Self-Organizing Maps for Durability Prediction of Fly Ash Geopolymer in Chloride Environment

by

Fong Wen Lee
(21020482)

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DECLARATION

I hereby declare that the work in this thesis was carried out in accordance with the regulations of Universiti Malaysia Sarawak. Except where due acknowledgements have been made, the work is that of the author alone. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.

Signature 

Student Name: Fong Wen Lee

Matric No: 21020482

Date: 30 March 2026

Faculty of Engineering
Universiti Malaysia Sarawak (UNIMAS)

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ABSTRACT

Geopolymer concrete offers a promising alternative to traditional Portland cement concrete, exhibiting comparable mechanical and durability performance, while reducing environmental impacts. However, its mechanical properties and durability depend on many factors such as the water/binder ratio, activator concentration, and curing temperature. This study utilized a Self-Organizing Map (SOM), an unsupervised artificial neural network, to model experimental data to predict the factors controlling geopolymer concrete's durability in chloride environments. The research specifically investigated how variations in the water-to-binder ratio and activator molarity impact performance. The model was trained on data obtained from cylindrical samples that were heat-cured, matured for 28 days, and then tested for chloride migration. This modeling approach effectively highlighted patterns and correlations within the dataset, offering essential insights into the chloride migration behavior that governs geopolymer concrete's durability in chloride environment. A key quantitative finding was the validation of the SOM and GSOM models' reliability, as cross-validation confirmed their high prediction accuracy and their clustering patterns closely corresponded with empirical trends. Based on the analysis of 2,268 data points from 9 different recipes, the study confirms that a mix of 12 M molarity and a 0.5 water-binder ratio offers the highest chloride resistance, providing an optimal recipe for durable geopolymer concrete.

Keywords: Geopolymer concrete, durability, artificial neural network (ANN), self-organizing map (SOM), chloride

Peta Penyusunan Kendiri untuk Ramalan Ketahanan Geopolimer Abu Terbang dalam Persekitaran Klorida

ABSTRAK

Konkrit geopolimer menawarkan alternatif yang menjanjikan kepada konkrit Portland tradisional, dengan menunjukkan prestasi mekanikal dan ketahanan yang setanding, serta mengurangkan kesan alam sekitar. Namun, sifat mekanikal dan ketahanannya bergantung pada banyak faktor seperti nisbah air/pengikat, kepekatan pengaktif, dan suhu pengawetan. Kajian ini menggunakan Peta Penyususan Kendiri (SOM), sejenis Rangkaian Neural Buatan (ANN) tanpa penyeliaan, untuk memodelkan data eksperimen bagi meramal faktor yang mengawal ketahanan konkrit geopolimer dalam persekitaran klorida. Penyelidikan ini khusus menyiasat bagaimana variasi dalam nisbah air-kepada-pengikat dan kemolaran pengaktif mempengaruhi prestasi. Model tersebut telah dilatih menggunakan data yang diperoleh daripada sampel silinder yang diawet haba, dimatangkan selama 28 hari, dan kemudian diuji untuk migrasi klorida. Pendekatan pemodelan ini berjaya menonjolkan corak dan korelasi dalam set data, sekaligus memberikan pemahaman penting tentang tingkah laku migrasi klorida yang mengawal ketahanan konkrit geopolimer dalam persekitaran klorida. Satu penemuan kuantitatif utama ialah pengesahan kebolehpercayaan model SOM dan GSOM, di mana pengesahan-silang mengesahkan ketepatan ramalan yang tinggi dan corak pengelompokannya sejajar dengan tren empirikal. Berasaskan analisis terhadap 2,268 titik data daripada 9 resipi berbeza, kajian mengesahkan bahawa campuran dengan kemolaran 12 M dan nisbah air-pengikat 0.5 menawarkan rintangan klorida tertinggi, sekaligus menyediakan resipi optimum untuk konkrit geopolimer yang tahan lama.

Kata Kunci: Konkrit geopolimer, ketahanan, artificial neural network (ANN), self-organizing map (SOM), klorida

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LIST OF ABBREVIATIONS

CGS	Centre for Graduate Studies
UNIMAS	Universiti Malaysia Sarawak
GPC	Geopolymer Concrete
OPC	Ordinary Portland Cement
GGBS	Ground Granulated Blast Furnace Slag
NaOH	Sodium Hydroxide
Na_2SiO_3	Sodium Silicate
MPCMs	Microencapsulated Phase Change Materials
GPM	Geopolymer Mortars
RGAs	Recycled Geopolymer Aggregates
GRAC	Geopolymer Recycled Aggregate Concrete
GSOM	Growing Self-Organizing Map
PFs	Geopolymer Formworks
3DPGPC	3D-Printed Geopolymer Concrete
SGPC-M	Slag-based Geopolymer Concrete
SEM	Scanning Electron Microscopy
XRD	X-ray Diffraction analysis
SCMs	Supplementary Cementitious Materials
SOM	Self-Organizing Map
PFA	Pulverized Fuel Ash
FEA	Finite Element Analysis
FDM	Finite Difference Methods
ML	Machine Learning

CHAPTER 1:

INTRODUCTION

1.1 Background of Study

Ordinary Portland cement (OPC), which is frequently used in building, contributes around 7% of CO_2 emissions. To counteract this, environmentally acceptable cement replacements, including fly ash, ground granulated blast furnace slag (GGBS), and metakaolin, have been investigated. The adoption of these alternatives could significantly reduce the CO_2 emissions associated with construction activities.

Geopolymer binders are cement alternatives synthesized from aluminosilicate materials like fly ash or slag using alkaline activators such as sodium hydroxide. This results in a concrete with advantages over conventional Portland cement, including increased strength, decreased permeability, and improved durability (Chen et al., 2021; Zhang et al., 2021).

One of the most important factors influencing concrete durability is its resistance to chloride ion penetration, which can cause corrosion of reinforcement bars and, ultimately, structural failure. Consequently, the assessment of the durability of geopolymer concrete in chloride-rich environments represents a significant area of research (Pasupathy et al., 2021; Turner et al., 2013).

Testing chloride migration durability is more time-consuming than measuring compressive strength. To address this, our research adopts machine learning tools to accelerate the process, the accuracy of which will be evaluated and discussed. Machine learning is a powerful tool for developing predictive models for complex systems such as concrete durability. It is possible to identify patterns and relationships that can be used to predict the behavior of new materials under different conditions by training a model on an extensive set of experimental data (Melchers et al., 2020; Alzeebaree et al., 2023).

It is essential to compile a comprehensive dataset of experimental results obtained from multiple sources to develop a machine learning algorithm capable of predicting the durability of geopolymer concrete in chloride-rich environments. This dataset should include information on the composition of the concrete, preparation technique, testing conditions, and results of chloride ion penetration tests (Wong et al., 2022; Idir et al., 2011).

Following the collection of the dataset, a variety of machine-learning algorithms can be used to create predictive models. These include decision trees, self-organizing maps (SOM), support vector machines (SVM), and artificial neural networks (ANN). The accuracy of each model can be measured statistically using measures, such as the mean squared error or coefficient of determination, and the best-performing models can be used to forecast new materials (Farahzadi et al., 2023; Huynh et al., 2020).

The development of a machine learning model aimed at predicting the durability of geopolymer concrete in chloride-rich environments has a significant impact on the construction industry. This could help improve the safety and chloride durability of concrete structures in the future by providing engineers and designers with a more accurate understanding of the behavior of these materials (Nagajothi et al., 2022).

1.2 Problem Statements

Geopolymer concrete is a novel construction material that employs industrial by-produces or recyclables rich in silica and alumina as a substitute for traditional Portland cement. The geopolymerization method involves the interaction of the source materials with an alkaline activator solution to create a durable three-dimensional network of interconnected polymeric chains. This unique chemistry not only reduces the environmental footprint, but also offers geopolymer concrete remarkable attributes, including exceptional fire resistance (Venkatesan et al., 2024), rapid early strength development (Amran et al., 2021), and formidable resistance to chemical aggression (Shill et al., 2020; Nanthini et al., 2024).

Chloride diffusion in concrete is a crucial process that influences the durability and lifespan of reinforced concrete structures, especially in marine environments or regions exposed to de-icing salts. The infiltration of chloride ions into concrete can result in the corrosion of steel reinforcement, leading to structural degradation. Key factors affecting

chloride diffusion in concrete include concrete composition. The type of cement, water-to-cement ratio, and the use of supplementary cementitious materials can significantly impact chloride penetration. The lack of precise and reliable models for predicting chloride permeability in geopolymer concrete presents a significant challenge to the development of environmentally friendly materials.

Unlike traditional Portland cement concrete, which has been extensively studied and modelled for decades, geopolymer concrete is a relatively new material with complex chemical interactions that are not yet fully understood. This lack of understanding impedes the proper prediction of chloride ion penetration and its impact on the long-term durability of geopolymer concrete structures.

Therefore, one solution to encourage confidence in the use of geopolymers is the development of reliable predictive models. This effort requires extensive research and data collection over extended time periods. Hence, this study aimed to use a machine learning technique to predict the chloride permeability durability of geopolymer concrete. This thesis employs machine-learning techniques, specifically artificial neural networks, to create predictive models with extensive datasets.

1.3 Study Objective

The main objectives of this thesis are,

a) To assess the fly ash geopolymer durability in chloride environment as a function of water/binder ratio and the concentration of the alkali activator.

b) To adopt an artificial neural network (ANN) to predict the durability of geopolymers in chloride environments.

In order to achieve these goals, this study sought to increase knowledge about geopolymer concrete (GPC), optimize its properties, and promote its adoption as a sustainable and viable alternative to conventional OPC in the construction sector.

1.4 Chapter Summary

This chapter establishes the environmental impetus for the research, highlighting that ordinary Portland cement (OPC) is a major contributor to global CO_2 emissions. As a sustainable alternative, geopolymer concrete synthesized from industrial by-products like fly ash using alkaline activators is introduced. This material not only reduces the carbon footprint but also exhibits superior properties, including enhanced strength and durability.

The main challenge is the absence of precise models to predict the resistance of geopolymer concrete against chloride assaults. This study uses machine learning (ML) to address the issue. An Artificial Neural Network (ANN) will be used to develop a prediction model after the study examines the effects of activator concentration and water-to-binder ratio on chloride resistance. Optimizing geopolymer concrete and making it a reliable, sustainable alternative to conventional cement is the ultimate objective.

CHAPTER 2:

LITERATURE REVIEWS

2.1 Overview of Geopolymers

In recent decades, geopolymers, a novel class of inorganic polymers, have attracted considerable interest owing to their exceptional mechanical qualities, environmental advantages, and promise as sustainable substitutes for ordinary Portland cement (OPC). Geopolymers are generally produced via the alkaline activation of aluminosilicate precursors, including fly ash, metakaolin, or slag, and display a three-dimensional amorphous to semi-crystalline structure. Their distinctive chemical compositions and bonding provide exceptional compressive strength, thermal stability, and resistance to chemical assaults, rendering them suitable for many applications in construction, waste encapsulation, and fire-resistant materials (Tekin et al., 2020; Shi et al., 2023).

Geopolymer concrete (GPC) has been developed as a viable sustainable alternative to conventional Portland cement-based concretes. Primarily composed of industrial wastes such as fly ash, metakaolin, and slag activated by alkaline solutions, GPC presents numerous advantages, including lower carbon emissions, repurposing of waste materials, and improved performance in adverse situations. Its distinctive attributes, including its elevated mechanical strength, chloride durability, thermal stability, and minimal shrinkage, render it highly appropriate for use in infrastructure, precast components, and industrial structures (He et al., 2023; Mayhoub et al., 2021).

However, the extensive implementation of geopolymer concrete encounters numerous obstacles. This encompasses the necessity for standardized testing techniques, variability in raw material quality, and issues related to the management of alkaline activators. Therefore, it is crucial to conduct further research to explore optimize mix formulations, and enhance the properties of geopolymer concrete to unlock the full potential of geopolymer concrete and advancing its use in sustainable construction.

2.1.1 Definition and Composition of Geopolymers

Geopolymers are inorganic polymeric substances created by chemical reactions between aluminosilicate precursors and alkaline activators, leading to a three-dimensional network of Si-O-Al links. This network is defined by its amorphous to semicrystalline structure, which differentiates geopolymers from conventional crystalline ceramics and organic polymers. The term "geopolymer" was introduced by Davidovits in the 1970s to characterize alkali-activated polymers that possess qualities similar to natural rock-forming minerals (Davidovits et al., 2020).

Alumino silicate precursors, which are rich in silicon (Si) and aluminium (Al) and made from materials like fly ash, metakaolin, slag, and natural pozzolans, are essential components of geopolymers. Fly ash is especially characterized for its high silica and alumina content. These precursors are dissolved and polymerisation is started using alkaline activators, such as solutions of silicates (e.g., sodium silicate) or alkali hydroxides (e.g., NaOH and KOH), which have a major impact on the mechanical and chemical characteristics of the final geopolymer. During geopolymerization, water serves as a solvent for ion dissolution and transport; however, too much water can degrade the material's strength and microstructure. The geopolymerization process involves dissolving aluminosilicate precursors in a highly alkaline medium, forming oligomers that undergo polycondensation into a solid gel, which eventually hardens into a durable polymer with excellent mechanical strength, thermal stability, and chemical resistance (Duxson et al., 2007; Ismail et al., 2014;Klima et al., 2022). The chemical structure of a geopolymer is described by the following general formula:

$$M_n\,[-(SiO_2)_z\text{-}AlO_2)]_n \cdot wH_2O \qquad \text{Equation 2.1}$$

Where M represents alkali cations (e.g., Na^+ and K^+), z is the Si/Al ratio, and w is the water content. For the n, a measure of the molecular weight and the chain length of the geopolymer.

Geopolymers are frequently characterized as "sustainable materials" owing to their reduced carbon emissions in comparison to conventional cement. Their manufacture releases up to 80% less CO_2 and incorporates industrial wastes, such as fly ash, promotes sustainable construction methods (Asim et al., 2024; Wijesekara et al., 2025). The distinctive

amalgamation of environmental and performance characteristics renders geopolymers viable substitutes for traditional building materials.

2.1.2 Advantages of Geopolymers over Ordinary Portland Concrete

Considering its improved performance in a number of areas and ability to handle important environmental issues, GPC has become a viable substitute for OPC. Using slag or fly ash, two industrial by-products, as the main binders, GPC exhibits important environmental benefits over OPC, which depends on energy-intensive clinker production. This can result in a carbon footprint reduction of up to 80% (Manzoor et al., 2023; Golafshani et al., 2024).

Compared to OPC, which clinkers at 1450°C, the manufacturing process for geopolymer concrete needs much lower temperatures (ambient to 80°C), resulting in considerable energy savings of 60–70%. In mechanical terms, GPC maintains greater dimensional stability with less drying shrinkage while demonstrating equivalent or superior compressive strength (35–100 MPa), increased flexural strength (10–15% higher), and improved bond strength with reinforcement (Turner et al., 2013; Jamal et al., 2025; Asadi et al., 2022).

An estimated 8% of global CO_2 emissions are caused by the manufacture of cement alone, making the building sector a pivotal point in the global fight to combat climate change (Thomas et al., 2022; Cong et al., 2021). The need for environmentally friendly building materials has increased as countries work to satisfy the Paris Agreement's strict carbon reduction goals. GPC is one of the most promising substitutes. It is a novel material that offers significant environmental benefits in addition to comparable structural performance to conventional OPC concrete. These advantages which place GPC at the forefront of the shift to green construction include significantly fewer carbon emissions, lower energy use, efficient waste management, and increased chloride durability performance.

The fundamental difference in the chemistry of geopolymer concrete is the first factor contributing to its exceptional environmental qualities. In contrast to OPC, which uses the energy-intensive calcination of limestone to produce clinker, geopolymers are made from industrial wastes including fly ash, slag, and metakaolin. With 0.9–1.2 kg of CO_2 released per kilogram of cement, the manufacture of clinker alone is responsible for over 90% of

OPC's carbon footprint, making this distinction crucial (Aygörmez et al., 2023). With 0.53 kg of CO_2 added for every kilogram of clinker, the calcination process, which converts limestone ($CaCO_3$) into lime (CaO) and CO_2, is intrinsically carbon-intensive (Huntzinger et al., 2009; Shobeiri et al., 2021). Furthermore, an additional 0.35 to 0.45 kg of CO_2 are added per kilogram of cement due to the burning of fossil fuels needed to keep cement kilns operating at 1400–1500°C (Hasanbeigi et al., 2012; Asadi et al., 2022).

In contrast, geopolymer concrete uses alkali activation to polymerise industrial waste materials at room temperature or slightly higher temperatures (60–80°C), doing away with the requirement for clinker completely. In comparison to OPC, this method uses 60–80% less thermal energy and emits just 0.15–0.25 kg of CO_2 per kg of binder (Chen et al., 2021). According to studies by Chen et al. (2021)., GPC is one of the best methods for decarbonising the construction industry and its broad implementation might reduce gigatons of CO_2 emissions yearly.

GPC offers stronger tensile and bending strength in addition to compressive strength because of its denser microstructure and larger interfacial transition zone (ITZ) between particles and binder. In contrast to OPC, geopolymer matrices have smaller pore structures and reduced porosity, which improves the bond strength with reinforcing steel, an important consideration for structural applications. According to Chokkalingam et al. (2022), GPC concrete has a greater elastic modulus than OPC concrete of the same strength grade, which is usually 10–30% higher. This results in better stiffness under load (Chokkalingam et al., 2022).

The superior durability of GPC distinguishes it from conventional concrete. Unlike OPC, which contains calcium hydroxide ($Ca(OH)_2$), a phase highly susceptible to corrosive chemicals. GPC exhibits exceptional resistance to sulfates, chlorides, and acids (Noushini et al., 2018). This makes it particularly suitable for demanding environments such as industrial flooring, wastewater treatment facilities, and marine construction. Additionally, while OPC concrete suffers significant strength loss at temperatures above 400°C, GPC retains 70–80% of its compressive strength even when exposed to 800–1200°C. Its ceramic-like structure prevents the explosive spalling typical of OPC at high temperatures, further enhancing its thermal durability (Thomas et al., 2022; Kong et al., 2010).

In harsh conditions, GPC performs noticeably better than conventional OPC concrete due to its exceptional resistance to chemical deterioration (Fu et al., 2021; Hassan et al., 2019). Its exceptional performance results from its distinct aluminosilicate polymer structure, which is free of the chemically attackable calcium silicate hydrate (C-S-H) and portlandite ($Ca(OH)_2$) phases found in OPC. OPC expands and cracks as a result of gypsum crystallisation and damaging ettringite production brought on by sulfate exposure. In sulfate-rich settings, GPC retains its structural integrity. Study shows that after a year in a 5% Na_2SO_4 solution, it expands by less than 0.5%, while OPC expands by 3-5%. GPC is ideal as sulphate attack frequently occurs in sewage systems, chemical storage facilities, and marine structures (Shiju et al., 2019).

Chloride diffusion coefficients are 5–10 times lower in GPC than in OPC due of its dense microstructure (Geise et al., 2013). According to electrochemical studies conducted in simulated maritime conditions, this significantly slows the corrosion of steel reinforcement, extending corrosion onset periods by 300–400% (Qin et al., 2024). While OPC usually surpasses critical levels (0.4% by mass) after 5 years, field tests of GPC in tidal zones show little chloride penetration (0.05% by mass) during 10-year exposure (Noushini et al., 2020).

According to Wang et al. (2020), GPC exhibits 150–200% greater freeze-thaw endurance than OPC. Its mesoporous structure (pore size 2-50 nm) lowers internal cracking pressures by enabling regulated water absorption and ejection. After 300 cycles, accelerated weathering tests (ASTM D4792) reveal a strength loss of less than 5%, whereas OPC shows a loss of 20–30%.

GPC is now at the forefront of sustainable building solutions due to the environmental requirement to decarbonise the construction sector. OPC which contributes to over 8% of global CO_2 emissions, has a startling environmental effect that requires immediate attention as the world struggles with the global warning crisis (Farahzadi et al., 2023). GPC represents a transformative advancement in sustainable construction, offering the potential to fundamentally mitigate the environmental footprint of the building industry. This thesis offers a thorough analysis of GPC's environmental sustainability, examining how it could be able to solve three important aspects: better lifetime sustainability, industrial waste valorisation, and radical carbon footprint reduction.

GPC's long-term environmental advantages go much beyond its manufacturing stage. The material's intrinsic resilience leads to service lifetimes that frequently double or treble that of OPC structures, especially in harsh situations like maritime settings or chemical exposure conditions (Albitar et al., 2017). This durability in chloride has a beneficial knock-on impact on the environment by reducing the frequency of reconstructions and the associated material usage. For example, GPC's ability to withstand chloride penetration in marine conditions keeps its structural integrity for decades longer than OPC, significantly reducing the environmental effect of coastal infrastructure during its duration (Noushini et al., 2018). GPC is positioned as a key technology for sustainable building in the twenty-first century because of its longer service life and possibility for genuine closed-loop recycling at end-of-life.

Although GPC has a strong environmental justification, there are a number of obstacles to its wider implementation, which this thesis thoroughly explores. These include regulatory gaps that now favour conventional concrete, economic difficulties in competing with existing OPC supply chains, and technological obstacles pertaining to standardisation and scale. Nevertheless, new approaches like carbon-negative formulations, activators made from biomass, and 3D printing applications show how quickly innovation is taking place in this area. Furthermore, favourable conditions for the implementation of GPC are being created by changing policy landscapes, such as carbon pricing systems and green procurement requirements.

Ultimately, this thesis provides a comprehensive framework for understanding GPC's role in building materials by systematically examining its properties, economic implications, and lifecycle characteristics. The findings offer important insights for legislators, industry professionals, and researchers evaluating GPC as a construction material. The analysis positions GPC as a notable option for infrastructure development based on its technical and practical merits.

2.2 Fly Ash as raw material for geopolymer

Fly ash, a by-product generated from coal combustion in thermal power plants, has become a popular choice of raw material for geopolymer synthesis owing to its accessibility, cost-effectiveness, and favourable chemical composition. Fly ash, predominantly consisting of silica (SiO_2) and alumina (Al_2O_3), functions as an ideal aluminosilicate precursor for the

geopolymerization process, which underlies geopolymer materials (Javed et al., 2022). Its application not only alleviates environmental concerns associated with disposal but also fosters the advancement of sustainable construction materials.

Fly ash particles are predominantly spherical, with diameters ranging from 2 to 14 μm, and are generally finer than Portland cement (Nizar et al., 2007). This quality improves its pozzolanic reactivity, which is an essential characteristic that enables fly ash to chemically interact with alkaline activators at ambient temperatures to produce cement-free concrete (de Oliveira et al., 2022). Fly ash is categorized into two types according to its chemical composition: Class F (low-calcium fly ash with less than 10% CaO) and Class C (high-calcium fly ash). Class F fly ash, characterized by elevated silica and alumina levels, is especially favored for geopolymer synthesis owing to its capacity to create a strong aluminosilicate network (Venkatesan et al., 2024; Owino et al., 2023).

The features of fly ash can be classified into physical and chemical characteristics. The spherical morphology enhances the workability and fluidity of new geopolymer mixes, decreases water requirements, and mitigates problems such as plastic shrinkage and breaking (Temuujin et al., 2009). Fly ash possesses pozzolanic characteristics, allowing it to be combined with alkaline solutions to produce robust and stable geopolymer binders. This reaction is expedited by alkaline activators, including sodium hydroxide or sodium silicate, which are crucial for geopolymerization.

The mineralogical and chemical characteristics of fly ash are significantly influenced by the coal source and the combustion process. Fly ash predominantly comprises non-crystalline (amorphous) glassy particles along with a minor proportion of crystalline substances generated during the rapid cooling of coal combustion residues (Temuujin et al., 2009). The heterogeneity in the composition highlights the necessity of choosing suitable fly ash sources for geopolymer synthesis to guarantee consistent performance.

Incorporating fly ash into geopolymers enables the construction sector to utilize its small shrinkage, reduced carbon emissions, and resistance to acid and sulfate attacks, thereby enhancing the chloride durability of concrete structures. Moreover, the utilization of fly ash adheres to the tenets of a circular economy, converting industrial waste into valuable construction materials, and fostering sustainable development.

In conclusion, fly ash is a multifaceted and ecologically advantageous precursor for geopolymer synthesis. Its distinctive physical and chemical characteristics, along with its ability to minimize waste and carbon emissions, make it an essential element in the advancement of resilient and sustainable construction materials.

2.3 Mechanism of geopolymerization

In the process of geopolymerization, aluminosilicate oxides react chemically with a solution of alkali metal silicate under extremely alkaline environments to create the linkage of Si–O–Al, forming 3-D polymers which can be amorphous to semi-crystalline in nature (Ng et al., 2016). The exothermic reaction of geopolymerization developed below atmospheric pressure and below 100 °C (Davidovits et al., 2020).

Synthetic polymers are constructed by the coordinated binding of silicon, aluminum, and free oxygen ions. Davidovits used the 'sialate' terminology to define aluminosilicate compounds, designating Si-O-Al bonds as sialate bonds and Si-O-Si links as siloxo bonds (Giacobello et al., 2022; Matsimbe et al., 2022).

Aluminosilicate precursors, like fly ash or slag, must dissolve in a strongly alkaline medium as the initial stage in the geopolymerization process. The glassy phases of these raw materials decompose at high pH levels (usually using NaOH, KOH, or sodium silicate solutions), releasing reactive silicate (Si^{4+}) and aluminate (Al^{3+}) species into the solution. Silicic acid ($Si(OH)_4$) and aluminate ions ($Al(OH)_4^-$) are formed when the alkali hydroxide (OH^-) ions attack the Si-O-Si and Si-O-Al bonds in the amorphous structure of fly ash or slag. This dissolving phase is important because it supplies the monomers required for the subsequent polycondensation reactions that create the geopolymer's distinctive three-dimensional aluminosilicate network. A number of variables affect the dissolution kinetics and overall production of the geopolymer, including temperature, alkali content, and the inherent reactivity of the precursor. It is a crucial step in the synthesis process because without it, the geopolymer gel network cannot form (Yang et al., 2023).

In the second stage of geopolymerization, known as polycondensation, a first aluminosilicate gel network is formed by the reaction of dissolved silicate ($Si(OH)_4$) and aluminate ($Al(OH)_4^-$) species. The backbone of the geopolymer structure is formed by Si–O–Al bonds, which are formed when Si–OH and Al–OH groups condense, releasing water

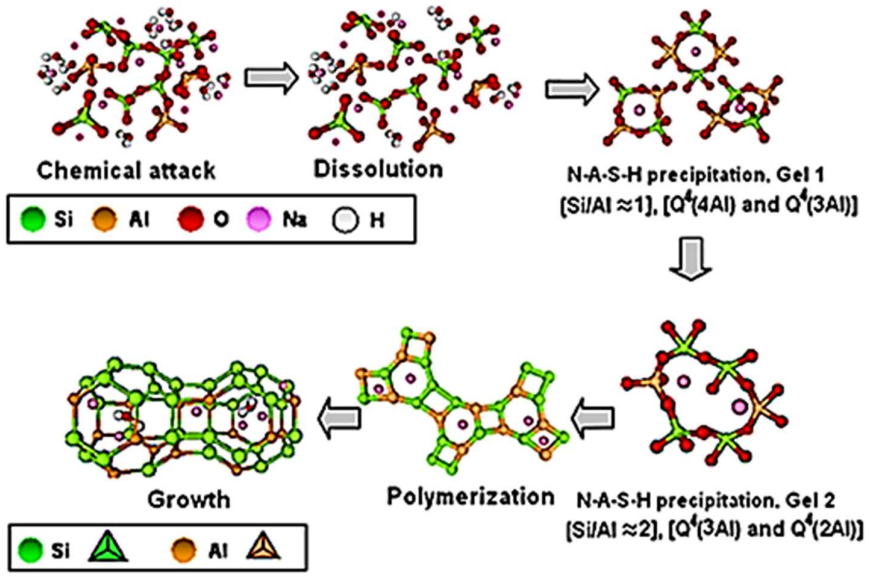
(H_2O) as a byproduct (Tanyildizi et al., 2021; Amran et al., 2021). Short-chain oligomers make up the resultant gel, which is usually chaotic and progressively connects to create a three-dimensional structure. An N-A-S-H gel (sodium aluminosilicate hydrate), which is the main result of sodium-based systems (with fly ash as the precursor), is distinguished by a strongly crosslinked aluminosilicate network with charge-balancing Na^+ ions. comparable to a modified C-A-S-H gel (calcium aluminosilicate hydrate), which is present in standard cement but has a higher degree of Al substitution in the silicate chains, the gel structure in calcium-rich systems (such slag-based geopolymers) is comparable. The gel remains weakly linked at this point and keeps reorganising and becomes stronger over time as a result of more polymerisation and densification. The final geopolymer material's mechanical characteristics and durability are ultimately influenced by the pace and degree of polycondensation, which is dependent on variables like the alkali content, curing temperature, and Si/Al ratio, as illustrated in Table 2-1.

Re-polymerization is the third and last stage of geopolymerization, during which the aluminosilicate gel that was first created develops and stabilises into a stronger, longer-lasting network. Heat or moisture curing frequently speeds up this step, which is characterised by the progressive change of the loosely attached gel into a denser, more crosslinked structure (Duxson et al., 2007; Shi, et al., 2011). The weakly bound Si–O–Al connections are rearranged to create a three-dimensional structure that is strongly linked and has improved Si–O–Al–O–Si connectivity. The alkaline environment causes the residual unreacted particles from the precursor material to dissolve further, releasing more silicate and aluminate species that combine with the expanding matrix to increase its homogeneity and mechanical strength. Concurrently, the gel experiences structural reorganisation, changing from a disorganised configuration to a more compact and ordered one, which lowers faults and improves performance, as per Figure 2-1. A refined microstructure with reduced permeability and increased durability is produced when the gel densifies, filling micropores and reducing microcracks. The final strength, stability, and resistance to environmental deterioration ofalanf the geopolymer are determined by the alkali activator concentration, precursor composition, and curing conditions, which include temperature, humidity, and time.

Table 2-1: Processes involved in geopolymerization (Wong et al., 2022)

Process in geopolymerization	Description
1. Dissolution	Dissolution of aluminosilicate atoms from solid precursor in an alkaline condition.
2. Rearrangement	Rearrangement and exchanging of dissolved ions between species from aluminosilicate source and activator solution.
3. Gel nucleation	Rearrangement and exchange led to the development of two types of gels: calcium aluminate silicate hydrate (C-A-S-H) from high-calcium precursors (1) and sodium aluminate silicate hydrated (N-A-S-H) from low-calcium precursors (2).
4.Polycondensation	The monomer gels combine to form polymers through the process of polycondensation. The polymer gel then solidifies, hardens and develops strength.

Figure 2-1: Conceptual paradigm of geopolymerization (Shi, et al., 2011)



2.3.1 Factors Influencing the Geopolymerization Process

Numerous factors affect the formation of oligomers, dissolution of aluminosilicate precursors, and final characteristics of the geopolymer during the geopolymerization process. Understanding these elements is essential for refining the synthesis procedure and customizing the geopolymer for specific uses. The following are the main variables affecting geopolymerization:

The chemical makeup of the precursor material, namely the ratio of silica (SiO_2) to alumina (AlO_3), has a significant impact on the geopolymerization process. For the geopolymer network to build steadily and sustainably, an ideal Si/Al ratio, usually between 2 and 4, is essential (Javed et al., 2022; Kim et al., 2023). Changes from this range may cause polymerisation to break down, resulting in uneven gel formation and weakened structural integrity. Additionally, by encouraging the production of calcium silicate hydrate (C-S-H) phases in addition to the main aluminosilicate geopolymer matrix, the inclusion of calcium in precursors like Class C fly ash adds even more complexity (Kim et al., 2023). Kim et al. (2023) points out that this dual-phase system can drastically change the mechanical characteristics and long-term durability of the final geopolymer, hence careful precursor chemistry optimisation is required for the intended performance.

Precursor dissolution processes and polymerisation behaviour are strongly impacted by the choice and concentration of alkaline activators, which are crucial in controlling the geopolymerization process. The chemical route and gel formation kinetics are determined by the activator selection, which can be sodium hydroxide (NaOH), potassium hydroxide (KOH), or sodium silicate (Na_2SiO_3). Sodium silicate, for example, improves polymerisation efficiency by providing more soluble silicate monomers, encouraging polycondensation and fortifying the aluminosilicate network (Haq et al., 2016; Valencia et al., 2023). The activator concentration, which establishes the alkalinity (pH) of the reaction environment, is equally important. High concentrations can accelerate dissolution rates and geopolymerization, but they can also induce excessive shrinkage and microcracking due to the rapid gel formation and water ejection (Mayhoub et al., 2021).

The curing temperature has a significant impact on the geopolymerization process; higher temperatures (usually between 60°C and 90°C) speed up the reaction rate and encourage faster strength growth. On the other hand, extreme heat can cause water to evaporate quickly, which can cause microcracking and weaken the structure (Danish et al., 2024). In order to avoid early moisture loss and guarantee full geopolymerization, it is also essential to maintain an appropriate humidity level during curing. Due to insufficient chemical bonding, low humidity levels might impede the reaction process and result in less-than-ideal mechanical qualities (Shamsah et al., 2025; Lekshmi et al., 2022). Thus, attaining desired geopolymer performance requires optimising both temperature and humidity levels.

The workability and microstructural properties of geopolymer composites are significantly influenced by the water-to-solid ratio. Since it directly affects the dissolution of aluminosilicate precursors and the ensuing polycondensation processes that control the production of geopolymers, striking an ideal balance in this ratio is crucial. A lack of water may interfere with the alkali activation process, resulting in poor polymerisation and partial raw material dissolution, which would impair mechanical performance. On the other hand, too much water might cause more porosity as a result of water evaporating during curing, which would weaken the geopolymer matrix and lower its compressive strength (Khalil et al., 2020). In order to provide sufficient workability for processing while preserving the intended structural integrity and mechanical qualities of the finished geopolymer product, careful optimisation of the water-to-solid ratio is required (Abdellatief et al., 2023).

Given that it directly controls the aluminosilicate source's reactivity and dissolution kinetics, the precursor materials' particle size distribution has a big impact on the geopolymerization process. Finer particles facilitate more effective geopolymer gel formation by increasing the dissolving rate in alkaline solutions because of their higher specific surface area (Hajimohammadi et al., 2017; Bernal et al., 2014). A greater degree of polycondensation is encouraged by this rapid dissolution, which improves the cured geopolymer's mechanical qualities. More homogenous and comprehensive geopolymerization is also made possible by an increased interfacial contact area between the precursor particles and the alkaline activator solution. Finely ground materials' increased surface reactivity guarantees improved ion exchange and gel network formation, which eventually produces a denser and more resilient geopolymer matrix. Nevertheless, very tiny particles can also cause problems like higher water requirements or quick setting, therefore careful particle size distribution optimisation is required for best results.

Although it guarantees the even distribution of the precursor material and alkaline activator, the completeness of mixing has a significant impact on the homogeneity of the geopolymer matrix. Inconsistent geopolymerization and heterogeneous microstructural development might arise from localised differences in chemical composition caused by inadequate mixing intensity or duration. Weak interfacial zones, decreased mechanical strength, or variable shrinking behaviour are some examples of this non-uniformity. In order to create a well-dispersed system that facilitates the thorough dissolution of aluminosilicate precursors and subsequent polycondensation into a durable geopolymer network, it is

necessary to carefully select the optimal mixing parameters. The ultimate density and pore structure of geopolymer composites are largely determined by the molding and compaction procedures. A denser and more structurally sound material results from proper compaction, which also lowers overall porosity, improves particle packing, and minimises trapped air gaps. According to research by Lyu et al., insufficient compaction causes increased porosity and weakened interfacial bonding, which have an adverse impact on durability and compressive strength (Lyu et al., 2022). On the other hand, the best compaction pressure guarantees better particle-to-particle contact, which strengthens the development of the geopolymer gel and creates a more uniform microstructure. The structural integrity of the final product is further enhanced by the use of appropriate moulding techniques, such as vibration-assisted casting or uniaxial pressing, which decrease defects and increase dimensional stability.

The speed of reaction and ultimate characteristics of geopolymer composites can be greatly impacted by the addition of additional aluminosilicate components, such as metakaolin or ground granulated blast furnace slag (GGBFS). In addition to providing more reactive silica and alumina sources, these mineral additions also aid in the creation of secondary reaction products that promote microstructural growth within the geopolymer matrix. While slag addition can increase mechanical strength and durability by forming calcium aluminosilicate hydrate (C-A-S-H) phases alongside the primary sodium aluminosilicate hydrate (N-A-S-H) gel, metakaolin's high pozzolanic reactivity helps create a more homogeneous geopolymer gel (Duxson et al., 2007; Bayrak et al., 2023). These additives' combined actions frequently lead to increased resistance to chemical attack, decreased shrinkage, and improved thermal stability, making them useful ingredients in specially designed geopolymer formulations for certain technical uses.

In conclusion, the water-to-binder ratio and the kind of alkaline activator employed are the primary determinants of the characteristics of geopolymer concrete. In order to ensure appropriate chemical interactions without producing a weak, porous structure, the water-to-binder ratio needs to be properly controlled. At the same time, the strength of the final geopolymer network and the rate of the chemical reaction are directly controlled by the activator selection (e.g., sodium hydroxide or sodium silicate).

2.4 Durability of Fly Ash Geopolymers

The superior mechanical qualities and environmental advantages of fly ash geopolymers make them viable substitutes for conventional Portland cement. A strong cementitious binder is produced by alkaline-activating fly ash, a byproduct of burning coal. One of the main benefits of fly ash geopolymers is their durability, they are more resistant to chemical attacks, such as exposure to sulfate and acid, and are less prone to alkali-silica interactions than regular concrete. Furthermore, they function better over the long-term under challenging conditions owing to their strong thermal stability and low permeability. To maximize their effectiveness for broad use, more studies are required, because variables such as fly ash content, curing conditions, and mix design might affect durability (Mehta et al., 2017; Mustafa et al., 2011).

2.4.1 Durability Characteristics of Geopolymers in Chloride

Due to a naturally thick and low-permeability microstructure, geopolymers are more resistant to chloride penetration than traditional cementitious materials. Chloride ion diffusion is hindered by the tortuous pathway created by the three-dimensional aluminosilicate network structure of geopolymers; reported chloride diffusion coefficients are usually an order of magnitude lower than those found in regular Portland cement (Zofia et al., 2013; Noushini et al., 2015; Chen et al., 2024). This feature is especially helpful for transportation components, coastal infrastructure, and marine constructions exposed to de-icing salts, where corrosion caused by chloride poses a serious durability risk. The ability of geopolymers to bind chloride enhances their protective qualities since the aluminosilicate matrix may chemically deactivate chloride ions through ionic interactions within its framework structure. Furthermore, even in cases when there is little chloride penetration, the pore solution chemistry of geopolymers, which is distinguished by strong alkalinity (pH usually >13), preserves a passive layer on embedded steel reinforcement, offering intrinsic corrosion protection.

The geopolymer matrix does more than just physically prevent chloride intrusion; it also produces an electrochemical environment that effectively passivates steel surfaces (Gunasekara et al., 2019). A stable iron oxide passive layer is encouraged by the high pH pore solution (Equation 3), and the cathodic reaction rate is constrained by the thick geopolymer matrix's decreased oxygen permeability (Equation 5). Additionally, other

chloride-binding processes from the typical Friedel's salt production in cement systems may be made possible by the special chemistry of geopolymers, which might provide more stable long-term chloride immobilisation (He et al., 2023; Feng et al., 2024). According to recent research, steel reinforcing in geopolymer concrete greatly increases service life in harsh settings by maintaining passivity at chloride threshold values that are two to three times greater than those seen in conventional concrete. Optimising the geopolymer formulation, especially by regulating the alkali activator composition and adding additional cementitious materials with particular chemical properties to customise the pore solution chemistry and microstructure for optimal durability, can further improve the corrosion protection performance.

Anodic Reaction (Iron Dissolution):

$$Fe \rightarrow Fe^{2+} + 2e^{-} \qquad \text{Equation 2.2}$$

Oxidation to Fe^{3+} and Passive Layer Formation:

$$2Fe^{2+} + 3H_2O \rightarrow Fe_2O_3 + 6H^{+} + 2e^{-} \qquad \text{Equation 2.3}$$

Or

$$3Fe^{2+} + 4H_2O \rightarrow Fe_3O_4 + 8H^{+} + 2e^{-} \qquad \text{Equation 2.4}$$

Cathodic Reaction (Oxygen Reduction):

$$O_2 + 2H_2O + 4e^{-} \rightarrow 4OH^{-} \qquad \text{Equation 2.5}$$

Chloride attacks represent a critical durability issue for concrete and geopolymer structures, especially in marine environments or regions utilizing de-icing salts. Chlorides can infiltrate the material, resulting in the corrosion of the embedded steel reinforcement and subsequent structural degradation. The mechanisms of chloride attack vary between conventional concrete and geopolymers, which is attributed to their different chemical compositions and microstructures.

Chloride ingress occurs when chloride ions penetrate concrete through its porous structure, which is facilitated by diffusion, capillary action, or permeation. The ingress rate

is influenced by variables such as the water-to-cement ratio, curing conditions, and existence of cracks (Mehta et al., 2017).

One of the major issues with durability of concrete is the corrosion of embedded steel reinforcement, especially in situations with high levels of chloride, including underwater applications or areas that use de-icing salts. When chloride ions enter the concrete matrix and break down the passive oxide layer (FeO_3/FeO_4) that protects steel surfaces in alkaline environments, this degradation mechanism starts (Broomfield et al., 2004). Through an electrochemical mechanism, the corrosion process produces expansive corrosion products that usually fill 2–6 times the volume of the original steel. Anodic iron dissolution ($Fe \rightarrow Fe^{2+} + 2e^-$) interacts with cathodic oxygen reduction ($O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$) (Bertolini et al., 2013). Through a positive feedback loop of increasing reinforcement exposure, these volumetric expansions cause significant internal stresses that eventually cause the concrete cover to crack and spall, speeding up structural degradation.

In terms of reducing the corrosion of reinforcement, geopolymer binders exhibit a number of intrinsic benefits over traditional Portland cement systems. According to Wang et al. (2020), their thick aluminosilicate gel microstructure retains enough alkalinity (pH 10–12) to protect the steel's passive layer while drastically lowering chloride diffusivity. Additionally, the aluminum-rich makeup of many geopolymers encourages the immobilisation of chlorides by forming Friedel's salt ($3CaO \cdot Al_2O_3 \cdot CaCl_2 \cdot 10H_2O$), which effectively lowers the concentration of free chlorides that might cause corrosion (Albitar et al., 2017).

According to recent studies, in accelerated chloride exposure testing, geopolymer concretes can increase the time-to-corrosion start by 300–50% when compared to regular Portland cement systems (Babaee et al., 2016). Regarding long-term performance under coupled environmental stresses, there are still significant information gaps, especially with regard to the possibility of carbonation-induced corrosion in lower-pH geopolymer formulations. For structural applications in harsh environments, where conventional corrosion prevention techniques would not be sufficient during multi-decadal service lifetimes, these factors are especially pertinent.

In contrast, geopolymers provide better resistance to corrosion caused by chloride than conventional concrete. Since the stable aluminosilicate network created during

geopolymerization produces a more impermeable barrier, its thick microstructure and low permeability considerably lower the rate of chloride penetration (Noushini et al., 2020; Yashwanth et al., 2023). Furthermore, geopolymers have a greater ability to bind chlorides, which chemically immobilises them inside the aluminosilicate matrix. This binding process is more resilient and less reversible than the less stable Friedel's salt formation found in standard concrete, which further reduces the danger of corrosion stable (Mayhoub et al., 2021). Furthermore, the passivation layer on steel reinforcement is maintained by the naturally high alkalinity of geopolymers (pH > 12), which offers an extra line of defence against chloride attack.

Due to their lower chloride diffusion coefficient, which considerably slows down chloride ingress and improves long-term durability, geopolymers show better resistance to chloride assault than conventional concrete (Lekshmi et al., 2022; Manzoor et al., 2023). Their strong chloride-binding ability, high alkalinity (pH > 12), and thick aluminosilicate microstructure all work together to postpone the onset of corrosion in reinforced structures (de Oliveira et al., 2022). Geopolymers chemically immobilise chlorides in a more long-lasting way, decreasing their mobility and corrosivity, in contrast to traditional concrete, where chlorides form less stable Friedel's salt.

Protective coatings, additional materials, and mix design modifications are important tactics to further maximise chloride resistance. While adding slag or metakaolin improves chloride binding and pore refinement (Bernal et al., 2012; El Moustapha et al., 2023), optimising the Si/Al ratio and alkali activator concentration increases the stability and impermeability of the geopolymer matrix. Surface coatings can offer an extra defence against chloride penetration in high-exposure settings (Broomfield et al., 2004; Kim et al., 2023), enhancing the natural durability of geopolymers for demanding applications.

In conclusion, although geopolymers and traditional concrete are both vulnerable to chloride attack, geopolymers are more resistant to chloride attack because of their alkaline environment, high chloride binding capacity, and dense microstructure. Designing long-lasting and robust structures, particularly in environments with high chloride concentrations, requires an understanding of the principles underlying chloride assault.

In applications such as marine structures, coastal defences, and infrastructure exposed to de-icing salts, fly ash-based geopolymers are good substitutes for traditional

Portland cement because of their remarkable resilience in chloride-rich environments. Their resistance to chloride ingress, thick microstructure, and distinct chemical makeup give them endurance. The following are the main factors influencing the resilience of fly ash geopolymers in chloride environments.

2.4.1.1 Reduced Chloride Permeability

A very dense and uniform microstructure with greatly decreased porosity is the end product of the geopolymerization process. Reducing chloride permeability requires this structural refinement because the formation of a well-integrated three-dimensional aluminosilicate network effectively restricts the entry of hostile ions (Mousavinejad et al., 2021; Noushini et al., 2021). In comparison to traditional cementitious systems, geopolymers' compact nature, which is a result of the polycondensation of aluminosilicate precursors, leads to fewer linked pores, improving resistance to chloride penetration.

Additionally, research shows that fly ash-based geopolymers have a significantly lower chloride diffusion coefficient than concrete made with regular Portland cement (OPC). A slower rate of chloride ion migration is suggested by this decrease in diffusivity, which is crucial for reducing the danger of corrosion in reinforced structures (Ekaputri et al., 2019; Wong et al., 2022). The enhanced durability performance is a result of geopolymeric gels' refined pore structure and chemical stability, which restrict chloride transport modes such ionic diffusion and capillary absorption. As a result, geopolymers offer a viable substitute for conventional concrete in settings like coastal and marine applications that are vulnerable to chloride-induced degradation.

2.4.1.2 Elevated Chloride Binding Capacity

Geopolymers based on fly ash have a strong ability to chemically bind chloride ions, which greatly lowers the amount of free chlorides that might cause corrosion. According to Falaciński et al. (2021), this suspension happens when chlorides are incorporated into the aluminosilicate framework and form stable, chemically bonded complexes instead of continuing to exist as free, reactive species. The geopolymer matrix, composed of a highly cross-linked network of Si-O-Al links, efficiently lowers the diffusivity of chlorides and decreases their corrosion susceptibility by offering active sites for chloride trapping (Falaciński et al., 2021).

Additionally, geopolymers exhibit a more robust and stable chloride retention mechanism than traditional Portland cement systems, where chloride binding is mainly controlled by the formation of Friedel's salt, a calcium chloroaluminate hydrate phase that can dissociate under changing pH or moisture conditions (El Moustapha et al., 2023). Instead of being physically adsorbed or weakly bonded in layered double hydroxides (LDHs), chlorides are incorporated into the three-dimensional aluminosilicate structure in geopolymers, which results in less reversible chemical binding. Even in the face of harsh environmental exposures like carbonation or cyclic wetting-drying, this durable binding guarantees long-term chloride suspension. As a result, geopolymers provide exceptional resistance to corrosion caused by chloride, which makes them especially useful for infrastructure situated in maritime or de-icing salt settings.

2.4.1.3 Alkaline Environment Passivation of Steel

Fly ash geopolymers' naturally high alkalinity (pH > 12) is essential for preserving the passivation of embedded steel reinforcement and offering an extra line of defence against corrosion brought on by chloride. A persistent and impermeable oxide layer, mostly made up of γ-FeO_3 or FeO_4, develops and remains on the steel surface in such a very alkaline environment, thereby serving as a barrier to electrochemical corrosion processes (Cong et al., 2021; Temuujin et al., 2009). At high pH, this passive layer maintains its thermodynamic stability, greatly postponing the depassivation threshold, or the critical concentration of chloride needed to start corrosion.

The geopolymer matrix shows a more resilient capacity to sustain alkalinity over time than regular Portland cement (OPC) systems, where carbonation or chloride incursion can locally lower pH and destabilise the passive layer. This is explained by the aluminosilicate gel structure's ability to act as a buffer, preventing acidification and extending the steel reinforcement's protective period (Pacheco-Torgal et al., 2012; Tennakoon et al., 2017). Additionally, geopolymers' alkaline nature and poor permeability work together to provide dual protection by preventing the diffusion of corrosive substances and limiting the entry of chlorides. According to empirical research, steel in geopolymer concretes may tolerate 2-3 times greater chloride concentrations before corrosion starts than OPC, highlighting their potential in challenging settings as industrial or maritime settings (Babaee et al., 2016).

2.4.1.4 Resistance to Damage Caused by Corrosion

In comparison to traditional concrete systems, fly ash geopolymers' better chloride binding ability and naturally low permeability greatly minimise corrosion-induced degradation processes, leading to noticeably fewer instances of spalling and cracking. This remarkable performance results from the material's capacity to chemically disable chlorides inside its three-dimensional network and physically prevent chloride penetration through its thick aluminosilicate matrix (Saha et al., 2018). These characteristics become especially important in harsh settings with high chloride concentrations, such as highway systems exposed to de-icing salts or marine infrastructure, as they successfully maintain structural integrity and prolong the maintenance-free service life of reinforced elements.

Fly ash-based geopolymers are great at protecting reinforced structures because they can resist water penetration and have a natural alkaline environment. These features works together to make the structure last much longer. According to research, even when exposed to chloride concentrations beyond typical threshold levels, these materials may sustain the passivation of steel reinforcement for noticeably longer periods of time than concretes made with Portland cement. Improved durability performance leads to considerable lifecycle cost savings by lowering the frequency of maintenance interventions and the need for premature structural replacements. When compared to their conventional equivalents, field investigations of geopolymer concrete buildings in maritime settings have shown service life extensions of 50–100%, confirming their promise as a sustainable option for important infrastructure projects where long-term durability is crucial (Albitar et al., 2017).

2.4.1.5 Efficacy in Marine Environments

Given their thick microstructure and resistance to chloride penetration, fly ash geopolymers have shown remarkable efficacy in maritime construction, including seawalls, breakwaters, and offshore platforms. They endure severe maritime conditions, including chemical assault, tidal pressures, and seawater immersion, with little deterioration over time, in contrast to traditional concrete. They are perfect for constructions needing minimum maintenance and a long service life since long-term field tests verify their durability, demonstrating minimal material disintegration even after years of exposure (Khan et al., 2023; Noushini et al., 2021).

The material's resistance to corrosion, alkali leaching, and sulfate attack especially in high-risk regions like tidal and splash areas is what makes it successful in marine settings. Workability and early strength have been further enhanced by mix design advancements, allowing for wider use in large-scale projects. For vital maritime infrastructure, fly ash geopolymers provide a high-performance, sustainable substitute by lowering lifespan expenses and maintenance requirements (Noushini et al., 2018).

2.5 Influence of Activator Choice in Geopolymer Reaction

The selection of an alkaline activator is a pivotal element in the geopolymerization process because it directly affects the dissolution of aluminosilicate precursors, the creation of oligomers, and the ultimate characteristics of the geopolymer. Alkaline activators, including sodium hydroxide (NaOH), potassium hydroxide (KOH), and sodium silicate (Na_2SiO_3), create elevated pH conditions essential for the dissolution of silica (SiO_2) and alumina (Al_2O_3) from the precursor material, thereby initiating polymerization reactions that establish the geopolymer network (Mustafa et al., 2011; Golafshani et al., 2024)

The nature and concentration of the activator profoundly influence the kinetics of geopolymerization, microstructure of the resultant geopolymer, and its mechanical and durability characteristics. Sodium silicate enhances the polymerization process by supplying extra silicate monomers, resulting in an increased compressive strength and enhanced durability (Wong et al., 2022; Manzoor et al., 2023). In contrast, the exclusive use of NaOH may lead to diminished reaction kinetics and mechanical performance.

Understanding the impact of activator selection is crucial for enhancing the geopolymerization process and customizing the geopolymer characteristics for certain applications. This section examines the function of several activators in geopolymer synthesis, emphasizing their influence on the reaction mechanism and resultant material characteristics.

2.5.1 Types of Alkaline Activators and Their Effects

The dissolution of aluminosilicate precursors, creation of oligomers, and final characteristics of the geopolymer were all directly impacted by the alkaline activator selection, making it a crucial step in the geopolymerization process. The characteristics of

the final material and the geopolymerization process are affected differently by several alkaline activators, including sodium hydroxide (NaOH), potassium hydroxide (KOH), and sodium silicate (Na_2SiO_3). An outline of the common alkaline activator types and their effects can be found below.

2.5.1.1 Sodium Hydroxide (NaOH)

Sodium hydroxide (NaOH) effectively dissolves alumina (AlO_3) and silica (SiO_2) from aluminosilicate precursors by breaking down Si-O-Si and Al-O-Al bonds in its high pH environment, initiating the geopolymerization process (Xu et al., 2000; Hajimohammadi et al., 2017; Tanyildizi et al., 2021). NaOH produces slower reaction kinetics than sodium silicate, which is advantageous for real-world applications as it gives greater control over workability and setting time.

Although the compressive strength of NaOH-activated geopolymers is generally mild, their mechanical characteristics can be improved by adjusting the concentration of NaOH and the curing conditions (Niyazuddin et al., 2023; Dash et al., 2023). In the synthesis of geopolymers, NaOH is a versatile activator that strikes a compromise between structural performance and reaction speed.

2.5.1.2 Potassium Hydroxide (KOH)

Potassium hydroxide (KOH), a potent alkaline activator, is just as effective as sodium hydroxide (NaOH) for dissolving silica and alumina from aluminosilicate source materials and starting the geopolymerization process. Rheological tests, however, have demonstrated empirically that KOH solutions have a substantially greater viscosity than NaOH solutions at comparable molar concentrations (Ozkan et al., 2022). In order to retain sufficient processability for building applications, this high viscosity directly affects the workability parameters of new geopolymer mixes, sometimes requiring formulation modifications through water content change or superplasticizer addition. The higher ionic radius of K^+ relative to Na^+, which influences solvation dynamics and ion mobility in the alkaline media, may be the cause of the unique dissolving behaviour of KOH.

Vicat needle and isothermal calorimetry tests have repeatedly shown that KOH-activated geopolymer systems exhibit faster reaction kinetics than their NaOH-activated equivalents, which is reflected in much shorter setting times (Cai et al., 2020; Klima et al., 2022). Although it could be difficult for large-scale placement operations, this quick reaction

profile has clear benefits for applications that call for the development of strength at an early age. Microstructural analyses have revealed a more homogeneous and densely cross-linked aluminosilicate gel formation, and extensive mechanical testing has further shown that KOH-activated geopolymers typically achieve 10–20% higher compressive strength values compared to NaOH systems (Xu et al., 2000; Cai et al., 2020). The potassium ion's function in charge balancing within the aluminosilicate framework, which encourages the formation of a more stable and structurally connected geopolymer matrix, is essentially responsible for the improved mechanical performance.

2.5.1.3 Sodium Silicate (Na_2SiO_3)

Sodium silicate (Na_2SiO_3), often known as water glass, serves as a particularly potent alkaline activator in geopolymer systems by providing readily available silicate monomers (Lu et al., 2023). These additional silicate species significantly enhance the geopolymerization process by encouraging the formation of a more extensive and interconnected aluminosilicate network. Greater cross-linking within the geopolymer gel phase is encouraged by the increased availability of reactive silica, which results in better structural integrity. Moreover, sodium silicate's alkaline properties aid in the breakdown of precursor materials and provide necessary silicate anions that blend into the expanding three-dimensional structure. Compared to hydroxide-based activators, this dual functionality not only speeds up reaction rates but also creates a more uniform and mechanically stable microstructure.

As demonstrated by shorter setting times and quicker heat development during early-stage geopolymerization, the use of sodium silicate as an activator usually produces noticeably faster reaction kinetics in comparison to NaOH or KOH (Huseien et al., 2020; Abdellatief et al., 2023). Applications needing strong early-age strength, such precast components or quick repair materials, benefit greatly from this accelerated reaction profile. The instant availability of soluble silicate species, which avoid the lengthier dissolution-reprecipitation phases connected to hydroxide activators, is the mechanism underlying the increased reactivity. Therefore, as compared to their hydroxide-activated counterparts, sodium silicate-activated geopolymers continuously exhibit higher compressive strength and long-term durability (Poloju et al., 2020; Eryılmaz et al., 2024). The denser and more stable aluminosilicate matrix created by the addition of more silicate monomers, which

successfully lower porosity and increase the overall structural integrity of the geopolymer network, is directly responsible for these improved mechanical capabilities.

2.5.1.4 Hybrid Activators

A common and very successful method in geopolymer synthesis is the combination of sodium hydroxide (NaOH) and sodium silicate (Na_2SiO_3) as alkaline activators, which capitalises on the complementing advantages of each component. While Na_2SiO_3 produces reactive silicate species that directly engage in polycondensation processes, NaOH offers the high alkalinity (pH >13) required to start the dissolution of aluminosilicate precursors. The extra silicate monomers from Na_2SiO_3 fill coordination sites within the geopolymer framework, improving the cross-linking density and facilitating the creation of a more extensive and chemically stable aluminosilicate network. As a result, geopolymers made with a combination of activators often exhibit better mechanical qualities, such as increased compressive strength (usually 20–40% greater than systems made with NaOH alone) and much better resistance to dimensional instability and chemical attack (Wong et al., 2022; Jamal et al., 2025). Since the instantaneous availability of silicate anions from Na_2SiO_3 shortens the induction period usually seen in hydroxide-only systems, the synergistic impact of these activators also encourages more effective reaction kinetics.

Through careful optimisation of the NaOH:Na_2SiO_3 ratio, a crucial parameter governing both processing behaviour and final material properties, the performance characteristics of mixed-activator geopolymers may be accurately adjusted. Although numerous empirical studies have established a weight ratio of 1:2.5 (NaOH:Na_2SiO_3) as a standard reference value ideal ratios can vary greatly (usually ranging from 1:1 to 1:3.5) based on the requirements of a given application and the chemistry of the precursor (Matsimbe et al., 2022; Anitha et al., 2023). In contrast, higher concentrations of Na_2SiO_3 improve microstructure density but might speed up setting times beyond practical handling limitations. Higher NaOH content typically speeds up dissolving rates but may impair workability and ultimate strength due to excessive alkalinity. A thorough analysis of these factors has shown that well-balanced activator mixtures can produce outstanding hardened-state performance (50-90 MPa compressive strength) and desirable fresh-state properties (e.g., 2-4 hour workability windows) at the same time. This makes them especially well-suited for high-performance construction applications where processability and mechanical reliability are crucial.

2.5.1.5 Impacts on Microstructure and Durability

The distribution of porosity and microstructural development in geopolymer matrices are greatly influenced by the alkaline activator selection. Mercury intrusion porosimetry and nitrogen adsorption methods demonstrate that sodium silicate (Na_2SiO_3) activation consistently yields geopolymers with 15–30% lower porosity than hydroxide-based activators, according to thorough microscopic investigations by Matsimbe et al. (2022). Two basic mechanisms underlie this microstructural superiority: the optimal Si/Al ratio attained through silicate activation favours the formation of a highly cross-linked N-A-S-H gel phase, and the instantaneous availability of soluble silicate species from Na_2SiO_3 encourages more thorough polycondensation reactions. However, because of inadequate polycondensation and the volatilisation of surplus water during curing, NaOH and KOH-activated systems usually have larger mesoporosity (2–50 nm range), resulting in capillary holes that jeopardise structural integrity. In backscattered electron microscopy, these microstructural variations are especially noticeable. Hydroxide-activated specimens frequently exhibit distinct interfacial transition zones and microcracking, whereas silicate-activated specimens exhibit a homogeneous phase distribution with few unreacted particles.

These geopolymers are especially resistant to harsh environmental exposure because of the improved microstructural density brought about by sodium silicate activation, which also translates into excellent durability performance. After 300 cycles of sulfate attack (5% Na_2SO_4 solution), Na_2SiO_3-activated specimens retain over 90% of their initial compressive strength, according to accelerated durability testing, while their NaOH-activated counterparts exhibit a 25–40% strength reduction under the same circumstances (Bayraktar et al., 2023; Ghassan Humur et al., 2022). Reduced permeability (water absorption levels usually <5% by mass) and the thermodynamically stable aluminosilicate network created during silicate-enhanced polymerisation act in concert to provide this remarkable chemical resistance. The better pore refinement of silicate-activated geopolymers is further confirmed by chloride diffusion coefficients evaluated using potentiostatic techniques, which show values an order of magnitude lower (10^{-13} m^2/s range) than hydroxide-activated systems. These characteristics make sodium silicate-activated geopolymers particularly suitable for use in marine applications, wastewater containment systems, and other scenarios requiring exceptional resistance to ionic penetration and chemical degradation. The material's capacity to generate secondary reaction products that can self-heal microcracks through continuous

pozzolanic reactions under service circumstances adds even further durability benefits (Matsimbe et al., 2022).

In conclusion, the selection of an alkaline activator is an important step in the geopolymerization process, as it affects the mechanical characteristics, durability, reaction kinetics, and precursor dissolution. While NaOH and KOH provide versatility in regulating reaction kinetics and workability, sodium silicate is frequently chosen for its capacity to improve the mechanical performance and polymerization.

2.5.2 Impact of Activator Concentration and Modulus on Geopolymer Properties

The alkaline activator concentration and modulus (the ratio of SiO_2 to NaO or K_2O) are crucial factors that have a significant impact on the geopolymerization process and the characteristics of the end product. These elements affect the microstructure of the final geopolymer, oligomer formation, and dissolution of aluminosilicate precursors. The outline of their impacts is as follows:

2.5.2.1 Concentration of Activator

Increasing the concentration of alkaline activators, such as sodium hydroxide (NaOH), potassium hydroxide (KOH), and sodium silicate (Na_2SiO_3), greatly improves the dissolution of aluminosilicate precursors. These activators promote the breakdown of silica (SiO_2) and alumina (AlO_3) from the precursor materials by increasing the pH of the solution.

Starting geopolymerization requires this accelerated dissolving process because it increases the availability of reactive species and the mixture's overall reactivity (Wang et al., 2020). The geopolymer paste's setting time is shortened by higher alkaline activator concentrations, which typically result in quicker reaction kinetics. Excessively high concentrations may result in early setting, which makes the combination challenging to handle during casting, even if this might be beneficial for quick strength growth. Furthermore, because of the sudden release of extra heat and moisture, such circumstances may cause microcracking and fast shrinkage (Sun et al., 2021; Manzoor et al., 2024). As a result, maintaining ideal response rates while guaranteeing acceptable workability requires regulating the activator concentration.

The concentration of the alkaline activator has a significant impact on the compressive strength of geopolymers. Strength may be increased with the right concentration increase by ensuring complete precursor breakdown and encouraging effective polycondensation. However, partial reactions might happen if the concentration is higher than the ideal threshold, which would result in weaker gel formation and worse mechanical performance (Mousavinejad et al., 2021; Javed et al., 2022). To maximise structural integrity while preventing negative consequences such excessive brittleness or cracking, the optimal activator dosage must be determined.

2.5.2.2 Activator Modulus Definition and Calculation

The molar ratio of SiO_2 to Na_2O (or K_2O) in the alkaline activator solution is known as the activator modulus, and it is a crucial factor in defining the reaction kinetics and ultimate characteristics of the geopolymer. Depending on how they are made, commercial sodium silicate (Na_2SiO_3) solutions usually have moduli between 1.0 and 3.3 (Khalil et al., 2020). More soluble silicate monomers are provided by a higher modulus (which denotes a higher SiO_2/Na_2O ratio), which encourages polycondensation and helps to create a denser and more resilient aluminosilicate gel network. Long-term durability and increased mechanical strength are the outcomes of this (Soong et al., 2022; Jaji et al., 2023).

The activator's modulus has a major impact on fresh-state characteristics including workability and setting time. Reactions involving dissolution and polycondensation are accelerated by activators with a low modulus, which have a larger NaO concentration than SiO_2. Faster setting may result from this, but it may also lessen workability, making the mixture more challenging to manage during placement (Duxson et al., 2007; Dehkordi et al., 2022). On the other hand, because of slower reaction kinetics, activators with a high modulus (excess SiO_2) tend to postpone setting. However, they also increase workability by retaining a more fluid paste for a longer amount of time. Therefore, in order to balance processability and early-age strength growth in geopolymer systems, activator modulus optimisation is crucial.

2.5.2.3 Optimization of Concentration and Modulus for Performance

Alkaline activator concentration and modulus (SiO_2/Na_2O ratio) optimisation are crucial for geopolymer performance; sodium silicate solutions with modulus 1.5–2.5 exhibit the optimum trade-off between mechanical strength and workability (Wang et al., 2015; Hadi

et al., 2019). While improper ratios can result in either quick setting or delayed reaction kinetics, proper optimisation guarantees full precursor dissolution and encourages the development of a dense, homogenous microstructure through controlled geopolymerization.

The durability and structural integrity of the material are directly impacted by the synergistic effects of modulus and concentration. While variations result in flaws like microcracking or partial polymerisation, ideal combinations create strong geopolymer networks that are impervious to chemical assault (Gunasekara et al., 2019). Therefore, maintaining desired fresh and hardened qualities while customising geopolymers to particular application needs requires careful management of these factors.

2.5.2.4 Pragmatic Considerations

The desired application and the particular aluminosilicate precursor used must be taken into consideration when choosing the alkaline activator concentration and modulus (SiO_2/Na_2O ratio). Custom activator formulations are necessary because different precursor materials have different reactivity profiles. For example, fly ash-based geopolymers usually require different alkaline activation conditions than metakaolin-based systems because of differences in their amorphous content and dissolution kinetics (Temuujin et al., 2009; Cai et al., 2020). Additionally, there is a considerable interaction between these activator factors and curing conditions. For example, high temperatures can work in concert with high activator concentrations and moduli to promote geopolymerization and strength growth (Zhuang et al., 2016).

The microstructure and macroscopic characteristics of the final binder are ultimately determined by the concentration and modulus of alkaline activators, which are essential parameters controlling the geopolymerization process. To attain the best possible balance between mechanical performance, workability, and long-term durability, these aspects must be precisely optimised. High-performance geopolymers appropriate for structural applications are produced when these parameters are calibrated correctly, since they facilitate full precursor dissolution, efficient polycondensation, and the development of a dense aluminosilicate matrix. The significance of thorough mix design studies to determine formulation-property connections for various precursor-activator combinations is highlighted by the interconnected nature of these factors.

In conclusion, the geopolymerization process and the properties of the final material are mostly controlled by the concentration and modulus (SiO_2/Na_2O ratio) of alkaline activators. The ideal ranges for these values vary depending on the precursor composition and curing circumstances, and they have a direct impact on reaction kinetics, microstructure formation, and final mechanical performance. Complete precursor dissolution, efficient polycondensation, and the creation of a robust, thick aluminosilicate matrix are all made possible by their appropriate balance.

But unworthy formulation can result in compromised properties, inappropriate moduli can lead to poor workability or incomplete reactions, while high concentrations can induce fast setting and microcracking. These elements are highly interdependent, which emphasises the need for methodical optimisation to get customised performance. In the end, creating high-performance geopolymers with exceptional strength, workability, and chemical resistance for structural applications requires exact control over activator chemistry.

2.5.3 Optimizing Activator Selection for Enhanced Durability

The choice of alkaline activators is essential for improving the endurance of geopolymers, particularly in harsh environments subjected to chlorides, sulfates, or acids. The selection of the activator, its concentration, and its modulus (SiO_2/Na_2O or SiO_2/K_2O ratio) substantially affect the chemical stability, microstructure, and long-term efficacy of geopolymers. The methods are essential for optimizing the activator selection to improve durability.

2.5.3.1 Selection of Activator Type Sodium Silicate (Na_2SiO_3)

Sodium silicate (Na_2SiO_3) is the most effective alkaline activator for durable geopolymers. It provides alkalinity and extra silicate monomers, forming a compact, stable network with low permeability and high chemical resistance. In contrast, NaOH and KOH dissolve aluminosilicate precursors effectively but lack additional silicates, leading to porous structures and reduced durability. Mixed systems combine sodium silicate with NaOH/KOH to balance quick dissolution (from hydroxides) and polymerization (from silicates), allowing optimized geopolymer properties for various applications (Song et al., 2023; Eryılmaz et al., 2024).

2.5.3.2 Enhancing Activator Concentration

The alkaline activator's concentration is critical in geopolymerization. Moderate to high levels enhance the dissolution of raw materials, forming a dense, durable matrix. However, excessive concentrations cause rapid setting and microcracks from shrinkage, compromising integrity. Optimizing this balance is key, ensuring sufficient reactivity without the detrimental effects of overly high alkalinity for a durable final product (Aygörmez et al., 2023; Manzoor et al., 2024).

2.5.3.3 Enhancing Activator Modulus

The silicate-to-alkali ratio (SiO_2/M_2O) is crucial for geopolymers. A higher ratio fosters a denser, more stable network, significantly improving resistance to chemicals, sulfates, and chlorides for use in harsh environments. However, this can reduce workability by increasing viscosity. An optimal ratio between 1.2 and 2.5 balances superior long-term durability with practical handling. Modern admixtures now help mitigate workability issues, allowing for more flexible and high-performance mix designs (Hadi et al., 2019; Shiju et al., 2019).

2.5.3.4 Increasing Resistance to Chloride

Sodium silicate-activated geopolymers excel at binding chlorides, outperforming those made with just NaOH or KOH. The extra silicate content enables both chemical and physical binding, reducing free chlorides that cause steel corrosion. This is enhanced by a denser, less permeable microstructure that further blocks chloride ingress. This dual-action protection makes sodium silicate the preferred activator for durable structures in coastal or chloride-exposed environments (Lee et al., 2019; Bagheri et al., 2021; Soong et al., 2022).

In conclusion, optimizing alkaline activators, particularly sodium silicate, is crucial for developing durable geopolymers. By carefully adjusting activator concentration and modulus to suit the precursor, engineers can create matrices highly resistant to chlorides, sulfates, and acids, enabling sustainable, robust materials for demanding infrastructure.

2.6 Predictive Modeling for Geopolymer Durability

Predictive modeling is a powerful tool for assessing geopolymer durability in harsh environments. By using machine learning and computational simulations on experimental

data, these models forecast long-term performance against chlorides, sulfates, and acids. This allows engineers to optimize mix designs and preempt durability issues, accelerating development. This section reviews current methods from analytical models to machine learning evaluating their strengths, limitations, and future potential in replacing lengthy field tests and enabling geopolymers' widespread adoption (Soong et al., 2022; Dash et al, 2023).

2.6.1 Existing Prediction Methods for Concrete Durability

Accurately forecasting the long-term durability of concrete and geopolymers is vital for infrastructure in harsh environments. Predictive methods are diverse, falling into categories like meta-analysis, analytical models, numerical simulations, and machine learning. Meta-analysis, for instance, statistically combines data from numerous studies to identify robust trends and create empirical models. It has successfully predicted key durability indicators like chloride diffusion, helping to optimize mix designs for specific exposure conditions and ensure performance standards are met (Bagheri et al., 2020; Owino et al., 2023).

Despite its value, meta-analysis in geopolymer research is limited by inconsistent source data. Variations in material properties and experimental methods introduce uncertainty, while a lack of standardized testing complicates direct comparisons. To enhance accuracy, future efforts must prioritize high-quality datasets and advanced statistics. A rigorous four-step methodology—involving systematic data collection, normalization for curing variables, multivariate regression modeling, and thorough statistical validation can mitigate these issues, successfully quantifying how mix design controls durability (Prem et al., 2019; Mohtasham et al., 2023; Ali et al., 2024;).

While this analytical model improves geopolymer durability assessment, it faces operational challenges. Its accuracy depends on consistent reporting of material properties, like precursor composition from quantitative XRD. The lack of standardized testing also requires careful use of conversion factors. Future integration of machine learning could enhance predictions by capturing complex, non-linear relationships (Nukah et al., 2023; Gomaa et al., 2024).

Separately, numerical simulations like FEA and CFD are vital for modeling long-term degradation from chlorides or sulfates. These tools solve complex equations to simulate

coupled physicochemical processes over time. However, their reliability hinges on accurate input parameters and significant computational resources. When properly executed, they provide invaluable insights for predicting service life and designing durable infrastructure (Toufigh et al., 2021; Barbhuiya et al., 2023; Saeed et al., 2024).

In conclusion, a variety of current concrete durability prediction techniques are available, ranging from straightforward empirical models to sophisticated computer simulations. The particular application, data at hand, and required degree of precision all influence the method selection. Each approach has its advantages and disadvantages. Engineers can guarantee long-term durability by optimizing the design and maintenance of concrete structures using these techniques.

2.6.2 Machine Learning Approaches in Durability Prediction

Machine learning (ML) has emerged as a potent instrument for forecasting the durability of construction materials such as concrete and geopolymers. Utilizing algorithms to examine extensive datasets, machine learning models can discern intricate, non-linear correlations among material characteristics, environmental factors, and long-term performance. These methodologies are proficient in managing high-dimensional data and delivering precise predictions without requiring specific physical or chemical models (Ford et al., 2022).

The prevalent machine learning methodologies employed in durability forecasting include regression analysis, neural networks, decision trees, and support vector machines. These methodologies have been effectively utilized to forecast essential durability metrics, including chloride diffusion, sulfate resistance, and carbonation depth, providing insights that are challenging to obtain using conventional empirical or analytical models (Nazar et al., 2023). This section examines the utilization of machine learning in durability forecasting, emphasizing its capacity to transform the design and upkeep of resilient construction materials.

Over the past five years, machine learning has been increasingly applied to study geopolymer concrete, as evidenced by the body of research summarized in Appendix 1. The table offers an overview of studies focused on geopolymer concrete and its composites. Geopolymers have demonstrated significant promise as environmentally friendly substitutes

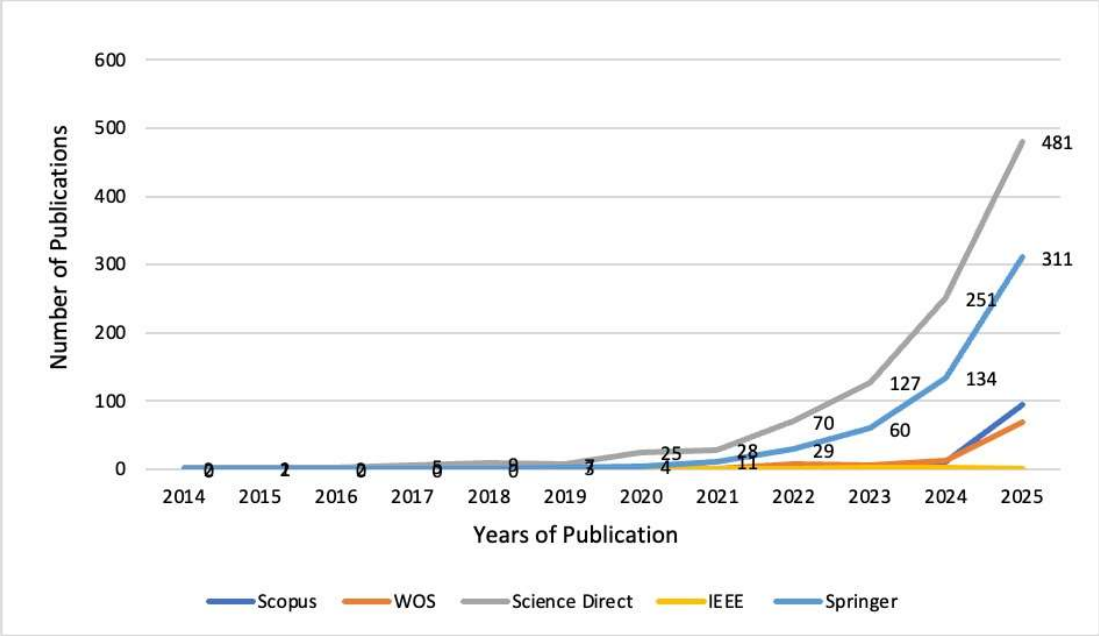
for conventional Portland cement-based concrete, owing to their exceptional resistance to chemical assaults and chloride intrusion. However, because of the interaction of several variables, including mix design, curing conditions, and environmental exposure, forecasting their long-term durability in harsh situations remains a difficult task. Researchers are increasingly turning to machine learning (ML) approaches to tackle this problem because they offer powerful tools for analysing complex information and predicting material performance.

Machine learning models provide a data-driven approach for understanding the relationships among material properties, environmental conditions, and durability outcomes. Large datasets are used by these models to find patterns, correlations, and prediction linkages that are hard to find with conventional analytical or empirical approaches. This section provides an overview of how machine learning is applied to predict and optimize the durability of geopolymers, setting the stage for a deeper exploration of specific ML techniques in the following subsections.

Over the past eleven years, the use of machine learning (ML) in geopolymer research has grown significantly. The number of research has increased from just two in 2014 to 251 in 2024 and 481 in 2025 (as of the most recent statistics), according to publications indexed in Scopus, Web of Science, Science Direct, IEEE, and Springer, as outlined in Figure 2-2. This exponential increase demonstrates the increasing understanding of ML's value in forecasting material qualities, improving sustainability, and optimising geopolymer formulations.

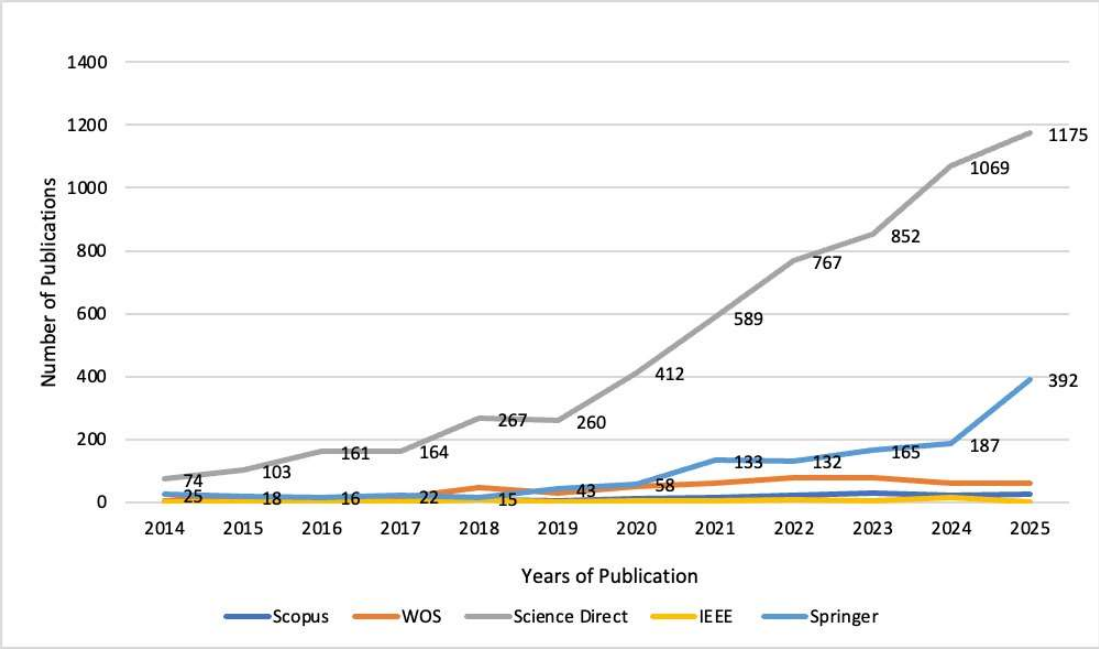
Science Direct had the most articles of any database examined, demonstrating its importance as a major forum for sharing ML-driven geopolymer research. This pattern highlights how, in recent years, the scientific community has placed a greater emphasis on using data-driven methods to develop geopolymer technology.

Figure 2-2: Number of Publication from 2014-2025 based on Adoption of ML on Geopolymer



Research production across key academic platforms has significantly increased between 2014 and 2025, according to a review of papers on geopolymers (with an emphasis on paste, mortar, and concrete applications). With publications rising from 74 in 2014 to 1,157 in 2025, a 15-fold increase over the decade. Science Direct has shown the most impressive growth, as per the Figure 2-3. This strong presence emphasises how important Science Direct is as the premier forum for sharing geopolymer research.

Figure 2-3: Numerous Machine Learning Studies based on geopolymer form (paste, mortar, and concrete) were conducted between 2014 and 2025



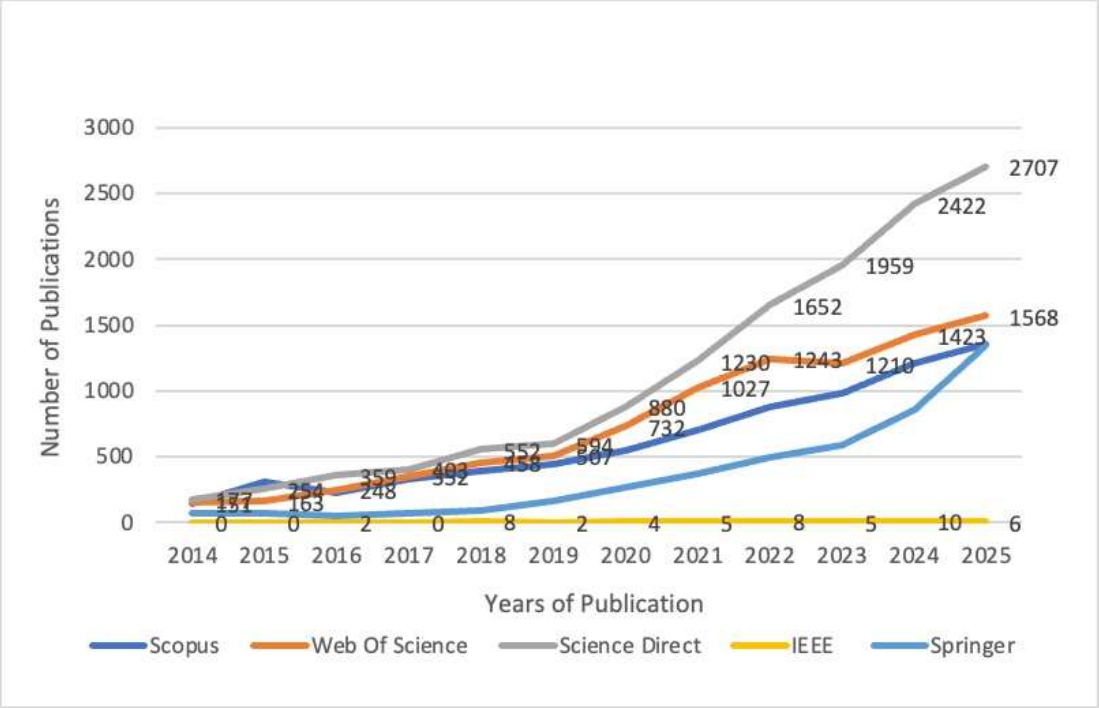
The exponential expansion across research platforms indicates that machine learning is becoming increasingly popular worldwide for geopolymer applications. This increase is a result of geopolymers' growing popularity as environmentally friendly substitutes for traditional cementitious materials. Deeper research into their uses in paste, mortar and concrete compositions has been prompted by the growing need for environmentally friendly building solutions.

A paradigm change in sustainable building materials is reflected in the exponential growth in research papers on geopolymer-based concrete from 2014 to 2025, as shown in Figure 2-4. With 2,707 and 1,568 articles in 2025 alone, a startling rise over previous years. Science Direct and Web of Science have become the top repository for this research among the main academic platforms.

Geopolymer research has seen an increase in machine learning (ML) applications, which is indicative of its transformational potential in sustainable building. ML has become a vital tool for developing environmentally acceptable solutions as traditional cement manufacturing comes under fire for its carbon footprint. ML's relevance in deciphering geopolymer complexities, from composition to performance, is highlighted by the increasing number of research available on sites like ScienceDirect and Web of Science. ML simplifies the creation of long-lasting, low-carbon materials by facilitating quicker analysis of big

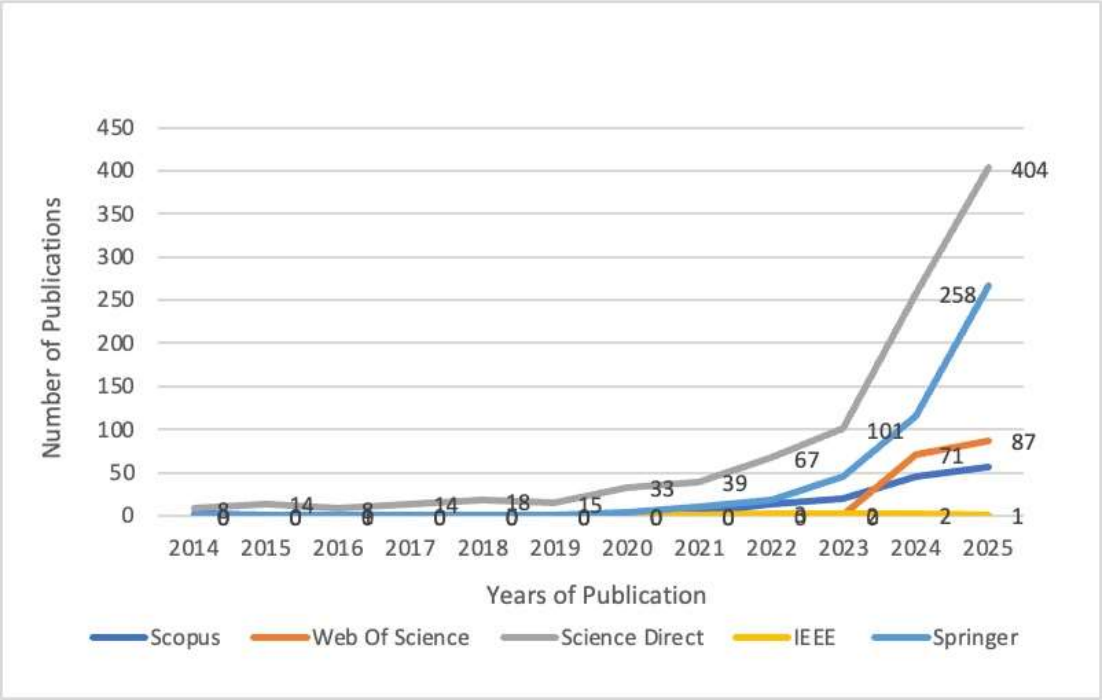
datasets and predictive insights. This pattern establishes machine learning as a key component of next-generation construction research and demonstrates an evolution towards data-driven innovation.

Figure 2-4: Numerous Machine Learning research projects utilising geopolymer-based concrete were carried out from 2014 to 2025



Its revolutionary importance in sustainable building is demonstrated by the exponential development in machine learning (ML) applications for fly ash-based geopolymers, which went from 8 to 404 yearly publications, as per Figure 2-5. The fact that ScienceDirect is the most widely used platform is a testament to machine learning's vital ability to handle fly ash unpredictability and enhance geopolymer performance. Today, complex algorithms outperform conventional trial-and-error techniques in the accurate prediction of material characteristics. This increase, especially after 2020, corresponds with advances in deep learning, speeding up both basic research and commercial implementation. In order to move fly ash geopolymers from lab-scale invention to workable, environmentally acceptable substitutes for traditional cement, machine learning has become essential.

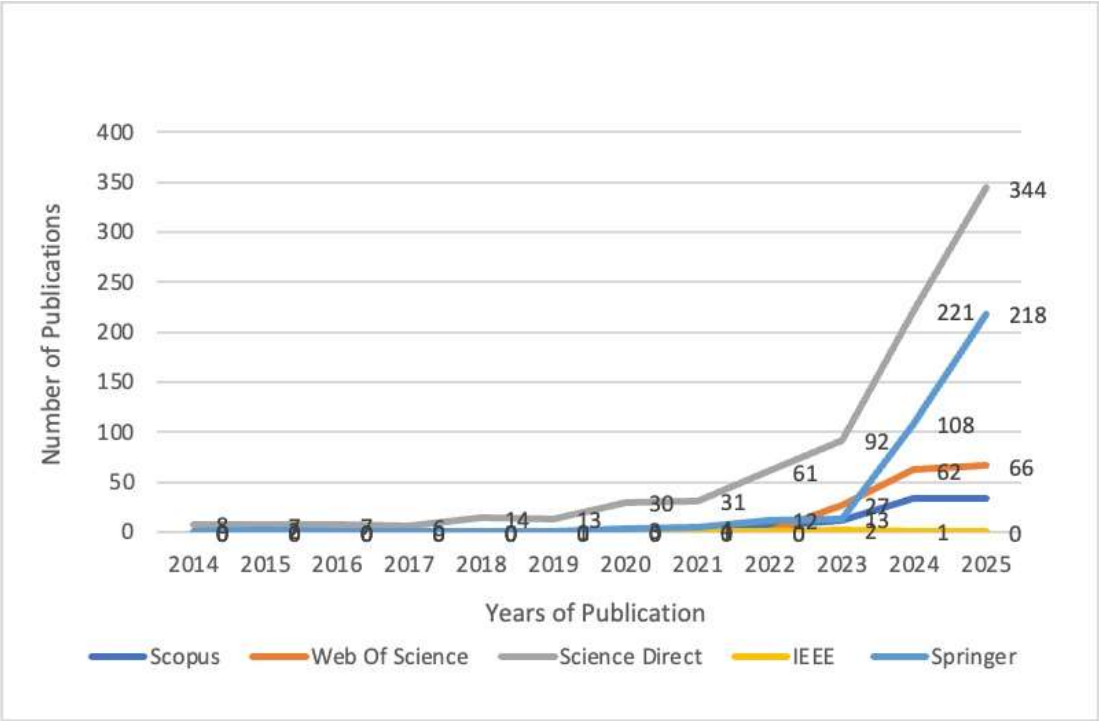
Figure 2-5: Number of studies using Fly Ash as a Geopolymer Concrete precursor in machine learning application analysis



The number of papers examining machine learning applications in geopolymer concrete using slag as a precursor is shown in Figure 2-6. According to the statistics, there is an important variation in the amount of research output between databases; in 2025, ScienceDirect had 344 articles, while Springer had only 218. The increasing significance of machine learning (ML) in materials science is reflected in this trend, which shows a rise in recent research investigating ML for slag-based geopolymer optimisation.

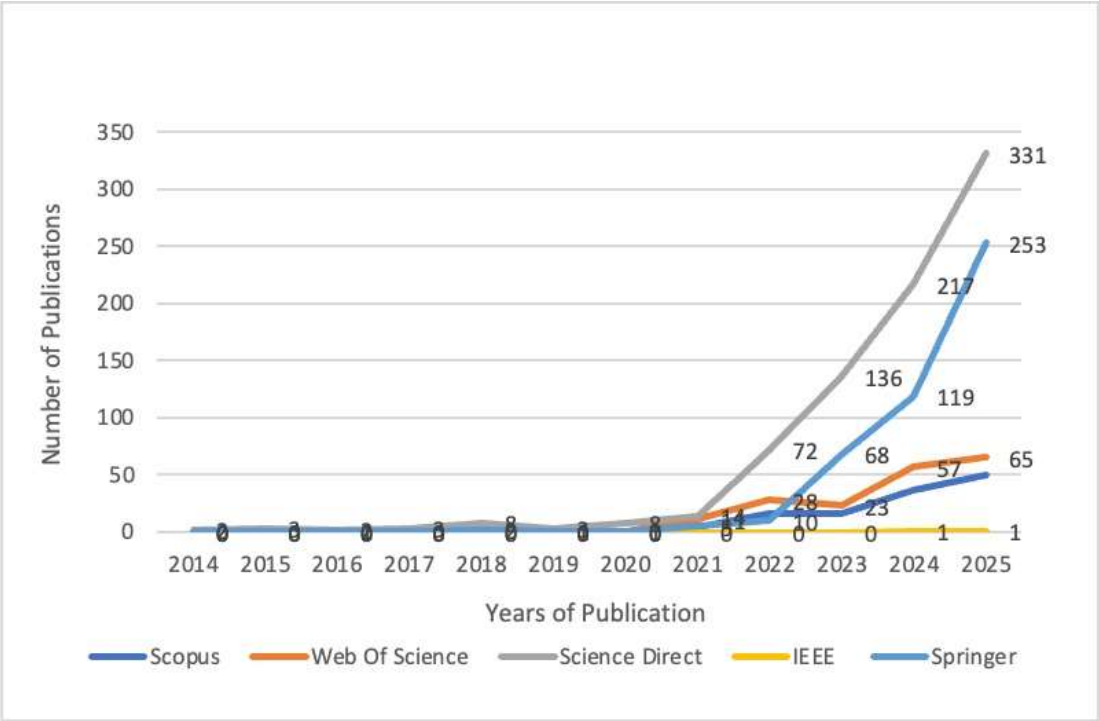
The remarkable benefits of machine learning (ML) in the analysis of geopolymer concrete, including faster data processing, better predictive modeling, and more efficient mix design, are the reason for its widespread use in this industry. Researchers are now able to discover intricate connections between material qualities and performance because to the growing popularity of machine learning techniques in recent years. This change demonstrates how ML can revolutionise the development of sustainable building materials.

Figure 2-6: Number of publications based on the investigation of machine learning applications using slag as a precursor type



Regression analysis's broad use in geopolymer research demonstrates how well it handles intricate, multifaceted material datasets. This approach is being used more and more by researchers to describe the links between mechanical characteristics and mix design factors, provide more accurate performance predictions, and effectively analyse big experimental datasets. Its increasing use, shown by a jump from two papers in 2014 to 331 in 2025, indicates how important it is to contemporary geopolymer research, as shown in Figure 2-7. In an area where nonlinear material interactions dominate important difficulties, regression approaches allow for decreased experimental iterations, formulation optimisation, and pattern detection in high-parameter spaces. Regression-based machine learning, which connects basic research with real-world material creation, has emerged as a crucial tool for developing sustainable building materials as an investigative and predictive tool. Its versatility and computational efficiency keep pushing the boundaries of geopolymer research.

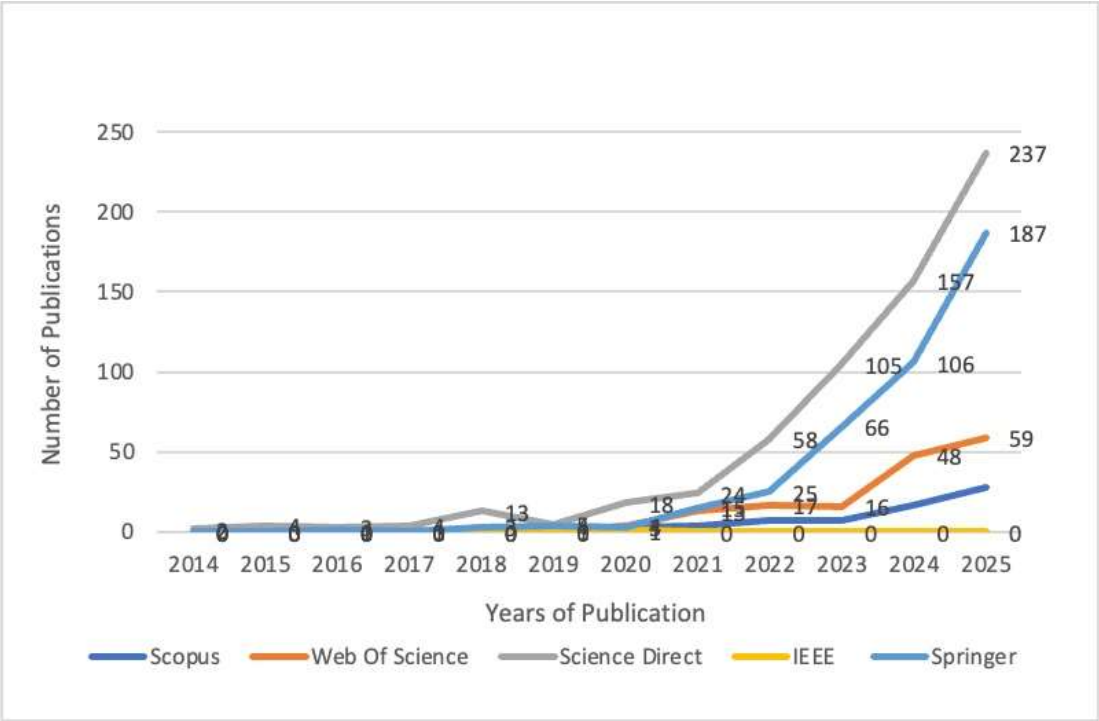
Figure 2-7: Total publications from 2014 to 2025, geopolymer concrete based on regression using machine learning algorithms



According to publishing trends across major databases, the use of machine learning (ML), and specifically artificial neural networks (ANN), in geopolymer concrete research has increased significantly over the last eleven years. Figure 2-8, with 237 articles in 2025, ScienceDirect has the most publications, followed by Springer with 187 papers. This higher trend is a result of the growing use of ANN and other ML approaches to improve sustainability evaluations, forecast mechanical characteristics, and optimise geopolymer mix designs.

ScienceDirect's publications increased from 58 papers in 2022 to 105 in 2023 before reaching a high in 2024, indicating a noticeable acceleration in research interest. Despite having smaller quantities, Scopus, IEEE, Web of Science, and Springer all exhibit consistent growth. This pattern highlights how the scientific community is moving towards data-driven strategies to get around the challenges of geopolymer formulations, such changing curing conditions and precursor compositions.

Figure 2-8: Total publications between 2014 and 2025, ANN-based geopolymer concrete using machine learning methods



The accuracy of it in simulating nonlinear connections in geopolymer systems is demonstrated by the prevalence of ANN-based research. It is anticipated that as machine learning techniques advance, they will be increasingly integrated into geopolymer research, facilitating more effective material design and wider industrial usage. The dramatic increase of publications after 2022 points to a turning point that is probably being fueled by the need for quick material innovation, growing sustainability regulations, and improvements in processing capacity.

In summary, the durability of building materials has been successfully predicted using conventional machine learning models such as ensemble methods, decision trees, support vector machines, neural networks, and regression analysis (Padmapoorani et al., 2023; Seki et al., 2024). These models provide various methods for managing various data types and degrees of complexity, offering insightful information for maximizing material performance and guaranteeing long-term durability (Baduge et al., 2022; Rusna et al., 2022).

2.6.3 Self-Organizing Maps (SOMs) and Growing Self-Organizing Maps (GSOMs) Comparison

Self-organizing Maps (SOMs) and growing self-organizing maps (GSOMs) are sophisticated machine-learning methodologies recognized for their capacity to manage intricate, high-dimensional data and deliver intuitive visual representations. Unsupervised learning methods are very effective for clustering, pattern recognition, and dimensionality reduction, rendering them ideal for forecasting the durability of construction materials, such as geopolymers.

2.6.3.1 Self-Organizing Maps (SOMs)

Self-organizing maps (SOMs) are a type of artificial neural network that uses unsupervised learning to simplify complex, high-dimensional data into an interpretable two-dimensional format. In geopolymer research, SOMs effectively identify hidden patterns and correlations, helping to classify formulations based on their durability performance against sulfate attack or chloride penetration. This provides a powerful visual tool for optimizing mix designs by revealing non-obvious relationships between composition, processing, and long-term material behavior (Kohonen et al., 1998; Taşdemir et al., 2009).

2.6.3.2 Growing Self-Organizing Maps (GSOMs)

An improved version of the classic Self-organising Maps (SOMs), Growing Self-organising Maps (GSOMs) provide dynamic expansion during training for more flexibility in data representation. In order to better represent the underlying data distribution, GSOMs start with a limited set of neurones and gradually expand by adding additional neurones, in contrast to SOMs, which depend on a fixed grid layout (Alahakoon et al., 2000). A predetermined threshold controls the growth process, wherein the algorithm assesses the error distribution and enlarges the map in areas that surpass it, producing a more accurate and comprehensive data representation (Coulson et al., 2023).

GSOMs have proven to be very helpful in predicting durability, especially when assessing how well geopolymers function when exposed to chloride. They can manage complicated and heterogeneous datasets, such as various mix designs and climatic circumstances, thanks to their dynamic expansion capabilities. GSOMs are a useful technique for spotting intricate patterns in high-dimensional data because of their adaptability (Anima et al., 2021).

2.6.3.3 Comparison SOM & GSOM

Growing Self-Organising Maps (GSOMs) provide greater flexibility than standard SOMs by dynamically adapting their structure during analysis. This makes them superior for uncovering complex patterns in high-dimensional data, such as optimising geopolymer compositions for durability. While GSOMs offer more detailed and accurate visualisations, this enhanced capability comes at the cost of higher computational demands. The choice between the two methods ultimately balances the need for in-depth, adaptable analysis against available processing resources (Alahakoon et al., 2000; Jayaratne et al., 2021).

SOM and GSOMs, surpass traditional statistics by identifying hidden, non-linear patterns in complex geopolymer data. Their key strength is transforming high-dimensional information into intuitive, two-dimensional color-coded maps (Coulson et al., 2023). These visualizations effectively cluster and display trends, outliers, and relationships, such as how composition affects chloride resistance, making complex material behavior instantly understandable. This powerful visual insight allows researchers to optimize mix designs for superior durability more effectively than conventional analytical methods (D'Urso et al., 2020; (Nazar et al., 2023).

GSOMs offer superior adaptability over standard SOMs. Their dynamic structure expands during training to better represent complex data with diverse features, leading to more accurate pattern recognition for heterogeneous material systems. Both models are highly tunable, allowing researchers to tailor parameters like learning rates for specific studies.

A key advantage is their ability to model intricate, non-linear relationships, such as how composition and environmental exposure jointly affect degradation, which linear models miss. This significantly boosts prediction accuracy for long-term performance. Furthermore, they are robust against imperfect, noisy data, making them suitable for real-world applications.

In practice, these tools are extensively applied to durability forecasting. They successfully predict critical behaviors like chloride diffusion rates. By simultaneously evaluating multiple interacting factors, they enable a comprehensive durability assessment and guide the development of geopolymers with enhanced resilience for demanding environments (Kumar et al., 2024).

In conclusion, self-organising maps and its expanding variations provide significant benefits for geopolymer durability prediction due to their interpretability and capacity to handle intricate, high-dimensional information. While clustering algorithms uncover innate patterns in material behaviour, their topological mapping skills facilitate the efficient visualisation of multidimensional interactions. Traditional analytical approaches frequently miss nonlinear relationships between composition, environmental exposure, and degradation processes, which these techniques excel at capturing.

2.7 Gaps in Current Research

Despite considerable progress in geopolymer research, significant deficiencies continue to impede their broader application. A primary concern is the insufficient comprehension of long-term durability, as current knowledge is largely derived from controlled laboratory studies that fail to replicate the complex conditions of real-world environments. There is a critical lack of longitudinal field data, especially from harsh settings, which hinders accurate service life predictions. Furthermore, the field suffers from a lack of standardised testing protocols and performance benchmarks specifically designed for geopolymers' unique chemistry. The absence of these established standards prevents reliable material comparison and quality control, ultimately obstructing the transition from successful laboratory research to widespread, confident use in construction projects (Prusty et al., 2022).

Current geopolymer mix design lacks comprehensive optimization. While basic compositional relationships are understood, systematic studies are needed to balance durability, strength, and sustainability simultaneously. A major hurdle is the high environmental impact of traditional alkaline activators, necessitating research into low-carbon alternatives. Furthermore, accurately predicting long-term durability remains a challenge. Existing models often fail to capture the complex, nonlinear relationships within the material. Advancing predictive capabilities requires sophisticated multi-scale modeling that integrates machine learning with simulations, bridging data from molecular interactions to macroscopic performance for reliable life-cycle forecasts (Iftikhar et al., 2022).

In conclusion, although considerable advancements have been achieved in comprehending the durability of geopolymers, significant inadequacies remain in existing studies. Rectifying such shortcomings is crucial for enhancing the efficacy of geopolymers,

establishing standardized testing protocols, and promoting their extensive use in construction. Future research must concentrate on extensive field studies, sophisticated predictive modeling, alternate activators, and application-specific optimization to fully harness the promise of geopolymers as sustainable and lasting construction materials.

2.7.1 Limited Understanding of Long-Term Durability

A major deficiency in geopolymer research is the inadequate comprehension of their long-term durability, especially under actual environmental conditions. Although laboratory investigations have shown that geopolymers may surpass ordinary concrete in terms of their tensile characteristics and chemical resistance, complete data on their long-term performance are lacking.

Current understanding of geopolymer durability is limited by a heavy reliance on controlled lab tests, which cannot replicate real-world conditions. The critical lack of long-term field data from actual infrastructure creates major uncertainty about their performance over time. Key aging mechanisms, such as microcracking from stress or chemical degradation, remain poorly understood outside the laboratory (Jaji et al., 2023; Kanagaraj et al., 2023). This gap hinders the development of reliable predictive models and performance standards. Without validation from real-world applications, confidence in using geopolymers for demanding infrastructure projects remains limited, underscoring the urgent need for comprehensive long-term field studies (Justnes et al., 2016).

Significant omissions in long-term performance data, especially with regard to microstructural development and interactions with steel reinforcement, impede a thorough knowledge of geopolymer durability. Reliable service-life forecasts are limited by the lack of documentation about the development of microcracks and changes in the pore structure under combined mechanical and environmental stress over time. Furthermore, there are significant concerns regarding the alkaline geopolymer matrix's long-term protective stability and how the crucial steel-geopolymer link changes over decades, even if it initially shields implanted steel from corrosion. Confidence in the use of geopolymers for long-term, reinforced concrete constructions is now hampered by these information gaps about microstructural alterations and interfacial behavior (Vu et al., 2018; Eryılmaz et al., 2024).

In summary, an inadequate comprehension of the long-term durability of geopolymers is a substantial deficiency in contemporary studies. Bridging this gap necessitates extensive longitudinal field research, thorough examination of aging mechanisms, and an enhanced comprehension of microstructural alterations and interactions with reinforcement. Addressing these knowledge gaps is crucial for enhancing the performance of geopolymers and promoting their extensive utilization in construction.

2.7.2 Challenges in Predicting Geopolymer Behavior in Aggressive Environments

Forecasting the long-term performance of geopolymers in hostile environments like those containing chlorides, sulfates, or acids remains a significant challenge due to complex chemical and physical interactions. Key issues include understanding intricate chemical processes, such as the long-term stability of bound chlorides and the kinetics of sulfate reactions that cause expansion. Furthermore, predicting microstructural evolution including pore network changes and crack propagation under combined chemical and mechanical stress is difficult (Chen et al., 2021). The interdependence of these degradation pathways necessitates advanced characterization and multiphysics models that integrate chemical data with fracture mechanics. Overcoming these forecasting limitations is essential for enabling the confident use of geopolymers in critical infrastructure (Shi et al., 2011).

Predicting the corrosion of steel reinforcement within geopolymer concretes is complex due to the unique interfacial chemistry between the steel and the aluminosilicate matrix. Key uncertainties persist regarding the stability of the protective passive layer in high-pH geopolymer environments, including corrosion initiation thresholds and long-term propagation rates. Furthermore, the bond strength between steel and geopolymer may evolve differently than in traditional concrete, potentially affecting long-term structural performance. Compounding these challenges is a critical lack of standardized testing methods and durability benchmarks specifically designed for geopolymers. The absence of these established protocols hinders reliable material comparison, quality control, and the transition from research to widespread structural application (Noushini et al., 2021; Romanazzi et al., 2023).

Accurately predicting geopolymer performance in harsh environments remains a significant challenge. Current predictive models are limited because they often fail to capture

the complex, nonlinear interactions between material composition, microstructural changes, and environmental exposure. While advanced computational techniques like machine learning and multiscale modeling offer promise, their effectiveness is hampered by a critical shortage of reliable, long-term experimental data for validation. Overcoming these limitations requires a coordinated effort to generate high-resolution durability datasets and develop sophisticated modeling frameworks. Establishing these accurate prediction tools is essential for enabling the confident, widespread use of geopolymer technology in demanding infrastructure applications (Alexander et al., 2023).

2.7.3 Need for Advanced Predictive Models like SOMs and GSOMs

Conventional prediction methods are challenged by the complicated, multi-factor nature of geopolymer durability, which is impacted by composition, stress, and environmental exposure. To solve this, sophisticated computational methods such as Self-Organizing Maps (SOMs) and their variations are crucial. These neural networks are particularly good at simulating the non-linear relationships that control long-term performance, handling high-dimensional input, and identifying hidden patterns (Kohonen et al., 1998). Their capacity to simplify complicated data into understandable, visual representations is a major advantage. This maintains important topological correlations, which enables researchers to pinpoint the crucial factors influencing durability and deterioration, leading to more precise forecasts and well-informed material design.

For the analysis of geopolymer durability, Self-Organizing Maps (SOMs) and their expanding variations (GSOMs) offer strong, user-friendly tools. They use color-coding to graphically illustrate patterns, clusters, and performance trends across various material compositions by converting complicated, high-dimensional data into two-dimensional topological maps. They are excellent at automatically recognizing hidden structures and classifying related geopolymer formulations without the requirement for pre-existing labels because they are unsupervised learning models. Additionally, GSOMs' versatility is a major benefit; parameters may be adjusted for certain research objectives, and its structure can be dynamically adjusted to a variety of datasets. They are particularly useful for identifying complex correlations in materials science because of their intuitive visualization, strong pattern recognition, and flexibility (Kaski et al., 1998; Dike et al., 2018; Stryhal et al., 2023).

Self-Organizing Maps (SOMs) significantly enhance the predictive accuracy for geopolymer durability by modeling the complex, non-linear relationships between material composition, environmental exposure, and degradation. They are particularly effective for specific applications, accurately forecasting critical issues like chloride penetration, sulphate attack, and carbonation. A key strength is their ability to integrate multi-scale data, effectively bridging the gap between controlled laboratory results and real-world field performance. This provides a more reliable method for predicting long-term degradation patterns. Ultimately, these computational models enable the development of optimized geopolymer mixes and support proactive, data-driven decisions for infrastructure design and maintenance (Alahakoon et al., 2000; Colantonio et al., 2021).

In conclusion, the intricacy of geopolymer behavior in hostile environments and the shortcomings of conventional models are the main drivers of the need for sophisticated predictive models, such as SOMs and GSOMs. These cutting-edge techniques have special powers for managing high-dimensional data, producing clear visuals, and identifying intricate, non-linear relationships. Researchers can optimize the mix designs, guarantee the long-term performance of geopolymer structures, and provide important insights into geopolymer durability by utilizing SOMs and GSOMs.

2.8 Chapter Summary

This chapter offers a thorough analysis of geopolymers, emphasizing their durability, composition, and sophisticated prediction models such as Self-Organizing Maps (SOMs). Fly ash, an industrial waste recognized as an affordable and environmentally acceptable precursor for producing sustainable binders as an alternative to conventional cement, is a crucial element mentioned.

The analysis goes on to describe these materials' remarkable resilience in harsh environments, where their alkaline chemistry and dense microstructure offer strong resistance to acids, sulphates, and chlorides. The chapter emphasizes the need for advanced computational tools to precisely forecast this intricate, long-term performance. Models such as SOMs and GSOMs are stressed for their capacity to manage high-dimensional data, identify hidden patterns, and bridge the essential gap between laboratory outcomes and real-world field performance.

Alkaline activators, such as sodium hydroxide, potassium hydroxide, and sodium silicate, are essential because they directly regulate the geopolymerization process and the characteristics of the finished product. The best material for increasing durability is frequently sodium silicate.

It is difficult to forecast this long-term durability, though. The intricate, non-linear relationships between a geopolymer's composition, exposure to the environment, and breakdown over time are difficult for conventional techniques like regression analysis to understand. More advanced computational frameworks are desperately needed to overcome the shortcomings of these traditional approaches in order to produce accurate service-life estimations.

Although geopolymers are a viable, sustainable substitute for conventional concrete, knowledge gaps about their long-term durability prevent them from being widely used. To get around this, sophisticated computational models like Self-Organizing Maps (SOMs) are essential. These techniques are excellent at deciphering hidden patterns in complicated data, allowing for precise durability projections and material composition optimization.

A targeted research approach is necessary for future advancement. Long-term field research, standardized testing procedures, and the advancement of prediction models are all part of this. Conducting thorough environmental studies and investigating other activators at the same time is essential. By methodically following these paths, we can ensure that geopolymers fulfill the performance requirements for sustainable infrastructure and promote their wider use by bridging the gap between laboratory research and real-world application.

CHAPTER 3:

RESEARCH METHODOLOGY

3.1 Research Design

This study employed a comprehensive mixed-method research design that integrates experimental investigations with advanced data-driven modeling techniques, specifically leveraging Self-Organizing Maps (SOMs), to assess and forecast the durability of fly ash-based geopolymer concrete (GPC) in chloride-laden settings. The research design was structured to address the complex interactions among the material composition, environmental exposure, and durability performance of geopolymer concretes. The methodology was divided into two primary components: experimental analysis and computational modeling. The experimental component focused on the preparation, testing, and evaluation of the geopolymer concrete samples under controlled chloride exposure conditions. This is complemented by the computational component, which utilizes SOMs to analyze the experimental data, identify patterns, and forecast the long-term resilience of geopolymer concretes. The combination of these methodologies guarantees a comprehensive understanding of the elements affecting the performance of geopolymer concrete under hostile chloride conditions.

The research design is guided by the following objectives:

1. To examine the impact of material composition, including fly ash, metakaolin, and alkaline activators, on the durability of geopolymer concrete.

2. To evaluate the performance of geopolymer concretes under accelerated chloride exposure conditions.

3. To develop a predictive model using SOMs that can accurately forecast the durability of geopolymer concrete based on the experimental data.

4. To establish correlations between material properties, environmental conditions, and durability outcomes.

5. To validate the result by comparing the model's forecasts against result from laboratory durability testing.

In addition to offering a prediction tool for maximising the performance of geopolymer concretes in chloride-laden settings, our study strategy guarantees a methodical and rigorous approach to comprehending the durability mechanisms of these materials by merging experimental and computational approaches.

3.2 Experimental Framework

An experimental framework for this study was created to comprehensively assess the durability of fly ash-based geopolymer concretes during chloride contamination. It consists of a series of well-defined stages including material selection, sample preparation, curing, and accelerated chloride exposure testing. Each stage was carefully controlled to ensure consistency, reproducibility, and relevance to the real-world conditions.

3.2.1 Material Selection

This study utilized fly ash as the principal precursor to improve the mechanical and durability characteristics of geopolymer concrete. Alkaline activators, such as sodium hydroxide (NaOH) and sodium silicate (Na_2SiO_3), where NaOH to Na_2SiO_3 is 1:0.5, were selected due to their effectiveness in activating the geopolymerization process. The ratios of these materials were refined through initial experiments to attain appropriate equilibrium of workability, strength, and durability.

3.2.2 Sample Preparation

Geopolymer concrete samples were prepared using a standardized mixing procedure to ensure uniformity and reproducibility. The mix design was governed by key molar ratios, with the specific values selected based on established principles for high-strength, low-efflorescence binders and finalized after an initial series of nine trial mixes to optimize fresh properties and mechanical performance. The target ratios were: a SiO_2/Al_2O_3 (Si/Al) molar

ratio of 2.4 to promote a dense poly(sialate-siloxo) network (Davidovits et al., 2020), a Na_2O/SiO_2 molar ratio of 0.22 to balance precursor dissolution and long-term stability (Bernal et al., 2014), and a H_2O/Na_2O molar ratio of 11.5 to ensure sufficient workability. The alkaline activator was synthesized by first dissolving sodium hydroxide pellets in distilled water, then adding sodium silicate solution to achieve the specified Na_2O/SiO_2 ratio. This activator was combined with the solid precursors (fly ash, metakaolin) in a mechanical mixer to produce a homogeneous paste, which was poured into cylindrical molds (100 mm diameter × 200 mm height) and compacted to eliminate air voids.

3.2.3 Curing Regime

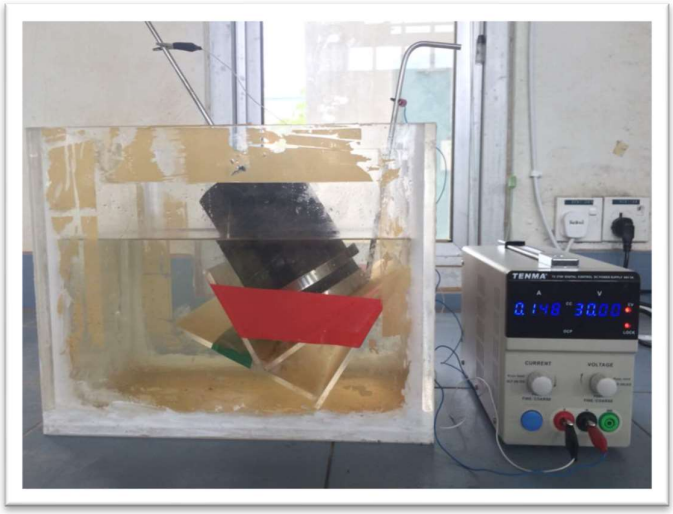
Based on established protocols for low-calcium aluminosilicate precursors like fly ash and metakaolin, which require accelerated reaction kinetics for practical strength development, the samples were subjected to a two-stage curing regime to facilitate geopolymerization (Duxson et al., 2007). An initial elevated temperature cure at 80°C for 24 hours in an oven was employed to rapidly drive the dissolution, gelation, and network-forming reactions, ensuring sufficient early-age mechanical integrity. This was followed by ambient curing until evaluation to allow for continued long-term polymerization and microstructural refinement. This specific temperature was selected as it is within the optimal 60–90°C range reported to maximize the degree of reaction and final compressive strength for heat-cured fly ash-based geopolymers, while avoiding excessive pore pressure or microcracking associated with higher temperatures (Bernal et al., 2014).

3.2.4 Chloride Exposure Testing

To assess their durability in aggressive chloride environments typical of marine conditions, cured geopolymer concrete samples were subjected to an accelerated chloride migration test. This evaluation was conducted in strict accordance with the Nordtest NT BUILD 492 standard, "Concrete, mortar and cement-based repair materials: Chloride migration coefficient from non-steady-state migration experiments." The test employed cylindrical specimens (Ø100 mm x 50 mm) that were initially vacuum-saturated. Each specimen was then placed in a test cell, where a constant external electrical potential (30V DC) was applied for 24 hours to drive chloride ions from a 10% NaCl catholyte solution into the concrete, as per Figure 3-1.

Following the exposure period, the specimens were axially split. The chloride penetration depth was determined visually by spraying a 0.1 M silver nitrate ($AgNO_3$) solution onto the freshly split surface, causing a colorimetric reaction. The measured penetration depth was used to calculate the non-steady-state migration coefficient, a direct and quantitative indicator of the concrete's resistance to chloride ingress. This systematic methodology provides a reliable, accelerated assessment of chloride diffusion, yielding high-quality, comparable data that is essential for a thorough evaluation of the durability performance of geopolymer concretes, as per Figure 3-4.

Figure 3-1: Setup for NordTest (NTBuild 492)



3.3 Modeling and Data Analysis

Advanced data analysis methods will be used to examine the information gathered from the experimental experiments including:

3.3.1 Self-Organizing Maps (SOM)

To find trends and connections between the different contributing elements affecting the durability of geopolymer concrete in chloride settings, self-organising maps will be used. Clustering samples according to performance attributes and visualizing complex datasets were made easier using this unsupervised learning technique.

3.3.2 Growing Self-Organizing Maps (GSOM)

An improved variant of classic self-organizing maps (SOM) and growing self-organizing maps (GSOM) overcomes some of the drawbacks of the original algorithm, especially when working with complicated, sizable, or unknown datasets. The GSOM dynamically modifies its structure during training, enabling it to expand as necessary, depending on the complexity of the input data, in contrast to the normal SOM, where the grid size is predetermined.

The proposed GSOM procedure for geopolymer concrete analysis involved mainly nine (9) steps.

In Step 1, the GSOM is initialized with two nodes or clusters, where a random-valued prototype weight vector $\boldsymbol{w}_j = [w_{j,1}, \dots, w_{j,p}], j = \{1,2\}$, is assigned as the centroid of the cluster.

In Step 2, the collected dataset is fed for learning the created cluster. The dataset consists of n data samples with p parameter settings of water/binder ratio, molarity, activator NaOH, activator Na_2SiO_3, water, and chloride diffusion coefficient, where each parameter value is normalized to a range of $[0,1]$ to ease the similarity test in the next step. The normalization was conducted by dividing the real parameter value by the maximum constant.

In Step 3, the learning of the GSOM begins with a similarity test on a data sample, $\boldsymbol{x}_i = [x_{i,1}, \dots, x_{i,p}]$, on the available clusters using Eq. 6.

$$d(\boldsymbol{x}_i, \boldsymbol{w}_j) = \sqrt[2]{\sum_{k=1}^{p} (x_{i,k} - w_{j,k})^2} \qquad \text{Equation 3.1}$$

In step 4, a winner, J, is selected among the clusters, where

$$J = \arg\min_j d(\boldsymbol{x}_i, \boldsymbol{w}_j) \qquad \text{Equation 3.2}$$

In Step 5, the winner cluster and its adjacent clusters are updated using Eq. 8-9, where h_{jJ} is the topological-based learning rate obtained by calculating the distance between the adjacent j-th node (N_j) and the winner J-th node (N_J) on the topological map. Let $j = J$ of Eq. Three to update the weight vector of the winner cluster, (w_J), and h_{JJ} in Eq. The

maximum learning rate ($h_{JJ} = \alpha$). In contrast, an adjacent node's prototype weight vector ($\boldsymbol{w}_j$) is updated with a lower $h\_JJ < \alpha$ for the self-organizing feature. $\alpha, \sigma \in [0,1]$ are the learning rate and adjacent width, respectively, which are monotonically reduced over the learning period.

$$\boldsymbol{w}_j = \boldsymbol{w}_j + h_{jJ}(\boldsymbol{x}_i - \boldsymbol{w}_j) \quad \text{Equation 3.3}$$

$$h_{jJ} = \alpha \exp\left(-\left(N_j - N_J\right)^2 \Big/ 2\sigma^2\right) \quad \text{Equation 3.4}$$

In Step 6, a hit sample counter of N_J was incremented to determine the size of the cluster.

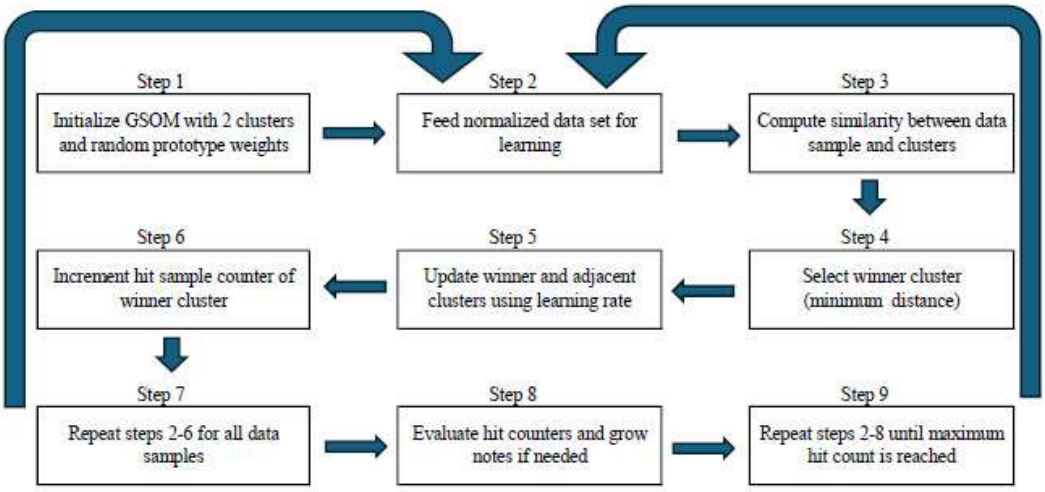
In step 7, go to step 2 with the subsequent data sample $\boldsymbol{x}_i, i = i + 1$, until $i = n$.

In step 8, the hit sample counters were evaluated for node growth. A row or column of new nodes is inserted to retain the topological features of the previous map. The rows of nodes were inserted on the west side of the row with the maximum total hit sample counts, and their prototype weight vectors were initiated from the rows. Otherwise, a column of nodes is inserted on the north side of the column with the maximum total hit sample count, and their prototype weight vectors are initiated from the columns.

In step 9, go to step 2 fetch $\boldsymbol{x}_i, i = 1$.

These steps are recursively conducted until the hit sample count of all the nodes does not exceed the maximum count. A summary of these steps is shown in Figure 3-2.

Figure 3-2: Flow Chart of Growing SOM



3.4 Material And Mix Design

Geopolymer concrete preparation involves the use of carefully selected raw materials, each of which contributes to the overall performance and properties of the final product. The materials used in this study are categorized as aluminosilicate sources, alkaline activators, aggregates, and water. A detailed description of each material, along with its specifications and role in the geopolymerization process, is provided below.

3.4.1 Materials

3.4.1.1 Aluminosilicate Source

Class F fly ash, a fine powdery byproduct produced when pulverized coal is burned in thermal power plants, served as the main source of aluminosilicate in this investigation. In particular, the Sejingkat Power Station in Kuching, Sarawak, Malaysia provided the fly ash used in this investigation. Class F fly ash is characterized by its low calcium content (typically less than 10%) and high concentrations of silica (SiO_2) and alumina (Al_2O_3), which together make up more than 70% of its chemical composition. These properties render it highly suitable for geopolymerization, a process in which silica and alumina react with alkaline activators to form a robust geopolymer binder.

Owing to its well-known pozzolanic qualities, fly ash can help cementitious materials become stronger and last longer. The principal precursor ingredient for geopolymer concrete is fly ash, which dissolves when exposed to alkaline solutions like sodium hydroxide (NaOH) and sodium silicate (Na_2SiO_3). The three-dimensional aluminosilicate gel created as a result of this reaction serves as the binding phase in the geopolymer concrete. Fly ash, a byproduct of industrial waste, not only enhances the final geopolymer's mechanical and durability properties but also promotes sustainability and lessens the environmental impact of traditional cement production. The unique chemical and physical characteristics of sejingkat fly ash, such as its fineness, reactivity, and particle size distribution, were thoroughly examined to ensure that they were appropriate for this investigation. This thorough investigation offers a strong basis for understanding the function of fly ash in the geopolymerization process and optimizing the mix design.

3.4.1.2 Chemical Composition

X-ray fluorescence (XRF) analysis was used to assess the chemical composition of the fly ash; the results are shown in Table 3-1. Iron oxide (FeO_3), silicon dioxide (SiO_2), and aluminum oxide (AlO_3) are the main oxides found in fly ash and are crucial for geopolymerization. The fly ash complied with the requirements of ASTM C618 for Class F fly ash, indicating its suitability for use in geopolymer concretes.

Table 3-1: Chemical composition of fly ash by XRF (%)

Precursor	MgO	Al_2O_3	SiO_2	P_2O_5	SO_3	K_2O	CaO	TiO_2	MnO	Fe_2O_3	Rb_2O_2	SrO	ZrO
Fly Ash	0.500	15.700	53	1.440	0.144	4.710	5.210	1.570	0.295	17.100	0.081	0.372	0.000ppm

3.4.1.3 Alkaline Activators Sodium Hydroxide (NaOH)

Due to its critical function in the geopolymerization process, sodium hydroxide pellets were used as the alkaline activator in this investigation. The high alkalinity of NaOH facilitates the breakdown of the silicon-oxygen and aluminum-oxygen bonds found in fly ash particles. The reactive silicate and aluminate species released by this chemical dissolution subsequently polymerise to create the three-dimensional geopolymer network. To systematically investigate the impact of alkali concentration on material attributes, three distinct NaOH molarities—8M, 10M, and 12M—were selected for study. These specific

concentrations were determined based on preliminary trial mixes, which targets compressive strength. The work has been published by another team member of this project (Teo et al., 2026).This variation in molarity enables a detailed examination of how alkali concentration influences the mechanical performance and microstructural development of the resultant geopolymer concrete, thereby helping to identify the ideal activation conditions for achieving the necessary engineering properties in the final product.

3.4.1.4 Alkaline Activator Sodium Silicate (Na_2SiO_3)

Solid-phase sodium silicate was used in the study as an additional activator to speed up the geopolymerization process. While speeding up the kinetics of the polymerisation step, the sodium silicate component greatly enhanced the aluminosilicate matrix's binding capabilities. Additionally, this addition enhanced the geopolymer concrete specimens' overall mechanical strength and long-term durability. Sodium silicate and sodium hydroxide were mixed in an exact mass ratio of 0.5 parts to 1 part, respectively—a ratio selected based on an initial phase of nine trial mixes to optimize activation efficiency. Effective precursor material dissolving was guaranteed by this precisely calibrated ratio, which also preserved the fresh geopolymer mixture's desirable workability and setting properties. The development of a strong and high-performing geopolymer concrete appropriate for structural applications required the use of sodium silicate as a secondary activator.

3.4.1.5 Fine Aggregate

As fine aggregate, river sand was sieved through a 4.75 mm sieve to ensure consistent grading. The fine-to-coarse aggregate ratio was optimized to 0.5:1 based on a series of nine initial trial mixes, which evaluated the combined effects on packing density, workability, and strength. This well-balanced blend preserved appropriate placement properties while enhancing interfacial bonding inside the geopolymer matrix. The controlled particle size distribution significantly improved the concrete's mechanical performance and structural integrity by balancing handling characteristics and durability requirements. Achieving consistent quality in the finished geopolymer concrete product required uniformity in the composite material, which was assured by this grading.

3.4.1.6 Coarse Aggregate

Crushed granite was used as the coarse aggregate because of its well-known strength and durability. The substance had an estimated specific gravity of 2.7 and a maximum particle size of 20 mm. According to IS 383 criteria, the aggregate grading met construction standards and ensured the right particle size distribution for the best possible concrete performance. The structural integrity of the geopolymer concrete was enhanced by this meticulously chosen and graded coarse aggregate, which also preserved the proper workability properties during mixing and installation procedures. The mechanical performance of the composite was improved by the natural qualities of granite and standardised grading, which encouraged efficient bonding within the geopolymer matrix.

3.4.1.7 Water

Water has two main functions and is an essential ingredient in the creation of geopolymer concrete.

(1) Preparation of Alkaline Solution: Potable water, free from impurities, was used to dissolve the sodium hydroxide pellets and prepare the alkaline activator solution.

(2) Curing: Water was used to cure the geopolymer concrete samples to maintain the moisture levels necessary for proper geopolymerization and strength development.

3.4.2 Geopolymer Design Mix

The design mix for geopolymer concrete in this study was meticulously developed to ensure optimal performance, durability, and workability. The precise function of each component in the geopolymerization process and its impact on the mechanical and structural characteristics of the end product were considered when determining the mix proportions. The following is a summary of the main components of the design mix.

Table 3-2: Geopolymer Mix Proportions

No.	WBR	Molarity	Aggregate (kg)	Sand (kg)	Fly Ash (kg)	NaOH (kg)	Na_2SiO_3 (kg)	Water (ml)
1	0.3	8	12.96	6.485	3.23	0.311	0.155	972
2	0.4	8	12.96	6.485	3.23	0.414	0.207	1296
3	0.5	8	12.96	6.485	3.23	0.518	0.259	1620
4	0.3	10	12.96	6.485	3.23	0.388	0.194	972
5	0.4	10	12.96	6.485	3.23	0.518	0.259	1296
6	0.5	10	12.96	6.485	3.23	0.648	0.324	1620
7	0.3	12	12.96	6.485	3.23	0.466	0.233	972
8	0.4	12	12.96	6.485	3.23	0.622	0.311	1296
9	0.5	12	12.96	6.485	3.23	0.780	0.390	1620

3.5 Geopolymer Mixing Procedure

The following steps will be followed to prepare the geopolymer concrete mixes:

a) Alkaline solution preparation: Sodium hydroxide (NaOH) and sodium silicate (Na_2SiO_3) were dry-mixed with sand and gravel before combined with the other ingredients. They were weighed according to the mix recipe weights, as shown in Table 3-2.

b) Mixing Procedure**:** Dry ingredients such as fly ash, metakaolin, and aggregates were well combined in a concrete mixer. After the alkaline solution was gradually added to the dry mix, the mixture was stirred until a consistent consistency was reached.

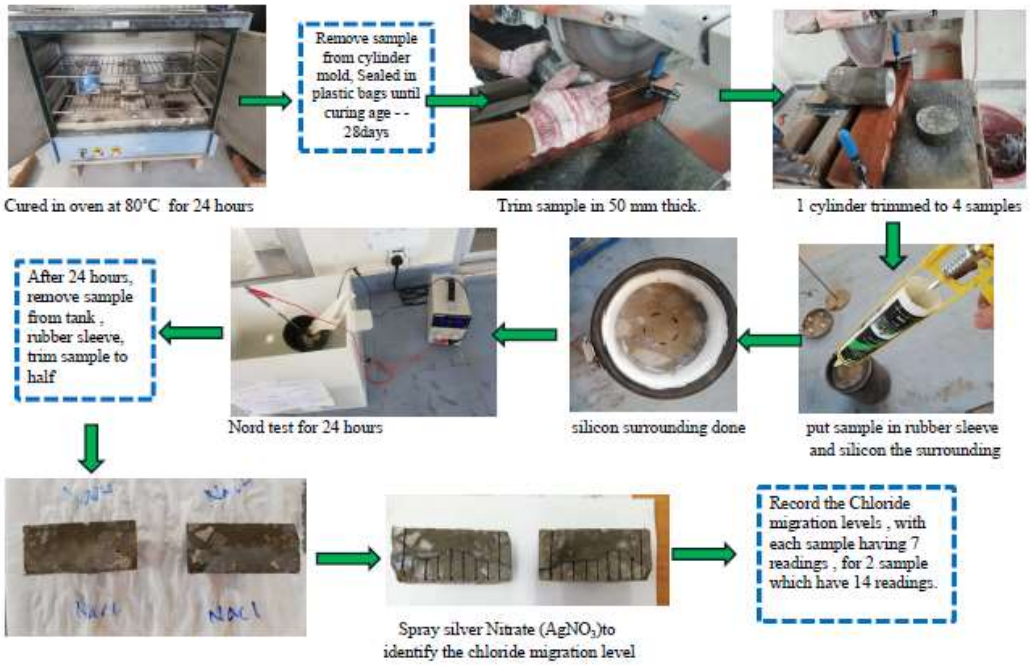
c) Casting and Curing: To test for durability, fresh geopolymer concrete was poured into molds of the right size (cylinder: 100 mm in diameter and 200 mm in height). To ensure compaction and remove air spaces, the samples were vibrated. To accelerate the initial setting phase, the molds were placed in an oven for 24 h after casting, as illustrated in Figure 3-3.

d) Sample Preparation for Chloride Exposure: After initial 24-hour oven curing, the samples were demolded and cured for 28 days. The samples were cut into 100 mm diameter × 50 mm thick slices after the curing procedure was completed. The Nord test, a standardized procedure used to assess the resistance of concrete to chloride penetration, was then applied to the formed slices. To replicate the

circumstances observed in real-world situations, the samples were subjected to a chloride-rich atmosphere during the Nord test. This was accomplished either by the direct application of chloride salts or by immersion in a chloride solution. The test findings provide insights into the long-term performance and durability of geopolymer concrete in settings where corrosion caused by chloride is an issue (Di Bella et al., 2011).

Figure 3-3: Sample Preparation and Test Procedure

Figure 3-4: NordTest Flow Chart



3.6 Machine Learning Techniques (Algorithms and Justification)

Effective tools for evaluating intricate datasets are provided by machine learning (ML) approaches, particularly in civil engineering applications such as forecasting the durability in chloride of geopolymer concrete. The endurance of geopolymer concrete, particularly under chloride conditions, was modelled and predicted in this study using a variety of machine learning techniques. The chosen methods were supported by their advantages, suitability, and effectiveness in managing properties of the dataset.

An artificial neural network, called a self-organizing map (SOM), is ideal for grouping and displaying high-dimensional data. SOM was utilized in this work to determine trends and connections among important variables affecting the durability in chloride of geopolymer concrete, especially in areas with high chloride levels.

Justification and application of SOM are as follows;

a) Dimensionality Reduction and Visualization: SOM simplifies the complex relationships between variables such as NaOH molarity water-to-binder ratio, and chloride penetration depth, mapping them into a lower-dimensional space.

This visualization will help identify clusters of data points with similar durability characteristics.

b) Pattern Recognition: SOM automatically clusters data based on underlying patterns, revealing trends that traditional methods may overlook.

c) Insights: Analyzing the SOM output will provide valuable insights into which factor combinations enhance or reduce concrete durability, guiding the optimization of mix designs.

d) Handling Non-linear Relationships: SOM excels in managing non-linear relationships common in material science, making it particularly useful for this study.

e) Effective Visualization: The SOM's ability to create a 2D representation of multidimensional data simplifies the interpretation of complex results, aiding both academic research and practical applications.

3.6.1 Feature Selection

Feature selection is the process of identifying and retaining the most relevant variables that significantly influence the durability of geopolymer concretes in chloride environments. This step reduces the complexity of the dataset, improves model efficiency, and enhances interpretability. The feature selection process used in this study included the following techniques.

To determine the connections between the input characteristics and goal variables (such as compressive strength and chloride penetration depth), a correlation analysis was performed. NaOH molarity and curing temperature were among the features that were given priority for inclusion in the model because of their high connections to the target variable. This stage lowers the noise and increases the accuracy of the model by ensuring that only the most significant variables are considered.

Techniques such as those based on decision trees or principal component analysis (PCA), have been employed to rank features based on their predictive power. This ranking aids in determining which factors, such as the type of precursor material or water-to-binder

ratio, have the greatest effects on the durability of geopolymer concrete. The model becomes more effective and comprehensible by focusing on these high-impact characteristics.

Dimensionality reduction methods such as PCA and t-distributed stochastic neighbor embedding (t-SNE) were used to further reduce the dataset. These techniques make it easier to handle and increase the computational efficiency of the SOM model by reducing the number of features, while maintaining the most crucial information.

3.6.2 Conclusion

This work makes certain that the Self-organising Map (SOM) model is trained on high-quality, meaningful data by carefully preparing the data and choosing the most pertinent characteristics. These procedures improve the precision and dependability of the model while also offering a better understanding of the variables affecting the durability of geopolymer concrete under chloride conditions. The systematic approach to data preprocessing and feature selection lays a strong foundation for subsequent analyses, enabling the development of a robust predictive tool for optimizing the performance of geopolymer concrete under challenging conditions.

3.7 Model Training and Validation

To guarantee that the model can efficiently learn from the data and precisely forecast the durability of geopolymer concretes in chloride settings, model training and validation are essential stages in the use of the Self-organising Map (SOM) for this study. These actions are necessary to create a solid and reliable prediction tool that can determine the connections between different input elements (such as material composition, curing conditions, and exposure to the environment) and the durability performance of geopolymer concrete. While validation evaluates the capacity of the model to generalize to new, unknown data, training allows the SOM to discover patterns and structures within the data. When combined, these procedures guarantee the precision, dependability, and usefulness of the model.

3.7.1 Model Training

The model training phase involves teaching the SOM to recognize and organize patterns within the dataset, enabling it to map the relationships between the input variables and the durability of geopolymer concrete. This phase consists of the following steps:

3.7.1.1 Training Data

Two subsets of the dataset were separated: a testing set (20–30% of the data) and a training set (usually 70–80% of the data). The SOM learned how several parameters, including NaOH molarity, water-to-binder ratio, curing temperature, and chloride exposure conditions, affect the durability of geopolymer concrete using a training set. This separation maintains a distinct subset for validation while guaranteeing that the model learns from a representative sample of data.

3.7.1.2 Learning Process

For the SOM to function, the input data must be arranged in a grid of neurons, each of which represents a collection of related data points. To reduce the distance between the input data and related neurons, SOM iteratively modifies the weights of these neurons during training. This process, known as competitive learning, allows SOM to group similar data points and identify patterns that reflect the impact of specific factors on durability. For example, the model might learn that a higher NaOH molarity combined with elevated curing temperatures leads to an improved chloride resistance.

3.7.1.3 Convergence

The training process proceeded until the model achieved convergence, at which point additional iterations had little effect on how the data were organized. SOM has successfully discovered the underlying correlations and patterns in the training data, offering a reliable and accurate depiction of the input factors and how they affect durability.

3.7.2 Model Validation

To guarantee SOM's dependability and forecast accuracy, the validation step assesses its capacity to extrapolate its learned patterns to fresh, untested data. The following actions are part of this phase:

3.7.2.1 Testing Data Evaluation

After training, the SOM was tested on a reserved testing dataset that was not used during the training phase. This step assesses how well the model can predict outcomes based on new data, simulating real-world scenarios in which the model must analyze unfamiliar inputs.

3.7.2.2 Validation Metrics

Topographic errors and quantization were the two validation criteria used to assess SOM performance. How effectively the SOM reflects the data is shown by the quantization error, which calculates the average distance between the data points and the neurons that correspond to them. The preservation of the topological structure of the data is evaluated by topographic error, which ensures that comparable data points are mapped to neighboring neurons. These metrics offer a numerical assessment of the dependability and accuracy of a model.

3.7.2.3 Cross-Validation

Cross-validation techniques were used to ensure the model robustness. This involves partitioning the dataset into multiple subsets and training the model on different combinations of these subsets. Cross-validation helped find any discrepancies or overfitting by evaluating the model on several data partitions, guaranteeing that the SOM predictions were dependable and consistent across datasets.

3.7.3 Conclusion

This study ensured that the SOM correctly represented the main variables affecting the durability in chloride of geopolymer concrete under chloride conditions by methodically training and validating the model. While the validation step verified the capacity of the model to generalize and provide accurate predictions, the training phase allowed the model to discover and arrange intricate patterns within the data. In addition to improving the accuracy of SOMs, this meticulous technique offers insightful information on how to best design and execute geopolymer concretes, which will eventually aid in the creation of more resilient and environmentally friendly building materials.

CHAPTER 4:

FINDINGS AND DISCUSSIONS

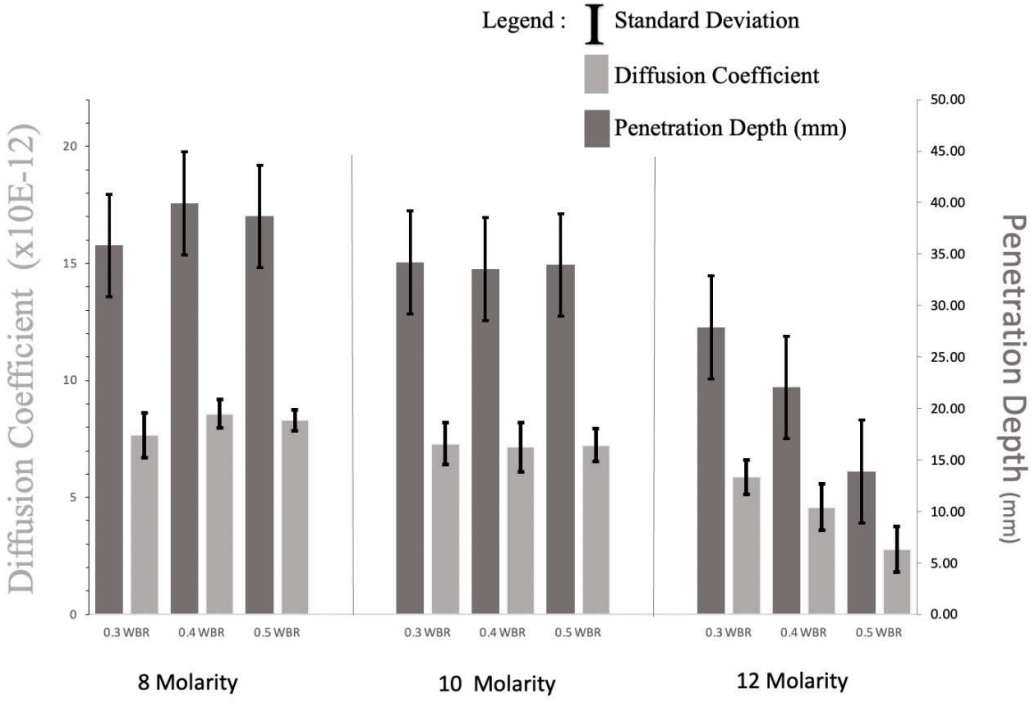
4.1 Chloride Penetration and Migration

Figure 4-1 illustrates the relationship between the chloride penetration depth and chloride diffusion coefficients in geopolymer concrete samples as a function of the water-to-binder (w/b) ratio and molarity. The graph presents data from 162 samples used in the Self-Organizing Map (SOM) prediction model. These two datasets are shown in the figure. The molarities of the alkaline activator solution (8M, 10M, and 12M) and water-to-binder ratios (0.3, 0.4, and 0.5) were plotted against both parameters. The graph demonstrates how these two factors (w/b ratio and molarity) influence the chloride penetration depth and diffusion coefficient of the geopolymer concrete. The impact of various mix designs on the chloride resistance characteristics of geopolymer concrete samples may be easily compared owing to this visualization. The data presented in this figure serves as the foundation for subsequent SOM analysis, enabling a deeper exploration of the complex relationships between the mixing design elements and chloride permeability in geopolymer concrete.

The observed trends are explained by their influence on the geopolymer microstructure. A higher molarity (e.g., 12M) typically enhances the dissolution of aluminosilicate precursors (fly ash/metakaolin), leading to a more complete geopolymerization reaction and a denser, less porous binder matrix with refined pore structure. This densification reduces the pathways available for chloride ion migration, thereby decreasing both the diffusion coefficient and penetration depth (Ekaputri et al., 2019; Noushini et al., 2020). Conversely, an increase in the w/b ratio introduces excess water into the mix. This water, not consumed in the chemical reaction, eventually evaporates, leaving behind a network of capillary pores and microcracks. This coarsened pore structure facilitates the ingress and transport of chloride ions, resulting in higher measured diffusion coefficients and greater penetration depths (Vu et al., 2018; Noushini et al., 2021).

The graph most likely shows trends in the relationship between the chloride resistance in geopolymer concrete and the molarity of the alkaline activator solution and water-to-binder ratio. These trends suggest that better chloride resistance is often achieved with higher molarities or lower water-to-binder ratios. Visualization may also draw attention to any possible interactions between these two elements, offering suggestions for the best mix design to increase the durability in chloride of geopolymer concrete in areas with high chloride levels.

Figure 4-1: Chloride penetration depth and diffusion coefficients as a function of activator molarity and water binder ratio



4.2 Validation of Results

In the current study, the optimized geopolymer concrete mix with a **0.5 water-binding ratio and 12 Molarity** achieved a diffusion coefficient of **5.3012 × 10^{-12} m^2/s**, representing the best chloride resistance observed in this study. This outcome supports Nanthini's findings, which showed that GPC typically has better chloride resistance than CC. The exceptionally low diffusion coefficient in the current study can be attributed to the optimized mix design, which further enhances the performance of the material (Nanthini et al., 2024).

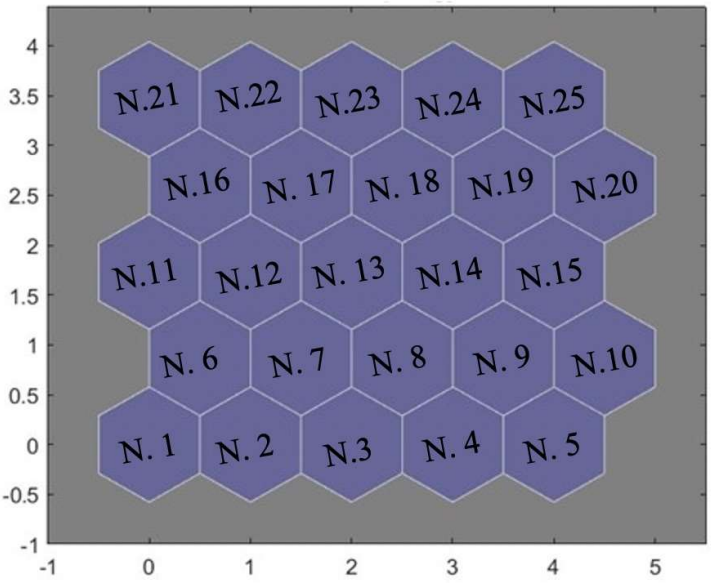
Additionally, Steel fibers added to GPC (SFRGPC) marginally improved the chloride penetrability, according to Nanthini, although it still performed better than CC and SFRC. This observation highlights a potential trade-off between mechanical reinforcement and chloride resistance, which should be considered in future optimizations.

The reliability of the present findings confirmed how well geopolymer concrete repelled chloride intrusion. This validation underscores the potential of GPC for use in chloride-exposed environments such as marine structures or roadways exposed to de-icing salts. Future work should focus on refining mix designs to balance chloride resistance with other performance metrics, such as mechanical strength and durability, while exploring the impact of additives such as steel fibers.

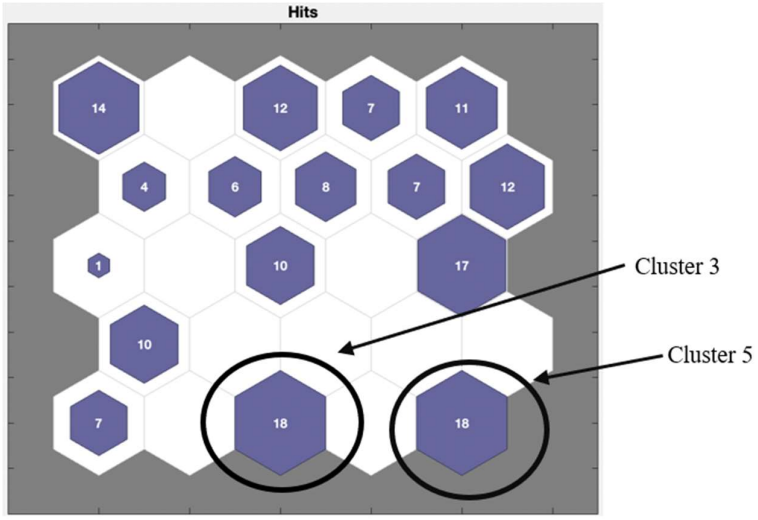
4.3 SOM simulation

Using MATLAB, the SOM model was trained using a 5 × 5 map size, resulting in a grid of 25 neurons arranged in a hexagonal structure, as shown in Figure 4-2. Each neuron represents a specific combination of the activator dosage and chloride permeability. The hexagonal topology allows for information exchange between adjacent neurons, aiding self-organization and learning.

Figure 4-2: Self-organizing map (SOM) topology; (a)5 x 5 map and (b) hit map



(a)



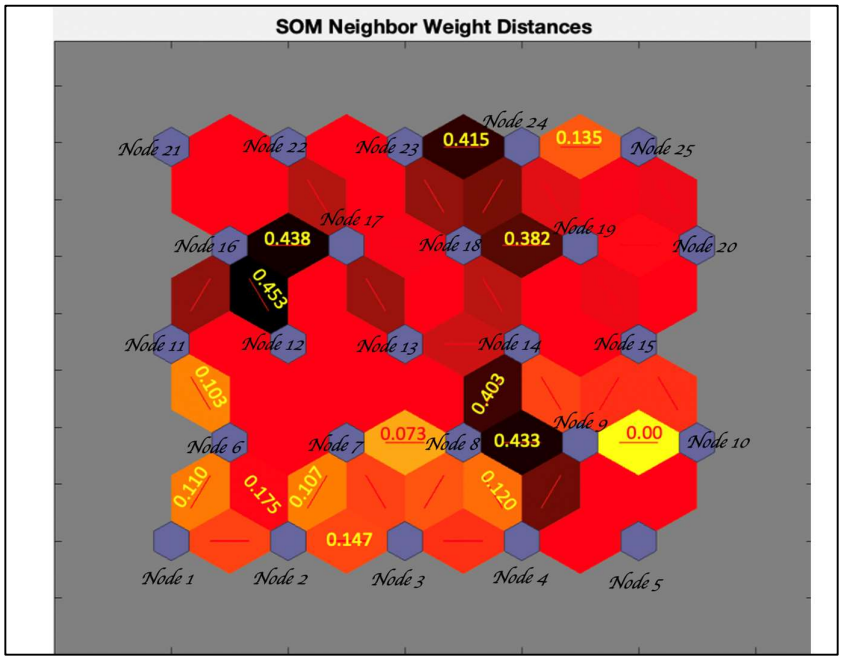
(b)

To assess the effectiveness of the model, hit maps were generated, as shown in Figures 4.2 (a) and (b), revealing how the input data were distributed within clusters. These maps also assessed the quality of clustering, with Clusters 3 and 5 receiving more hits, indicating a better representation of common patterns in the data. However, some clusters lacked associated datasets, suggesting that the chosen number of clusters may not have been ideal for capturing distinct variations in data. Overall, SOM analysis offers valuable insights into mixing design patterns, emphasizing the importance of precise mix design considerations for achieving durable and structurally sound geopolymer concrete composition.

Meanwhile, SOM neighbor weight distance (Figure 4-3) analysis assesses the likeness or disparity between neighboring neuron weight vectors, which determines the influence of the inputs on each neuron's output. The weight distances were calculated using the Euclidean distance in Eqs. 1.

Using the SOM library in MATLAB, these neighbor weight distances are visualized using a colormap, as depicted in Figure 4-3, where the darker shade represents the least relevance between the nodes, while the lightened shade represents the highest relevance of the nodes. This color map provides a graphical illustration to identify clusters of similar information or relevant geopolymer concrete characteristics. For example, r_9 and r_10 are the relevant nodes indicated in the color map.

Figure 4-3: SOM Neighbour Weight Distances



Deriving insights from a trained SOM requires post-processing to create a cluster "recipe," chosen for its accuracy in predicting the durability of geopolymer concrete under various chloride exposure conditions. Ensuring alignment with experimental data and providing reliable recommendations for achieving specific durability levels is crucial. The robustness of the recipe was also considered with the aim of offering reliable suggestions for datasets beyond those used for training.

4.4 Growing SOM simulation

Growing Self-Organizing Maps (GSOM) are a variant of Self-Organizing Maps (SOM) that possess the ability to dynamically adjust their size during the learning process. Unlike traditional SOMs, GSOMs can grow or shrink in response to the input data, allowing them to adapt to and represent complex structures more effectively (Alahakoon et al., 2000). The primary advantage of the GSOM is its capability to automatically expand the map size in regions of high data density, thereby enhancing the ability of the map to capture intricate patterns (Coulson et al., 2023).

4.4.1 Key Features of GSOM

4.4.1.1 Flexible Network Growth

GSOM begins with a small map and grows automatically based on the complexity of the data. This means that the map adds new nodes that are required to better capture the patterns in the data. GSOM can adjust its structure to the fundamental complexity of the input data according to this dynamic development process, which produces a more accurate depiction of the underlying patterns. Flexible network expansion also enables the GSOM to handle datasets of varying sizes and dimensions without the need to predetermine the map size. Therefore, GSOM can effectively capture both local and global data structures, offering a more thorough and nuanced understanding of data properties.

4.4.1.2 Better Data Fit

GSOM adapts to the shape and distribution of the data rather than compressing it into a fixed-size map, giving the information a more realistic and accurate representation, Figure 4-4(a) GSOM sample hits, expanded to 8x9 sample hits. The adaptive nature of GSOM allows it to overcome the limitations associated with fixed-size maps, such as data distortion and the loss of important features. This flexibility enhances the ability of the model to reveal subtle relationships and hierarchies within complex datasets, potentially uncovering insights that may be overlooked by more rigid clustering methods. Furthermore, the self-organizing property of the GSOM enables it to automatically identify and highlight areas of high data density or sparse regions, thereby providing useful details regarding the structure and distribution of incoming data.

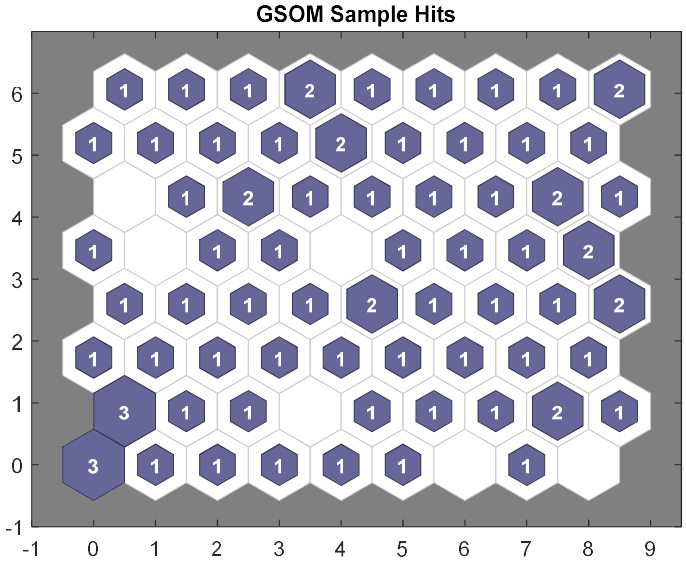
4.4.1.3 Focused Clustering

The GSOM creates more detailed clusters where the data are dense and simplifies the map to less crowded areas, making it easier to identify meaningful groups in the data. GSOM's adaptive clustering approach not only provides a more accurate representation of data but also offers computational efficiency by allocating resources where they are most needed. This dynamic allocation allows for the faster processing of large datasets while maintaining high-quality results.

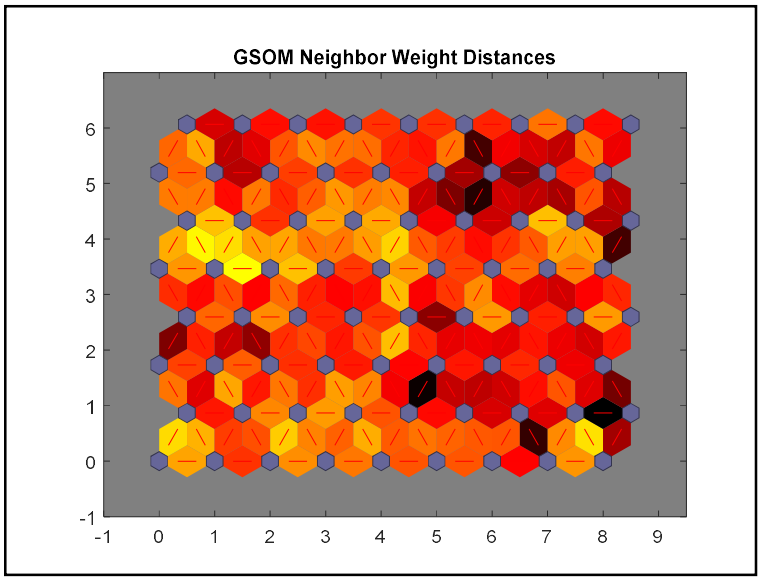
4.4.1.4 Customizable Detail

The extent of map expansion can be regulated by modifying a "spread factor." Increased values result in more intricate details, whereas decreased values result in a more compact and straightforward map. The adaptive nature of the GSOM allows for a more efficient use of computational resources, as it only expands in areas where additional details are required. This flexibility can be particularly useful when dealing with high-dimensional or complex datasets, where traditional fixed-size maps may struggle to capture all the relevant patterns.

Figure 4-4: Growing Self-organizing map(GSOM): (a) GSOM Sample Hits and (b) GSOM Neighbor Weight Distances



(a)



(b)

4.4.2 Summary

The Growing Self-Organizing Map (GSOM) offers several advantages over traditional SOMs, including flexible network growth, better data fit, focused clustering, and customizable details. These features allow GSOM to adapt its structure to the inherent characteristics of the data, making it particularly well-suited for analysing complex and high-dimensional datasets. Deeper insights and more effective data analysis are made possible by GSOM's more precise and efficient representation of data patterns, which is achieved by dynamically expanding and concentrating on dense regions. The ability to control the level of detail by using the spread factor further enhances its versatility, making it a valuable tool for a wide range of applications.

4.5 Prediction of durability

SOM and GSOM revealed a clear analysis that suggests the lowest possible chloride diffusion coefficient in the formulation of geopolymer concrete. This optimal mix proportion is a harmonious blend of a water binding ratio of 0.5, coupled with a molarity of 12, as per the SOM suggested above. The optimal combination is cluster 21 (highlighted in bold), as depicted in Appendix 3, diffusion coefficient = $5.3012e^{-12}$. The specific combination became evident, as it outperformed the other tested formulas. This finding underscores the potential

of this particular formula to significantly mitigate the diffusion coefficient, positioning it as a standout solution with superior capabilities compared with its counterparts.

The comparison between SOM and GSOM, as illustrated in Appendix 3 (WBR = 0.5, Molarity = 12; chloride diffusion coefficient = 5.3012×10^{-12}) and Appendix 4 (WBR = 0.5, Molarity = 12; chloride diffusion coefficient = 5.37×10^{-12}), shows closely aligned results. This similarity confirmed that the GSOM effectively validated the findings obtained from the SOM. Drawing from the data provided, SOM has demonstrated its value as an effective method for clustering geopolymer concrete data and visualizing intricate relationships on a two-dimensional plane. This feature allows for an understanding of how parameters interact and supports the efficient examination of large parameter spaces.

For superior chloride durability, SOM analysis indicated an optimal mix design with the following specifications: NaOH Concentration, 12M - Water-to-binder ratio 0.4, NaOH quantity, 790 g; and Na_2SiO_3 quantity, 390 g. This formulation was expected to yield the lowest chloride diffusion.

4.6 Verification and Validation

This section focuses on the verification and validation of the results obtained from the clustering analysis and the proposed cluster formula for predicting the chloride permeability in fly ash geopolymer concrete. Two main methods were used to guarantee the correctness and dependability of the results: (1) statistical analysis using the Coefficient of Determination (R2) and Mean Absolute Error (MAE) and (2) new validation utilizing experimental chloride migration testing. These methods were used to confirm the robustness of the cluster formula and to validate its predictions under specific conditions.

4.6.1 Statistical Evaluation: MAE and Coefficient of Determination

To verify the accuracy of the cluster formula derived from clustering analysis, a **5-fold cross-validation process** was conducted. The purpose of this procedure was to assess how well the suggested mixing scheme and activator dosage predicted chloride permeability. The performance of the model was assessed using two crucial validation metrics: the Mean Absolute Error (MAE) and Coefficient of Determination (R^2).

4.6.1.1 Mean Absolute Error (MAE)

The model's prediction accuracy is clearly shown by MAE, which calculates the average absolute difference between the expected and actual values.

The formula for MAE is:

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

Equation 4.1

Where y_i is the actual value, $\hat{y}_i$ is the predicted value, and n is the number of samples.

A lower MAE indicates a higher model performance as there are less discrepancies between the anticipated and actual values.

4.6.1.2 Coefficient of Determination (R^2)

The percentage of variance in the dependent factor (chloride permeability), which can be predicted from the independent variables (such as molarity and the water-binder ratio), is measured by R^2. It ranges from 0 to 1, where 1 indicates perfect fit.

The formula for R^2 is:

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

Equation 4.2

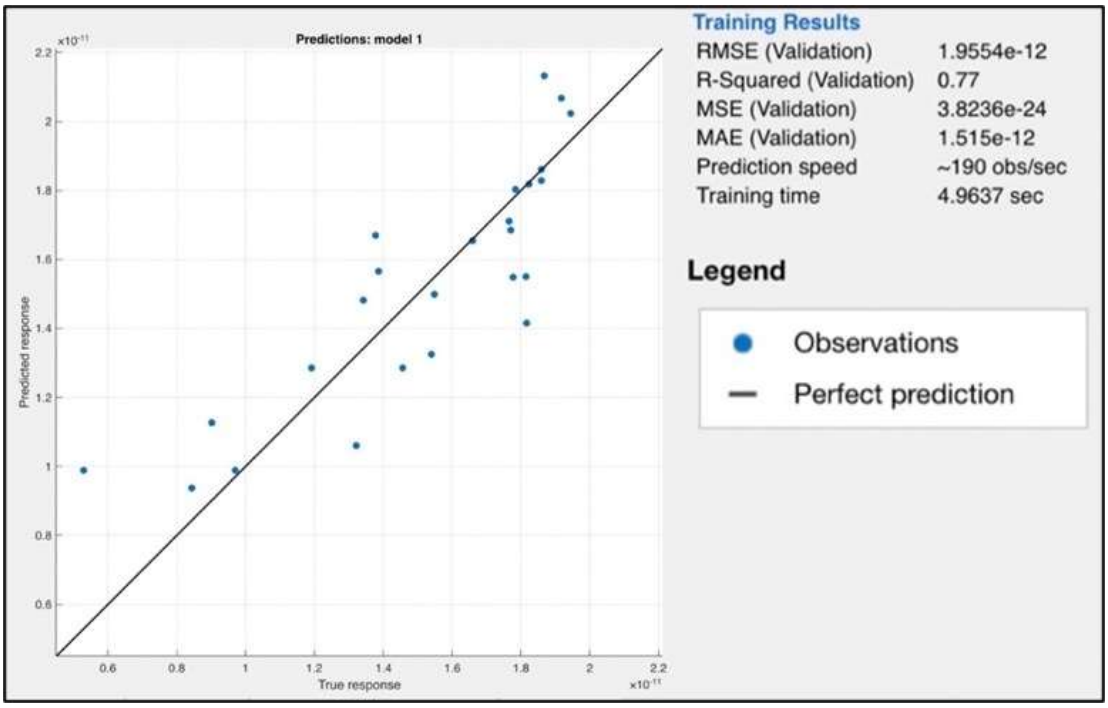
Where $\bar{y}$ is the mean of the actual values.

An R^2 score of approximately 1 indicated that a significant amount of data variability could be explained by the model, confirming its predictive capability.

The results of the 5-fold cross-validation process yielded an **MAE of 1.515e-12** and an **R^2 value of 0.77**. These results demonstrate that the cluster formula effectively forecasts the chloride permeability based on the recommended mixing design and activator dosage. The dependability of the cluster formula is confirmed by the low MAE and high R^2 values, which show significant agreement between the predicted and experimental results. These

validation outcomes instill confidence in the capacity of the cluster formula to guide the selection of optimal mixing designs and activator dosages, thereby ensuring the desired chloride resistance in fly ash geopolymer concrete. Figure 4-5 displays the results of the validation.

Figure 4-5: Performance of the clustering formula generated from the clustering analysis



4.6.2 Fresh Validation: Chloride Migration Testing

To further validate these findings, **fresh experimental testing** was conducted on fly ash geopolymer concrete samples with a **0.5 water-binder ratio (WBR)** and **12 Molarity (12M)** activator concentrations. These specific conditions were chosen based on the cluster formula predictions, which suggested that this combination would exhibit low chloride-ion penetrability.

The predictions of the clustering formula were validated by the chloride migration test results, and the measured chloride penetration depths for the 0.5 WBR and 12M samples were significantly lower than those of the other combinations, indicating superior chloride

resistance, as compare to Figure 4-1 result of Chloride Penetration depth of other combinations.

This finding aligns with the cluster formula's prediction that a higher molarity (12M) and a moderate water-binder ratio (0.5) would result in a denser and more durable geopolymer matrix, reducing the permeability to chloride ions.

The experimental results strongly support the prediction of the cluster formula that the 0.5 WBR and 12M combination exhibits low chloride-ion penetrability. The accuracy of the cluster formula in forecasting the durability in chloride of fly ash geopolymer concretes in chloride environments was strengthened by this validation.

4.6.3 Discussion

The cluster formula for forecasting the chloride resistance of fly ash geopolymer concrete was shown to be accurate and reliable during verification and validation procedures. While new experimental testing confirmed the model's predictions under particular situations, statistical analysis utilizing MAE and R^2 showed that the model produced accurate and consistent predictions.

The accurate validation of the 0.5 WBR and 12M combination demonstrates the cluster formula's promise as a formidable tool for mix design optimization and long-term durability prediction of geopolymer concretes. This study offers a solid foundation for evaluating the performance of fly ash geopolymer concrete in chloride-rich settings by fusing computational modeling with experimental validation.

4.7 Chapter Summary

This section presents the verification and validation of the cluster formula using statistical metrics and experimental testing. The low MAE and high R^2 values confirmed the predictive accuracy of the model, whereas chloride migration testing validated the model's predictions for specific mix designs. The results demonstrate that the cluster formula is a reliable and effective method for predicting the chloride resistance of fly ash geopolymer concrete, providing valuable insights for optimizing mix designs and enhancing durability in chloride-exposed environments.

CHAPTER 5:

CONCLUSION AND RECOMMENDATIONS

This thesis applies an Artificial Neural Network (ANN), specifically the Self-Organizing Map (SOM) algorithm, to achieve its dual objectives of (a) assessing durability as a function of key mix parameters and (b) predicting chloride resistance.

Addressing Objective (a): The SOM was employed to systematically analyze the complex, multi-dimensional dataset generated from this study, where the chloride diffusion coefficient—a key durability metric—was assessed as a function of the water/binder (W/B) ratio and alkali activator concentration (molarity). The SOM's pattern recognition capability was pivotal in identifying and visualizing the hidden correlations within this data.

Addressing Objective (b): The core predictive function of the ANN/SOM model was its ability to cluster and forecast performance. The analysis specifically revealed a distinct, optimal cluster indicating that the mix design combination of a 0.5 W/B ratio and 12M NaOH activator consistently resulted in the lowest chloride diffusion coefficients. This identified optimal formula was not merely a statistical output but was rigorously validated through fresh experimental chloride migration tests, confirming the model's predictive accuracy for durability in chloride environments.

Summary of AI Contribution: The application of SOM served three critical functions in meeting these objectives:

1. Efficient Data Synthesis: It processed the complex dataset (linking W/B ratio, molarity, and diffusion results) to reveal patterns not easily discernible through conventional analysis.

2. Predictive Pattern Recognition: It successfully identified the optimal parameter combination (0.5 W/B, 12M) for minimizing chloride penetrability, fulfilling the predictive aim of the ANN adoption.

3. Resource-Efficient Optimization: By pinpointing this optimal mix, the model provides a direct pathway for designing durable geopolymer concrete, enabling targeted use of materials and reducing trial-and-error in future mix development.

In conclusion, this case study demonstrates that the SOM is an effective ANN tool for both assessing the influence of mix parameters on chloride durability and reliably predicting optimal mix designs for enhanced performance, thereby achieving the core objectives of this research. The validated optimal formulation offers a reliable reference for engineers seeking to improve the long-term durability of geopolymer concrete in chloride-prone environments.

5.1 Contributions to knowledge

The data-driven method in this study introduces the optimization of mix designs for enhanced chloride resistance, which provides a substantial addition to the area of geopolymer concrete. This work offers a novel and effective method of predicting the lifespan of fly ash geopolymer concrete in scenarios with high chloride levels by creating a cluster formula and applying the Self-organising Maps & Growing Self-organising Maps (GSOM) model. With the use of these tools, the best mix parameters, such as the water-binder ratio and activator concentration, can be found to improve the resistance of the material to chloride penetration. The results establish a solid framework for creating geopolymer concrete with exceptional long-term performance, particularly in challenging environments, and offer engineers and researchers useful practical insights. This work promotes the creation of more robust and sustainable building materials while also advancing our understanding of the durability of geopolymer concretes.

5.2 Recommendations for Future Work

5.2.1 Studies on Long-term Durability

Long-term durability studies could involve monitoring the performance of concrete under various environmental conditions such as marine environments, de-icing salt exposure, or industrial settings with high chloride concentrations. Accelerated aging tests can also be employed to simulate long-term exposure within a short time frame. Chloride diffusion coefficients, modifications to mechanical characteristics (such as compressive and tensile strength), and microstructural changes using methods such as scanning electron microscopy (SEM) and X-ray diffraction (XRD) are the main factors to be assessed.

In addition, a comparison of the long-term performance of fly ash geopolymer concrete with that of conventional Portland cement-based concrete highlights its advantages and limitations. Such studies would not only validate the suitability of the material for chloride-exposed environments, but also provide data to refine predictive models and design guidelines, ensuring safer and more durable infrastructure.

5.2.2 Expanded Dataset

To enhance the reliability and generalizability of findings related to fly ash geopolymer concrete, it is advisable to include a more extensive and varied dataset. A greater variety of factors, such as curing conditions, should be included in this dataset (e.g., ambient curing, heat curing, or steam curing), temperature variations (e.g., extreme cold or hot climates), and exposure to other aggressive agents such as sulfates, acids, or fire.

A more thorough knowledge of how these variables affect a material's mechanical strength, durability, and resistance to chloride permeability is possible with an extended dataset. For instance, varying the curing conditions can significantly affect the geopolymerization process, which in turn affects the concrete microstructure and long-term performance. Similarly, exposure to sulfates or high temperatures could reveal potential vulnerabilities or strengths that are not apparent under standard testing conditions.

Predictive models would be more accurate and laboratory results would be further validated if real-world data, such as structures exposed to industrial or marine environments, were included. Patterns, correlations, and the best mix designs for certain environmental

circumstances can then be found using advanced data analytics and machine learning approaches.

To ensure that fly ash geopolymer concrete is suitable for a wider range of infrastructure projects and environmental concerns, researchers may provide more comprehensive recommendations for its practical implementation by increasing the dataset. Ultimately, this will aid in the development of stronger and more sustainable building materials.

5.2.3 Alternative Activators

Future studies should concentrate on the application of different activators or innovative activator combinations to further develop fly ash geopolymer concretes. Although they are often employed in geopolymerization, traditional activators like sodium hydroxide (NaOH) and sodium silicate (Na_2SiO_3) may have drawbacks in terms of price, environmental effect, and performance under particular circumstances. Exploring alternative activators, such as potassium-based solutions, calcium-rich compounds, or even waste-derived materials (e.g., rice husk ash or slag), could lead to more sustainable and efficient geopolymer systems.

Optimization of the geopolymerization process using alternative activators can enhance the chloride resistance of the material by improving its microstructure and reducing its porosity. To prevent chloride infiltration and the corrosion of implanted reinforcements, activators with varying alkali concentrations or chemical compositions may encourage the development of a denser and more durable geopolymer matrix. Additionally, combining multiple activators or incorporating supplementary materials such as nanomaterials or industrial by-products can further refine the properties and performance of geopolymers.

Future work should also explore the environmental and economic implications of using alternative activators, including their carbon footprint, availability, and scalability for large-scale applications. Researchers can identify the best formulations that strike a compromise between performance, sustainability, and cost-effectiveness by methodically assessing how various activators affect the geopolymerization process, mechanical characteristics, and durability. This will pave the way for the development of next-generation

geopolymer concrete with enhanced chloride resistance and broader applicability in aggressive environments.

5.2.4 Machine Learning Enhancements

Future studies should concentrate on utilizing cutting-edge machine-learning (ML) approaches to further enhance the forecasting capacities for chloride permeability in fly ash geopolymer concrete. This study demonstrates how techniques such as deep and ensemble learning can be used to increase the precision and resilience of prediction models; however, there is significant scope for expanding and refining these approaches to achieve even greater performance and reliability.

Future research should investigate how Self-organising Maps (SOMs) may be integrated with more sophisticated machine learning techniques, including gradient boosting machines (GBMs), recurrent neural networks (RNNs), and convolutional neural networks (CNNs). These methods can be used in conjunction with SOMs, which are useful for grouping and visualizing high-dimensional data, to reveal intricate patterns and connections within a dataset. For instance, SOMs can be used as a preprocessing step to identify clusters of similar data points, which can then be fed into neural networks or support vector machines (SVMs) for more accurate predictions.

Additionally, to combine the advantages of several models and lower prediction errors, the use of ensemble techniques, such as stacking, AdaBoost, and random forests, should be studied. Ensemble techniques can improve model robustness by mitigating the limitations of individual algorithms and enhancing the generalization to unseen data.

Another promising direction is the application of deep learning models that can automatically extract intricate features from raw data, such as microstructural images or chemical compositions, to predict the chloride permeability. To increase the forecast accuracy and identify non-linear interactions, these models can be trained using vast, varied datasets.

Future studies should concentrate on model interpretability and uncertainty quantification to ensure the dependability of these models. Bayesian methods or Monte Carlo simulations can be used to quantify the uncertainty in the predictions, whereas Shapley

Additive explanations (SHAP) or Local Interpretable Model-agnostic Explanations (LIME) can be used to explain model predictions.

Finally, a more thorough knowledge of chloride transport pathways in geopolymer concrete may be possible with the creation of hybrid models that blend data-driven machine learning approaches with physics-based concepts. Such models would integrate domain knowledge with the predictive power of ML, leading to more accurate and physically meaningful predictions.

Future research can significantly improve the precision, resilience, and applicability of chloride permeability predictions by developing machine learning techniques and combining them with domain-specific knowledge. This will ultimately aid in the development of more resilient and environmentally friendly building materials.

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APPENDICES

Appendix 1:
An Overview of Research Studies On Geopolymer Concrete and Its Composites Using Machine Learning

Author	Year	Raw Material	Focused parameters	Test method	Main outcome
Gomaa et al.	2024	Class C fly ash, Alkali activators ($NaOH/Na_2SiO_3$), Aggregates	Slump flow, Compressive strength	Rheometry (slump), Compression testing (ASTM C39), XRD, SEM	Random Forest (RF) model identified optimal activator ratios ($Na_2SiO_3/NaOH$ = 1.5–2.0) and mixing energy (≥500 rpm) for strength (↑30%) and workability (↑25%)
Zhang et al.	2024	Fly ash concrete (FA: 0–40%), NaCl solution	Free Cl^- concentration, Exposure time, Penetration depth	Potentiometric titration (ASTM C1218), XRD	1D-CNN outperformed MLP/SVR in predicting Cl^- distribution, especially at low concentrations (<0.1%). Validated against Fick's law (↑30% accuracy)
Emad Golafshani et al.	2024	Fly ash, GGBFS, Natural aggregates, $NaOH/Na_2SiO_3$ activators	Elastic modulus (EGC), Compressive strength (CS), Chemical composition (22 input variables)	Uniaxial compression tests (ASTM C469), XRD, SEM	XGBoost-MOGWO hybrid outperformed traditional models, identifying optimal SCM blends (Fly ash/GGBFS = 70/30) and curing conditions (CT = 60°C, HTCD = 1 day) for maximal EGC (↑28.5 GPa)
Tanyildizi et al.	2021	Fly ash, $NaOH/Na_2SiO_3$ activators	Geopolymerization peak time, Geopolymerization peak heat, Dissolution peak time, Dissolution peak heat	Isothermal calorimetry (ASTM C1679)	Deep LSTM outperformed SVR/kNN in predicting reaction kinetics, capturing nonlinear time-dependent heat flow patterns.
Ding et al.	2023	Multiple solid wastes (fly ash, slag, red mud, rice husk ash, steel slag, etc.)	Compressive strength, Chemical composition (Al_2O_3, CaO, SiO_2)	Uniaxial compression tests, XRD, SEM	XGBoost model identified optimal waste combinations (high CaO + moderate SiO_2) for maximum strength (↑45MPa) while SHAP analysis revealed CaO content as most critical parameter.
Mohammed et al.	2025	Natural fibers (jute, hemp, flax, sisal) + Concrete	Compressive strength, Flexural strength, Toughness, Crack resistance	Compression tests (ASTM C39), Flexural tests (ASTM C78), SEM/XRD for microstructure	AI models overcome variability in fiber properties and optimize fiber-matrix bonding for enhanced mechanical performance.
Chen et al.	2024	Recycled Concrete Aggregate (RCA), Recycled Brick Aggregate (RBA), Fly Ash (FA), Alkali activators (NaOH + Na_2SiO_3), Construction & Demolition Waste (C&DW) sources	Morphological: Axial coefficient, angularity, sphericity, Physical/Mechanical: Crushing value, water absorption, apparent density, Physical/Mechanical: Crushing value (GB/T 14685), water absorption, apparent density	Image processing + Machine Learning (Decision Tree)	Optimal SiO_2/Na_2O molar ratio (Ms = 1.4) for FGP coating: ↑ Apparent density (2.3–2.6%); ↓ Crushing value (21.6–22.2%); ↑ Water absorption (2.1–5.8%) due to coating thickness/geopolymerization.

Appendix 2:
Weight vectors of 5x5 nodes rounded to the nearest 4 decimal places from SOM in MATLAB

j	$w_{j,1}$	$w_{j,2}$	$w_{j,3}$	$w_{j,4}$	$w_{j,5}$	$w_{j,6}$
1	1.0000	0.6667	0.6641	0.6641	1.0000	0.8546
2	0.8947	0.6686	0.6115	0.6115	0.8947	0.8678
3	0.8000	0.6667	0.5308	0.5308	0.8000	0.8916
4	0.6909	0.6667	0.4587	0.4580	0.6909	0.8355
5	0.6000	0.6667	0.3987	0.3974	0.6000	0.8174
6	0.9744	0.7564	0.7325	0.7325	0.9744	0.8118
7	0.8000	0.8333	0.6641	0.6641	0.8000	0.8237
8	0.8000	0.7500	0.5974	0.5974	0.8000	0.8127
9	0.6000	0.6667	0.3987	0.3974	0.6000	0.4619
10	0.6000	0.6667	0.3987	0.3974	0.6000	0.6702
11	1.0000	0.8333	0.8308	0.8308	1.0000	0.7429
12	0.8974	0.8675	0.7754	0.7754	0.8974	0.7049
13	0.8000	0.8333	0.6641	0.6641	0.8000	0.6459
14	0.6741	0.8457	0.5666	0.5666	0.6741	0.7314
15	0.6000	0.8333	0.4974	0.4974	0.6000	0.7951
16	1.0000	1.0000	1.0000	1.0000	1.0000	0.4399
17	0.8000	1.0000	0.7974	0.7974	0.8000	0.6032
18	0.8000	0.8333	0.6641	0.6641	0.8000	0.5438
19	0.6000	1.0000	0.5974	0.5974	0.6000	0.6462
20	0.6000	0.8333	0.4974	0.4974	0.6000	0.6525
21	1.0000	1.0000	1.0000	1.0000	1.0000	0.2347
22	0.9034	1.0000	0.9022	0.9022	0.9034	0.3885
23	0.8000	1.0000	0.7974	0.7974	0.8000	0.4155
24	0.6667	1.0000	0.6641	0.6641	0.6667	0.5433
25	0.6000	1.0000	0.5974	0.5974	0.6000	0.5404

Appendix 3:
Predicted Chloride Diffusion Coefficients from SOM 5 x 5 nodes

Cluster	WBR	Molarity	NaOH (g)	Na_2SiO_3 (g)	Water (ml)	Chloride Diffusion Coefficient (m^2/s)
1	0.5	10	648	324	1620	$1.8170e^{-11}$
2	0.5	8.9697	581.0303	290.5152	1620	$1.7847e^{-11}$
3	0.5	8.0000	518.0000	259.0000	1620	$1.8673e^{-11}$
4	0.4548	8.0000	471.0323	235.5161	1473	$1.9165e^{-11}$
5	0.4	8.0000	414	207	1296	$1.9443e^{-11}$
6	0.5	10.0000	648	324	1620	$1.5490e^{-11}$
7	0.4658	9.1053	545.3684	272.6842	1509	$1.7656e^{-11}$
8	0.4567	8.8667	518.0000	259.0000	1479	$1.8233e^{-11}$
9	0.3452	8.0000	357.5161	178.4839	1118	$1.8592e^{-11}$
10	0.3452	8.0000	357.5161	178.4839	1118	$1.8592e^{-11}$
11	0.5	10	648	324	1620	$1.3425e^{-11}$
12	0.4400	10.5333	600.5333	300.2667	1425	$1.5398e^{-11}$
13	0.4000	10.000	518.0000	259.0000	1296	$1.8148e^{-11}$
14	0.3400	9.1000	405.3500	202.4500	1101	$1.6593e^{-11}$
15	0.3000	8	311.0000	155.0000	972	$1.7699e^{-11}$
16	0.5000	12	780	390	1620	$9.6929e^{-12}$
17	0.4000	12.0000	622	311	1296	$1.3216e^{-11}$
18	0.4000	10	518	259	1296	$1.3857e^{-11}$
19	0.3000	9.7143	377.0000	188.4286	972	$1.3776e^{-11}$
20	0.3000	10.000	388	194	972	$1.7781e^{-11}$
21	**0.5000**	**12**	**780**	**390**	**1620**	$\mathbf{5.3012e^{-12}}$
22	0.4515	12.0000	703.3939	351.6970	1462	$8.4333e^{-12}$
23	0.4000	12	622	311	1296	$9.0224e^{-12}$
24	0.3000	12	466	233	972	$1.1914e^{-11}$
25	0.3000	12	466	233	972	$1.4555e^{-11}$

Appendix 4:
Predicted chloride diffusion coefficients from GSOM

Cluster	WBR	Molarity	NaOH (g)	Na_2SiO_3 (g)	Water (ml)	Chloride Diffusion Coefficient (m^2/s)
1	0.5	10	648	324	1620	$1.810e^{-11}$
2	0.5	8.9697	581.0303	290.5152	1620	$1.7847e^{-11}$
3	0.5	8	518	259	1620	$1.88e^{-11}$
4	0.4531	8.0000	469.25	234.625	1468.125	$1.91e^{-11}$
5	0.4	8.0000	414	207	1296	$1.96e^{-11}$
6	0.5	10.0000	648	324	1620	$1.57e^{-11}$
7	0.4684	9.1053	548.789	274.3947	1517.684	$1.765e^{-11}$
8	0.4567	8.8667	518	259	1485.931	$1.82e^{-11}$
9	0.3468	8.0000	359.281	179.375	1123.875	$1.83e^{-11}$
10	0.3468	8.0000	359.281	179.375	1123.875	$1.83e^{-11}$
11	0.5	10	648	324	1620	$1.34e^{-11}$
12	0.4433	10.5333	604.866	302.433	1436.4	$1.53e^{-11}$
13	0.4	10.000	518	259	1296	$1.82e^{-11}$
14	0.3494	9.1000	404.8684	202.2100	1099.894	$1.65e^{-11}$
15	0.3	8	311	155	972	$1.77e^{-11}$
16	0.5	12	780	390	1620	$9.699e^{-12}$
17	0.4	12.0000	622	311	1296	$1.356e^{-11}$
18	0.4	10	518	259	1296	$1.39e^{-11}$
19	0.3	9.7143	377.00	188.4285	972	$1.386e^{-11}$
20	0.3	10.000	388	194	972	$1.7651e^{-11}$
21	**0.5**	**12**	**780**	**390**	**1620**	**$5.37e^{-12}$**
22	0.45	12	701	350.5	1458	$8.373e^{-12}$
23	0.4	12	622	311	1296	$9.024e^{-12}$
24	0.3	12	466	233	972	$1.1514e^{-11}$
25	0.3	12	466	233	972	$1.4555e^{-11}$

Appendix 5:
Publications

1. **Fong Wen Lee** , Chang Wui Lee, Teo Siaw Hui, Tay Kai Meng, Annisa Jamali, Mohamad Nazim bin Jambli , and Idawati Ismail (2025), Factors Controlling Durability of Geopolymer Concretes in Chloride Determined via Growing Self-Organizing Maps. *Pertanika Journal of Science and Technology*,
2. **Fong Wen Lee**, Chang Wui Lee, Teo Siaw Hui, Nur Fadhilah Mohamad Tahan, Tay Kai Meng, Annisa Jamali, Mohamad Nazim Bin Jambli, Rehman Ullah Khan and Idawati Ismail (2024), Optimal Curing Temperature for Determination of Compressive Strength of Geopolymer Concrete via Artificial Neural Network (ANN), presented at *4th International Conference on Science, Engineering and Technology, Bandung, Indonesia 10-11 Julai 2024*

Appendix 6:
SOM Code

```
clear all; clc;
folderDir = ''; % set folder directory
fileName = 'DATA.xlsx'; % set filename
sheetName = 'Sheet1'; % set sheetname for excel.
colRange = 'A2:D181'; % set column range for excel.

data = excelDataExtraction(folderDir, fileName, sheetName, colRange); %
extract data from external file.
x = data./max(data); % normalise data.

%% SOM clustering.
for m1 = 1:5
for m2 = 1:5
map_sz = [m1,m2]; % define SOM network map size.
cluster_no = map_sz(1) * map_sz(2); % determine number of clusters from
map size.
net = selfOrganisingMap(x, map_sz);
% net = selforgmap(map_sz); % set initialise SOM learning architecture.
% [net,tr] = train(net , x'); % SOM network training/learning
y = net(x'); % obtain data class from clusters.
data_cluster = vec2ind(y)'; % extract data class in numerical indexing.
w = net.IW{:}; % obtain cluster weight vectors.
%writematrix(w, strcat('Result_in_ExcelA2:C181/SOM-data-A2:C181-',
num2str(m1), 'x', num2str(m2), '.xlsx'), 'Sheet','Protytope Weight');
w2 = net.IW{:}.* max(data); % obtain cluster recipe.
%writematrix(w, strcat('Result_in_ExcelA2:C181/SOM-data-A2:C181-',
num2str(m1), 'x', num2str(m2),'.xlsx'), 'Sheet','SOM Recipe');
% plot sample hit map
%saveas(plotsomhits(net,x'), strcat('Result_in_ImageL4:R543/SOM-sampleHit-
A2:C181-', num2str(m1), 'x', num2str(m2),'.png'));
% plot sample hit map
%saveas(plotsomplanes(net), strcat('Result_in_ImageL4:R543/SOM-
mapPlane-A2:C181-', num2str(m1), 'x', num2str(m2),'.png'));
% plot map neighbouring distance
%saveas(plotsomnd(net), strcat('Result_in_ImageL4:R543/SOM-
neightbourDistance-A2:C181-', num2str(m1), 'x', num2str(m2),'.png'));
end
end
```

Appendix 7:
GSOM Code

```
function GSOM
close all; clear all;
% GHSOM starts with 2x2 map size.
% after training, hit sample is counted.
% IF average hit samples in a row is maximum, add a new row below it.
% new weight initiated from the top row.
% IF average hit samples in a column in maximum,add new column to the right,
% To control the growth, limit the spliting with a constant threshold.

% x = iris_dataset;
inputFolder = ''; % select local folder.
% fileName = 'FYP RAW DATA.xlsx'; % data file name.
fileName = 'DataSet.xlsx';
tab = 'Jas'; % tab
col = 'A2:P80'; % columns that contains data.
% col = 'B4:G33';
data = fmeaDataExtraction(inputFolder, fileName, tab, col);
% data is the training data.
%% normalise data into [0,1] range.
x = data./max(data);
x = x';
a = 1;
b = 1;
epoch = 200;
nn = a*b;
grow = 1;
hit_threshold = 9;
net = selforgmap([a b]);
x = x./max(x')';
% x = x(1:3,:);
net = configure(net, x);

% while ep <= 200

net.trainParam.epochs= epoch;
[net, y] = TypicalSOM(a,b,x, net, grow);
%net.IW{:}

save(strcat('GHSOM/result/mat/somnet-',num2str(grow),'.mat'),
'net','a','b','x'); while max(sum(y,2)) > hit_threshold
% stop growing when maximum hit sample hit a threshold.
newnodtop = [];
grow = grow + 1
```

```
B = reshape(sum(y,2),[a,b]);
net_row = sum(B,1);
net_col = sum(B,2);
if find(net_row == max(max(net_row), max(net_col)))
% find high hit nodes horizontal map
ind = find(net_row == max(max(net_row), max(net_col)));
% get the row number for expansion
nodtop = reshape(1:a*b, [a,b]);
if ind > 1
newnodtop(:,1:ind) = nodtop(:,1:ind);
newnodtop(:,ind+1:size(nodtop,2)+1) = nodtop(:,ind:end);
else
newnodtop = [nodtop(:,ind), nodtop];
end
ordering = reshape(newnodtop,[numel(newnodtop),1]);
wold = net.IW{1};
w = wold(ordering,:);
 [a,b] = size(newnodtop);

net = selforgmap([a b]);
net = configure(net,w');
net.IW{1} = w;
net.trainParam.epochs= epoch;

%new_weight1 = net.IW{1}
 [net, y] = TypicalSOM(a,b,x, net, grow);
save(strcat('GHSOM/result/mat/somnet-',num2str(grow),'.mat'),
'net','a','b','x');
%new_weight2 = net.IW{1}
elseif  find(net_col == max(max(net_row), max(net_col)))
% find high hit nodes vertical map
ind = find(net_col == max(max(net_row), max(net_col)));
% get the column number for expansion
nodtop = reshape(1:a*b, [a,b]);
if ind > 1
newnodtop(1:ind,:) = nodtop(1:ind,:);
newnodtop(ind+1:size(nodtop,1)+1,:) = nodtop(ind:end,:);
else
newnodtop = [nodtop(ind,:);nodtop];
end

ordering = reshape(newnodtop,[numel(newnodtop),1]);
wold = net.IW{1};
w = wold(ordering,:);
[a,b] = size(newnodtop);
net = selforgmap([a b]);
```

```
net = configure(net,w');
net.IW{1} = w;
net.trainParam.epochs= epoch;
%new_weight1 = net.IW{1}
[net, y] = TypicalSOM(a,b,x, net,grow);
save(strcat('GHSOM/result/mat/somnet-',num2str(grow),'.mat'), 'net','a','b','x');
%new_weight2 = net.IW{1}
end

end

getWeightVector(net,max(data));

end

function [net,y] = TypicalSOM(a,b,x, net,grow)
% read learnsom matlab file.
% net.IW{1}
[net,tr] = train(net,x);
y = net(x);
cluster_index = vec2ind(y);
% plotsomtop(net);
figure(1),plotsomhits(net,x);
saveas(gcf,strcat('GHSOM/result/hitsample/hitsample-', num2str(grow), '.png'));
% plotsomnc(net);
figure(2),plotsomnd(net);
saveas(gcf,strcat('GHSOM/result/noderelation/nodeRelation-',
 num2str(grow), '.png'));
% plotsomplanes(net);

w = net.IW{1};
clf(figure(3));
figure(3),hold on;

% plot3(w(:,8),w(:,2),w(:,3),'xk', 'MarkerSize', 12, 'linewidth', 2);
% plot3(x(8,:), x(2,:),x(3,:), '.r', 'MarkerSize', 12);
% % % for j = 1:size(x,2)
% % %     text(x(1,j), x(2,j), num2str(find(y(:,j)==1)), 'FontSize', 12,
'FontName', 'Times', 'Color', [128 128 128]/255);
% % % end
% % % for j = 1:size(w,1)
% % %     text(w(j,1), w(j,2), num2str(j), 'FontSize', 28,
'FontName', 'Times', 'Color', 'k');
% % % end
topomap = reshape(1:a*b,[a,b]);
% for j = 1:a
```

```
%for k = 1:b
%if k+1 <= b
%plot3([w(topomap(j,k),8);w(topomap(j,k+1),8)],[w(topomap(j,k),2);
w(topomap(j,k+1),2)],[w(topomap(j,k),3);w(topomap(j,k+1),3)],'-r');
%end
%if k-1 > 0
%plot3([w(topomap(j,k),8);w(topomap(j,k-1),8)],[w(topomap(j,k),2);
w(topomap(j,k-1),2)],[w(topomap(j,k),3);w(topomap(j,k-1),3)],'-r');
%end
%if j+1 <= a
%plot3([w(topomap(j,k),8);w(topomap(j+1,k),8)],[w(topomap(j,k),2);
w(topomap(j+1,k),2)],[w(topomap(j,k),3);w(topomap(j+1,k),3)],'-r');
%end
%if j-1 > 0
%plot3([w(topomap(j,k),8);w(topomap(j-1,k),8)],[w(topomap(j,k),2);
w(topomap(j-1,k),2)],[w(topomap(j,k),3);w(topomap(j-1,k),3)],'-r');
%end
%end
% end
saveas(gcf,strcat('GHSOM/result/data/Data-', num2str(grow), '.png'));
end

function data = fmeaDataExtraction(inputFolder, fileName, tab, col)
%this function read excel file.
%extract columns from file.
num = readmatrix(strcat(inputFolder,fileName), 'Sheet',tab,'Range',col);
% row is the training data.
% here we combne left and right measurement feature as single input vector.

data = num;
end

function getWeightVector(net, norm)
w = net.IW{:};
recipe = w.*norm;
end
```