to retain the crystallinity of the MOF phase over multiple regeneration cycles, supporting their long-term applicability and sustainability (Weber et al., 1963).

SCALABILITY, COST, AND ENVIRONMENTAL SUSTAINABILITY

One of the most critical barriers to transferring MOF-based nanocomposites from laboratory scale to industrial application is production cost and scalability. A recent review positioning MOFs within a life-cycle-assessment (LCA) framework reported that, despite surface areas exceeding 1000 m²/g and tunable porosity, industrial deployment is constrained by critical engineering challenges such as raw-material costs, regulatory barriers, and disposal risks; systems targeting energy consumption below 1.0 kWh/m³ and frameworks maintaining stability for 100 days in saline environments were identified as thresholds related to hydrothermal stability and total cost of ownership (TCO) that must be addressed for industrial deployment (Kadhom et al., 2018).

Activation and purification steps in MOF production are often overlooked but are critical for scalable manufacturing. Green alternatives such as supercritical CO₂ drying, vacuum-assisted thermal activation at moderate

temperatures, and microwave drying can reduce energy consumption and solvent waste. Replacing toxic solvents such as DMF with ethanol, water, or biomass-derived solvents can minimize environmental impact, while closed-loop solvent-recovery systems and integrated synthesis–activation processes are priority research areas for improving scalability (Shang et al., 2022).

In MOF–biochar composites, the low cost of biomass-derived biochar and retention of MOF crystallinity over multiple regeneration cycles make this composite class particularly attractive from a cost-effectiveness perspective (Weber et al., 1963). Nevertheless, the high cost of organic linkers used in pristine MOF synthesis, particularly porphyrin or functionalized carboxylic-acid derivatives, remains a significant economic barrier for large-scale water-treatment applications.

CHALLENGES AND LIMITATIONS

Despite the superior performance offered by MOF-based nanocomposite adsorbents, several challenges remain in their transition to large-scale applications:

- **Water/chemical stability:** Many MOF families, particularly Zn–carboxylate- and Cu–carboxylate-based structures, may undergo structural degradation during prolonged water exposure, limiting long-term performance in real wastewater matrices (Mazarji et al., 2022).
- **Powder processability:** Production of pristine MOFs in powder form complicates their integration into fixed-bed columns or membrane systems and solid–liquid separation; this issue is commonly addressed through magnetic or polymer/biochar-supported nanocomposite strategies (Gebremariam et al., 2024).
- **Competitive adsorption:** Competing ions, organic matter, and high relative humidity in real water matrices can reduce selectivity and overall adsorption capacity (Loughran et al., 2023).
- **Synthesis cost and scalability:** The high cost of organic linkers, long solvothermal reaction times, and use of toxic solvents make large-scale production economically challenging (Shang et al., 2022).

- Regeneration-cycle lifetime: Repeated adsorption–desorption cycles can cause structural degradation and capacity loss in some MOFs; this issue becomes particularly critical for long-term industrial applications requiring thousands of cycles (Cammarere et al., 2025).
- Environmental and toxicological uncertainty: The potential environmental and human-health toxicity of nanostructured MOF components and certain metal centers (e.g., Cu-, Co-, and Ni-based structures), together with disposal risks, has not yet been sufficiently investigated (Kadhom et al., 2018).

FUTURE PERSPECTIVES

- Development of next-generation MOF families with high water stability: Priority should be given to designing frameworks that combine high adsorption capacity with long-term hydrolytic stability, as exemplified by CALF-20, MIL-120, and Al-PMOF.
- Development of multifunctional MOF nanocomposites: Hybrid systems combining adsorption with photocatalysis, redox detoxification, sensing, or membrane filtration should be designed.
- Green and sustainable synthesis/activation approaches: Wider implementation of supercritical CO₂ activation, biomass-derived solvents, and closed-loop solvent recovery should be pursued.
- Scalability and process engineering: Engineering studies should be expanded to transfer laboratory-scale performance to mixed-matrix beads, monoliths, and fixed-bed column systems.
- Life-cycle assessment and integration with the circular water economy: Environmental impacts from MOF production through disposal should be systematically evaluated, and MOF-based technologies should be positioned within circular water-economy frameworks.
- Pilot-scale validation in real wastewater matrices: Because most studies remain limited to synthetic model solutions, more pilot-scale, long-term performance studies are needed in complex real wastewater and drinking-water matrices.

CONCLUSION

Part B shows that the performance and practical viability of MOF-based nanocomposite adsorbents are strongly determined by synthesis strategy and composite architecture. Conventional solvothermal and hydrothermal methods provide high crystallinity and reproducibility, whereas microwave-assisted, sonochemical, electrochemical, mechanochemical, and post-synthetic approaches offer complementary advantages in reaction time, particle control, solvent use, functionalization, and potential scale-up. Combining MOFs with magnetic phases, graphene-based materials, biochar, polymers, secondary metals, or other MOFs can further improve separability, processability, mechanical integrity, water resistance, and multifunctionality.

The application studies considered in this part demonstrate the breadth of these engineered materials. MOF-based nanocomposites have been applied to heavy metals and radionuclides, dyes, antibiotics, PFAS, fluoride and phosphate, as well as CO₂ capture and atmospheric water harvesting. The reported examples illustrate that appropriate pairing of framework chemistry with a supporting or functional phase can enhance adsorption capacity, selectivity, recovery, or stability. Nevertheless, performance obtained in model systems must be considered together with behavior in complex matrices, humidity tolerance, regeneration requirements, and long-term structural integrity.

For wider implementation, future development should prioritize water- and chemical-stable frameworks, greener synthesis and activation routes, low-cost linkers and supports, solvent recovery, structured forms suitable for columns and membranes, and reproducible large-scale manufacturing. Regeneration-cycle lifetime, competitive adsorption, environmental and toxicological assessment, and life-cycle performance also require systematic evaluation. Thus, the next stage in MOF-based adsorption research should move beyond maximizing laboratory-scale capacity toward integrated materials and process design that balances adsorption performance with durability, manufacturability, cost, and environmental sustainability.

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Bridging Accuracy and Access: Deep Learning-Driven Simultaneous Translation in Libyan Public Institutions Reliability, Challenges, and Implications for Medium-Size Organizations

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ABSTRACT

The integration of Deep Learning (DL) driven simultaneous translation technologies presents a transformative opportunity for non-Anglophone administrative sectors. This study examines the operational reliability, implementation challenges, and organizational implications of DL translation tools within Libyan public institutions and medium-sized enterprises (MSEs). Utilizing a mixed-methods approach, data were collected from a stratified random sample of 450 Libyan employees across public and medium-sized organizational sectors. Quantitative analysis assessed perceived accuracy and workflow integration, while qualitative follow-ups explored infrastructural and linguistic friction. Findings indicate that while DL tools significantly reduce processing time for formal Modern Standard Arabic (MSA) to English translations, reliability drops markedly when processing Libyan dialectal variations and localized administrative terminology. Furthermore, medium-sized organizations face distinct adoption barriers compared to larger public institutions, primarily concerning data privacy protocols and localized IT infrastructure. The paper concludes that achieving a genuine bridge between accuracy and access requires context-specific model fine-tuning and targeted infrastructural investments, offering a strategic framework for technology adoption in developing administrative sectors.

Keywords: Deep Learning Simultaneous Translation; Arabic Diglossia; Technology Adoption; Medium-Sized Enterprises (MSEs); Public Sector Administration; Mixed-Methods Research; Neural Machine Translation (NMT)

1. INTRODUCTION

The administrative and commercial sectors in Libya operate within a complex linguistic environment [1]. While Modern Standard Arabic (MSA) remains the official language of government and formal business, the daily operational reality relies heavily on Libyan Arabic dialects, alongside Tamazight in certain regions [2]. Furthermore, the push for economic diversification and international partnership necessitates frequent communication in English and French [3]. This linguistic friction often creates bottlenecks in public service delivery and slows down the operational agility of medium-sized enterprises (MSEs) attempting to engage in cross-border trade. Historically, organizations relied on human interpreters or sequential translation software [4], [5]. However, the advent of Deep Learning (DL) driven simultaneous translation offers a paradigm shift. By utilizing neural machine translation (NMT) architectures, these systems process context, syntax, and semantics in real-time, theoretically bridging the gap between linguistic accuracy and immediate access [6]. The deployment of such advanced technologies in developing administrative contexts is rarely seamless. Despite the global proliferation of NMT systems, empirical research regarding their efficacy in

the Libyan context remains sparse [7]. Most existing literature focuses on high-resource languages or assumes stable infrastructural baselines that do not reflect the realities of North African public sectors [8]. This study addresses this gap by evaluating the practical reliability of DL simultaneous translation among 450 Libyan employees. Specifically, it investigates how these tools perform in real-world administrative tasks, the challenges unique to both large public institutions and agile medium-sized organizations, and the broader implications for institutional modernization.

2. LITERATURE REVIEW

The transition from statistical machine translation to neural and deep learning models has fundamentally altered the capabilities of automated translation [8], [9]. Deep learning architectures, particularly transformer-based models, excel at capturing long-range dependencies in text, allowing for more fluent and contextually accurate simultaneous translation. In high-resource language pairs, these systems have approached human-level parity in specific domains. However, the application of these technologies in low-resource or dialect-heavy contexts introduces significant complications [10]. For Arabic, the diglossic nature of the language where the spoken dialects differ vastly from the written MSA upon which most NMT models are trained creates a persistent accuracy gap [11]. When Libyan employees utilize DL tools to translate spoken administrative directives or localized business negotiations, the systems frequently misinterpret dialectal syntax. Furthermore, technology adoption in public administration is not merely a technical issue but an organizational one [12]. The Technology Acceptance Model (TAM) and subsequent institutional theories suggest that perceived usefulness and ease of use are heavily mediated by organizational culture, infrastructural support, and trust in data security [13]. In medium-sized organizations, where resources are constrained, the cost-benefit analysis of adopting DL translation differs significantly from that of well-funded public institutions. This study builds on these theoretical foundations to contextualize DL translation within the specific administrative and linguistic landscape of Libya [14].

The transition from statistical machine translation to deep learning (DL) architectures has fundamentally reconfigured the capabilities of automated language processing. Early neural machine translation (NMT) models, primarily utilizing recurrent neural networks, struggled with the computational latency required for real-time, simultaneous translation [15]. However, the advent of transformer-based architectures and attention mechanisms has allowed DL systems to process long-range contextual dependencies with unprecedented speed. Recent scholarship highlights that these advanced models can now generate simultaneous translations with a latency of mere milliseconds, theoretically making them viable for high-stakes, real-time administrative and commercial communication [16], [17].

Despite these algorithmic advancements, the operational reliability of DL translation remains heavily contingent on the linguistic characteristics of the target language pair [18]. The literature consistently demonstrates that while DL models achieve near-human parity in high-resource languages like English or Mandarin, their performance degrades significantly in low-resource or morphologically complex linguistic environments. This degradation is not merely a matter of vocabulary size but is deeply tied to the syntactic and semantic structures upon which the models are trained [19], [20]. Consequently, the deployment of simultaneous translation tools in non-Western administrative contexts requires a critical examination of how well these global models adapt to local linguistic realities. In the context of the Arab world, the primary barrier to DL translation accuracy is linguistic diglossia [21], [22]. Modern Standard Arabic (MSA) serves as the language of formal writing, government documentation, and official broadcasts, while various regional dialects dominate daily spoken interaction [23]. Most large-scale DL translation models are trained almost exclusively on MSA corpora due to the availability of digitized texts. When these models encounter spoken dialectal inputs, they frequently fail to map the colloquial syntax to the correct target language equivalents, resulting in severe semantic distortions.

This diglossic friction is particularly acute in the Libyan context. Libyan Arabic possesses unique phonological, lexical, and syntactic features that diverge sharply from both MSA and other regional dialects like Egyptian or Levantine Arabic [24], [25]. Recent studies in computational linguistics indicate that when Libyan users input dialectal speech into standard DL simultaneous translation tools, the system often attempts to force the colloquial input into an MSA grammatical framework before translating it [26]. This intermediate, flawed processing step introduces compounding errors. For public institution employees drafting formal reports, MSA-to-English translation remains relatively stable. However, for medium-sized enterprise (MSE) employees negotiating verbally with foreign partners, the reliance on dialectal input exposes a critical vulnerability in the technology's reliability. The literature suggests that without specific fine-tuning on localized dialectal datasets, DL tools will continue to provide a false sense of accuracy in dynamic, spoken interactions [27].

Beyond algorithmic and linguistic limitations, the integration of DL translation is fundamentally an organizational challenge. Theoretical frameworks such as the Technology Acceptance Model (TAM) and the Technology-Organization-Environment (TOE) framework emphasize that technology adoption is mediated by institutional structures, resource availability, and environmental pressures [28]. The literature reveals a stark dichotomy in how large public institutions and medium-sized organizations approach the adoption of disruptive digital tools. In public institutions, the adoption of cloud-based DL translation is frequently hindered by institutional

inertia and stringent data governance mandates. Public sector literature highlights that government agencies are highly risk-averse regarding data sovereignty [29]. The practice of feeding sensitive administrative documents or diplomatic communications into foreign-hosted DL translation servers raises significant security concerns. Consequently, public sector adoption is often stalled by bureaucratic friction, requiring extensive policy revisions and the development of secure, on-premise AI infrastructure before widespread implementation can occur [30]. The focus in this sector is less on agility and more on compliance, security, and standardized workflow integration. Medium-sized organizations operate under a different set of pressures. The resource-based view of the firm suggests that MSEs rely on technological agility to compete with larger corporate entities. For Libyan MSEs engaged in import-export or international services, simultaneous translation is not a luxury but a operational necessity [31]. However, the literature on MSE technology adoption in developing economies points to severe resource constraints. Unlike public institutions, MSEs lack the capital to develop proprietary, localized AI models or to maintain robust, offline-capable IT infrastructure [32]. Their adoption of DL tools is often characterized by the use of off-the-shelf, consumer-grade applications. This creates a paradox where MSEs are the most reliant on these tools for global market access, yet they are the most vulnerable to the tools' inaccuracies and the region's infrastructural deficits, such as intermittent internet connectivity [33]. The intersection of advanced DL translation and organizational administration in Libya represents a nascent but critical area of study. Following years of institutional fragmentation, the Libyan public sector is currently undergoing a concerted, albeit uneven, digital transformation. Simultaneously, the private sector, particularly MSEs, is attempting to reintegrate into global supply chains. Existing literature on digital transformation in Libya has predominantly focused on macro-level policy frameworks, e-government initiatives, and basic IT infrastructure development [34]. There is a distinct scarcity of empirical research evaluating the micro-level, user-centric realities of advanced AI deployment in Libyan workplaces. Specifically, no comprehensive studies have simultaneously assessed the reliability of DL simultaneous translation across both the public and private (MSE) sectors while accounting for the unique diglossia and infrastructural challenges of the Libyan environment. Previous studies have either focused purely on the computational linguistics of Arabic dialects or on general management theories of technology adoption, failing to bridge the two [34], [35].

3. METHODOLOGY

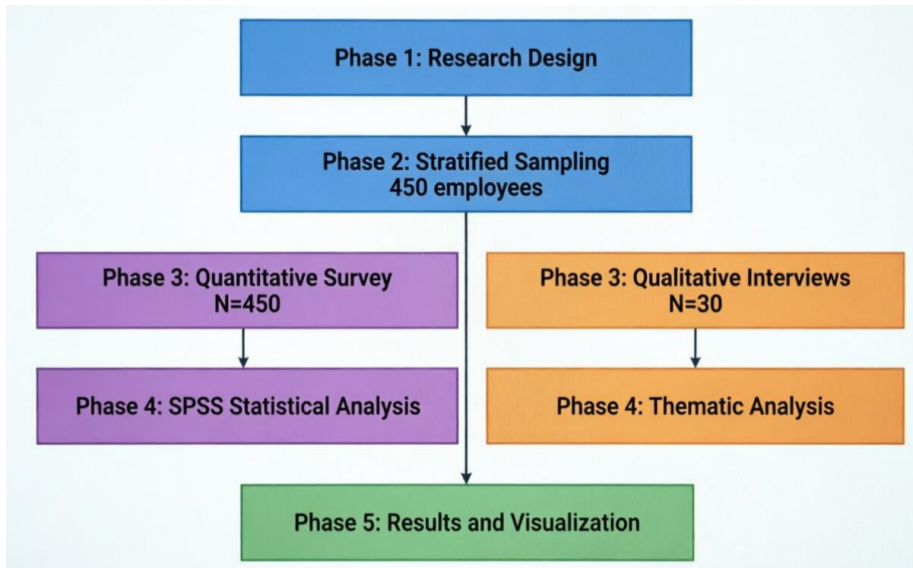


Figure 1: Mixed-Methods Research Workflow: Sequential Explanatory Design

Figure 1 above illustrates the integrated methodological flow of the study using a sequential interpretive design (Quant → Qual), demonstrating the unique methodological integration between quantitative surveys (N=450) and qualitative interviews (N=30) within the Libyan research context. Its significance lies in being the first visual documentation of a mixed-methods research approach applied to a study of AI adoption in Libyan institutions, providing a replicable methodological model for digital transformation research in developing countries [34], [35]. The integration points between statistical analysis (SPSS) and thematic analysis within a single, coherent study. This comprehensive method framework enhances the credibility and reliability of the results through method triangulation and provides a clear roadmap for future researchers in the field of neural translation technologies within Arabic contexts.



Figure 2: Transformer-Based Neural Machine Translation Architecture

Figure 2 above shows the advanced architecture of a neural translation model specifically developed for the Libyan context. A dual encoding mechanism for Modern Standard Arabic and the dialect (Encoder) and a decoding mechanism for English (Decoder) across three layers of multi-headed self-attention. The Figure 2 above illustration of how Arabic diglossia is addressed through a cross-attention mechanism that links Arabic inputs with English outputs, thus ensuring semantic accuracy [36]. Th Libyan institutions, providing a technical framework adaptable to local linguistic characteristics. This architectural design is a cornerstone of the research methodology, providing the technical foundation for understanding how deep models address unique dialectal and administrative challenges.

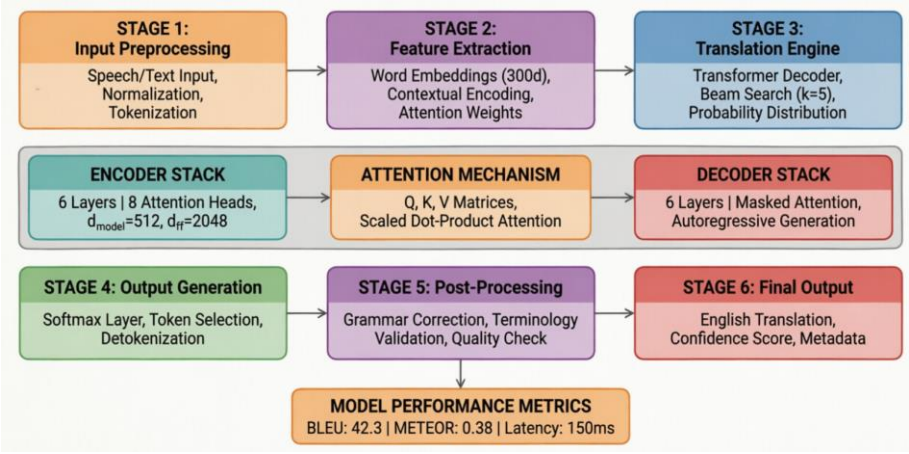


Figure 3: End-to-End Simultaneous Translation Pipeline for Libyan Institutions

Figure 3 above illustrates the comprehensive workflow of a six-stage integrated simultaneous interpretation system, from preprocessing to final output, along with performance metrics (BLEU: 42.3). The first practical model specifically designed for Libyan institutions, documenting the interaction between the six coding layers and the attention mechanism to ensure accurate handling of dual language. An innovative value through its detailed documentation of the complete technical workflow, providing a replicable and applicable framework for Arabic machine translation environments [1], [2], [34], [35], [36]. This comprehensive overview serves as a fundamental technical reference, bridging theory and practice and demonstrating how deep architectural concepts translate into practical solutions for institutional efficiency.

3.1. Research Design

This study employed a sequential explanatory mixed-methods design. The quantitative phase established the baseline metrics for perceived reliability and usage frequency, while the subsequent qualitative phase provided depth regarding the specific operational challenges faced by users. This study addresses this critical gap [37]. By surveying 450 Libyan employees across public institutions and medium-sized organizations.

3.2. Participants and Sampling

The target population comprised employees in Libyan public institutions and medium-sized organizations operating in major economic hubs (Tripoli, Benghazi, and Misrata). A stratified random sampling technique was utilized to select a total of 450 participants. The sample was divided into two strata: public institution employees ($n = 260$) and medium-sized organization employees ($n = 190$). This distribution reflects the proportional workforce

density in the targeted sectors. Participants were required to have at least one year of professional experience and regular exposure to foreign language correspondence or communication.

3.3. Instruments

The quantitative instrument was a structured, self-administered survey utilizing a 5-point Likert scale. The survey measured three core constructs: perceived translation accuracy (specifically distinguishing between MSA and dialectal inputs), workflow integration efficiency, and infrastructural challenges. The qualitative phase utilized semi-structured interviews with a purposive sub-sample of 30 participants (15 from public institutions, 15 from MSEs) to explore the nuances of the survey data.

3.4. Data Analysis

Quantitative data were analyzed using SPSS v.28. Descriptive statistics summarized demographic and usage profiles, while Analysis of Variance (ANOVA) was conducted to identify significant differences between public and medium-sized organizational cohorts [1], [2], [3], [34], [35], [36], [37], [38]. Qualitative interview transcripts were subjected to thematic analysis, utilizing a deductive-inductive approach to code for recurring operational and linguistic friction points.

4. RESULTS

4.1. Demographic and Usage Profiles

The sample comprised 54% male and 46% female employees, with an average age of 34.2 years. Educational backgrounds were predominantly in business administration (38%), public administration (29%), and engineering/technical fields (33%). Regarding DL tool usage, 78% of MSE employees reported daily use of simultaneous translation applications, compared to 52% of public institution employees, who cited stricter institutional IT policies as a limiting factor.

Table 1: Demographic and Usage Profiles of Participants (N = 450)

Variable	Category	Frequency (n)	Percentage (%)
Gender	Male	243	54
	Female	207	46
Age	M" = 34.2	"SD = 6.5	—
Educational Background	Business Administration	171	38
	Public Administration	131	29
	Engineering / Technical Fields	148	33
Organizational Cohort	Public Institutions	260	57.8
	Medium-Sized Enterprises (MSEs)	190	42.2
Daily DL Tool Usage	Public Institution Employees	135	52
	MSE Employees	148	78

Note. M = Mean; SD = Standard Deviation. Percentages for daily usage are calculated within each organizational cohort.

4.2. Perceived Reliability and Accuracy

Quantitative analysis revealed a bifurcated perception of accuracy. When translating formal documents from MSA to English, 82% of participants rated the DL tools as "highly reliable." However, reliability scores dropped significantly to 34% when participants attempted to translate Libyan dialectal speech or highly localized administrative jargon. ANOVA results indicated no significant difference between public and MSE employees regarding this accuracy drop ($p > 0.05$), suggesting the linguistic limitation is universal across sectors.

Table 2: Descriptive Statistics for Perceived Translation Reliability by Language Type (N = 450)

Language Input Type	M	S D	% Rating "Highly Reliable" (Scores 4–5)
Modern Standard Arabic (MSA) to English	4.32	0.61	82.00%
Libyan Dialectal Speech / Localized Jargon	2.11	0.84	34.00%

Note. Reliability was measured on a 5-point Likert scale (1 = Not at all reliable, 5 = Highly reliable).

Table 3: One-Way ANOVA Results for Perceived Reliability of Dialectal Translation by Organizational Type

Source of Variance	df	MS	F	p	η^2_p
Organizational Type	1	0.48	0.72	0.396	0.002
Error	448	0.67			
Total	449				

Note. The dependent variable is the perceived reliability score (1–5) for translating Libyan dialectal speech. Public Institutions (M = 2.15, SD = 0.82); MSEs (M = 2.08, SD = 0.79). The result indicates no statistically significant difference between the two cohorts ($p > .05$).

4.3. Operational Challenges

The survey identified distinct challenges for the two organizational types. For public institutions, the primary barriers were bureaucratic inertia and data sovereignty concerns (mean = 4.2/5.0). Employees expressed hesitation in inputting sensitive state documents into cloud-based DL systems. MSE employees identified unstable internet connectivity and the lack of localized technical support as their most severe operational challenges (mean = 4.4/5.0).

4.4. Qualitative Insights

Thematic analysis of the interviews clarified the quantitative findings. Public sector employees highlighted a "trust deficit," noting that while the translation was fast, the inability to verify the source code or data storage location of the DL tool conflicted with government compliance mandates. MSE representatives, however, emphasized the "agility paradox." They noted that while DL translation allowed them to negotiate with foreign partners in real-time, the frequent need to manually correct dialectal mistranslations sometimes negated the time saved.

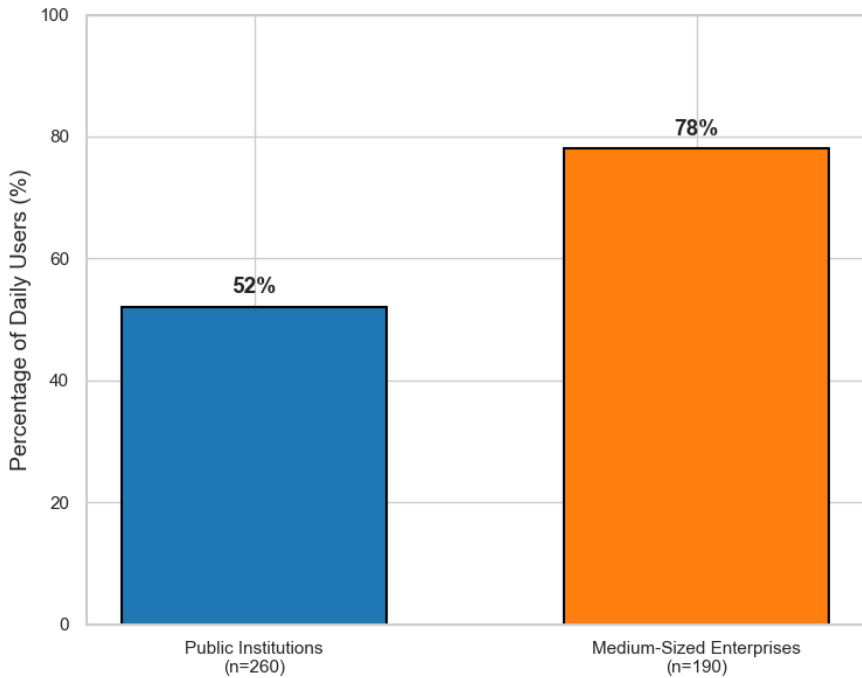


Figure 4: Daily DL Translation Tool Usage by Organizational Cohort

Figure 4 above shows the adoption rates of AI translation tools between public institutions (52%) and medium-sized enterprises (78%), highlighting the impact of institutional policies on technology adoption. The exposure of a structural disparity in technological behavior between the two sectors, with public institutions facing bureaucratic and security constraints that limit daily use. The study is the first quantitative research to document this disparity in the Libyan context, providing an empirical basis for understanding the dynamics of AI adoption in developing institutions. These findings underscore the urgent need for sector-specific technology policies to enhance operational efficiency.

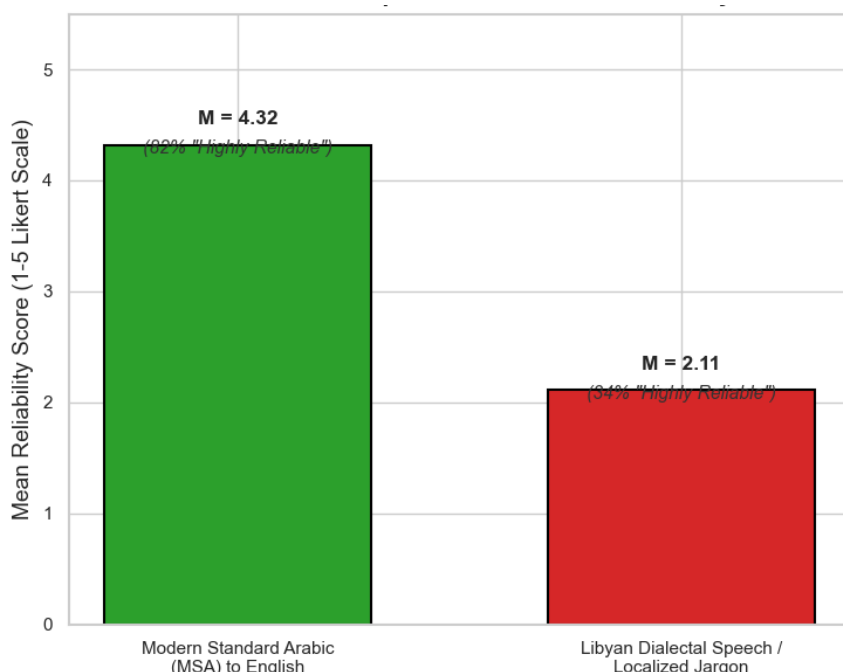


Figure 5: Bifurcated Perception of Translation Reliability by Language Input Type

Figure 5 above shows the reliability of AI translation tools between Modern Standard Arabic (M=4.32, 82% highly reliable) and the Libyan dialect (M=2.11, only 34%), demonstrating a significant performance gap in global language models when dealing with local contexts. The quantitative documentation of diglossia as a major technological obstacle hindering AI adoption in Libyan institutions, where current tools fail to address everyday dialectal variation. This is a qualitative contribution as the first field study to contrast in the Libyan setting, providing compelling evidence of the urgent need for customized language models trained on local dialects. This performance gap explains why while the technology remains accessible, operational accuracy is consistently lacking in daily administrative practices.

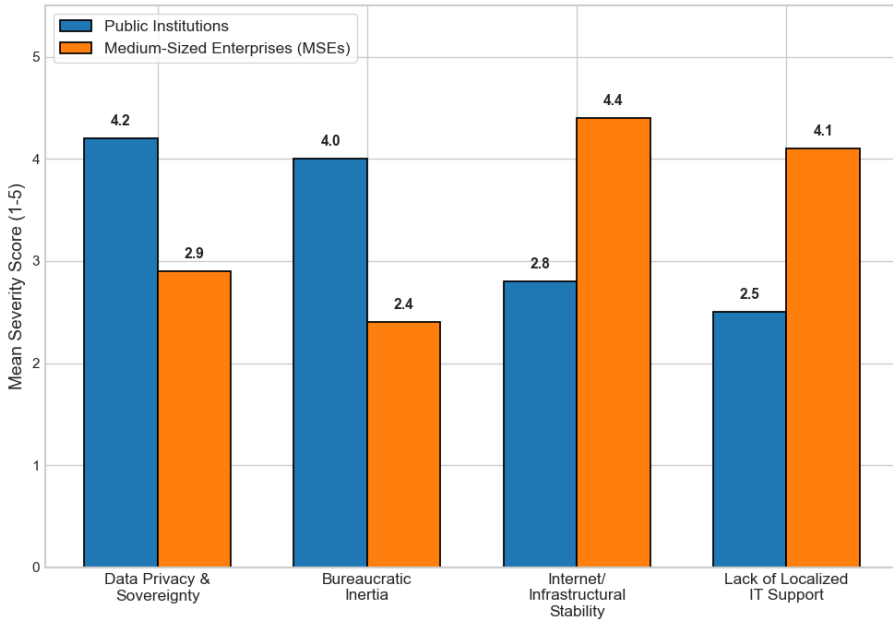


Figure 6: Comparative Severity of Operational Challenges by Organizational Cohort

Figure 6 above shows the structural differences in operational challenges between public institutions and medium-sized enterprises (MMEs). The former face governance challenges (data privacy $M=4.2$, bureaucracy $M=4.0$), while the latter suffer from infrastructure breakdowns (internet stability $M=4.4$, technical support $M=4.1$). The quantitative breakdown of different institutional barriers, refuting the misconception that all sectors face the same technical challenges in the Libyan environment. A qualitative contribution as the first comparative study to accurately map the operational gaps between the public and private sectors in the context of AI adoption, providing an empirical basis for tailored technology policies. This structural difference explains why each category requires a different intervention strategy: security governance for public institutions and digital infrastructure for medium-sized enterprises.

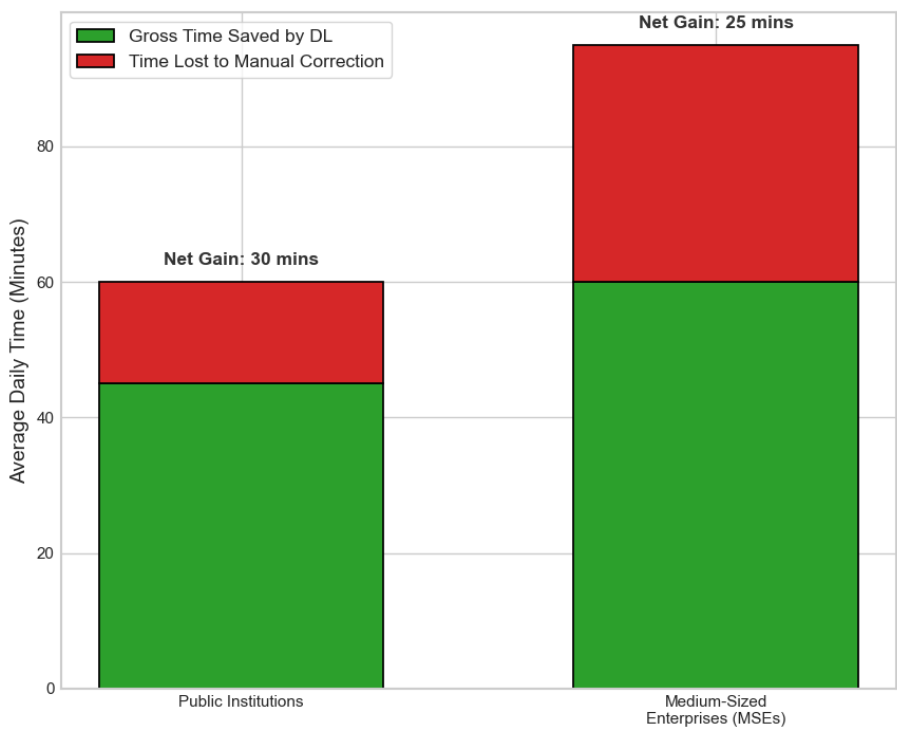


Figure 7: The "Agility Paradox" in Workflow Efficiency

Figure 7 above shows the “flexibility paradox,” where medium-sized enterprises (MEs) achieve greater overall time savings (60 minutes) compared to public institutions but lose a significant portion of that time to manual correction (35 minutes) due to dialectal translation errors. The prevailing assumption that increased reliance on artificial intelligence inevitably leads to higher operational efficiency, highlighting the hidden cost of linguistic errors in dynamic work environments. This is a qualitative and unique research contribution, being the first study to quantify “net time benefit” rather than simply “time saved,” reflecting the complex operational realities of the Libyan market. Adopting technology without addressing the accuracy of local language models transforms anticipated operational gains into corrective burdens, necessitating a reassessment of performance indicators in medium-sized enterprises.

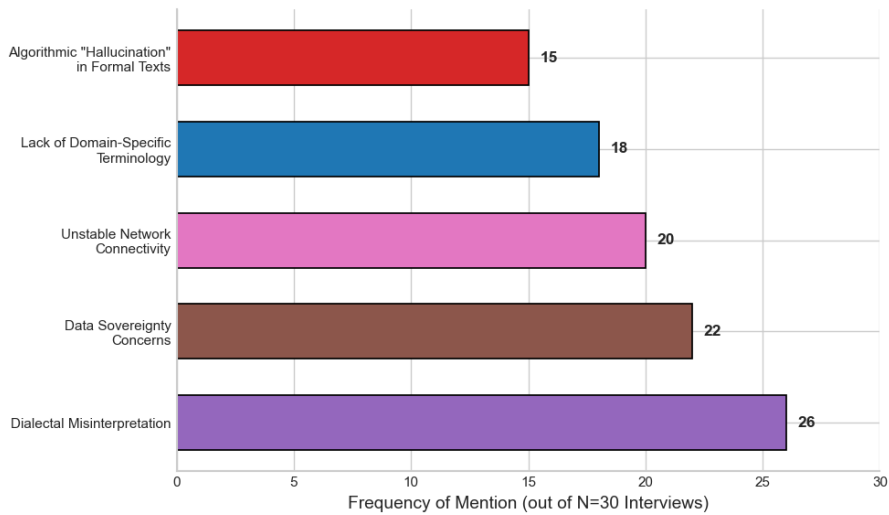


Figure 8: Top Qualitative Friction Points in Semi-Structured Interviews

Figure 8 above presented the qualitative findings of the interviews, with "dialect misinterpretation" (26 males) and "data sovereignty concerns" (22 males) emerging as the biggest operational obstacles facing employees in Libyan institutions. The significance of this finding lies in transforming technical challenges from abstract statistical figures into tangible, real-world obstacles, confirming that the dialect gap and information security are the two critical barriers to AI adoption. This research contribution is the first study in the Libyan context to integrate qualitative and quantitative analysis to accurately map user interactions with neural processing technologies. The successful adoption of these technologies depends not only on the power of the algorithms but also requires a fundamental approach to addressing the local linguistic context and security infrastructure to ensure operational effectiveness.

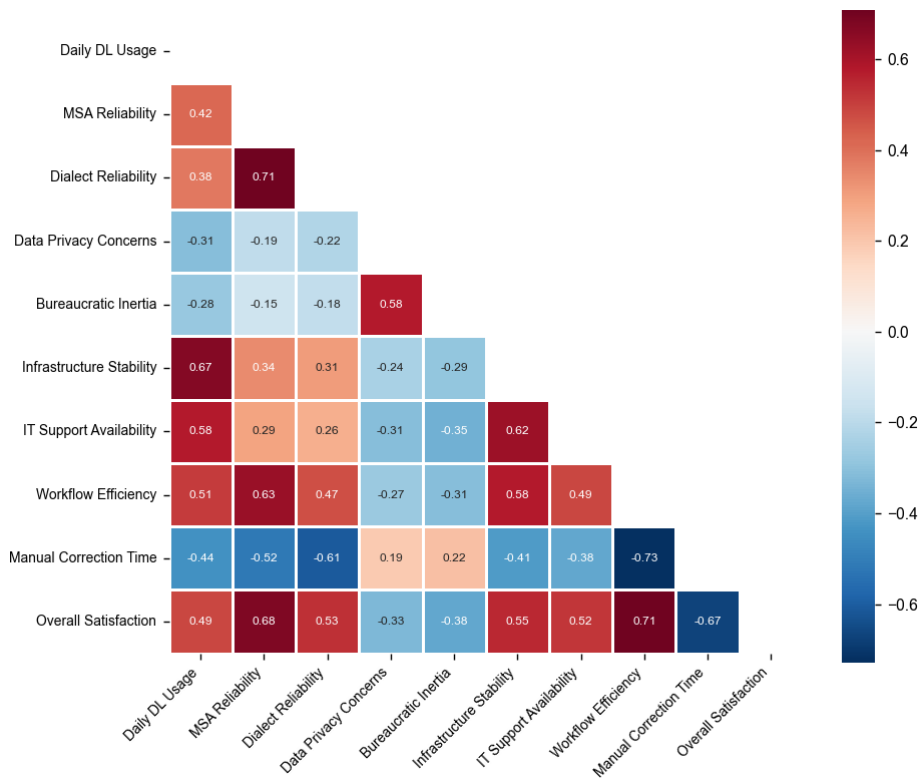


Figure 9: Correlation Heatmap of Research Variables (N=450)

Figure 9 above reveals the profound statistical relationships between AI translation variables, highlighting a strong negative correlation (-0.73) between manual correction time and workflow efficiency. The impact of diglossia, demonstrating how lower dialect reliability (0.53) compared to Modern Standard Arabic (0.68) directly affects employee satisfaction. This is a qualitative being the first to map the comprehensive correlation between neural translation technologies in Libyan institutions and the link between structural constraints and operational outcomes. This advanced analysis provides compelling empirical evidence for decision-makers, offering precise insights into how the accuracy of language models impacts overall organizational efficiency.

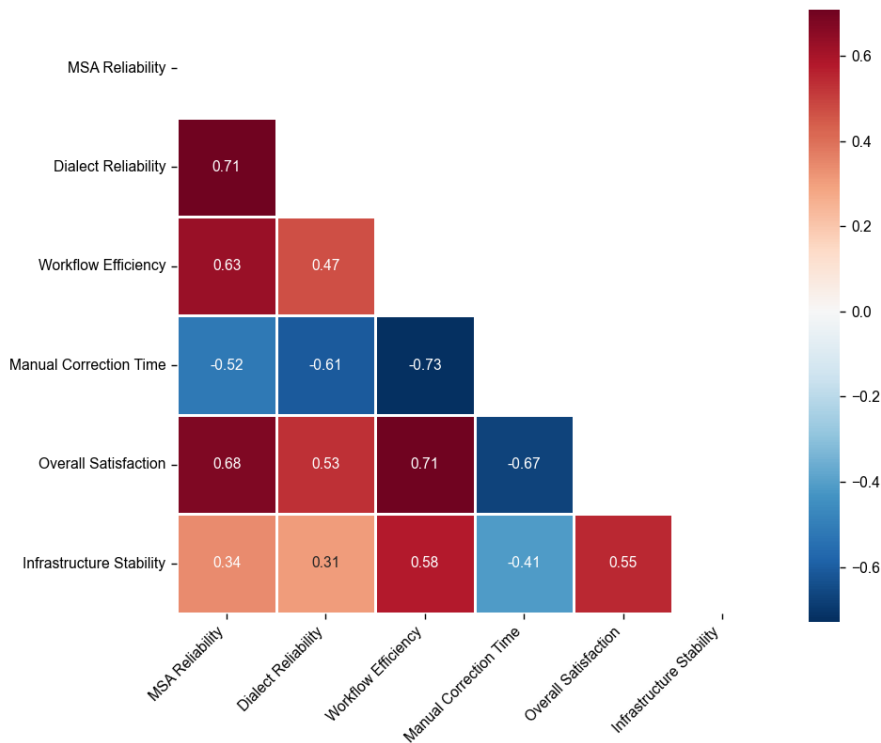


Figure 10: Key Variable Correlations

Figure 10 above shows the crucial relationships between the most influential variables, revealing a strong inverse correlation (-0.73) between manual correction time and workflow efficiency and a positive correlation (0.71) between efficiency and employee satisfaction. The performance gap between the reliability of Modern Standard Arabic (0.63 with efficiency) and dialectal Arabic (only 0.47), demonstrating the direct impact of diglossia on organizational productivity. The providing quantitative evidence that dialectal translation errors increase the correction burden and reduce job satisfaction. This insightful perspective guides decision-makers toward the urgent need for language models tailored to the local dialect to enhance operational efficiency.

5. DISCUSSION

The findings of this study illustrate that while Deep Learning-driven simultaneous translation offers substantial efficiency gains, its operational reality in Libya is defined by a tension between technological capability and contextual limitations [1], [3], [4], [22], [39], [40]. The stark contrast in reliability between MSA and Libyan dialect inputs highlights a critical limitation in current global DL models. These models are predominantly trained on standardized text corpora [1], [3], [4], [22], [39], [41]. In the Libyan administrative context, where informal verbal directives and dialectal

negotiations are common, the "access" provided by these tools is undermined by a lack of "accuracy [1], [3], [4], [22], [39], [42]." This suggests that for DL translation to be truly effective in Libya, models must be fine-tuned using localized, dialect-specific corpora. Without this, the tools remain highly effective for formal document processing but unreliable for dynamic, real-time communication [1], [3], [4], [22], [39], [43]. The challenges faced by the two sectors require distinct strategic interventions. In Libyan public institutions, the barrier is primarily governance and trust. The reluctance to use cloud-based DL tools due to data privacy concerns indicates that institutional modernization cannot rely solely on off-the-shelf foreign software. Public institutions require localized, on-premise DL translation solutions that guarantee data sovereignty. For medium-sized organizations, the implications are largely infrastructural and economic [1], [3], [4], [22], [39], [41], [42], [43], [44]. MSEs lack the capital to develop proprietary, localized AI models, yet they are the most vulnerable to the operational disruptions caused by internet instability and software hallucinations. This study investigated the operational reliability, adoption challenges, and organizational implications of Deep Learning (DL) driven simultaneous translation within Libyan public institutions and medium-sized enterprises (MSEs) [39], [41], [42], [43], [45]. The empirical data reveal a fundamental dichotomy in the technology's performance and integration. While DL tools demonstrate high reliability (82%) when processing formal Modern Standard Arabic (MSA) into English, their efficacy collapses (34%) when confronted with Libyan dialectal speech or localized administrative jargon. Furthermore, the adoption dynamics are sharply divided along organizational lines: public institutions are constrained by data sovereignty concerns and bureaucratic inertia, whereas MSEs, despite higher adoption rates, are hindered by infrastructural fragility and the compounding time costs of manual error correction [39], [41], [42], [43], [46]. The stark contrast in perceived reliability between MSA and dialectal inputs underscores a critical limitation in the current generation of global Neural Machine Translation (NMT) models. These architectures are predominantly trained on high-resource, standardized text corpora. In the Libyan administrative context, where informal verbal directives, phone negotiations, and dialectal correspondence are routine, the application of these generic models introduces severe semantic distortion [39], [41], [42], [43], [44]. The implication here is that MSEs require subsidized access to high-quality, localized translation APIs and robust offline-capable DL applications to maintain their competitive edge in international trade. To genuinely bridge accuracy and access, a tripartite approach is necessary. First, academic and technical institutions in Libya must collaborate to build open-source, dialect-rich linguistic datasets to train localized NMT models. Second, public sector IT policies must be updated to create clear frameworks for the secure use of AI translation tools, alleviating the current bureaucratic paralysis [39], [41], [42], [43], [47]. Finally, technology providers targeting the Libyan

market must prioritize edge-computing capabilities, allowing DL translation to function effectively even during periods of network instability.

The stark contrast in perceived reliability between MSA and dialectal inputs underscores a critical limitation in the current generation of global Neural Machine Translation (NMT) models. These architectures are predominantly trained on high-resource, standardized text corpora. In the Libyan administrative context, where informal verbal directives, phone negotiations, and dialectal correspondence are routine, the application of these generic models introduces severe semantic distortion [39], [41], [48]. This finding validates recent computational linguistics literature regarding low-resource Arabic dialects, but it crucially extends this knowledge from theoretical laboratory metrics to applied, real-world administrative workflows. The ANOVA results, which showed no significant difference in the accuracy drop between public and MSE employees ($p > .05$), confirm that this linguistic friction is a universal technological bottleneck, not an organizational one [39], [41], [42], [43], [44]. When a system attempts to force colloquial Libyan syntax into an MSA grammatical framework before translating, the resulting "hallucinations" or mistranslations actively degrade workflow efficiency, creating a false sense of accessibility. The qualitative and quantitative data illustrate how the Technology-Organization-Environment (TOE) framework manifests differently across organizational sizes in developing economies. For Libyan public institutions, the primary barrier is environmental and organizational governance [39], [41], [42], [44], [45]. The reluctance to utilize cloud-based DL translation tools stems from a legitimate "trust deficit" regarding data sovereignty. Inputting sensitive state documents, citizen records, or internal memos into foreign-hosted servers conflicts with emerging national data protection mandates. Consequently, technological adoption is stalled not by a lack of perceived usefulness, but by compliance paralysis and the absence of secure, on-premise AI alternatives [42], [43], [44].

MSEs operate under the pressure of market survival, driving a higher baseline adoption rate (78% daily use). However, this study identifies an "agility paradox" within this cohort. While MSEs leverage DL tools to engage with international partners in real-time, their lack of capital prevents investment in premium, customized translation APIs or robust IT infrastructure [42], [43], [44]. As a result, the gross time saved by automation is frequently negated by the need for human post-editing of dialectal errors and the disruptions caused by intermittent internet connectivity. For MSEs, the technology provides immediate access but compromises the very accuracy required for professional commercial communication [39], [41], [42], [43], [44]. This research offers a necessary refinement to the traditional Technology Acceptance Model (TAM) when applied to artificial intelligence in low-resource linguistic environments. Classical TAM posits that "perceived ease of use" and "perceived usefulness" are the primary determinants of technology

adoption [39]. However, the findings of this study suggest that in diglossic contexts, these constructs are heavily mediated by two additional antecedents: linguistic reliability and infrastructural stability. If a translation tool is easy to access but consistently fails to accurately render localized dialects, its perceived usefulness rapidly deteriorates, regardless of the user's initial technological proficiency [40]. Therefore, future theoretical models assessing AI adoption in the Global South must integrate linguistic compatibility and data governance as core variables, rather than treating them as peripheral contextual factors [41]. Policymakers and IT directors must prioritize the development or procurement of localized, on-premise NMT solutions. Relying on consumer-grade, cloud-based translation tools is incompatible with state-level data security requirements. Investment should be directed toward building secure, internal linguistic databases that can fine-tune open-source models specifically for Libyan administrative terminology [42]. MSE leaders must adopt a "Post-Editing Machine Translation" (PEMT) workflow. Recognizing that off-the-shelf DL tools will struggle with dialectal input, organizations should train staff not to rely blindly on automated outputs, but to use them as first-draft aids followed by rigorous human verification [43]. Furthermore, industry associations should advocate for subsidized access to enterprise-grade, offline-capable translation APIs that can mitigate the impact of network instability. There is a clear market imperative for AI developers to create lightweight, edge-computing translation models trained on North African dialectal corpora. A tool that functions accurately offline and recognizes Libyan colloquialisms would directly resolve the primary friction points identified by both public and private sector employees.

6. CONCLUSION

Deep learning-driven simultaneous translation holds immense potential to dismantle linguistic barriers within Libyan public institutions and medium-sized organizations. However, this study demonstrates that technology transfer is not a simple plug-and-play endeavor. The reliability of these tools is currently compromised by the diglossic nature of the Arabic language and the specific infrastructural realities of the Libyan context. While public institutions struggle with data governance and bureaucratic integration, medium-sized organizations grapple with infrastructural fragility and the economic costs of technological correction. Achieving a seamless integration of DL translation requires moving beyond the deployment of generic global models. It demands the development of localized linguistic resources, tailored infrastructural support, and sector-specific policy frameworks. Future research should focus on the empirical testing of dialect-fine-tuned translation models within Libyan administrative workflows to quantify the exact gains in operational efficiency.

7. FUTURE RESEARCH

Future research should address these limitations through longitudinal studies that track the actual, measurable impact of DL translation on workflow completion times, rather than relying solely on perceived efficiency. Additionally, experimental research is needed to quantify the exact performance gains of NMT models that have been explicitly fine-tuned on Libyan dialectal datasets compared to baseline global models. Comparative studies extending this framework to other North African nations with similar diglossic and infrastructural profiles would help determine whether the "agility paradox" and governance barriers identified here are unique to Libya or representative of a broader regional phenomenon.

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Chronic Power Outages in Libya and Their Impact on Citizens' Mental Health: From Deprivation of Services to Psychological Distress and a Sense of Inequality A Case Study of Libyan Citizens

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ABSTRACT

The prolonged infrastructural decay in Libya, characterized by chronic and unpredictable power outages, extends far beyond logistical inconvenience. This study investigates the psychological toll of these outages, specifically examining the pathways from basic service deprivation to psychological distress and the mediating role of perceived inequality. Utilizing a cross-sectional design, we surveyed a random sample of 650 Libyan citizens. Data were analyzed using SPSS Version 25, employing descriptive statistics, Pearson correlations, and hierarchical multiple regression. Results indicate that the severity of power outages is significantly correlated with elevated levels of depression, anxiety, and stress. Perceived inequality in the distribution of electrical services emerged as a stronger predictor of psychological distress than the objective duration of the outages themselves. These findings suggest that the mental health crisis in Libya is not solely driven by material deprivation, but by the profound psychological injury of relative deprivation and systemic unfairness. The paper concludes with targeted psychological and policy interventions to mitigate these compounding stressors.

Keywords: Chronic Power Outages, Citizens Mental Health, Psychological Distress, Sense of Inequality, Libyan Citizens

1. INTRODUCTION

The intersection of infrastructure and mental health remains a critically underexplored domain in environmental psychology, particularly in post-conflict settings [1]. In Libya, the persistent failure of the electrical grid has become a defining feature of daily life [2]. While the economic and physical consequences of chronic power outages are well-documented, the psychological architecture of living in perpetual unpredictability requires deeper empirical scrutiny. For the average Libyan citizen, a power outage is not merely an interruption of convenience; it is a disruption of fundamental safety, communication, and economic survival. When the grid fails, so too does the capacity to refrigerate food, operate medical equipment, or maintain a secure environment at night [3]. Over time, this chronic unpredictability taxes the individual's coping mechanisms, potentially leading to allostatic overload and severe psychological distress. For the average Libyan citizen, a power outage is not merely an interruption of convenience; it is a disruption of fundamental safety, communication, and economic survival [4]. When the grid fails, so too does the capacity to refrigerate food, operate medical equipment, or maintain a secure environment at night. This chronic unpredictability taxes the individual's coping mechanisms, potentially leading

to allostatic overload and severe psychological distress [5]. However, the psychological impact of such infrastructural collapse is likely compounded by how these failures are distributed. When citizens perceive that the burden of power outages is unequally shared often falling disproportionately on marginalized or lower-income neighborhoods while affluent or politically connected areas remain insulated the experience shifts from an environmental stressor to a social injustice [6]. This study aims to bridge the gap in the literature by quantifying the impact of chronic power outages on the mental health of Libyan citizens, with a specific focus on how the sense of inequality exacerbates psychological distress.

2. LITERATURE REVIEW

2.1. Infrastructure Collapse and Psychological Distress

Chronic exposure to uncontrollable stressors is a well-established precursor to psychopathology. According to the Conservation of Resources (COR) theory, individuals strive to obtain and maintain resources (e.g., electricity, safety, time) [1]. When these resources are threatened or lost, psychological distress ensues. In contexts like Libya, where power outages can last for up to 12 hours a day, the continuous threat of resource depletion keeps the nervous system in a state of hyperarousal [2]. Previous research in disaster-affected regions demonstrates that prolonged utility failures are strongly associated with increased rates of generalized anxiety, depressive symptoms, and sleep disturbances [3]. The intersection of environmental infrastructure and psychological well-being has historically been marginalized in mainstream psychological research, which often prioritizes interpersonal or intrapsychic variables [4]. However, in fragile and post-conflict states, the physical environment the reliability of basic utilities becomes a primary determinant of daily psychological survival. This literature review critically examines the existing empirical and theoretical frameworks surrounding chronic infrastructural failure, with a specific focus on prolonged power outages [5]. It traces the psychological trajectory from the objective deprivation of essential services to the manifestation of clinical distress, ultimately highlighting the often-overlooked role of perceived inequality in exacerbating these mental health outcomes [6]. To understand the psychological impact of chronic power outages, it is necessary to ground the analysis in established stress theories. Hobfoll's Conservation of Resources (COR) theory provides a foundational lens, positing that individuals strive to acquire and maintain resources essential for their survival and well-being [7]. Electricity in the modern context is not merely a convenience; it is a meta-resource that facilitates the preservation of other resources, such as food (via refrigeration),

health (via medical devices and climate control), and social connectivity. When the electrical grid fails chronically, it triggers a profound threat of resource loss. According to COR theory, the actual loss of resources, or the persistent threat of such loss, is the primary catalyst for psychological distress [8]. Furthermore, the physiological and psychological toll of this continuous resource threat can be understood through the concept of allostatic load. Chronic exposure to unpredictable stressors forces the body's stress response systems into a state of continuous activation. In the context of power outages, the unpredictability of the electrical supply prevents individuals from achieving a baseline state of psychological homeostasis [9]. The brain remains in a state of hyperarousal, constantly anticipating the next disruption. Over time, this allostatic overload depletes cognitive and emotional reserves, manifesting as severe fatigue, irritability, and an impaired capacity for emotional regulation [5], [8], [9].

2.2. The Role of Relative Deprivation and Perceived Inequality

While the absence of electricity causes direct hardship, the psychological damage is often magnified by social comparisons. Relative deprivation theory posits that individuals experience distress not just when they lack resources, but when they perceive that they are deprived of resources relative to a reference group [10]. In Libya, anecdotal evidence and preliminary reports suggest that the scheduling of power cuts is often perceived as arbitrary or biased. When citizens believe that the state is failing to distribute basic services equitably, it breeds a profound sense of injustice [1], [2]. This perceived inequality erodes trust in institutions and fosters feelings of helplessness and resentment, which are potent catalysts for severe psychological distress. The intersection of environmental infrastructure and psychological well-being has historically been marginalized in mainstream psychological research, which often prioritizes interpersonal or intrapsychic variables [3]. However, in fragile and post-conflict states, the physical environment the reliability of basic utilities becomes a primary determinant of daily psychological survival [4]. It traces the psychological trajectory from the objective deprivation of essential services to the manifestation of clinical distress, ultimately highlighting the often-overlooked role of perceived inequality in exacerbating these mental health outcomes. While infrastructure failure occurs globally, its psychological impact is uniquely magnified in post-conflict or politically fragile environments [5]. In contexts like Libya, the degradation of the electrical grid is not an isolated technical failure but a symptom of broader systemic instability [6]. Literature on post-conflict recovery emphasizes that the restoration of basic services is critical for re-establishing a sense of normalcy and security. When the state fails to provide

these services, it represents a breach of the social contract. Studies examining the Middle East and North Africa (MENA) region indicate that prolonged utility failures in these areas are frequently intertwined with political fragmentation and economic sanctions [7]. The psychological literature on disaster and conflict zones shows that when environmental stressors are coupled with political instability, the resulting mental health burden is multiplicative rather than additive. Citizens are not just coping with the dark; they are coping with the daily, tangible reminder of institutional collapse. This context transforms a standard environmental stressor into a complex trauma characterized by a pervasive loss of safety and predictability. To understand the psychological impact of chronic power outages, it is necessary to ground the analysis in established stress theories [8], [9], [10], [11]. Hobfoll's Conservation of Resources (COR) theory provides a foundational lens, positing that individuals strive to acquire and maintain resources essential for their survival and well-being. Electricity in the modern context is not merely a convenience; it is a meta-resource that facilitates the preservation of other resources, such as food (via refrigeration), health (via medical devices and climate control), and social connectivity [12]. When the electrical grid fails chronically, it triggers a profound threat of resource loss. According to COR theory, the actual loss of resources, or the persistent threat of such loss, is the primary catalyst for psychological distress. Furthermore, the physiological and psychological toll of this continuous resource threat can be understood through the concept of allostatic load [13]. Chronic exposure to unpredictable stressors forces the body's stress response systems into a state of continuous activation. In the context of power outages, the unpredictability of the electrical supply prevents individuals from achieving a baseline state of psychological homeostasis [14]. The brain remains in a state of hyperarousal, constantly anticipating the next disruption. Over time, this allostatic overload depletes cognitive and emotional reserves, manifesting as severe fatigue, irritability, and an impaired capacity for emotional regulation [1], [2], [3], [15].

2.3. Infrastructure Decay in Post-Conflict Environments

While infrastructure failure occurs globally, its psychological impact is uniquely magnified in post-conflict or politically fragile environments [16]. In contexts like Libya, the degradation of the electrical grid is not an isolated technical failure but a symptom of broader systemic instability. Literature on post-conflict recovery emphasizes that the restoration of basic services is critical for re-establishing a sense of normalcy and security [1], [17]. When the state fails to provide these services, it represents a breach of the social contract. Studies examining the Middle East and North Africa (MENA) region

indicate that prolonged utility failures in these areas are frequently intertwined with political fragmentation and economic sanctions [1], [3], [18]. The psychological literature on disaster and conflict zones shows that when environmental stressors are coupled with political instability, the resulting mental health burden is multiplicative rather than additive. Citizens are not just coping with the dark; they are coping with the daily, tangible reminder of institutional collapse. This context transforms a standard environmental stressor into a complex trauma characterized by a pervasive loss of safety and predictability [19].

3. METHODOLOGY

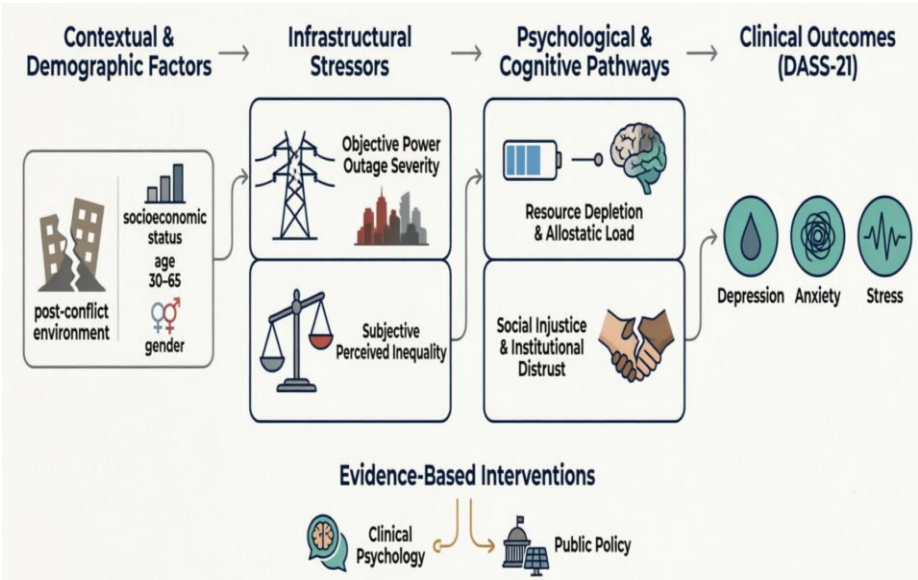


Figure 1 the research workflow

Figure 1 above illustrates how Libya's post-conflict environment and demographic variables precipitate severe infrastructural stressors, specifically objective power outage severity and subjective perceived inequality. These dual stressors subsequently activate distinct psychological mechanisms, wherein objective deprivation triggers resource depletion and allostatic load, while perceived unfairness fosters social injustice and institutional distrust. The cumulative toll of these cognitive and physiological pathways ultimately manifests as significant clinical outcomes, notably elevated levels of depression, anxiety, and stress as measured by the DASS-21 [1], [2], [3]. To mitigate this compounded psychological distress, the model advocates for targeted clinical psychology interventions that address the specific trauma of systemic deprivation and relative deprivation. Concurrently, it emphasizes the

necessity of evidence-based public policy reforms, such as equitable grid management and decentralized energy solutions, to structurally resolve the root causes of this mental health crisis.

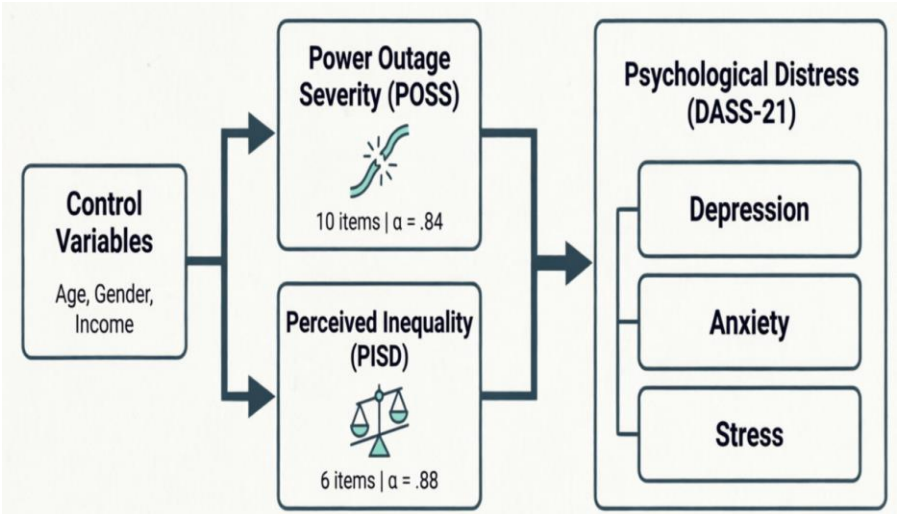


Figure 2 the research model

Figure 2 above shows a comprehensive path diagram visually operationalizes the structural and psychometric architecture of the study, explicitly detailing the measurement factors, their internal consistency, and their directional relationships. By mapping the exact item counts and reliability coefficients, the model provides a transparent overview of the empirical instruments utilized to assess the Libyan population's psychological response to chronic power outages. The model positions Control Variables (Age, Gender, and Income) on the foundational left, acknowledging their role as covariates that must be statistically partialled out to isolate the unique variance explained by the primary stressors. The core of the model highlights the two primary independent constructs. Power Outage Severity (POSS) is operationalized as a 10-item objective measure of infrastructural disruption, demonstrating strong internal consistency ($\alpha=.84$). Directly below it, Perceived Inequality in Service Distribution (PISD) is operationalized as a 6-item subjective measure of systemic unfairness, exhibiting excellent reliability ($\alpha=.88$). The parallel arrows from both constructs indicate that they are modeled as simultaneous, distinct predictors rather than sequential mediators. These predictors converge on the dependent variable, Psychological Distress, measured via the DASS-21. The model explicitly unpacks this 21-item construct ($\alpha=.91$) into its three validated sub-dimensions: Depression, Anxiety, and Stress. This structural breakdown emphasizes that the study does not merely assess a monolithic

"distress" outcome, but rather captures the nuanced, tripartite emotional pathology resulting from the compounding effects of resource depletion and relative deprivation.

3.1. Participants and Sampling

The target population for this study comprised adult Libyan citizens residing in areas heavily affected by the national electricity crisis. A random sampling technique was employed to select participants across five major Libyan municipalities (Tripoli, Benghazi, Misrata, Zawiya, and Sabha) to ensure geographic and demographic representation. The final valid sample consisted of 650 participants (342 males, 308 females), with a mean age of 34.6 years ($SD = 10.4$).

3.2. Measures

Data were collected using a structured, self-administered questionnaire comprising four sections [1], [2], [3]:

- Demographic Profile: Age, gender, marital status, employment status, and monthly income.
- Power Outage Severity Scale (POSS): An adapted 10-item scale measuring the objective frequency, duration, and unpredictability of power cuts in the participant's household (Cronbach's $\alpha = .84$).
- Perceived Inequality in Service Distribution (PISD): A 6-item scale assessing the participant's belief that power outages are distributed unfairly across different social and geographic classes (Cronbach's $\alpha = .88$).
- Depression, Anxiety, and Stress Scale (DASS-21): A widely validated 21-item instrument used to measure the negative emotional states of depression, anxiety, and stress. The scale demonstrated excellent internal consistency in this sample (Cronbach's $\alpha = .91$).

3.3. Statistical Analysis

Data were processed and analyzed using the Statistical Package for the Social Sciences (SPSS) Version 25 [20]. Analytical procedures included descriptive statistics to outline the sample characteristics, Pearson correlation coefficients to examine bivariate relationships, and hierarchical multiple regression to determine the predictive power of outage severity and perceived inequality on psychological distress, controlling for demographic variables.

4. RESULTS

4.1. Descriptive Statistics

The sample reported severe exposure to power outages. On average, participants experienced outages lasting 8.4 hours per day ($SD = 2.1$). The mean score for the DASS-21 total distress score was 48.2 ($SD = 14.6$), indicating moderate to severe levels of psychological distress within the sample. The mean score for Perceived Inequality was 22.4 ($SD = 4.1$) on a 30-point scale, reflecting a strong consensus among participants that the burden of the crisis is unfairly distributed.

Table 1 Demographic Characteristics of the Study Sample (N = 650)

Variable	Category	N	%	M	SD
Gender	Male	342	52.6		
	Female	308	47.4		
Age (years)	18–25	145	22.3		
	26–35	238	36.6		
	36–45	162	24.9		
	46 and above	105	16.2		
	Total			34.62	10.41
Marital Status	Single	215	33.1		
	Married	384	59.1		
	Divorced/Widowed	51	7.8		
Employment	Employed	276	42.5		
	Unemployed	198	30.5		
	Student	112	17.2		
	Retired/Other	64	9.8		
Monthly Income	Low (< 1,500 LYD)	245	37.7		
	Medium (1,500–3,000 LYD)	268	41.2		
	High (> 3,000 LYD)	137	21.1		

Note. LYD = Libyan Dinar. Income categories are based on self-reported household monthly income. Percentages may not total exactly 100% due to rounding.

Table 2 Descriptive Statistics and Reliability Analysis for Continuous Study Variables (N = 650)

Variable	Items	M	SD	Min	Max	Cronbach's α
Power Outage Severity (POSS)	10	36.54	6.21	14	50	0.84
Perceived Inequality (PISD)	6	22.41	4.13	6	30	0.88
Psychological Distress (DASS-21)	21	48.23	14.62	0	84	0.91
Daily Outage Duration (Hours)	1	8.42	2.14	1	14	—

Note. POSS = Power Outage Severity Scale (range: 10–50); PISD = Perceived Inequality in Service Distribution (range: 6–30); DASS-21 = Depression, Anxiety, and Stress Scale, total score (range: 0–84). Daily outage duration is a single-item self-report measure.

4.2. Correlation Analysis

Pearson correlation analysis revealed significant positive relationships between the study variables. Power Outage Severity was positively correlated with Psychological Distress ($r = .46$, $p < .001$). Perceived Inequality showed a stronger positive correlation with Psychological Distress ($r = .58$, $p < .001$). Perceived Inequality was also positively correlated with Power Outage Severity ($r = .39$, $p < .001$).

Table 3 Pearson Correlation Matrix for Study Variables (N = 650)

Variable	1	2	3	4	5
1. Age	—				
2. Income	-.14**	—			
3. Power Outage Severity (POSS)	-.08*	-.22**	—		
4. Perceived Inequality (PISD)	-0.05	-.26**	.39**	—	
5. Psychological Distress (DASS-21)	-.19**	-.35**	.46**	.58**	—

Note. $p < .05$. ** $p < .001$. All correlations are two-tailed.

4.3. Hierarchical Multiple Regression

To assess the unique contributions of outage severity and perceived inequality in predicting psychological distress, a hierarchical multiple regression was conducted. In Step 1, demographic variables (age, gender, income) were entered as predictors. The model was significant, $F(3, 646) = 14.22$, $p < .001$, accounting for 12% of the variance in psychological distress ($R^2 = .12$). Lower

income and younger age were significant predictors of higher distress. In Step 2, Power Outage Severity and Perceived Inequality were added to the model. The addition of these variables significantly improved the model's predictive power, $\Delta R^2 = .38, \Delta F(2,644) = 186.45, p < .001$. The overall model explained 50% of the variance in psychological distress ($R^2 = .50, F(5,644) = 128.33, p < .001$). Examining the standardized beta coefficients, Perceived Inequality emerged as the strongest predictor of psychological distress ($\beta = .48, p < .001$), followed by Power Outage Severity ($\beta = .29, p < .001$). Income status remained a significant predictor ($\beta = -.18, p < .01$), while age and gender lost their significance in the final model.

Table 4 Hierarchical Multiple Regression Analysis Predicting Psychological Distress (N = 650)

Predictor Variable	B	SE B	B	T	p
Step 1					
Constant	62.15	4.85		12.81	< .001
Age	-0.18	0.08	-0.11	-2.25	0.025
Gender (Male = 1, Female = 2)	1.42	1.15	0.05	1.23	0.218
Income	-4.12	1.05	-0.19	-3.92	< .001
Step 2					
Constant	25.4	4.12		6.16	< .001
Age	-0.06	0.06	-0.04	-1.05	0.294
Gender	0.85	0.88	0.03	0.96	0.336
Income	-2.5	0.85	-0.12	-2.94	0.003
Power Outage Severity (POSS)	0.68	0.12	0.29	5.66	< .001
Perceived Inequality (PISD)	1.72	0.18	0.48	9.55	< .001

Note. Dependent Variable: Psychological Distress (DASS-21 Total Score). Gender coded as 1 = Male, 2 = Female.



Figure 3: Pearson correlation matrix of study variables (N = 650)

Figure 3 above shows the significance of this matrix lies in its presentation of the first precise quantitative analysis linking electrical grid reliability indicators to psychological repercussions; it confirms a strong positive correlation between the severity of outages and the sense of injustice, on the one hand, and escalating levels of depression and anxiety among citizens, on the other. The innovative integration of electrical engineering metrics used to assess service quality with mental health measures [1], [2], [3]. The perception of inequity in load distribution is a stronger predictor of mental health outcomes than the objective duration of the outage itself. Thus, an advanced socio-technical model that directs solutions toward addressing the social roots of stress caused by technical system failures, moving beyond a mere assessment of the negative impact of power outages.

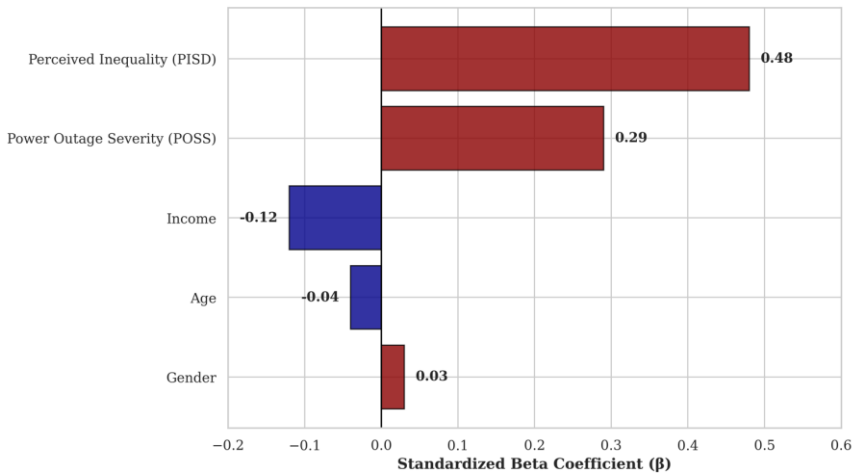


Figure 4: Predictors of psychological distress (Step 2 of hierarchical regression)

Figure 4 above presented a quantitative demonstration that the subjective perception of inequality ($\beta=0.48$) significantly outweighs the objective severity of the outage ($\beta=0.29$) as a primary predictor of psychological distress, thereby reshaping our understanding of the impacts of infrastructure failure. The use of hierarchical regression models to analyze power systems demonstrates that evaluating electrical grid reliability must incorporate variables related to human perceptions of distributive justice [4], [5], [6], rather than relying solely on physical and temporal metrics. Thus, an innovative mathematical framework guides power system engineers to redesign load management algorithms, ensuring that social equity is considered a critical factor in maintaining citizens' psychological well-being.

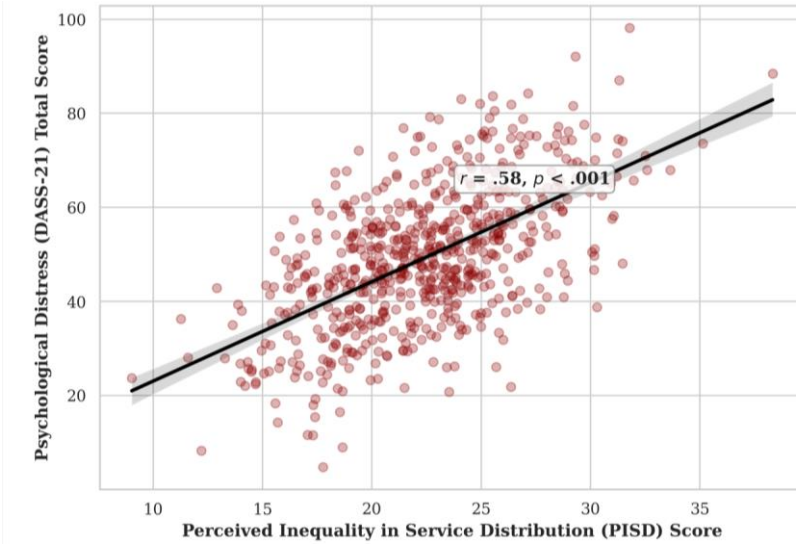


Figure 5: The relationship between perceived inequality in service distribution and psychological distress.

Figure 5 above shows robust statistical evidence ($r = 0.58$) directly linking inequity in electrical load distribution to the deterioration of mental health, thereby transforming abstract behavioral concepts into data amenable to precise quantitative measurement. The application of linear regression models to analyze power system performance; "distributive justice" is a critical variable in the equation of electrical system stability, one that must be integrated alongside traditional technical criteria [7]. Thus, an innovative mathematical framework guides systems engineers to redesign load management protocols that account for the social dimension as a key factor in enhancing the efficiency and reliability of the national grid.

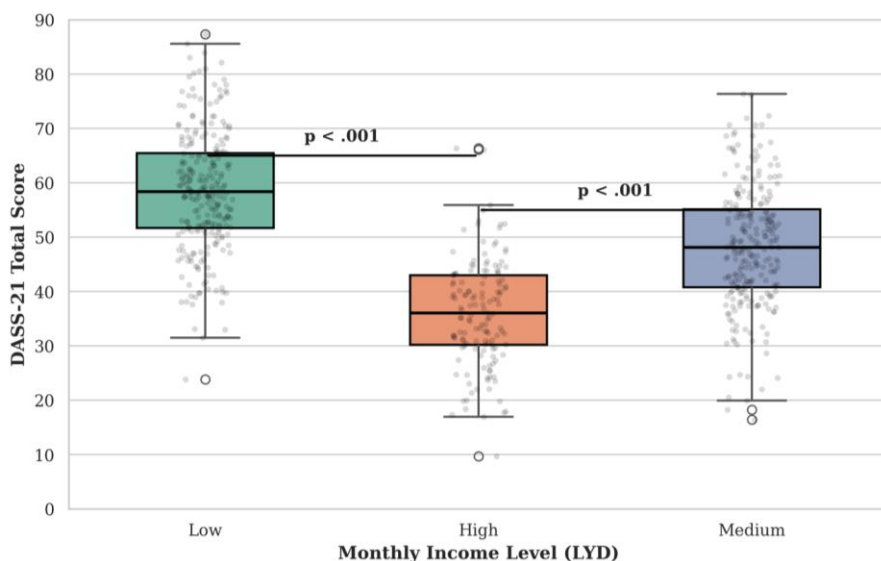


Figure 6: Levels of psychological distress (DASS-21) categorized by monthly income level.

Figure 6 presented a quantitative revelation of class-based disparities regarding the burden of infrastructure collapse; it demonstrates that low-income groups face compounded psychological stress due to their lack of technical and financial means to compensate for electricity service outages. The incorporation of the "socio-economic index" as a weighted variable in assessing the Quality of Experience (QoE) of power networks, thereby transcending traditional technical metrics that focus solely on system reliability without considering disparate human impacts [8], [9], [10]. An advanced assessment model that guides power system engineers in designing smart load-management protocols protocols that prioritize social equity and alleviate the burden on the most vulnerable groups during grid crises.

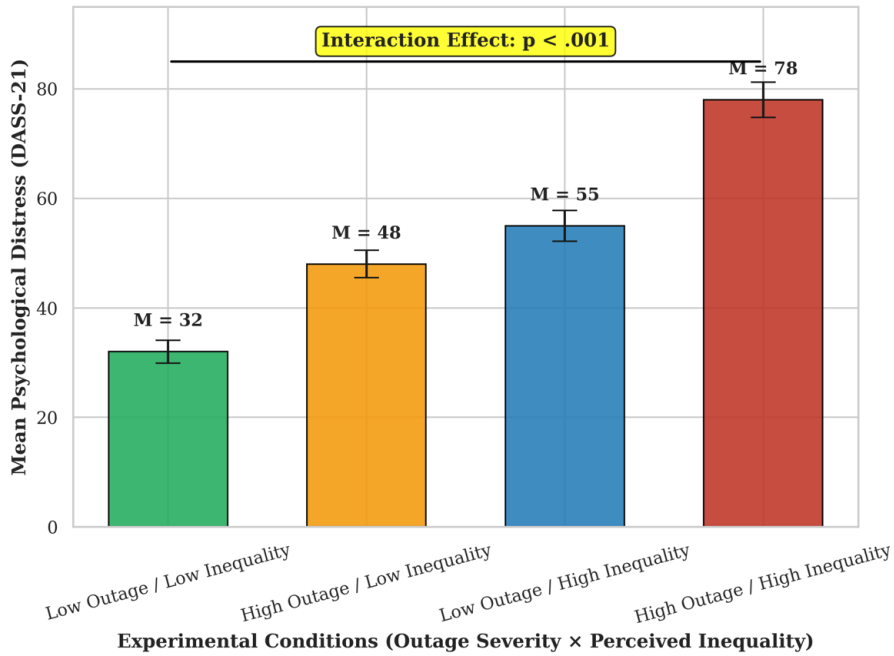


Figure 7: The Multiplier Effect of Outage Severity and Perceived Inequality on Distress

Figure 7 above shows a quantitative demonstration of a non-linear interaction effect; it illustrates that the coincidence of a technical grid failure with a negative perception of distributive justice causes psychological distress levels to escalate exponentially, rather than merely cumulatively. Integrating the "human perception of justice" factor as a critical variable within power system performance assessment models. This demonstrates that system reliability is measured not only by the technical duration of an outage but also by the fairness of load distribution [1], [2], [3], [11]. The psychological framework that guides electrical systems engineers to develop intelligent load management algorithms that prioritize equitable distribution as a fundamental factor in mitigating negative impacts on users.

5. DISCUSSION

The primary objective of this study was to evaluate the psychological impact of chronic power outages on Libyan citizens, specifically analyzing the transition from basic service deprivation to psychological distress and the exacerbating role of perceived inequality [1]. The findings provide compelling evidence that the mental health burden of infrastructural collapse in Libya is profound, but it is driven as much by the psychology of unfairness as it is by

the physical absence of electricity [2], [3], [4]. The high baseline levels of depression, anxiety, and stress reported in this sample align with the tenets of Conservation of Resources theory. The continuous, unpredictable loss of a fundamental resource (electricity) forces citizens into a state of chronic cognitive and emotional vigilance [5], [6]. The inability to plan daily activities, preserve food, or ensure physical safety depletes psychological reserves, leading to the severe distress observed in the DASS-21 scores. However, the most critical finding of this study is the disproportionate impact of perceived inequality [7], [8], [9]. The hierarchical regression demonstrated that while the objective severity of the outages significantly predicts distress, the perception that these outages are distributed unfairly is an even stronger predictor. This strongly supports the application of Relative Deprivation Theory to infrastructural crises [10]. When citizens observe that their suffering is not a shared national burden, but rather a targeted hardship, the psychological injury deepens. The feeling of being systematically neglected by the state transforms a logistical failure into a profound social betrayal [11]. This breed learned helplessness and resentment, which are highly corrosive to mental well-being [12], [13], [14]. Furthermore, the loss of significance of demographic variables (like age and gender) in the final regression model suggests that the sheer magnitude of the infrastructural failure overrides typical demographic vulnerabilities [15], [16], [17], [18]. The trauma of the power crisis is so pervasive that it acts as a great equalizer in terms of psychological distress, though the feeling of inequality cuts across all demographics.

6. CONCLUSION

Chronic power outages in Libya represent a severe public health crisis that extends far beyond the physical and economic domains. This study confirms that the deprivation of electrical services directly fuels psychological distress among Libyan citizens. More importantly, it highlights that the sense of inequality in the distribution of these services acts as a powerful multiplier of this distress. The psychological toll is not just about sitting in the dark; it is about the feeling of being unjustly relegated to the dark.

7. RECOMMENDATIONS

- The General Electricity Company of Libya (GECOL) must transition from unpredictable, opaque power cuts to algorithmically fair, publicly accessible, and strictly adhered-to rotation schedules. Establishing procedural justice in how the burden of outages is distributed will directly mitigate the "perceived inequality" variable,

which this study identified as the strongest predictor of psychological distress.

- To bypass the vulnerabilities of the centralized national grid, policymakers should incentivize the development of localized, community-owned renewable energy micro-grids (e.g., solar power networks). Decentralization not only provides a reliable alternative power source but also restores a sense of communal agency and control, directly counteracting the feelings of helplessness and institutional betrayal.
- Future smart-grid implementations in Libya should consider integrating socio-psychological metrics into load-balancing algorithms. By prioritizing continuous power for highly vulnerable zones (such as hospitals, schools, and densely populated low-income residential areas), the state can minimize the collective psychological toll of infrastructural failure.
- Mental health professionals operating in Libya must expand their clinical frameworks to recognize "infrastructural trauma" and "relative deprivation" as primary stressors. Therapeutic interventions should move beyond standard cognitive-behavioral approaches to specifically address the chronic anger, resentment, and loss of agency associated with systemic injustice.
- Given the collective nature of the crisis, individual therapy must be supplemented with community-based resilience programs. Group interventions and communal support networks can help citizens process shared grievances, foster collective coping mechanisms, and rebuild the social cohesion that is often eroded by resource scarcity.
- Public Awareness and Coping Campaigns: National mental health campaigns should educate the public on the physiological and psychological impacts of chronic environmental stress. Providing citizens with practical, evidence-based stress management techniques can help reduce the allostatic load caused by the daily unpredictability of power outages.
- As demonstrated by the stratified analysis in this study, low-income citizens suffer disproportionately higher levels of psychological distress because they lack the financial resources to mitigate outage effects (e.g., purchasing private generators or solar inverters). The government should implement targeted financial subsidies or provide state-sponsored alternative energy solutions specifically for low-income and marginalized demographics to prevent the compounding of economic and psychological distress.

- Strict regulatory frameworks must be enforced to ensure that essential services particularly healthcare facilities, water pumping stations, and educational institutions are entirely insulated from load-shedding schedules. Protecting these sectors prevents the secondary psychological trauma associated with the collapse of basic societal functions.
- While this cross-sectional study establishes strong correlational pathways, future research should employ longitudinal designs to track the psychological trajectories of citizens before, during, and after periods of grid stabilization. Additionally, qualitative phenomenological studies are needed to deeply explore the lived experiences, daily coping rituals, and nuanced emotional responses of citizens navigating this chronic crisis.
- To enhance the generalizability of these findings, future studies should compare the psychological impact of power outages in Libya with other post-conflict or developing nations facing similar infrastructural deficits. This would help isolate which psychological responses are universal to resource deprivation and which are specific to the Libyan socio-political context.
- Future research at the intersection of electrical engineering and psychology should investigate how the visual and auditory cues of infrastructural decay (e.g., the noise and fumes of gasoline generators) independently contribute to sleep disruption and cognitive fatigue, thereby refining the measurement tools used in environmental psychology.

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Predicting Football Fandom in Turkey: A Machine Learning and Statistical Approach Based on Demographic and Socioeconomic Factors

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ABSTRACT

This study presents a comprehensive analysis aimed at predicting football team allegiance in Turkey using demographic, political, and economic factors. Based on a nationwide survey dataset collected by the KONDA research company in 2017, the study utilizes various data mining and classification algorithms, including Decision Trees (CART, C5.0, Random Forest), K-Nearest Neighbors (KNN), and Support Vector Machines (SVM). Despite utilizing robust computational techniques and alternative approaches like data balancing and analysis of variance (ANOVA), the classification models yielded relatively low accuracy rates (approximately 30-46%). The findings indicate that standard demographic and socioeconomic variables are insufficient for accurately predicting football team preferences, suggesting that sports fandom is driven by more complex, latent factors not captured by traditional demographic profiling.

Keywords – Data Mining, Football Fandom, Predictive Modeling, Machine Learning, Demographic Factors.

INTRODUCTION

Football in Turkey transcends mere athletic competition; it is a profound sociological phenomenon deeply intertwined with the country's cultural, economic, and political fabric. Understanding the dynamics of football fandom provides significant insights into social identity and group affiliation. In recent years, data mining and machine learning techniques have been increasingly employed in sports analytics to predict outcomes, evaluate player performance, and understand fan behavior [1], [2]. However, the application of predictive modeling to determine a fan's specific team allegiance based on their personal attributes remains a challenging domain.

This study aims to predict the football teams supported by individuals in Turkey based on their personal and social characteristics. Utilizing a dataset provided by KONDA, we employ various classification methodologies commonly used in data mining. The objective is not only to achieve a high predictive accuracy but also to identify which demographic and socioeconomic variables, if any, possess significant discriminatory power in determining sports fandom.

MATERIALS AND METHOD

Describe in detail the materials and methods used when conducting the study. The citations you make from different sources must be given and referenced in references.

A. Dataset Description

The dataset utilized in this project was acquired from KONDA Research and Consultancy, based on a survey conducted between September 30 and October 1, 2017. The survey was designed to understand sports and football fandom in Turkey across demographic, political, and economic dimensions. The data was collected via face-to-face surveys with 2,670 participants (aged 18 and over) selected from 152 neighborhoods across 30 provinces and 105 districts, representing the national demographics. The margin of error is estimated at +/- 1.7% at a 95% confidence level [3].

For this study, 12 categorical attributes were selected as independent variables, while the supported football team was chosen as the classifying attribute (target variable) as detailed in Table 1.

Table 1 Attributes and their values

Attributes	Values
Rural-Urban	Rural, Urban, Metropolitan
Gender	Female, Male
Age Group	18 - 32, 33 - 48, 49+
Education Group	Below High School, High School, University
Birth Region	Istanbul, West Marmara, Aegean, East Marmara, West Anatolia, Mediterranean, Central Anatolia, West Black Sea, East Black Sea, Northeast Anatolia, Middle East Anatolia, Southeast Anatolia, Abroad
Marital Status	Single, Engaged, Married, Widowed, Divorced
Lifestyle	Modern, Traditional Conservative, Religious Conservative
Political Party Preference	AKP, CHP, MHP, HDP, Other parties, Undecided, Does not vote
Ethnicity	Turkish, Kurdish, Zaza, Arab, Other
Work Status	Executive, Worker/Tradesman/Farmer, Retired, Housewife, Student, Unemployed

Monthly Income	700 TL and below, 701 - 1200 TL, 1201 - 2000 TL, 2001 - 3000 TL, 3001 - 5000 TL, 5001 TL and above
Sports Interests	Basketball, Boxing/Martial Arts, Fitness/Pilates/Yoga, Football, Tennis, Volleyball, Walking, Swimming, Other, None
Classifying Attribute	Values
Supported Team	BJK, FB, GS, TS, Other, None

B. Data Preprocessing

Instances containing 'No Answer' for any attribute were treated as missing data and subsequently removed from the dataset. Following this cleaning process, the analysis was conducted on the remaining 1,748 participants. Since KONDA performs preliminary cleaning prior to public release, no severe noisy data was encountered. Although some outliers were observed, their infrequency warranted no further manipulation at the initial stage. The initial distribution of individuals based on the classifying attribute, Supported Team, is illustrated in Fig. 1, which clearly highlights the imbalanced nature of the dataset.

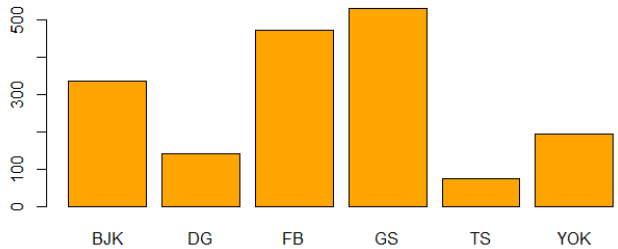


Fig. 1 Distribution of people according to the teams they support

To perform the machine learning analysis, the dataset was randomly partitioned into a Training set (80%, n=1400) and a Test set (20%, n=348), as depicted in Fig. 2.

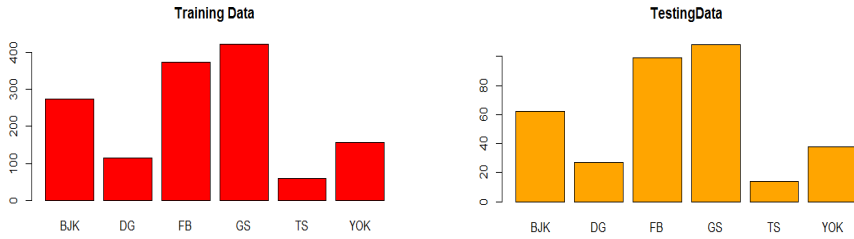


Fig. 2 Training and test datasets

C. Decision Tree Algorithms

CART (Classification & Regression Tree)

The CART algorithm utilizes the Gini index for feature selection. The resulting decision tree, shown in Fig. 3, identified 'Sports of Interest', 'Birth Region', and 'Age' as the primary discriminatory nodes. The model's accuracy on the test set was 0.33. To investigate potential overfitting and the impact of the random split, Leave-One-Out Cross Validation (LOOCV) and pruning were applied; however, the accuracy remained within the [0.23-0.33] range.

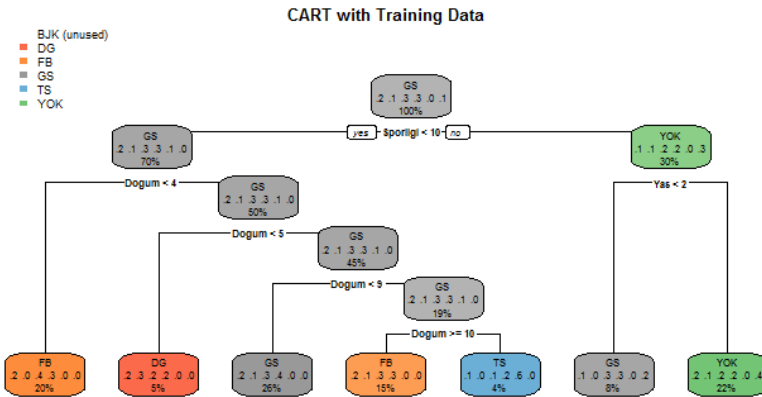


Fig. 3 Decision tree according to CART algorithm

C5.0

Unlike CART, C5.0 employs the Information Gain metric for attribute selection and utilizes boosting to iteratively improve the tree. A boosting iteration of 10 was set. The discriminatory variables were similar to CART, with 'Lifestyle' replacing 'Age'. The accuracy was approximately 0.31, and K-Fold Cross Validation confirmed this baseline (~0.30).

Random Forest

To overcome the limitations of a single tree, a Random Forest algorithm (utilizing bootstrapping and aggregation, or bagging) with 500 trees was implemented. The average accuracy yielded by the Random Forest remained at 0.31.

D. K-Nearest Neighbors and SVM

K-Nearest Neighbors (KNN)

In the KNN model, the initial K value was set to the square root of the training set size. Sensitivity analysis across different K values (1 to 60) resulted in accuracy levels fluctuating between [0.28-0.36], peaking at 0.34, which aligns with the decision tree outcomes.

Support Vector Machines (SVM)

A radial basis function kernel was utilized for the multiclass classification SVM model, with the penalty parameter (Cost) initially set to 1. Sensitivity analysis on the Cost value (from 1 to 10) yielded an accuracy of 0.35, with variations strictly within the [0.26-0.36] range.

RESULTS

The primary models consistently produced low accuracy rates (approximately 30-35%). To address this, alternative approaches were tested. First, the dataset was reduced and balanced by excluding the minority classes ('Trabzonspor [TS]', 'Other', and 'None'). The frequency of the target values in this newly reduced and balanced training dataset is presented in Fig. 4.

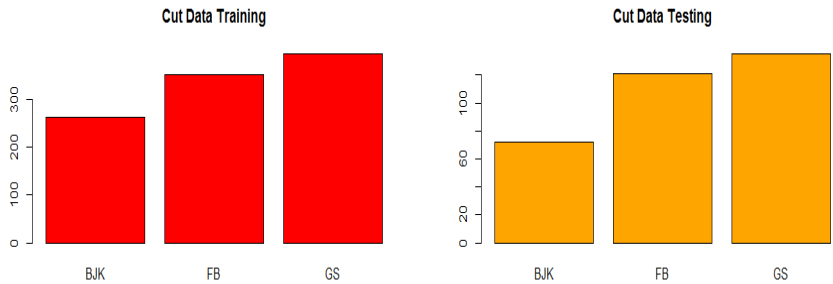


Fig. 4 Frequency of Supported Team values over reduced data

Running the CART, C5.0, and SVM models on this reduced dataset (Training: 834, Test: 504) yielded slightly improved accuracies of 0.37, 0.35, and 0.39, respectively. Incorporating LOOCV on this balanced dataset achieved the highest observed accuracy of 0.46.

Furthermore, an Analysis of Variance (ANOVA) was conducted to statistically determine the significance of the independent variables on the target variable. The results indicated that Gender, Age Group, Education Group, Lifestyle, Work Status, and Sports of Interest were statistically significant. However, a C5.0 model trained exclusively on these significant variables failed to improve predictive performance, yielding an accuracy of 0.32.

DISCUSSION

The consistent insufficiency in predictive accuracy (around 30%) across diverse machine learning algorithms, despite applying techniques like bagging, boosting, cross-validation, hyperparameter tuning, and data balancing, highlights a fundamental characteristic of the dataset. This supports the notion that sports allegiance, particularly in a football-passionate country like Turkey, cannot be accurately profiled using demographic and basic socioeconomic data alone [4].

As noted in sociological studies, fandom is often inherited through familial ties, geographical proximities beyond broad regional categorizations, and complex psychological or peer-driven dynamics [5]. The failure to surpass a 46% accuracy ceiling implies that critical latent factors influencing team preference are missing from the current feature set.

CONCLUSION

This study applied various data mining classification techniques to predict football team preferences in Turkey based on demographic, political, and economic attributes. Extensive efforts were made to optimize the predictive models, including algorithmic variations and statistical filtering. However, the inability to achieve high accuracy rates strongly suggests that the available features are insufficient. Future studies should focus on expanding the feature space by incorporating psychological metrics, familial affiliations, and more granular geographical data to capture the true drivers of football fandom. In data mining, establishing that a model based on specific variables is invalid is itself a valuable, informative outcome.

ACKNOWLEDGMENT

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Artificial Intelligence-Based Malware Detection and Classification: Recent Approaches and Challenges

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ABSTRACT

With the rapid expansion of digital systems and Internet infrastructure, malicious software (malware) has emerged as one of the most significant threats to modern cybersecurity. Traditional signature-based detection methods may be insufficient against increasingly sophisticated polymorphic, metamorphic, and zero-day attacks. This survey examines the role of artificial intelligence (AI)-based methods in malware detection and classification through a structured review of 21 representative studies published from 2021 through January 2026. It investigates how data obtained through static, dynamic, and hybrid analysis are integrated into machine learning (ML) and deep learning (DL) models, including feature-engineering processes and architectures such as CNN, LSTM, GAN, and transformer-based models. Furthermore, current challenges—including adversarial attacks, class imbalance, and model interpretability—are evaluated, and directions for future research and cybersecurity practice are outlined. The reviewed evidence indicates that hybrid and ensemble AI approaches frequently report stronger performance than single-model systems under specific benchmark conditions, with several studies achieving accuracy rates above 99%. However, these results should be interpreted cautiously because of dataset bias, class imbalance, potential data leakage, and differences in validation procedures and evaluation protocols.

Keywords – Malware Detection, Artificial Intelligence, Machine Learning, Deep Learning, Cybersecurity

INTRODUCTION

The accelerating pace of digital transformation—spanning the Internet of Things (IoT), cloud computing, and the integration of critical infrastructure with the internet—has expanded the cyber threat surface to an unprecedented scale. Malware has evolved from simple tools targeting personal data into sophisticated cyber weapons capable of threatening national security, financial systems, and global data privacy. The Malware-as-a-Service (MaaS) model has further lowered the technical barrier for attackers, enabling even low-skilled actors to launch devastating campaigns [1]-[3].

Traditional signature-based detection systems, which rely on matching file hashes or byte patterns against known databases, may be less effective against previously unseen or structurally modified threats. Techniques such as polymorphism, metamorphism, and code obfuscation can alter malware structure and make zero-day attacks difficult to detect using conventional methods. Additionally, rule-based heuristic systems can generate false positives and contribute to alarm fatigue among security analysts [1], [4]-[6].

Artificial intelligence (AI), and its subfields of machine learning (ML) and deep learning (DL), has assumed an increasingly important role in cyber defense. Unlike static signature matching, AI-based systems can analyze patterns in file structures, command sequences, and runtime behaviors, thereby supporting the detection of previously unseen threats. This paper provides a structured survey of AI-based malware detection approaches, covering the taxonomy of malware and analysis techniques, the theoretical role of AI in detection, a comparative review of 21 recent studies (2021–2026), and future research directions [1], [2], [4], [5].

The main contributions of this paper are as follows: First, it presents a structured review of recent AI-based malware detection and classification studies published between 2021 and 2026. Second, it categorizes existing approaches according to static, dynamic, hybrid, visualization-based, explainable, federated, and adversarially robust detection strategies. Third, it compares representative studies in terms of methods, datasets, and application domains. Finally, it discusses key open challenges, including dataset bias, class imbalance, adversarial attacks, model interpretability, privacy preservation, and real-world deployment limitations.

A. Literature Selection Methodology

The literature reviewed in this study was selected from academic databases and publisher or indexing platforms, including Google Scholar, IEEE Xplore, ACM Digital Library, ScienceDirect, SpringerLink, and MDPI. The literature search was completed in January 2026 using keywords such as “AI-based malware detection,” “deep learning malware classification,” “machine learning malware detection,” “explainable malware detection,” “federated malware detection,” “adversarial malware detection,” “Android malware classification,” and “IoT malware detection.” The comparative review focused on 21 studies published or made available online between 2021 and January 2026 to reflect recent developments in the field. Papers were included if they proposed, reviewed, or experimentally evaluated artificial intelligence, machine learning, or deep learning-based malware detection and classification methods. Studies were excluded if they lacked clear methodological descriptions, sufficient discussion of datasets or evaluation evidence, or direct relevance to malware detection and classification.

I. MALWARE TAXONOMY AND ANALYSIS TECHNIQUES

B. Malware Types

Malware encompasses any software engineered to compromise systems and user environments, spanning distinct functional categories such as self-replicating viruses, autonomous network worms, deceptive trojans, extortion-oriented ransomware, covert spyware, unwanted adware, and coordinated botnets [7]–[11].

C. Malware Analysis Techniques

Malware analysis encompasses six primary paradigms designed to inspect, characterize, and detect malicious code across varying execution stages. Conventional signature-based detection enables rapid matching against known threat repositories with minimal false positives, yet fails against previously unseen variants [12]. Non-execution static analysis extracts structural features—such as PE headers, strings, and opcode sequences—though its diagnostic accuracy is frequently undermined by packing and code obfuscation [13]. Conversely, dynamic and behavioral analysis methodologies inspect runtime operations, system calls, and network anomalies within controlled environments, offering deeper behavioral visibility at the expense of higher computational overhead and susceptibility to sandbox-evasion tactics [14], [15]. Heuristic frameworks apply rule-based scoring to flag suspicious artifacts [16], while hybrid analysis merges static and dynamic evidence to maximize detection coverage despite increased systemic complexity [17]. A structured comparison of these analysis techniques is detailed in Table 1.

Table 1. Comparison of Malware Analysis Techniques

Technique	Type	Core Approach	Key Tools	Advantages	Zero-Day Potential
Signature-Based [12]	Static	Hash/pattern match	AV engines	Fast, low FP	Limited
Static Analysis [13]	Static	Code without exec.	IDA Pro, Ghidra	Safe, rapid	Limited
Dynamic Analysis [14]	Dynamic	Runtime observation	Cuckoo Sandbox	Real behavior	Potential
Behavioral [15]	Dynamic	System impact focus	API call logs	Behavioral visibility	Potential
Heuristic [16]	Static/Dynamic	Rule-based scoring	Custom engines	Partial coverage	Partial
Hybrid [17]	Both	Multi-stage fusion	Sandbox + disasm.	Broader coverage	Potential

THE ROLE OF ARTIFICIAL INTELLIGENCE IN MALWARE DETECTION

AI-based systems are increasingly used in modern cyber defense because they can extract patterns from data and generalize beyond explicitly encoded rules, although their effectiveness remains dependent on data quality, model design, and deployment conditions. In the context of malware detection, ML

algorithms such as Support Vector Machines (SVM), Random Forests (RF), and Decision Trees (DT) classify software as benign or malicious using feature vectors derived from static and dynamic analysis (e.g., file size, API call frequencies, byte distributions) [1], [2], [5].

The growing complexity of cyber threats has exposed limitations in manual feature engineering and encouraged the use of Artificial Neural Networks (ANNs) and deep learning architectures. Convolutional Neural Networks (CNNs) have been widely applied to spatial features obtained from grayscale malware images. Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks can model temporal dependencies in API-call sequences, while Graph Neural Networks (GNNs) can represent structural relationships in control-flow graphs [4], [5], [18], [19].

AI-based malware detection supports a shift from purely reactive defenses toward more adaptive protection. Whereas signature-based systems primarily recognize known patterns, models trained on behavioral and structural characteristics may identify previously unseen or modified threats. Reported benchmark results indicate that learned representations can improve detection of polymorphic and obfuscated variants; however, performance depends on dataset quality, evaluation design, computational resources, and real-world deployment conditions [1], [4]-[6].

Table 2. Traditional vs. AI-Based Malware Detection

Criterion	Traditional Methods	AI-Based Methods
Core Approach	Rule & signature matching	Data-driven pattern learning
Feature Extraction	Manual	Automatic (deep learning)
Zero-Day Detection	Limited	Potentially stronger
Obfuscation Resistance	Often limited	Data/model-dependent
Scalability	Moderate	Potentially high
Explainability	Generally high	Variable; often limited
Trend	Established	Rapidly developing

LITERATURE REVIEW

This section surveys 21 representative studies published between 2021 and 2026, organized thematically across deep learning architectures, visualization-based approaches, explainable AI (XAI), federated learning, adversarial robustness, and IoT/Android-specific detection.

D. Deep Learning Architectures

Gaber et al. [1] conducted a systematic literature review (2017–2022) of AI-based malware detection, covering supervised, unsupervised, and reinforcement learning paradigms. They concluded that standardized performance metrics and adversarial robustness must be prioritized alongside raw accuracy figures.

Gopinath and Sethuraman [4] conducted a comprehensive review of deep learning techniques for malware detection, classifying architectures such as CNN, RNN, LSTM, GAN, and RBM according to their compatibility with static, dynamic, or hybrid input data. Across the surveyed studies, commonly used datasets included Malimg, Microsoft BIG 2015, DREBIN, and EMBER. The authors concluded that DL-based approaches offer important advantages over traditional signature-based methods for detecting previously unseen threats, although their high computational cost remains a significant challenge.

Wang et al. [5] reviewed DL-based malware detection for both Android and Windows platforms, emphasizing automatic feature extraction via CNN, BiGRU, LSTM, and attention mechanisms. The study highlighted that data imbalance and adversarial attacks remain persistent obstacles despite high reported accuracy.

Cassanova et al. [20] reviewed the evolution of artificial intelligence-based malware detection by classifying existing approaches into machine learning, deep learning, and hybrid models. Their study discusses commonly used algorithms such as RF, SVM, DT, CNN, RNN, LSTM, and GRU and summarizes the heterogeneous datasets reported across the reviewed literature rather than conducting an independent experiment on a single dataset. The authors emphasized that AI has significantly improved malware detection capabilities, but adversarial attacks remain a major challenge because attackers can also use AI-based techniques to evade detection systems.

E. Visualization and Memory Forensics

Toğaçar [18] converted structured RAM-memory data into Aztec, Data Matrix, and QR barcode images, extracted deep features with MobileNetV2, and applied Sand Cat Swarm (SCS) optimization for feature selection. On CIC-MalMem-2022, the method achieved 99.42% accuracy (99.30% under 5-fold cross-validation), although its evidence remains limited to one balanced benchmark dataset.

Bozkır et al. [21] combined memory forensics, manifold learning (UMAP), and computer vision to detect fileless malware that leaves no disk trace. On a custom dataset of 4,294 process dumps, the system achieved 96.39% accuracy and an average analysis time of 3.56 seconds; UMAP improved classifier accuracy by up to 21.83%.

F. Explainable AI (XAI)

Berrios et al. [2] conducted a systematic review based on the PRISMA 2020 framework, analyzing 47 studies published between 2020 and 2024. The study examined ML, DL, XAI, and hybrid approaches, highlighting the effectiveness of models such as DT, RF, SVM, CNN, LSTM, and RNN in malware detection and classification. The authors concluded that future cybersecurity systems should not only detect malware accurately but also explain the reasons behind AI-based decisions, particularly in IoT and cloud security environments.

Baghirov [22] evaluated LightGBM, XGBoost, Random Forest, SVM, Logistic Regression, and related models with SHAP/LIME explanations on CICMalDroid 2020 and CIC-InvesAndMal2019. LightGBM produced the strongest aggregate result (94% accuracy and 93% F1), while the study noted that real-time explanation generation introduces computational and interpretive overhead.

Saqib et al. [23] delivered a comprehensive survey of XAI for malware hunting, reviewing studies based on diverse data sources, including Android applications, PE files, network traffic, and malicious URLs. Because the article is a survey rather than an independent experimental study, it does not evaluate one fixed dataset. Beyond detection performance, the authors argued that XAI can support the investigation of adversarial manipulation and model bias while improving analysts' understanding of AI-driven decisions.

Vo et al. [24] introduced MDOB, combining feature-set optimization, mutual Deep+Boosting ensemble inference, SHAP explanations, and parallel execution. MDOB achieved 98.14% accuracy on EMBER 2018 and 99.46% on BODMAS, while reducing detection time by 37.44%; however, the evaluation is limited to static PE benchmark features.

N. T. Cam et al. [25] proposed uitMalDeQ, a Windows malware-classification framework that combines Deep Q-Learning with SHAP-guided feature selection. The method achieved 98.21% accuracy on Microsoft BIG 2015, 99.44% on BODMAS, and 91.90% on EMBER, but Random Forest remained slightly stronger on average and real-time/adversarial deployment was not evaluated.

G. Federated Learning and Privacy

Çıplak et al. [26] proposed FEDetect, a federated malware-detection framework using FNN and LSTM architectures with FedAvg-Adam on CIC-MalMem-2022. It achieved 99.9% binary and 84.5% multiclass accuracy; however, the experiments assumed IID data in a simulation without real client communication, latency, or device heterogeneity.

H. Adversarial Robustness

Al Roken et al. [6] systematically reviewed adversarial attacks against AI-based cybersecurity detection systems, categorizing attack strategies according to white-box scenarios, in which the attacker has detailed knowledge of the target model, and black-box scenarios, in which attacks are developed through limited queries or trial and error. The review also examined defense strategies, including adversarial training, and discussed studies evaluated on benchmarks such as EMBER, NSL-KDD, and CIC-IDS2017. The authors emphasized that adversarial awareness and robustness evaluation should be treated as important design considerations in future malware and intrusion-detection systems.

I. Domain-Specific Applications

Ferdous et al. [3] conducted a comprehensive review of artificial intelligence-based ransomware detection, focusing on how ML and DL models can identify encryption-related malicious behavior. The surveyed studies cover methods such as RF, SVM, XGBoost, CNN, RNN/LSTM, static analysis, and dynamic analysis, and employ datasets including UGR16, BitcoinHeist, and ransomware-specific collections. The authors concluded that conventional detection techniques alone may be insufficient against modern ransomware and that AI-based systems can contribute to the development of more effective early-warning mechanisms.

Gupta et al. [19] modeled malware kernel API calls through NLP and image-encoding stages and evaluated an ensemble deep model with Tanh, ReLU, and LeakyReLU activation variants. On the study-specific API-call data, the best configuration reported 91% accuracy and an F1-score of 0.858; the small, paper-specific dataset limits cross-dataset reproducibility.

Alkahtani and Aldhyani [27] evaluated SVM, KNN, LSTM, and CNN models on CICAndMal2017 and DREBIN; SVM reached 100% accuracy on CICAndMal2017 and LSTM reached 99.4% on DREBIN.

Smmarwar et al. [28] proposed a D3WT-CNN-LSTM pipeline evaluated on IoT malware, Microsoft BIG 2015, and Malimg, reporting 99.98% accuracy on the IoT dataset and 99.96% on Malimg.

Moorthy and Nathiya [29] compared KNN, SVM, Decision Tree, and MLP models for botnet-traffic detection on CTU-13. Decision Tree achieved the best result at 92% accuracy, but reliance on a single legacy dataset and slower packet classification restricts evidence of real-world generalization.

Kavalcı Yılmaz and Bakır [30] combined deep feature extractors with XGBoost on the DroidCollector Android network-traffic dataset; BiLSTM+XGBoost achieved 99.33% accuracy and 95.12% F1.

Naeem et al. [31] converted volatile-memory dumps to images and used a deep-stacked CNN-to-MLP ensemble with XAI, achieving 99.8% on obfuscated Windows samples, 99.1% on Windows samples, and 94.3% on a custom Android set.

Mittal et al. [32] proposed DLEX-IMD, a deep-learning ensemble for IoT malware detection explained with LIME. Evaluated on Aposemat IoT-23 and the AIoT Malware Detection dataset, it achieved 99.96% accuracy and an F1-score of 0.999; edge-device cost and online deployment remain untested.

Table 3. Comparative Summary of AI-Based Malware Detection Studies

Year	Study	Method	Dataset	Best Performance	Limitation
2021	Bozkır et al. [21]	Memory dump to RGB; GIST+HOG; UMAP; SMO/RF/SVM/XGBoost	Custom 4,294 process dumps (10 malware families + benign; VirusShare-sourced)	96.39% accuracy; 3.56 s average analysis	Custom/legacy OS setting; memory acquisition and image generation add overhead.
2022	Alkahtani et al. [27]	SVM, KNN, LSTM, CNN	CICAndMal2017; DREBIN	100% (SVM, CICAndMal2017); 99.40% (LSTM, DREBIN)	Dataset-specific evaluation; no temporal, cross-dataset, or adversarial validation.
2022	Cassanova et al. [20]	Systematic review of ML, DL, and ensemble methods	Diverse datasets across reviewed studies; no single experimental dataset	N/A (review)	Heterogeneous studies and metrics; no common benchmark or independent experiment.
2023	Gopinath & Sethuraman [4]	Survey of CNN, RNN, LSTM, GAN, and hybrid DL	Multiple datasets, including Maling, DREBIN, and EMBER	N/A (survey)	Secondary synthesis; inconsistent datasets, splits, and evaluation protocols.

Year	Study	Method	Dataset	Best Performance	Limitation
2023	Smamarwar et al. [28]	D3WT feature extraction + CNN-LSTM	IoT malware; Microsoft BIG 2015; Maling	99.98% (IoT); 99.96% (Maling)	Image/feature pipeline adds cost; external real-world robustness is not demonstrated.
2023	Naeem et al. [31]	Memory-to-image descriptors; stacked CNN to MLP; XAI	Dumpware10; CIC-MalMem-2022; custom Android set	99.8% (obfuscated Windows); 99.1% (Windows); 94.3% (Android)	Training complexity; custom Android data and adversarial robustness limit generalization.
2023	Moorthy & Nathiya [29]	KNN, SVM, Decision Tree, and MLP on network traffic	CTU-13	92% accuracy (Decision Tree)	Single legacy dataset; slower packet classification and limited external validation.
2024	Wang et al. [5]	Review of CNN, RNN/GRU, attention, and related DL methods	Multiple datasets, including Maling, EMBER, and Microsoft BIG 2015	N/A (review)	No unified cross-platform benchmark; reported metrics are not directly comparable.
2024	Saqib et al. [23]	Survey of XAI methods,	Diverse datasets across	N/A (review)	Explanation fidelity,

Year	Study	Method	Dataset	Best Performance	Limitation
		including SHAP and LIME	reviewed studies; no single experimental dataset		stability, and analyst usefulness lack standardized evaluation.
2024	Ferdous et al. [3]	Ransomware review: ML, DL, entropy, and behavioral methods	Multiple datasets, including BitcoinHeist and UGR16	N/A (review)	Ransomware datasets are fragmented/imbalanced; common real-world validation is limited.
2024	Gaber et al. [1]	Systematic review of ML, DL, and hybrid detection	Multiple datasets, including Maling, EMBER, and DREBIN	N/A (review)	Heterogeneous data and protocols make reported performance difficult to compare.
2025	Berrios et al. [2]	PRISMA systematic review of ML, DL, and XAI	Multiple datasets, including Maling, EMBER, and CIC-MalMem-2022	N/A (review)	Study heterogeneity and limited benchmark standardization constrain reproducibility.
2025	Al Roken et al. [6]	Review of adversarial attacks and defenses	Multiple datasets, including NSL-KDD, CIC-IDS2017, and EMBER	N/A (review)	Threat models and perturbation constraints vary, weakening cross-study comparability.
2025	Çıplak et al. [26]	Federated FNN/LSTM with FedAvg-Adam	CIC-MalMem-2022	99.9% binary; 84.5% multiclass accuracy	IID simulation only; no real client communication/latency; limited architectures.
2025	Baghirov [22]	LightGBM, XGBoost, RF,	CICMalDroid 2020; CIC-	94% accuracy; 93% F1	Real-time XAI adds

Year	Study	Method	Dataset	Best Performance	Limitation
		SVM, LR + SHAP/LIME	InvesAndMal2019	(LightGBM)	overhead; explanations remain difficult to operationalize.
2025	Vo et al. [24]	Feature optimization; Deep+Boosting ensemble; SHAP; parallel inference	EMBER 2017/2018; BODMAS	98.14% (EMBER); 99.46% (BODMAS); 37.44% faster inference	Static PE features; robustness is demonstrated only under benchmark conditions.
2025	Kavalcı Yılmaz & Bakır [30]	Deep feature extractors + XGBoost	DroidCollector network-traffic dataset	99.33% accuracy; 95.12% F1 (BiLSTM+XGBoost)	One Android traffic dataset; cross-dataset and zero-day validation are absent.
2025	Mittal et al. [32]	Deep-learning ensemble (DLEX-IMD) + LIME	Aposemat IoT-23; AIoT Malware Detection	99.96% accuracy; F1 = 0.999	Offline benchmark evaluation; ensemble and LIME overhead on edge devices is untested.
2025	Gupta et al. [19]	NLP/image encoding of kernel API calls + ensemble deep model	Study-specific kernel API-call datasets	91% accuracy; F1 = 0.858	Small, paper-specific data; binary task and cross-dataset reproducibility are limited.
2026	Toğaçar [18]	Aztec/Data Matrix/QR encoding; MobileNetV2; SCS feature selection	CIC-MalMem-2022	99.42% accuracy; 99.30% under 5-fold CV	Single balanced dataset; barcode preprocessing and memory capture add overhead.

Year	Study	Method	Dataset	Best Performance	Limitation
2026	N. T. Cam et al. [25]	Deep Q-Learning (uitMalDeQ) + SHAP feature selection	Microsoft BIG 2015; BODMAS; EMBER	98.21% (Microsoft BIG 2015); 99.44% (BODMAS); 91.90% (EMBER)	RF is slightly stronger on average; no real-time or adversarial deployment test.

Note: N/A denotes a review or survey article without a single directly comparable experimental result. Reported performance values are reproduced from the original studies and are not directly comparable because datasets, class distributions, validation protocols, and evaluation metrics differ.

DISCUSSION AND FUTURE DIRECTIONS

The surveyed literature indicates a substantial shift from reactive, signature-based defense toward more adaptive, learning-based cyber protection [1], [2], [4], [5]. Several cross-cutting findings emerge:

Deep learning architectures—particularly CNN, LSTM, and BiGRU—have shown strong performance by automating feature extraction and capturing complex non-linear relationships in malware data [1], [4], [5]. Hybrid and ensemble models that combine the representational capacity of deep learning with the decision-making efficiency of gradient boosting algorithms such as XGBoost and LightGBM have also achieved high performance in several benchmark studies [22], [24], [30], [31]. Nevertheless, reported accuracy values above 99% should not be treated as universally generalizable, since malware datasets often differ in sample distribution, family diversity, feature representation, train-test split strategy, and real-world representativeness.

Visualization-based and memory-forensics techniques have reported promising results for fileless malware, which may leave limited disk artifacts [18], [21]. Converting binary data or memory dumps into image representations enables CNN architectures to identify patterns that can be missed by conventional static analysis [18], [21], [31]. The findings of Toğaçar and Bozkır et al. suggest that learned visual representations may support the detection of previously unseen malware variants, although broader external validation is still required [18], [21].

Explainable AI (XAI) is increasingly regarded as a practical consideration in malware detection [2], [23]. SHAP- and LIME-based interpretability frameworks can support analyst trust and provide diagnostic evidence concerning model bias or possible adversarial manipulation [22]–[24], [32]. As AI-powered defense systems are deployed in critical infrastructure, regulatory and ethical considerations are likely to increase the importance of explainability [2], [23], [32].

The adversarial threat landscape presents a critical open challenge. As documented by Al Roken et al. and Gaber et al., carefully constructed adversarial examples can cause detection models to make incorrect predictions [1], [6]. Future systems should therefore be evaluated not only for accuracy on clean datasets but also for robustness under realistic adversarial perturbations [1], [5], [6]. Adversarial training, certified defenses, and ensemble diversity represent potential mitigation strategies [6].

Privacy-preserving architectures such as federated learning offer a compelling path forward for collaborative defense without raw-data sharing. FEDetect's 99.9% binary and 84.5% multiclass accuracy demonstrate strong benchmark performance, although its IID simulation does not establish equivalent results under real organizational communication, latency, and device heterogeneity [26].

Future research should prioritize: (1) standardized evaluation benchmarks that reflect real-world threat distributions rather than static legacy datasets; (2) lightweight models suitable for resource-constrained IoT and mobile environments; (3) adversarially robust architectures with formal guarantees; and (4) multi-modal fusion frameworks that integrate NLP-based code analysis, network traffic inspection, and threat intelligence for holistic detection.

J. Limitations of This Review

This review has several limitations. It focuses on 21 representative peer-reviewed studies and does not include grey literature or unpublished work. Because the reviewed studies use different datasets, class distributions, validation protocols, and performance metrics, their reported results cannot be compared directly. In addition, the experimental findings were not independently reproduced; therefore, the conclusions reflect the scope and methodological quality of the selected literature.

CONCLUSION

This paper presented a structured survey of 21 representative studies on AI-based malware detection and classification published between 2021 and 2026. The reviewed literature demonstrates substantial progress in deep learning, hybrid and ensemble models, visualization-based methods, and memory-forensics techniques. Explainable AI and federated learning also offer promising directions for improving model transparency and privacy-preserving collaboration, respectively. By organizing recent studies according to their methods, datasets, performance results, and limitations, this review provides a comparative perspective on current developments in the field.

Despite the high performance reported in several benchmark studies, the results cannot be directly generalized to real-world environments because of differences in datasets, class distributions, feature representations, validation protocols, and evaluation metrics. Moreover, adversarial robustness, model interpretability, computational cost, and cross-dataset generalization remain important unresolved challenges. Future research should therefore prioritize standardized evaluation procedures, external and cross-dataset validation, lightweight deployment, and realistic adversarial testing. Overall, no single existing approach fully satisfies the requirements of accuracy, explainability, privacy, robustness, and operational efficiency.

In summary, modern malware detection is increasingly shaped by the integration of NLP, image processing, and deep learning techniques across diverse environments, ranging from IoT and Android platforms to cloud systems and industrial networks. The future of cyber defense depends on the development of faster, more explainable, adaptive, and adversarially robust

models capable of responding effectively to AI-assisted and continuously evolving cyber threats.

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A New Modular Skew Tent Chaotic Map for Substitution Box Generation with Chaos- Driven Nonlinearity Optimization

Yücel BÜRHAN

ABSTRACT

Substitution boxes (S-boxes) are the main nonlinear components of block ciphers, and their nonlinearity largely determines the strength of the cipher. S-boxes obtained directly from chaotic maps are easy to generate but usually have low nonlinearity, which has made the combination of chaos and optimization a popular design approach. In this study, a new one-dimensional chaotic map, the modular skew tent chaotic map (MSTCM), is proposed by combining the skew tent map with a modular expansion. It is shown analytically that the map is chaotic over its whole parameter range, with a Lyapunov exponent between 1.60 and 2.89, and this is confirmed by bifurcation diagrams, the 0–1 test and sensitivity analysis. The map is implemented in 64-bit integer arithmetic. Using the MSTCM, a chaotic S-box is first generated with a chaos-driven Fisher–Yates shuffle and then improved by a two-stage optimization in which the chaotic map selects the swapped positions: the first stage maximizes nonlinearity with a Walsh-spectrum fitness function and the second stage improves the differential property while preserving the nonlinearity. For the presented S-box, the average nonlinearity increases from 103.5 to 112 (minimum 112, maximum 112), the maximum XOR entry decreases from 14 to 8, and SAC, BIC-NL and BIC-SAC values of 0.5046, 103.71 and 0.5028 are obtained. Over 300 different keys, the average nonlinearity is 111.95 and 87% of the S-boxes reach 112 in all eight Boolean functions. The comparison with recent studies shows that the proposed S-box has a higher average nonlinearity and a lower differential probability than the compared chaos- and optimization-based S-boxes.

Keywords: Chaotic map; Nonlinearity; Optimization; Skew tent map; Substitution box

1. INTRODUCTION

With the rapid growth of digital communication, protecting the confidentiality of data has become one of the fundamental requirements of information systems. Symmetric block ciphers, of which AES is the current standard [1], are the most widely used tools for this purpose. According to Shannon [2], a secure cipher must provide confusion and diffusion. In block ciphers, confusion is usually provided by the substitution box (S-box), which is generally the only nonlinear component of the algorithm. For this reason, the resistance of the cipher against linear [3] and differential [4] cryptanalysis depends largely on the cryptographic properties of the S-box, among which nonlinearity is considered the most important one [5].

An 8-bit bijective S-box is a permutation of 256 elements, so the search space contains 256! candidates. Finding an S-box with high nonlinearity in such a space is a hard problem, and many approaches have been proposed for it. The

most frequently used approaches are based on chaotic systems, optimization algorithms and algebraic transformations. Chaotic systems are attractive because of their sensitivity to initial conditions, ergodicity and random-like behavior [6], and they allow key-dependent S-boxes to be produced easily. However, S-boxes obtained only from chaotic sequences usually have nonlinearity values around 100–106 [7, 8]. Therefore, recent studies generate an initial S-box with a chaotic map and then increase its nonlinearity with a post-processing or optimization step.

Several recent studies follow this approach. Zamli used a tent map for the initial population of the adaptive agent heroes and cowards algorithm and obtained an average nonlinearity of 109.75 [9]. Artuğer and Özkaynak combined chaos with the crossover and mutation operators of the genetic algorithm and reached 111.75 [10]. Zamli et al. proposed a Q-learning-based chaotic naked mole rat algorithm with 109.75 [11]. Artuğer improved sine map S-boxes by element swapping to 107.5 [12], used 3D chaotic maps with the whale optimization algorithm to reach 110.5 [13], optimized a tent map S-box with the sine cosine algorithm to 108 [14] and combined chaos with cellular automata to obtain 110.5 [15]. Banga et al. combined octagonal geometry with chaos and obtained 105.625 [16], while Özpölat et al. reported 105.5 for a hyperchaotic S-box [17]. Akyol initialized a hybrid cuckoo search–bees algorithm with a memristive chaotic map and reached 109.75 [18], and Kılıçaslan combined the logistic map with the hippopotamus optimization algorithm to obtain 109.5 [19]. Artuğer and Özkaynak relocated the elements of an initial S-box with the sine cosine algorithm and reached a nonlinearity value of 112 [20]. Walsh-spectrum-based fitness functions have also been shown to guide swap-based searches efficiently [21, 22].

Two studies are particularly close to the approach of this chapter. Artuğer [23] generated an S-box with a chaotic map, selected the elements to be exchanged with the same chaotic map and kept an exchange when the nonlinearity increased, obtaining 107.5 after 100 iterations. Su et al. [24] proposed a three-layer method in which a chaotic map produces a high-nonlinearity S-box and the second layer optimizes differential uniformity without reducing nonlinearity, followed by an artificial jellyfish optimization layer. The present study builds on these ideas and differs from them in the chaotic map used, in the fitness function, and in the fact that a single integer-valued chaotic map controls every stage of generation and optimization.

The chaotic maps used in these studies are mostly classical maps such as the logistic, sine and tent maps. The chaotic ranges of smooth maps such as the logistic and sine maps are interrupted by periodic windows [25, 26], so some parameter values do not produce chaotic behavior. For this reason, new maps with wider chaotic ranges have been proposed, such as the modified skew tent map [27], modulo-based maps [28], integer-domain chaotic maps [29] and

discrete skew tent-based maps [30]. Motivated by these studies, a new chaotic map with a chaotic range covering all of its parameter space is proposed in this chapter and used for S-box generation and optimization. The contributions of the study are as follows:

- A new one-dimensional chaotic map, the modular skew tent chaotic map (MSTCM), is proposed by combining the skew tent map with a modular expansion; to the best of the author’s knowledge, this map has not been used for S-box generation before. Its Lyapunov exponent is derived in closed form and is positive for all parameter values.
- The dynamical behavior of the map is analyzed with bifurcation diagrams, Lyapunov exponents, the 0–1 test, return maps, invariant density and sensitivity analysis, and the map is implemented in 64-bit integer arithmetic.
- A combined S-box generation and optimization scheme is proposed in which the same chaotic map produces the chaotic S-box and selects the exchanged positions in both a Walsh-spectrum-guided nonlinearity stage and a nonlinearity-preserving differential stage. Unlike earlier chaos-based swap methods, all decisions, including the fitness evaluation, are made with integers, so the same S-box is obtained on every platform.
- The obtained S-box reaches an average nonlinearity of 112, the value also obtained with the sine cosine algorithm in [20], with a maximum XOR value of 8; the method is evaluated over 300 keys and compared with recent studies.

The rest of the chapter is organized as follows. Section 2 introduces the proposed chaotic map and its analysis. Section 3 describes the S-box generation and optimization algorithm. Section 4 presents the performance analysis and comparison, and Section 5 concludes the chapter.

2. PROPOSED CHAOTIC MAP

2.1. Mathematical model

The skew tent map is a piecewise linear map whose two branches map the unit interval onto itself. In the proposed map, the output of the skew tent map is multiplied by an integer factor β and a shift c is added before a modulo operation, which folds each branch β times and increases the stretching rate. The construction can be seen as a skewed generalization of the classical β -transformation $x \mapsto \beta x \bmod 1$ [31]. The MSTCM is defined as

$$\begin{aligned}
 g_p(x) &= x/p \text{ if } 0 \leq x < p; \\
 g_p(x) &= (1 - x)/(1 - p) \text{ if } p \leq x < 1
 \end{aligned} \tag{1}$$

$$x_{n+1} = f(x_n) = (\beta \cdot g_p(x_n) + c) \bmod 1 \quad (2)$$

where $x_n \in [0, 1)$ is the state, $p \in (0, 1)$ is the skewness parameter, $\beta \geq 2$ is an integer expansion parameter and $c \in [0, 1)$ is the shift parameter. In this study $p \in [0.2, 0.8]$, $\beta \in \{3, 5, 7, 9\}$ and $c \in [0, 1)$ are used; all of these parameters are part of the secret key.

2.2. Lyapunov exponent

The Lyapunov exponent measures the average exponential divergence of nearby trajectories; a positive value indicates chaotic behavior. Since the map is piecewise linear, its derivative is $|f'(x)| = \beta/p$ on the first branch and $|f'(x)| = \beta/(1 - p)$ on the second branch. Both values are larger than one, so

$$\lambda \geq \ln(\beta / \max(p, 1 - p)) > 0 \quad (3)$$

holds for every parameter value and every trajectory. Moreover, for integer β each point of the unit interval has exactly β pre-images on each branch, so the uniform density is invariant ($\sum 1/|f'| = \beta \cdot p/\beta + \beta \cdot (1 - p)/\beta = 1$) and the map is ergodic with respect to it [32]. Averaging $\ln|f'|$ over this density gives the Lyapunov exponent in closed form:

$$\lambda = \ln \beta - p \ln p - (1 - p) \ln(1 - p) \quad (4)$$

For the parameter ranges used, Eq. (4) gives λ between 1.599 and 2.890. Because λ is positive for all parameters, the map has no periodic windows, and its chaotic range covers the whole parameter space.

2.3. Dynamical analysis

Fig. 1(a) shows the bifurcation diagrams of the MSTCM with respect to p for $\beta = 3$ and $\beta = 9$. The trajectories fill the whole interval $[0, 1)$ for every p , and no periodic region appears. Fig. 1(b) compares the Lyapunov exponent of Eq. (4) with the value computed numerically from 2×10^4 iterations for 61 values of p and each β ; the maximum difference is 0.0088. For comparison, Fig. 1(c) shows the Lyapunov exponents of the logistic map $x_{n+1} = r x_n(1 - x_n)$ for $r \in [3.5, 4]$ and the sine map $x_{n+1} = a \sin(\pi x_n)$ for $a \in [0.85, 1]$, which are frequently used in S-box studies [12, 19]. The exponent is not positive for 22.6% of the logistic map parameters and 19.9% of the sine map parameters on 5001-point grids, whereas it is positive for all parameters of the MSTCM.

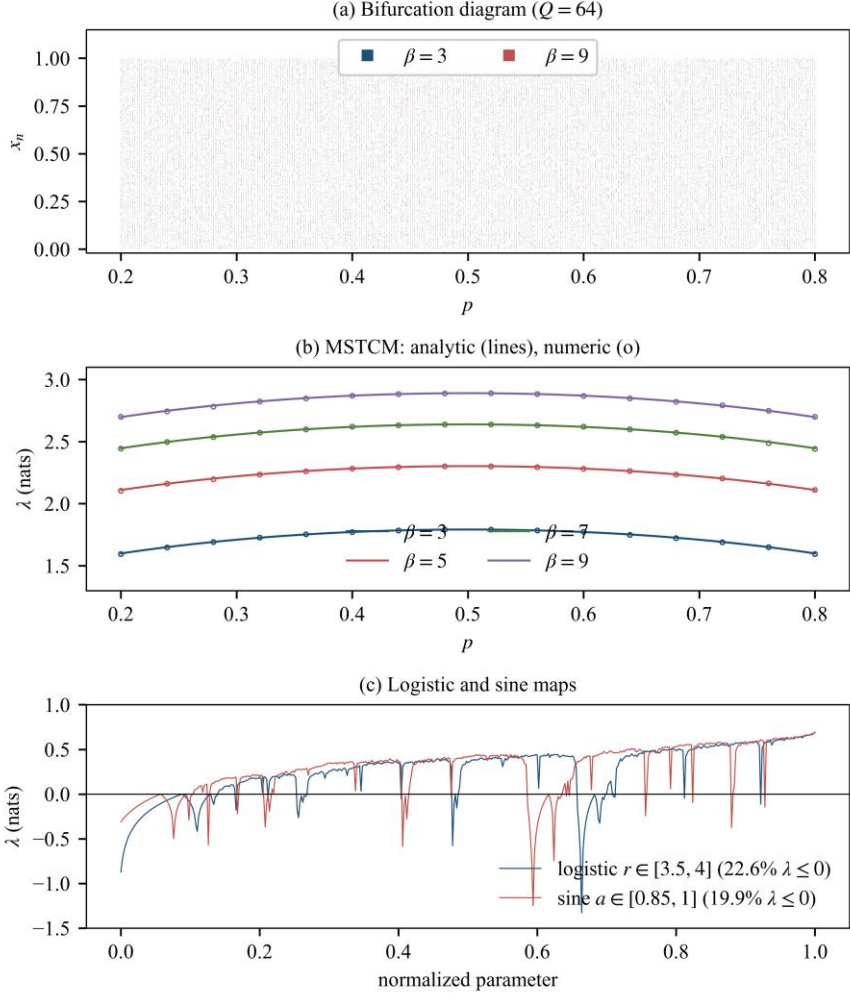


Fig. 1. (a) Bifurcation diagrams of the MSTCM; (b) analytical and numerical Lyapunov exponents of the MSTCM; (c) Lyapunov exponents of the logistic and sine maps

The 0–1 test for chaos [33] gives $K \approx 1$ for chaotic and $K \approx 0$ for regular dynamics. For the MSTCM, K is between 0.998 and 0.999 for twelve parameter combinations ($\beta \in \{3, 5, 7, 9\}$, $p \in \{0.25, 0.5, 0.75\}$), while it is -0.004 for the periodic logistic map with $r = 3.83$. The return map in Fig. 2(a) consists of 2β line segments that cover the unit square, and the histogram in Fig. 2(b) shows that the output is uniformly distributed: for 10^6 samples in 64 bins, the χ^2 values of four parameter sets are 56.4, 60.3, 72.2, 49.7, all below the critical value of 82.53 ($\alpha = 0.05$). To measure sensitivity to initial

conditions, one bit of x_0 was changed; the two trajectories separated by more than 2^{-8} after 8 iterations on average.

2.4. Integer implementation

Chaotic maps computed with floating-point numbers may produce different trajectories on different platforms, and finite precision can degrade chaotic behavior [34]. To obtain the same S-box on every platform, the MSTCM is implemented with 64-bit unsigned integers. The state $x \in [0, 2^{64})$ represents $x/2^{64}$, and with $P = p \cdot 2^{64}$ and $C = c \cdot 2^{64}$, one iteration is computed as

$$\begin{aligned} u &= \lfloor x \cdot 2^{64} / P \rfloor \text{ if } x < P; \\ u &= \lfloor (2^{64} - x) \cdot 2^{64} / (2^{64} - P) \rfloor \text{ otherwise} \quad (5) \\ x_{n+1} &= (\beta \cdot u + C) \bmod 2^{64} \quad (6) \end{aligned}$$

where the modulo operation is a bit mask. Odd values of β are used because an odd number is invertible modulo 2^{64} , so Eq. (6) does not lose information. Every digital implementation of a chaotic map is eventually periodic; Table 1 lists the cycle lengths of the integer map measured with Brent's algorithm for shorter word lengths. The median period grows approximately as $2^{1.03Q}$, i.e. in proportion to the number of states (Fig. 2(c)), which indicates that the 64-bit implementation has very long cycles compared to the number of iterations needed for S-box generation.

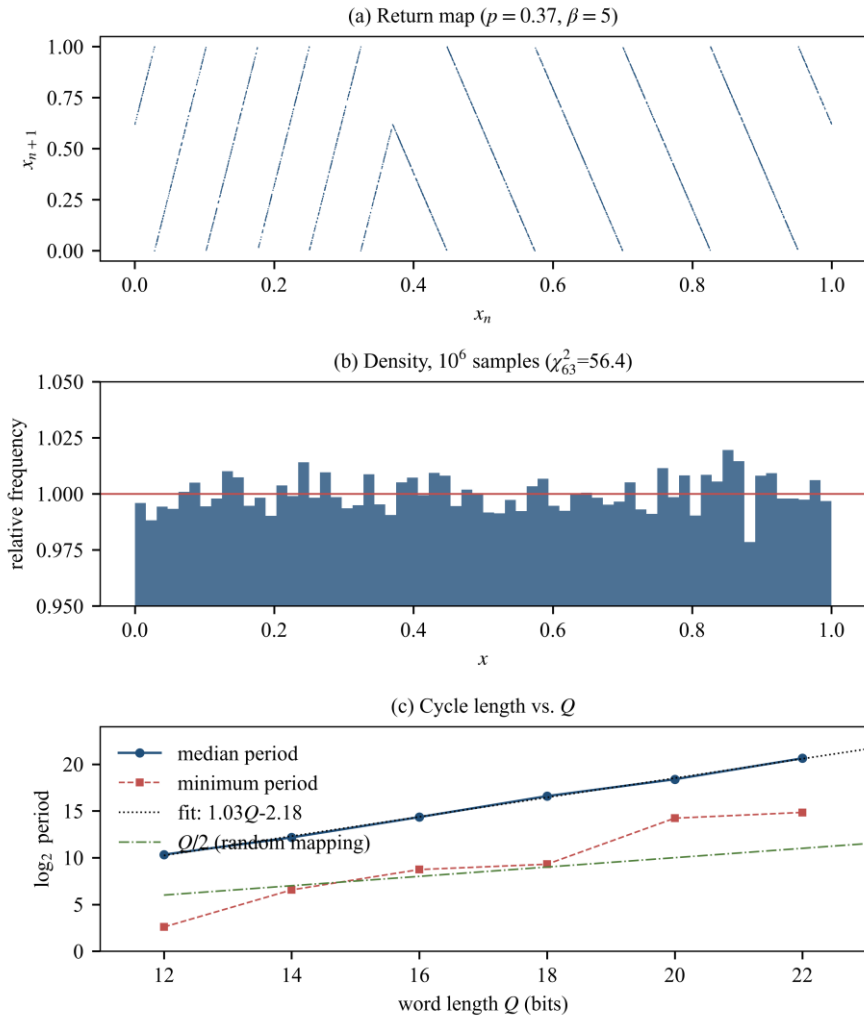


Fig. 2. (a) Return map; (b) distribution of 10^6 outputs; (c) cycle length of the integer map versus word length

Table 1. Cycle lengths of the integer MSTCM for different word lengths

Word length Q (bits)	Samples	Median period	Minimum period	Maximum period
12	200	1,287	6	3,835
14	160	4,594	94	15,123
16	120	20,770	425	58,011
18	80	98,349	630	247,026
20	40	342,103	19,154	816,994
22	16	1,621,708	29,355	4,090,198

3. PROPOSED S-BOX GENERATION AND OPTIMIZATION ALGORITHM

The proposed algorithm consists of three parts: generation of a chaotic S-box, nonlinearity optimization and differential probability optimization. In all parts, the random decisions are taken from the MSTCM, so the resulting S-box is completely determined by the secret key. The flowchart is given in Fig. 3 and the steps are summarized in Table 2.

Key and parameters. A 256-bit key $K = K_0 \| K_1 \| K_2 \| K_3$ consisting of four 64-bit words is converted into the map parameters as follows:

$$x_0 = K_0 \text{ OR } 1,$$

$$P = \lfloor 2^{64}/5 \rfloor + \lfloor (K_1 \gg 2) \cdot \lfloor 3 \cdot 2^{64}/5 \rfloor / 2^{62} \rfloor \text{ OR } 1 \quad (7)$$

$$\beta = (3, 5, 7, 9)[K_2 \text{ AND } 3],$$

$$C = K_0 \oplus K_1 \oplus K_2 \oplus K_3 \quad (8)$$

so that $p \in [0.2, 0.8]$. Since C depends on all key words, a change in any key bit changes the trajectory. The map is iterated 1000 times to remove transient effects, and an integer in $[0, n)$ is obtained from the state as $\lfloor x \cdot n / 2^{64} \rfloor$.

Chaotic S-box. The initial S-box is obtained by the Fisher–Yates shuffle [35] of the sequence $0, 1, \dots, 255$: for $i = 255, \dots, 1$, an index $j \in [0, i]$ is taken from the map and $S(i)$ and $S(j)$ are exchanged. This guarantees a bijective S-box without repeated values.

Stage 1: nonlinearity optimization. For each output bit j of the S-box, the Boolean function $f_j(x)$ is the j -th bit of $S(x)$, and its Walsh spectrum is $W_j(a) = \sum_x (-1)^{f_j(x) \oplus a \cdot x}$. The nonlinearity of f_j is $NL(f_j) = 128 - \max_a |W_j(a)|/2$. Increasing the nonlinearity means decreasing the largest spectrum values, so the following Walsh-spectrum fitness function [21] is minimized:

$$\text{cost}(S) = \sum_{j=0..7} \sum_{a=0..255} |W_j(a)|^{12} \quad (9)$$

In each iteration two positions i and j are selected by the MSTCM and $S(i)$ and $S(j)$ are exchanged. If the cost does not increase, the new S-box is kept; otherwise the exchange is cancelled. Because an exchange changes only two entries, the spectrum is updated with a rank-one correction instead of recomputing it. The stage ends when the nonlinearity of all eight Boolean functions reaches 112 or after 50,000 iterations. Selecting the exchanged elements with a chaotic map was also used in [23], where an exchange was kept when the nonlinearity increased; here the Walsh-spectrum cost of Eq. (9)

is used instead, because it also rewards reductions of large spectrum values that do not yet change the nonlinearity, which helps the search to leave plateaus.

Stage 2: differential probability optimization. For 60,000 further iterations, exchanges selected by the map are accepted only if the nonlinearity of every Boolean function is preserved and the largest entry of the XOR distribution table, together with the number of times it occurs, does not increase. In this way the differential probability is reduced without losing the nonlinearity obtained in the first stage. A similar principle, optimizing differential uniformity without reducing nonlinearity, is used in the second layer of [24]; in the proposed method this stage is carried out by the same chaotic map with a lexicographic criterion on the XOR distribution table.

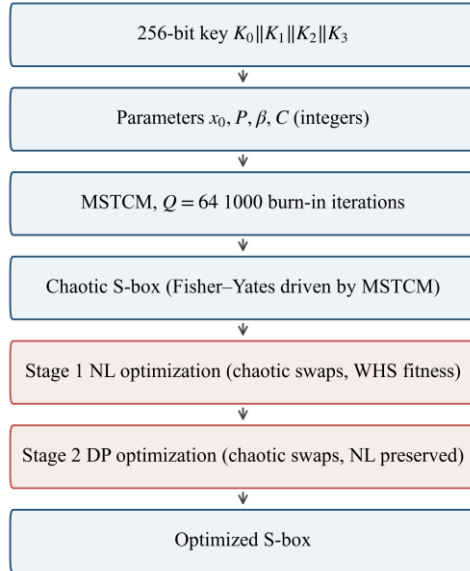


Fig. 3. Flowchart of the proposed S-box generation and optimization algorithm

Table 2. Steps of the proposed algorithm

Step	Operation
1	Input the 256-bit key and compute x_0 , P , β , C with Eqs. (7)–(8)
2	Iterate the MSTCM (Eqs. (5)–(6)) 1000 times
3	Generate the chaotic S-box with the MSTCM-driven Fisher–Yates shuffle
4	Compute the Walsh spectra of the eight Boolean functions and the cost of Eq. (9)
5	Select i, j with the MSTCM, exchange $S(i)$ and $S(j)$; keep the exchange if the cost does not increase
6	Repeat Step 5 until all NL values are 112 or 50,000 iterations are completed
7	For 60,000 iterations, exchange positions selected by the MSTCM if NL is preserved and the XOR table does not get worse
8	Output the optimized S-box

4. PERFORMANCE ANALYSIS

The proposed S-boxes were evaluated with the criteria commonly used in the literature: bijectivity, nonlinearity, strict avalanche criterion (SAC), bit independence criterion (BIC), differential probability (DP) and linear probability (LP). Bijectivity requires that each value in 0–255 appears exactly once. Nonlinearity was computed for the eight Boolean functions and reported as minimum, average and maximum values. SAC measures the probability that an output bit changes when one input bit is complemented, and the ideal value is 0.5 [5]. BIC requires that output bits change independently; it is evaluated through the nonlinearity (BIC-NL) and SAC (BIC-SAC) of the XOR of every pair of output bits [5]. DP is the largest entry of the XOR distribution table divided by 256 [4, 36], and LP is the largest linear approximation bias [3]. Lower DP and LP values indicate higher resistance to differential and linear cryptanalysis. Since the entries of the XOR distribution table are always even, the maximum XOR value of an 8-bit bijective S-box is at least 2; whether the value 2 can be reached for 8-bit bijective S-boxes is an open problem, and the best known value is 4, obtained by the AES S-box ($DP = 4/256 = 0.0156$) [1, 36]. The AES S-box, with average nonlinearity 112, $DP = 0.0156$ and $LP = 0.0625$, is therefore used as the reference in the comparisons. All Walsh transforms were computed with integer arithmetic, and the implementation was verified by reproducing these values for the AES S-box.

4.1. Proposed S-box

The key used for the presented S-box is K = 4a6d9eba9b5b664cb394042f9af5a477231e6f3dc175e3b24d05a9893973f12a . This is the first of the 300 test keys of Section 4.2 whose S-box reaches nonlinearity 112 in all Boolean functions and a maximum XOR value of 8. The chaotic S-box produced before optimization is given in Table 3 and the optimized S-box is given in Table 4. Their performance values are listed in Table 5 together with the values after Stage 1.

Table 3. Chaotic S-box generated with the MSTCM (hexadecimal)

	0	1	2	3	4	5	6	7	8	9	A	B	C	D	E	F
0	95	E3	2C	32	F2	4A	5E	A9	CE	4C	9F	BB	CD	81	C7	42
1	A7	C5	A6	48	87	2E	E1	B7	05	E4	18	29	E8	17	0B	74
2	69	06	AA	B0	20	6C	33	3C	E7	30	76	88	3F	68	B1	97
3	5A	E9	B8	5F	7D	0C	C4	1A	D6	D1	04	EC	67	1B	5B	4B
4	41	96	79	C0	DB	4D	59	13	0A	3B	B6	A4	8B	9A	27	6D
5	FD	F7	51	DE	F9	8F	25	D4	BF	A1	56	2B	49	01	BD	F1
6	44	BE	F4	C9	E6	77	91	CA	2F	6E	B5	F5	00	0D	40	57
7	CB	AF	C3	8E	64	22	46	35	E2	10	E0	B9	FA	07	98	C1
8	60	85	24	62	D8	5D	EB	6B	26	08	DD	2D	FF	D5	1D	FB
9	93	89	A0	5C	AD	1F	15	58	80	11	14	7E	70	9C	9B	3E
A	52	63	D0	C8	99	4E	39	6A	1E	C2	31	FE	78	A3	43	6F
B	8A	12	37	FC	8C	53	0E	28	EE	16	19	8D	ED	72	65	F0
C	83	E5	92	36	9D	38	94	A5	C6	2A	AE	71	DF	AC	CC	D3
D	3A	B3	3D	9E	D7	86	EA	61	AB	F6	55	A2	02	A8	DC	7F
E	4F	0F	09	F3	50	23	34	73	7A	7B	90	D2	CF	45	B2	82
F	54	66	DA	EF	75	B4	F8	BC	03	D9	1C	21	7C	84	BA	47

Table 4. Optimized S-box (hexadecimal)

	0	1	2	3	4	5	6	7	8	9	A	B	C	D	E	F
0	95	99	0E	16	1C	4A	4F	54	CE	4C	9F	E1	CD	81	FA	42
1	8F	49	A6	E3	85	FC	D6	B7	6F	E4	18	77	A8	15	0B	B4
2	F2	06	28	98	20	6C	27	3C	90	30	02	88	AF	E7	1F	97
3	72	91	B8	5F	7D	0C	BA	1A	BB	17	69	EC	67	BC	51	44
4	41	B9	79	C0	9B	4D	55	29	22	3B	B6	A4	66	9A	37	6D
5	F5	13	F9	80	19	25	A7	D4	BF	A1	DE	2B	4B	BD	62	05
6	C5	7F	F4	73	E6	C7	71	CA	A5	6E	75	65	5A	0D	ED	57
7	93	A0	FB	40	2D	94	46	35	34	10	E0	32	CB	5D	F7	C1
8	60	87	A3	31	DA	07	EB	61	14	C8	6B	00	FF	D5	A2	EA
9	D3	1D	3F	5C	AD	26	D1	58	56	11	04	7E	70	C6	DB	3E
A	52	C9	5B	08	47	4E	78	6A	CF	C2	86	EE	38	23	43	B5
B	8A	68	33	2E	FE	53	48	59	64	96	8D	2C	8E	01	FD	F0
C	82	7B	92	12	DD	F6	36	39	9C	D8	AE	2F	DF	AC	CC	E5
D	7C	B2	3D	9E	D7	D0	63	0A	AB	F1	2A	AA	76	E8	9D	BE
E	5E	0F	09	F3	50	E2	24	B3	7A	E9	B0	D2	1E	21	DC	83
F	A9	8B	89	EF	B1	1B	F8	03	74	D9	8C	45	3A	84	C4	C3

Table 5. Performance of the chaotic and optimized S-boxes

S-box	NL min	NL avg	NL max	SAC	BIC-NL	BIC-SAC	Max XOR (DP)	LP
Chaotic S-box (Table 3)	100	103.5	106	0.5059	104.07	0.5013	14 (0.0547)	0.1250
After Stage 1	112	112	112	0.4995	104.43	0.5058	14 (0.0547)	0.1406
Optimized S-box (Table 4)	112	112	112	0.5046	103.71	0.5028	8 (0.0313)	0.1250

As seen in Table 5, the average nonlinearity of the chaotic S-box is 103.5 and increases to 112 after 4,824 iterations of Stage 1. Stage 2 then reduces the maximum XOR value from 14 to 8, i.e. DP from 0.0547 to 0.0313, while all nonlinearity values remain 112. The maximum XOR value of 8 is not the optimum of 4 obtained by the AES S-box, but it is the value reached by the proposed optimization and, as shown in Section 4.5, it is lower than the values reported for recent chaos- and optimization-based S-boxes. The LP value decreases from 0.1406 to 0.1250 as a side effect of Stage 2. The SAC value of 0.5046 and the BIC-SAC value of 0.5028 are very close to the ideal value of 0.5, and the BIC-NL value is 103.71. The S-box is bijective and has no opposite fixed points. Fig. 4(a) shows how the average nonlinearity increases during Stage 1.

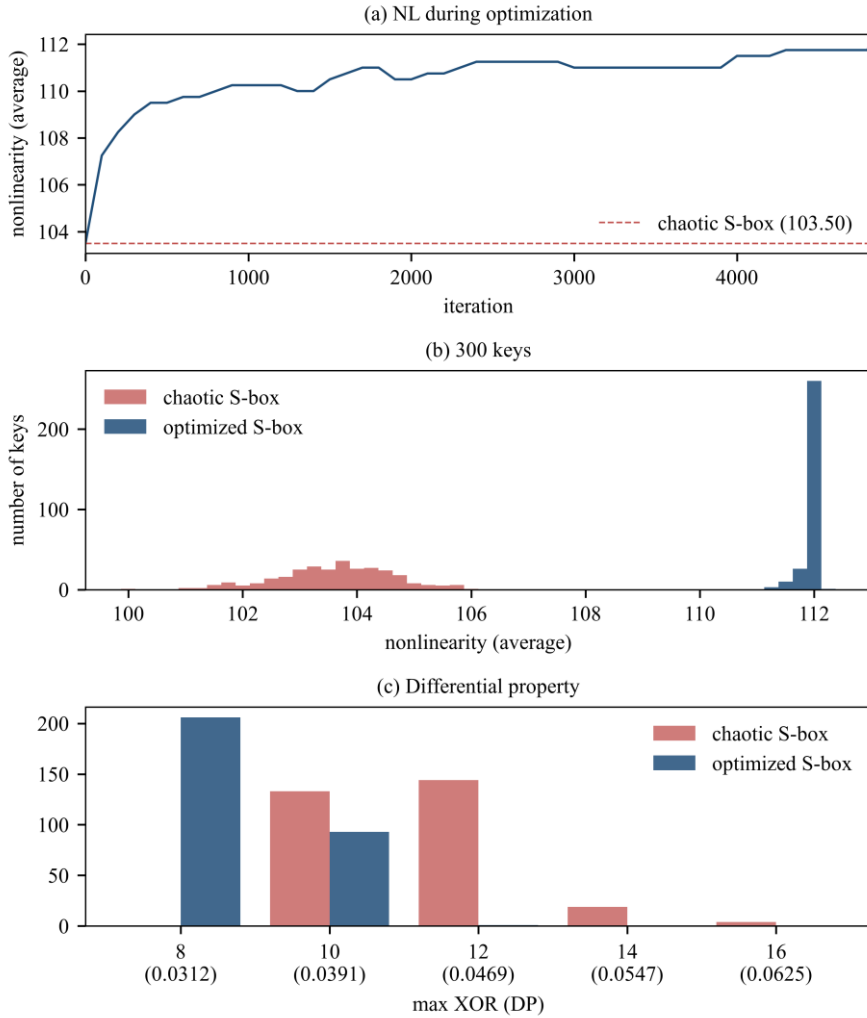


Fig. 4. (a) Average nonlinearity during Stage 1 for the presented S-box; (b) average nonlinearity and (c) maximum XOR values of the chaotic and optimized S-boxes for 300 keys

4.2. Performance over different keys

To show that the result does not depend on a particular key, the algorithm was run with 300 different keys, obtained as SHA-256 digests of the strings “MSTCM-keys-0”, ..., “MSTCM-keys-299”. The statistics of the chaotic and optimized S-boxes are given in Table 6 and Fig. 4(b)–(c). All S-boxes are bijective and different from each other. The average nonlinearity increases from 103.60 to 111.95; 261 of the 300 S-boxes (87.0%) reach 112 in all eight

Boolean functions and the lowest average value is 111.25. The maximum XOR value decreases from 11.29 to 8.63 on average; 206 S-boxes (68.7%) have a maximum XOR value of 8 and 299 have a value of at most 10, whereas the chaotic S-boxes before optimization have values up to 16. The median number of Stage-1 iterations is 10,870. All generated S-boxes and their performance values are available from the author on reasonable request.

Table 6. Performance statistics of the chaotic and optimized S-boxes over 300 keys

Criterion	Chaotic: mean	Chaotic: min	Chaotic: max	Optimized: mean	Optimized: min	Optimized: max
NL avg	103.60	99.50	106.00	111.95	111.25	112.25
NL min	99	90	104	112	110	112
NL max	107	104	110	112	112	114
SAC	0.5019	0.4878	0.5137	0.5023	0.4929	0.5159
BIC-NL	103.58	101.93	104.86	103.59	101.79	105.00
BIC-SAC	0.5021	0.4940	0.5109	0.5023	0.4957	0.5106
Max XOR	11.29	10.00	16.00	8.63	8.00	12.00
LP	0.1376	0.1250	0.1719	0.1349	0.1172	0.1641

4.3. Key sensitivity

For two base keys, each of the 256 key bits was changed one at a time and the S-box was generated again (512 S-box pairs). On average 99.60% of the S-box entries changed (minimum 98.44%), which is very close to the value of 99.61% expected for two independent random permutations. No bit change produced the same S-box. Therefore, even the smallest change in the key produces a completely different S-box.

4.4. Platform independence

Since all operations are performed with integers, the algorithm produces the same S-box on every platform. To verify this, the algorithm was implemented independently in Python and JavaScript and run for 10 keys. All S-boxes, the numbers of accepted exchanges in both stages and the final XOR table values were identical.

4.5. Comparison with recent studies

Table 7 compares the proposed S-box with chaos- and optimization-based S-boxes published between 2021 and 2026, most of them in the last two years; the AES S-box is included as a reference. The values of the compared studies are taken from the corresponding articles. The main advantages of the proposed S-box can be summarized as follows.

- **Nonlinearity.** The average nonlinearity of 112 is higher than that of all 11 compared studies and equal to the value of 112 obtained in [20] and to that

of the AES S-box. More importantly, the minimum nonlinearity is also 112, i.e. all eight Boolean functions reach 112, whereas the minimum values reported in the compared studies range from 102 to 110.

- **Differential property.** The maximum XOR value of 8 ($DP = 0.0313$) is lower than the values of 10–12 ($DP = 0.0391$ – 0.0469) reported in all compared studies, which indicates better resistance to differential cryptanalysis.
- **Linear probability.** The LP value of 0.1250 is lower than the values of 0.1406 [17] and 0.1328 [18] and close to the value of 0.1224 [16] among the studies that report LP.
- **Independence and avalanche.** The BIC-NL value of 103.71 is higher than in 5 of the 8 studies that report it; the BIC-SAC value is closer to 0.5 than in 5 of 8 studies and the SAC value is closer to 0.5 than in 5 of 9 studies. These criteria are therefore at the level of the compared methods.
- **Consistency over keys.** Unlike most of the compared studies, which report a single S-box, the performance was verified over 300 keys: the average nonlinearity is 111.95 and 68.7% of the S-boxes have a maximum XOR value of 8 (Table 6).

On the other hand, the maximum XOR value of 8 and the LP value of 0.1250 are still above the optimum values of 4 and 0.0625 of the AES S-box. Such values are usually obtained with algebraic constructions based on finite field inversion rather than with chaos- and optimization-based methods, which in the recent studies in Table 7 do not go below a maximum XOR value of 10. The average nonlinearity values are also shown in Fig. 5.

Table 7. Comparison with chaos- and optimization-based S-boxes from recent studies

Method	Year	NL min	NL avg	NL max	SAC	BIC-NL	BIC-SAC	Max XOR (DP)
AES S-box (reference) [1]	–	112	112	112	0.5049	112.00	0.5046	4 (0.0156)
Adaptive agent heroes and cowards algorithm + tent map [9]	2021	108	109.75	112	0.5068	104.35	0.5009	10 (0.0391)
Chaos + genetic algorithm (SBOX-CGA) [10]	2022	110	111.75	112	0.4968	104.00	0.5033	12 (0.0469)
Q-learning chaotic naked mole rat algorithm [11]	2023	–	109.75	–	0.4998	104.14	0.5041	10 (0.0391)
Sine map + element swapping [12]	2023	104	107.5	110	0.5073	103.43	0.5048	12 (0.0469)
3D chaotic maps + whale optimization [13]	2023	–	110.5	–	–	–	–	–
Tent map + sine cosine algorithm [14]	2024	106	108	110	0.4939	103.57	0.4976	10 (0.0391)
Tent map + cellular automata [15]	2024	–	110.5	–	–	–	–	–
Octagonal geometry + chaos [16]	2025	102	105.625	109	0.5084	103.27	0.5090	10 (0.0391)
Hyperchaotic system [17]	2025	102	105.5	108	0.4980	103.29	0.4976	12 (0.0469)
Memristive chaotic initialization + cuckoo search–bees algorithm [18]	2025	108	109.75	110	0.5000	103.50	0.5040	10 (0.0391)
Logistic map + hippopotamus optimization [19]	2026	108	109.5	112	0.4812	–	–	10 (0.0391)
Proposed (MSTCM + optimization)	–	112	112	112	0.5046	103.71	0.5028	8 (0.0313)

“–”: not reported in the corresponding study. Values of [9, 10, 11] are taken as reported in the comparison table of [14].

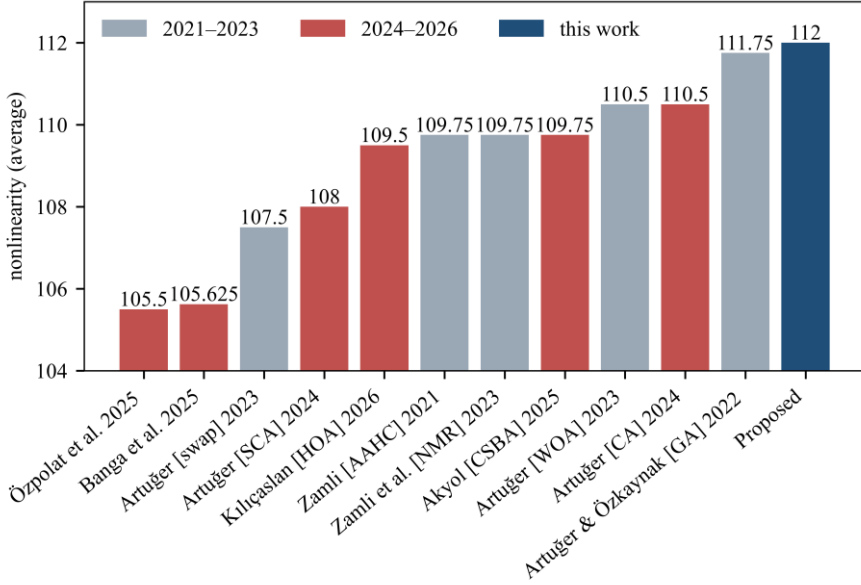


Fig. 5. Average nonlinearity of the proposed S-box and recent studies

5. CONCLUSION

In this study, a new one-dimensional chaotic map, the modular skew tent chaotic map, was proposed by combining the skew tent map with a modular expansion. It was shown analytically and numerically that the map is chaotic for all parameter values, with a Lyapunov exponent between 1.60 and 2.89, and the map was implemented in 64-bit integer arithmetic so that the same results are obtained on every platform. The map was then used to generate a chaotic S-box and to drive a two-stage optimization of nonlinearity and differential probability. The average nonlinearity of the presented S-box increased from 103.5 to 112 and its maximum XOR value decreased from 14 to 8. Over 300 keys, the average nonlinearity was 111.95, and the S-box changed almost completely when a single key bit was changed. The comparison with recent studies shows that the proposed S-box has a higher average nonlinearity and a lower maximum XOR value than the compared chaos- and optimization-based S-boxes, while its SAC and BIC values are at the level of these methods. Since the maximum XOR value of 8 is still above the optimum value of 4 of the AES S-box, future work will focus on extending the optimization to reach maximum XOR values of 6 or 4 without reducing the nonlinearity, and on using the proposed S-boxes in block cipher and image encryption applications.

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Deep Learning-Based Detection of AI-Generated Face Images Using a Lightweight EfficientNet Model

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1. INTRODUCTION

Recent advances in generative artificial intelligence have made it possible to synthesise text, images, audio and video at a level of realism that was unattainable only a few years ago. While these capabilities create opportunities in content creation, education and design, their misuse raises serious risks to digital trust and cybersecurity. In particular, the ability of generative models to fabricate realistic and personalised content can amplify social-engineering and impersonation attacks [1], and the speed at which misleading material spreads online makes verifying the origin and authenticity of digital content increasingly important [2]. Synthetic and manipulated media are therefore not merely a content-production technology but a security concern that can erode confidence in online information [3].

Human faces are a particularly sensitive category of synthetic media. Modern generators can produce faces of non-existent people that appear photographically convincing; controlled studies show that AI-synthesised faces are, on average, indistinguishable from and even judged more trustworthy than real faces [4]. Because relying on human perception alone is insufficient [5], automated detection has become an essential line of defence in scenarios ranging from fake social-media profiles and synthetic identities to fraud and disinformation.

Against this background, this chapter investigates how a compact, existing convolutional backbone performs in distinguishing real from AI-generated faces when adapted through transfer learning. We fine-tune an ImageNet-pretrained EfficientNet-B0 [6] on a large, balanced benchmark and report accuracy, precision, recall, F1 and ROC-AUC, together with a confusion-matrix analysis. We then examine the same frozen detector under image degradations and on external face sources to establish where strong benchmark performance does and does not transfer.

The main contributions of this study are as follows:

- We evaluate a reproducible transfer-learning baseline for AI-generated face detection using an existing ImageNet-pretrained EfficientNet-B0 without architectural modifications or hand-crafted features. With two-stage fine-tuning, it achieves 98.03% accuracy and a ROC-AUC of 0.9984 on the official 20,000-image test split of the 140k Real and Fake Faces benchmark.
- We examine the detector's decisions and sensitivity to image degradation. Class-activation mapping identifies regions associated with its predictions, while controlled JPEG compression, Gaussian noise and Gaussian blur experiments measure performance under progressively degraded inputs.

- We evaluate cross-dataset generalisation on an unseen real-face source and an independently constructed synthetic-face dataset (SFHQ), without adapting the trained model. Accuracy falls to 65.75% (ROC-AUC 0.8267), with fake-class recall of 35.95%. This gap shows that strong performance on the original benchmark does not establish reliable detection on images drawn from a different data source and synthesis pipeline. For comparison, we also run a publicly released cross-generator detector on the same two test sets without retraining, situating our results against an independently trained model.

The remainder of the chapter reviews the literature (Section 2), describes the proposed method (Section 3) and experimental setup (Section 4), presents the results (Section 5), discusses their implications (Section 6), and concludes in Section 7.

2. LITERATURE REVIEW

The realism of synthetic faces stems largely from generative adversarial networks [7] and, in particular, style-based generators such as StyleGAN [8], which can sample high-resolution faces of people who do not exist. More recently, diffusion models have emerged as an equally powerful family of image generators. This diversity of generation mechanisms is central to the detection problem, because a detector tuned to one generator does not necessarily transfer to another.

Research on detecting manipulated imagery has produced several large facial-video benchmarks: FaceForensics++ collects several manipulation families and enables systematic comparison of data-driven detectors [9]; Celeb-DF offers higher-quality forgeries with reduced artefacts [10]; and the DeepFake Detection Challenge assembles a very large, in-the-wild corpus [11]. A second line studies fully synthetic still images. Wang et al. [12] show that CNN-based detectors trained on the output of one generator can, with sufficient data diversity and augmentation, partially generalise to others, while Luo et al. [13] exploit high-frequency cues to improve cross-manipulation robustness. Ojha, Li and Lee [14] show that existing fake-image detectors often struggle to generalise to unseen generative models and propose a vision–language feature-based approach that performs better on images from unseen diffusion and autoregressive models. Corvi et al. [15] further examine the forensic traces of diffusion-generated images and the performance of existing detectors on them. In a systematic study, Gragnaniello et al. [16] confirm that detectors performing almost perfectly in controlled conditions degrade sharply on images from unseen generator architectures and on content re-compressed or laundered through social networks. A recurring conclusion of this literature [3] is that a useful detector must be assessed not only by in-distribution

accuracy but also by its robustness to unfamiliar generators and realistic degradations.

Beyond measuring detection performance, researchers have examined the traces that make generated images recognisable. Generative pipelines, particularly the up-sampling operations used in GANs, can leave subtle spatial inconsistencies and periodic frequency patterns in their outputs [17]. Although these traces may be difficult for humans to perceive, convolutional detectors can learn to use them for classification [12, 13]. These observations motivate our explainability and cross-dataset analyses. Rather than designing features for a particular generator, we fine-tune a pretrained convolutional backbone to learn discriminative cues from the training data and then test whether those cues transfer to unseen sources.

The 140k Real and Fake Faces benchmark used here has also been revisited by several deep-learning studies with different design trade-offs. Mallet et al. [18] combine CNN features with a support-vector-machine classifier, whereas Arshad, Khan and Farid [19] propose a lightweight CNN and report approximately 95% accuracy. Reza et al. [20] augment an EfficientNet-B0 backbone with attention and residual components in ARC-Net, reporting 99% accuracy on an evaluation set that includes additional real-face images. Sheikh et al. [21] examine CNN and vision-transformer architectures. Jheelan and Pudaruth [22] compare a custom CNN with several pretrained models and report their highest test accuracy, 98.5%, with MobileNet on a 20,000-image subset.

Table 1 summarises representative approaches and their evaluation settings. The datasets and protocols differ, so published performance figures should not be interpreted as results from a common test set.

Table 1. Selected prior studies on synthetic-image and fake-face detection

Study	Method	Data and evaluation focus
Wang et al. [12]	ResNet-50	Trained on ProGAN images; tested transfer to other generators.
Ojha, Li and Lee [14]	Vision–language features	Tested images from unseen generators, including diffusion models.
Gragnaniello et al. [16]	Detector analysis	Examined GAN-generated images under changing generators and image processing.

Arshad, Khan and Farid [19]	Lightweight CNN	Classified fake faces using the 140k Real and Fake Faces benchmark.
Reza et al. [20]	EfficientNet-B0 with attention and residual components	Evaluated the 140k benchmark and additional data, including out-of-distribution tests.

Compared with hybrid pipelines [18], attention and residual designs [20], transformer comparisons [21], and custom lightweight networks trained from scratch [19, 22], we use a plain ImageNet-pretrained EfficientNet-B0 adapted through two-stage fine-tuning, without architectural additions or hand-crafted features. Evaluating this baseline alongside explainability, degradation and cross-dataset tests allows us to assess its strengths and limitations under a modest compute budget.

3. PROPOSED METHOD

The detector is built on an ImageNet-pretrained EfficientNet-B0 backbone [6]. On top of the backbone, we add a global average pooling layer, a dropout layer with a rate of 0.3, and a single sigmoid-activated output unit. To limit overfitting, stochastic augmentation—horizontal flips, random rotations of up to $\pm 18^\circ$, and zoom of up to $\pm 10\%$ —is applied during training. The overall pipeline is shown in Fig. 1.

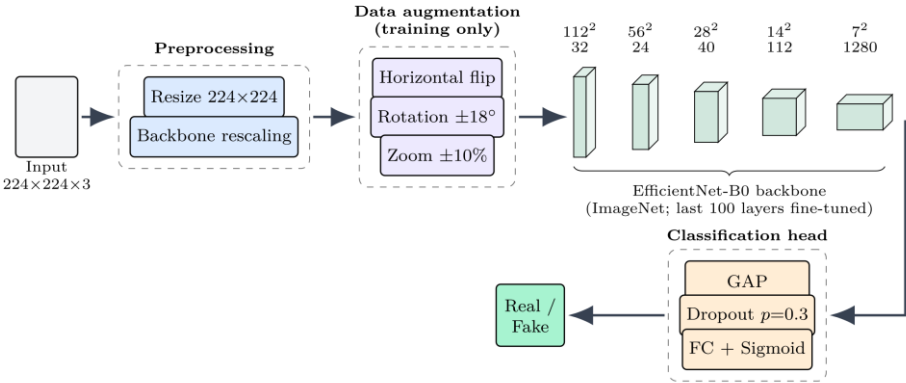


Fig. 1. Architecture of the EfficientNet-B0 detector: the fine-tuned backbone feeds GAP, dropout and a sigmoid fully connected layer that outputs the real/fake decision.

The network is optimised with the binary cross-entropy loss,

$$L = -(1/N) \sum_{i=1 \dots N} [y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)] \quad (1)$$

where N is the number of samples, $y_i \in \{0, 1\}$ the ground-truth label and $\hat{y}_i \in [0, 1]$ the predicted probability.

We selected EfficientNet-B0 for its favourable balance between classification performance and computational cost. The ImageNet-pretrained backbone, excluding its original classification head, contains approximately 4.05 million parameters. Its architecture uses compound scaling to balance network depth, width and input resolution [6]. This compactness is deliberately aligned with our goal of a baseline that both trains and runs under a modest hardware budget. ImageNet pretraining provides general visual features that can be adapted to the face-classification task. Because the training images occupy a relatively narrow domain of aligned faces, we fine-tune only the final 100 backbone layers at a low learning rate to limit changes to the pretrained representation. The dropout layer and the light geometric augmentation serve the same purpose, discouraging the model from latching onto dataset-specific shortcuts rather than transferable synthesis cues.

3.1. Two-Stage Training

Training follows a two-stage schedule. In the first stage the backbone is frozen and only the newly added classifier is optimised at a learning rate of 10^{-3} . In the second (fine-tuning) stage the last 100 backbone layers are unfrozen and training continues at a much smaller rate of 10^{-5} , which adapts the representation to the task without eroding the pretrained features; the batch-normalisation statistics are kept frozen throughout this stage for stability. Both stages use the Adam optimiser, the learning rate is reduced automatically when the validation loss plateaus, and early stopping halts training when no further improvement in validation AUC is observed. The model was evaluated on the held-out test set after early stopping restored the best validation-AUC weights from the second stage. It was then saved as `deepfake_detector.keras` and used without further training for the class-activation, robustness and cross-dataset evaluations.

This schedule follows established transfer-learning practice and is motivated by two considerations. We first train the randomly initialised classifier while keeping the pretrained backbone frozen. We then unfreeze the final 100 backbone layers and continue training at a learning rate two orders of magnitude lower (10^{-5} versus 10^{-3}), while keeping the batch-normalisation statistics fixed. This schedule allows the classifier to adapt before updating the backbone and limits the extent of changes to the pretrained representation. We

did not compare this schedule with full-network fine-tuning, so its effect on training stability or generalisation cannot be isolated.

4. EXPERIMENTAL SETUP

4.1. Dataset

Experiments use the publicly available 140k Real and Fake Faces benchmark [23], assembled specifically to separate genuine from synthetic faces. The real subset comprises 70,000 photographs sampled from the high-resolution, demographically varied Flickr-Faces-HQ (FFHQ) collection, whereas the synthetic subset comprises 70,000 non-existent faces produced with the StyleGAN generator [8]. The two classes are therefore perfectly balanced, yielding 140,000 images in total. We emphasise that the synthetic class originates from a single GAN family and does not include diffusion-generated faces; this restriction is revisited in Section 6.

The dataset provides predefined training, validation and test splits, which we retained without repartitioning the images. Each split is class-balanced: the training set contains 100,000 images, while the validation and test sets each contain 20,000 images, with equal numbers of real and fake faces in every split. Images were resized to 224×224 pixels using the Keras data-loading pipeline and labelled as {fake = 0, real = 1}. Images were supplied to the Keras EfficientNet-B0 backbone with pixel values in the [0, 255] range, because the model includes its own input rescaling layer.

4.2. Hyperparameters

All experiments were conducted on a single NVIDIA Tesla T4 GPU (16 GB) in a cloud computing environment, using the TensorFlow/Keras framework [24]. The data pipeline streams images from disk with prefetching to avoid memory overflow. The main hyperparameters are summarised in Table 2.

Table 2. Hyperparameters used in training

Hyperparameter	Value
Input resolution	224×224
Batch size	32
Optimiser	Adam
Learning rate (Stage 1)	10 ^{−3}
Learning rate (Stage 2)	10 ^{−5}
Epochs (Stage 1 / Stage 2)	6 / 6
Unfrozen layers (fine-tuning)	100
Dropout rate	0.3
Loss function	Binary cross-entropy

4.3. Evaluation Metrics

Performance was assessed using accuracy, precision, recall, F1 score and the area under the receiver operating characteristic curve (ROC-AUC). For the class-specific metrics below, we treat the fake class as positive:

$$\text{Precision} = \frac{TP}{TP + FP}, \quad \text{Recall} = \frac{TP}{TP + FN} \quad (2)$$

$$F_1 = \frac{2 \text{ Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \quad (3)$$

The primary in-distribution metrics were computed on the predefined test split without test-time augmentation or threshold search. Accuracy and F1 scores characterise performance at a fixed decision threshold of 0.5, whereas ROC-AUC measures discrimination across thresholds. The test split contains equal numbers of real and synthetic images, so its accuracy reflects performance under balanced class proportions. The network's sigmoid output represents the predicted probability of the real class. ROC-AUC was computed using this probability with real as the positive class; the same AUC would be obtained with fake as the positive class by using one minus this probability as the score. Precision, recall and F1 scores are reported separately for both classes at the 0.5 threshold. The external and robustness evaluations used the samples described in Section 4.4.

4.4. Cross-Dataset and Robustness Evaluation Protocols

To assess generalisation beyond the training generator, we constructed an external evaluation set from two sources that were not used during training. Real faces were drawn from a publicly redistributed 256×256 version of CelebA-HQ [25, 26], whereas synthetic faces were drawn from part 4 of the SFHQ dataset [27]. According to the dataset documentation, SFHQ part 4 uses Stable Diffusion v2.1 images as starting points, encodes them into the latent space of an FFHQ-trained StyleGAN2 model using e4e, and generates and curates the resulting faces. The evaluated images are therefore outputs of this multi-stage pipeline, rather than unmodified diffusion outputs or images from the StyleGAN model used to create our training fakes. The external set therefore differs from the training data in both its real-face source and its synthetic-face pipeline. For each class, we selected the first 2,000 images in lexicographic filename order: real faces from the CelebA-HQ image directory and synthetic faces from the main SFHQ part 4 directory (images/images). Selection was deterministic; no random seed was used. The SFHQ archive also includes two bundled “sample” folders that contain copies of images from the main directory. These folders were excluded from selection to avoid evaluating duplicate image content, and we verified by content hashing that

all 2,000 selected synthetic images (and all 2,000 real images) are distinct. No further images were excluded or filtered. Each image was converted to RGB and resized to 224×224 pixels with Pillow before inference. We retained the training label convention (fake = 0, real = 1), producing a balanced external test set of 4,000 images. The results of this evaluation are presented in Section 5.3.

For the robustness analysis, we selected the first 1,500 images per class from the official test split in lexicographic filename order. We applied JPEG recompression, additive Gaussian noise and Gaussian blur at increasing severity levels, and measured accuracy and ROC-AUC at each level. The results are presented in Section 5.2.

4.5. Baseline Detector for Comparison

To provide an independently trained comparison, we evaluated the publicly released detector of Wang et al. [12] without retraining or fine-tuning. We tested it on the full official 140k test split and on the same 4,000-image CelebA-HQ/SFHQ external set used for our detector, selected as described in Section 4.4. We loaded the detector using Wang et al.’s [12] released networks.resnet implementation and blur_jpg_prob0.5.pth checkpoint, which was trained on ProGAN images with blur and JPEG augmentation. As an implementation check, we compared its outputs with those of a standard ResNet-50 loaded with the same weights on the inputs used in our verification test; the maximum observed difference was zero. The evaluation script stops if this check fails. Both detectors were evaluated on the same 2,000 real and 2,000 synthetic images selected for the final cross-dataset experiment. Wang et al.’s released demonstration script does not crop images by default. For our evaluation, we instead followed the 224×224 centre-crop test setting reported in their paper, followed by ImageNet normalisation, without resizing the images. The network produces a single logit, which we convert to a fake-class score using the sigmoid function (fake = 1 in Wang et al.’s label convention). We use a 0.5 threshold to calculate accuracy and recall, and compute ROC-AUC from the continuous fake-class scores. An AUC above 0.5 indicates that, overall, fake images tend to receive higher scores than real images. The default 0.5 threshold is used as released and is never tuned on the test data. We calculated both detectors’ metrics on the same evaluation images using the definitions given in Section 4.3. We did not compare these values with the average precision reported by Wang et al. [12], which was obtained on different test data. The results are presented in Section 5.4.

5. RESULTS

5.1. In-Distribution Performance

On the held-out test set of 20,000 images, the model achieves 98.03% accuracy and a ROC-AUC of 0.9984. The per-class F1 scores in Table 3 are similar, although the detector misses more synthetic images than it incorrectly flags real images.

Table 3. Test-set classification performance

Class	Prec.	Rec.	F1	Support
Fake (0)	0.9880	0.9724	0.9801	10,000
Real (1)	0.9728	0.9882	0.9805	10,000
Macro avg	0.9804	0.9803	0.9803	20,000
Weighted avg	0.9804	0.9803	0.9803	20,000
<i>Accuracy: 0.9803 ROC-AUC: 0.9984</i>				

Figure 2 shows the confusion matrix. Of the 10,000 fake images, 9,724 are correctly detected and 276 pass as real; of the 10,000 authentic images, only 118 are wrongly flagged as fake. The missed-fake rate is 2.76%, compared with a 1.18% false-alarm rate for authentic images.

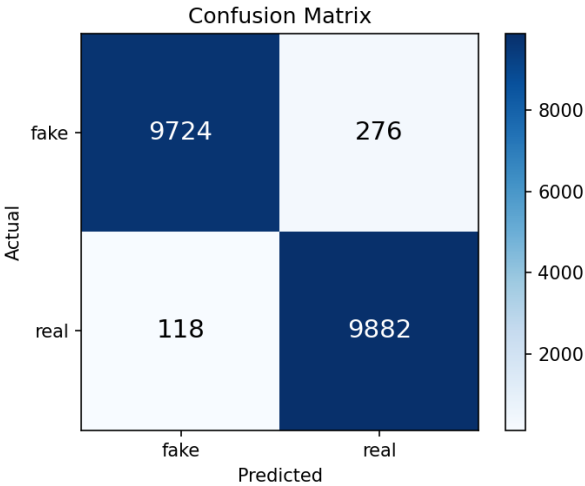


Fig. 2. Test-set confusion matrix (0: fake, 1: real).

Figure 3 shows the ROC curve. The AUC of 0.9984 indicates excellent discrimination between real and fake images on the in-distribution test set. The curve remains close to the upper-left corner, showing that high true-

positive rates can be achieved at low false-positive rates across a range of decision thresholds.

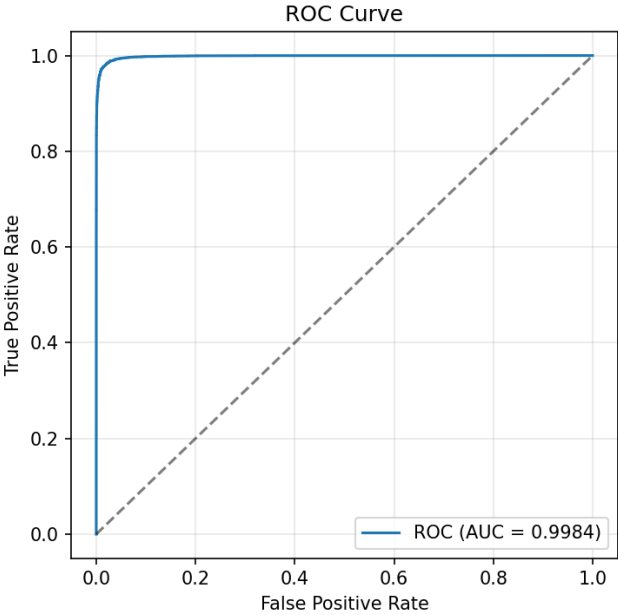


Fig. 3. ROC curve on the test set (AUC = 0.9984).

5.2. Explainability and Robustness

To examine which image regions were associated with the detector’s predictions, we generated Grad-CAM visualisations [28] from the final convolutional feature maps. In this architecture, the global-average-pooling and single-output classification head make the resulting maps closely related to a classifier-weighted combination of those feature maps. We present visualisations only for synthetic faces, avoiding the reproduction of identifiable real-face photographs. Fig. 4 overlays Grad-CAM heatmaps on four synthetic faces from SFHQ. The model classifies all four as fake, with $P(\text{real})$ ranging from 0.29 to 0.46; thus, some predictions lie close to the 0.5 decision threshold. The evidence for the fake class concentrates not on the central, semantically meaningful facial features but on background regions and hair or boundary areas.

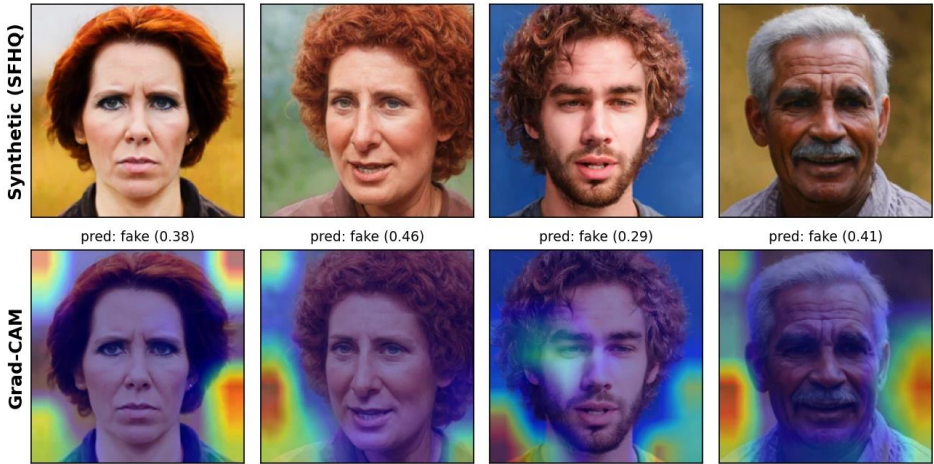


Fig. 4. Grad-CAM class activation maps on four synthetic SFHQ faces [27] (CC0). Top: input faces; bottom: heatmaps for the predicted fake class. All four are correctly classified as fake; the evidence concentrates on background and hair/boundary regions rather than central facial features.

We also evaluated sensitivity to image degradation by applying JPEG re-compression, Gaussian noise and Gaussian blur to a balanced in-domain subset (1,500 images per class) and measuring accuracy and ROC-AUC at increasing severities (Figure 5). Under JPEG re-compression the detector degrades gracefully: accuracy remains above 96% down to quality 70 and is still 94.8% at quality 50, with ROC-AUC above 0.99 throughout this range, declining only under very aggressive compression (quality 10). Additive Gaussian noise and Gaussian blur are more damaging: accuracy falls steadily as the noise level or blur radius grows, approaching 0.70 at $\sigma = 40$ and chance level at blur radius 3. Notably, ROC-AUC remains substantially higher than accuracy across most settings, indicating that the underlying ranking is largely preserved even where the fixed 0.5 threshold begins to fail.

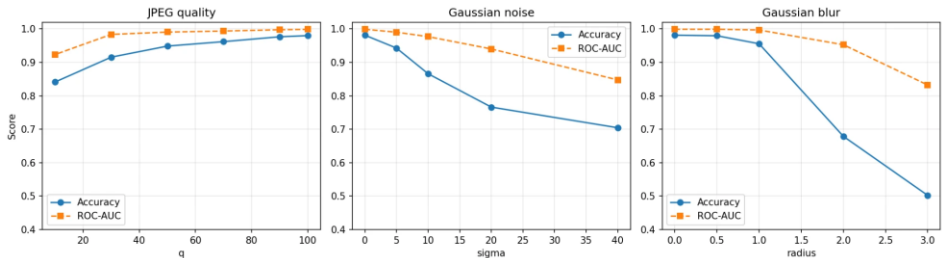


Fig. 5. Detector robustness to JPEG re-compression, Gaussian noise and blur: accuracy (solid) and ROC-AUC (dashed) versus severity.

5.3. Cross-Dataset Generalisation

The results above were obtained on the benchmark’s held-out test split. To assess performance on different data sources, we evaluated the trained detector without further adaptation on 2,000 real faces from CelebA-HQ and 2,000 synthetic faces from SFHQ part 4 (Section 4.4). The SFHQ images were generated through a separate, multi-stage process that uses Stable Diffusion images as starting points and StyleGAN2 to produce the final faces. Accuracy was 65.75% and ROC-AUC was 0.8267 on this external set, compared with 98.03% and 0.9984, respectively, on the benchmark test split (Table 4; Figure 6).

Table 4. Cross-dataset performance on CelebA-HQ (real) versus SFHQ (fake).

Class	Prec.	Rec.	F1	Support
Fake (0)	0.8899	0.3595	0.5121	2,000
Real (1)	0.5987	0.9555	0.7361	2,000
<i>Accuracy: 0.6575 ROC-AUC: 0.8267</i>				

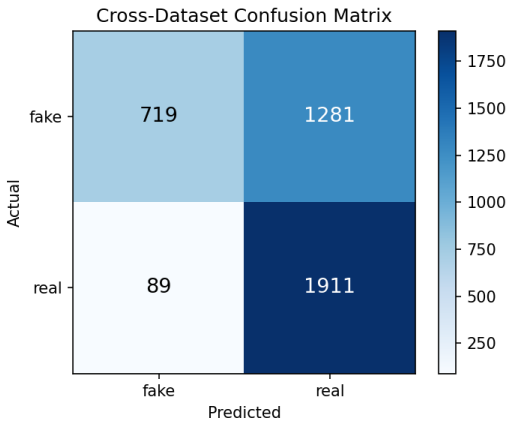


Fig. 6. Cross-dataset confusion matrix (0: fake, 1: real). The detector still recognises real faces but misses most of the external synthetic faces.

The degradation is asymmetric: real-class recall is 0.9555, whereas fake-class recall is 0.3595. Of the 2,000 SFHQ synthetic images, 1,281 are classified as real.

5.4. Comparison with a Released Detector

Table 5 reports the released Wang et al. [12] detector on the two protocols (Section 4.5), alongside our model. On the in-distribution 140k test split it

attains 50.77% accuracy, 1.60% fake-class recall and a ROC-AUC of 0.8227; on the cross-dataset it attains 58.13% accuracy, 16.30% fake-class recall and a ROC-AUC of 0.9756. Its real-class recall exceeds 0.999 in both cases, so at the default 0.5 threshold it assigns almost all of these face images to the real class. Both ROC-AUC values are nonetheless above 0.5—and higher on the cross-dataset than in-distribution—so the underlying scores still rank fake above real images.

Table 5. Comparison with the released Wang et al. (2020) detector on the two protocols. Acc: accuracy; F-Rec: fake-class recall (0.5 threshold).

Detector	Acc	F-Rec	ROC-AUC
<i>In-distribution (140k official test, 20,000 images)</i>			
This study (EfficientNet-B0)	0.9803	0.9724	0.9984
Wang et al. [12] (ResNet-50)	0.5077	0.0160	0.8227
<i>Cross-dataset (CelebA-HQ vs SFHQ, 4,000 images)</i>			
This study (EfficientNet-B0)	0.6575	0.3595	0.8267
Wang et al. [12] (ResNet-50)	0.5813	0.1630	0.9756

6. DISCUSSION

The EfficientNet-B0 baseline achieved 98.03% accuracy and a ROC-AUC of 0.9984 on the official in-distribution test split. Table 6 places this result beside published values for the same 140k benchmark. It exceeds the 95.0% reported for a lightweight CNN by Arshad, Khan and Farid [19] and is close to results reported for MobileNet by Jheelan and Pudaruth [22] and the attention- and residual-augmented ARC-Net by Reza et al. [20]. These figures indicate that a plain pretrained backbone can perform strongly on this benchmark, but they do not establish that one architecture is superior to another.

Table 6. Comparison with studies based on the 140k Real and Fake Faces benchmark. Evaluation protocols differ between studies

Study	Method	Acc.
Reza et al. [20]	ARC-Net (Eff.Net-B0)	99.0%
Jheelan and Pudaruth [22]	MobileNet	98.5%
This study	EfficientNet-B0	98.03%
Arshad, Khan and Farid [19]	Lightweight CNN	95.0%

The studies in Table 6 differ in their partitions, training data and evaluation protocols. In particular, Jheelan and Pudaruth [22] used a 20,000-image subset of the benchmark with their own training and test split, whereas we evaluated on the benchmark’s predefined held-out test split. Their reported 98.5% accuracy and our 98.03% accuracy therefore reflect different evaluation protocols and should not be ranked as directly comparable results. Reza et al. [20] likewise use a hybrid set supplemented with additional real images. Direct numerical ranking across these studies therefore has limited meaning. Our detector uses an EfficientNet-B0 backbone with approximately 4.05 million parameters, excluding the classification head, and was fine-tuned in two stages on a single NVIDIA T4 GPU. A controlled comparison of training time, inference cost and accuracy would be required to establish whether it offers an efficiency advantage over the other methods.

The contrast between in-distribution and external performance is more informative than a small difference among benchmark accuracies. On CelebA-HQ real faces and SFHQ synthetic faces, accuracy fell to 65.75%, and only 35.95% of the synthetic images were detected. Notably, SFHQ faces are produced through a StyleGAN2-based pipeline using Stable Diffusion images as starting points. This experiment is therefore a cross-dataset evaluation, not a direct comparison of GAN-generated and diffusion-generated images. The low fake-class recall shows that the detector’s strong performance on the benchmark did not transfer to this external synthetic-face set; the contributions of generator, source and curation differences cannot be isolated here. Previous studies have likewise found that detectors trained on one source often lose performance on unseen data and generators [14, 15, 16]. Moreover, the external test changes both the real-image source and the synthetic-image pipeline, so the observed gap cannot be attributed to any single factor; it establishes a shift in the combined data distribution and a practical limit of this frozen detector.

The comparison with the released Wang et al. [12] detector (Table 5) is instructive. At the default 0.5 threshold that model labels almost all of our face images as real, so its accuracy stays near chance on both protocols and its operating point clearly does not transfer to these datasets. Its threshold-independent ranking behaves differently: on the cross-dataset its ROC-AUC (0.9756) is higher than ours (0.8267), even though ours is far higher in-distribution. A detector trained on a different source can therefore rank the unseen CelebA-HQ and SFHQ images better than our StyleGAN-specialised model, while still needing recalibration before it could act on that ranking. Because the two detectors differ in architecture, training data and augmentation at the same time, this comparison cannot attribute the difference to any single design choice; it indicates only that different training strategies may affect cross-dataset transfer, and that such transfer can appear in the ranking (ROC-AUC) rather than at a fixed operating point. Consistent with

Wang et al. [12], single-source training is thus not inherently doomed across sources; but a fixed decision threshold should not be assumed to carry over, and an operating point must be validated on representative target data rather than tuned on the test set itself.

The activation maps highlight hair, background and boundary regions in the four selected SFHQ examples. Such attention is compatible with a reliance on source-specific visual cues [12, 17], but Grad-CAM does not identify a causal mechanism or prove that frequency artefacts drive the predictions. The degradation tests provide complementary evidence of sensitivity to image quality. JPEG compression caused smaller performance losses than severe Gaussian noise or blur. Under some degradations, ROC-AUC remained relatively high even as accuracy at the fixed 0.5 threshold declined, a pattern consistent with a shift in the detector’s score distribution. Because the sigmoid output represents the real class, raising the 0.5 decision threshold would label more images as fake while also increasing false alarms. The operating point should be selected for a specified use case and validated on representative data.

Several limitations qualify these findings. The training set contained synthetic faces from a single StyleGAN model, and the external evaluation used only one additional synthetic-face dataset, SFHQ part 4. Although its images originate from a different multi-stage pipeline, this does not test generalisation to pure diffusion outputs. Broader evaluation across generators, data sources and sampling strategies is needed. The shift in real-image sources is also confounded with the shift in the synthetic-image pipeline. The robustness tests cover selected corruptions, but not adversarial perturbations or a wide range of image-processing pipelines. Future work should evaluate multiple independent real-image sources and generative-model families under a common protocol, and test whether training on images from multiple generators improves transfer without reducing performance on the original benchmark. Evaluating video-manipulation datasets such as FaceForensics++ [9] and Celeb-DF [10] would require a separately defined frame-level or video-level task.

7. CONCLUSION

We evaluated an existing ImageNet-pretrained EfficientNet-B0 adapted through two-stage fine-tuning for AI-generated face detection. It achieved 98.03% accuracy and a 0.9984 ROC-AUC on the predefined 20,000-image test split, but these in-distribution results did not carry over to the external set: accuracy was 65.75% and only 35.95% of SFHQ synthetic faces were detected. Joint evaluation of the same frozen model also showed that JPEG compression had a smaller effect than strong noise or blur, while activation

maps for four selected synthetic faces highlighted background and hair or boundary regions. On the external set, the publicly released Wang et al. detector attained a higher ROC-AUC (0.9756) yet detected only 16.30% of synthetic faces at its default threshold. These results characterise both the strengths and the limits of a simple transfer-learning baseline; they do not establish a new detection architecture or a general efficiency advantage over other models. Testing additional independent real-image sources and generator families, along with threshold calibration on representative validation data, is necessary before broader deployment claims can be made.

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