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# Machine Learning–Driven Ultrasonic Characterization of Cement Mortar HydrationAcross Extended Temperature Ranges

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**Abstract- Backscattering study of ultrasonic waves is a non-destructive technique used in characterization of cement mortar during hydration. Experimentally measured Attenuation, acoustic impedance, amplitude and velocity of ultrasonic waves at 25C, 32C, and 42C temperatures are considered for analysis. The present study explores different Machine learning models and expands the experimental data recorded at 25C, 32C and 42C to a range of 20C to 45C. Three machine learning models: linear regression, backpropagation-based neural network and linear discriminant analysis (LDA) are used for extrapolation. The critical phase transitions during hydration of cement mortar was detected. For this the angular relationship between attenuation and impedance vectors, was analysed by the Sliding Window Principal Component Analysis (SW-PCA) approach. Further volatility angle was analyzed to distinguish stable, transitional, and decoupled microstructural states of mortar. The SW-PCA approach again used to evaluate the extended datasets generated by various machine learning models. From ultrasonic wave velocity and impedance, density of mortar is estimated for both experimental and predicted datasets. This study was incorporated with angular volatility trends to obtain threshold temperatures for effective setting in mortar. The present study signifies that 25C supports a controlled and consistent solidification. 32C corresponds to a kinetic transition state exhibiting an elevated instability in microstructure and 42C leads to accelerated but structurally weaker densification. Further in the chosen machine learning models, linear regression captures overall trends, LDA and neural network models more appropriately represent non-uniform hydration behaviour and effective capture of crossover effects. The proposed SW-PCA analysis along with the ML framework captures an improved insight into temperature-dependent microstructural evolution during hydration.**

**Keywords: Ultrasonic NDT, Sliding Window PCA, Angular Volatility.**

## I. INTRODUCTION

Mortar, a cementitious material, is a combination of cement, sand and water. Cement mortar is a commonly used material in the construction industry. As urban cities are developing more rapidly, now a days the demand for cement mortar is also increasing [1]. Hence, it is essential to ensure the two critical properties of the mortar, mechanical strength and hardness, which directly influence its performance and durability in civil infrastructure. These properties of mortar decide the structural integrity of any construction to withstand various environmental and service conditions in the long run. To fulfil these requirements, the real-time monitoring of cementitious materials during the early stages of hydration is essential [2].

In ultrasonic, the non-destructive testing is one of the important techniques to characterize materials, as it can evaluate many properties of a material without damaging the internal structure of the material. Hence, this evaluation of mortar provides a versatile tool for the durability and stability of construction materials and infrastructure [3]. The propagation of ultrasonic waves through cement mortar is governed by its elastic properties and internal heterogeneities [4]. Parameters such as ultrasonic wave attenuation, wave velocity and frequency-dependent response are sensitive to changes in density, stiffness, and microstructural development during hydration [5]. During hydration of cement, the formation of calcium silicate hydrate (C–S–H) and other products leads to a progressive increase in stiffness and reduction in porosity, this can be effectively captured through ultrasonic measurements [6].

While propagating inside the material, ultrasonic waves get attenuated and this in turn provides information about internal structure like voids, cracks and other discontinuities [7] which are important for determining resistance to freeze–thaw cycles, durability and mechanical degradation [8]. During the hydration process of cement mortar, the formation of solid phases increases stiffness and reduces porosity, which in turn affects the ultrasonic wave velocity and attenuation. Analyzing these changes over a wide range of temperatures makes measurement of different parameters complex and challenging [9]. To study this type of multi-parameter analysis [10], [11], machine learning techniques are efficient tools to extract meaningful information from high dimensional data. This data can be reduced dimensionally without damaging the major variance in the given dataset by using Principal Component Analysis (PCA), a valuable statistical tool.

Application of PCA to ultrasonic backscattered signals from mortar at different temperatures could retain more than 93% of the information in a reduced 2D space, with correlations between acoustic impedance and ultrasonic velocity exceeding 96% [9]. They reveal a constant progression from basic PCA applications to classy multi-parameter analysis systems. The usual single-parameter study may be inadequate in many complex material systems. Hence the combination of this multiple signal processing techniques and machine learning is an improvement in characterisation [12].

There are several factors of environment and real world conditions influencing the hydration of cement mortar systems. These factors include temperature, wind, moisture, precipitation, etc. Among these factors, temperature provides a simplest parameter whose influence can be recorded in laboratory environment and then by applying a machine learning model, it will project into the real world conditions. Therefore, the present study explores the methodology to apply the machine learning models on ultrasonic backscattering records on hydrating cement mortar to project the real world temperature conditions.

## II. LITERATURE SURVEY

Non-destructive evaluation using ultrasonic has been extensively used for the characterization and monitoring of cementitious materials. A comprehensive overview of ultrasonic pulse velocity (UPV) evaluation methods, covering measurement techniques and their correlations with mechanical properties was studied by Panzera et al. [4]. Yaman [14] investigated the effects of specimen geometry and transducer frequency (54, 82, and 150 kHz) on UPV measurements in mortar, finding that as path length increases, there is a significant reduction in measured UPV. Keskin et al. [15] demonstrated that choosing appropriate frequency and travel path distance is critical for monitoring UPV development in fresh cementitious materials during the first 24 hours after mixing. An ultrasonic Non-Destructive Testing (NDT) characterization was conducted using an ultrasonic reflection transducer with central frequency 0.5 MHz as reported by Lofti et.al.[16].

Sayers and Dahlin [6], in a foundational study, showed that ultrasonic compressional wave velocity decreases slightly during the first few hours after mixing, followed by a rapid rise as the solid phase becomes interconnected — demonstrating that ultrasonic waves are sensitive to the critical point at which the solid phase acquires load-bearing capacity. Qin and Li [1] developed embedded piezoelectric transducers for in-situ cement paste hydration monitoring, measuring wave velocity, amplitude, and dynamic modulus. Kamada et al. [17] confirmed that the maximum amplitude of ultrasonic waveforms reflects changes in shear resistance, while wave velocity correlates with the formation of ettringite crystals as observed by SEM and X-ray diffraction. Punurai et al. [9] developed an analytical model for predicting ultrasonic attenuation in cement paste containing randomly distributed spherical air voids. Treiber et al. [18] extended this to multiphase materials containing both sand inclusions and air voids. Molero et al. [19] showed that velocity information identifies changes in volume fraction of aggregates, whereas attenuation is more sensitive to aggregate size variations.

Wunderlich et al. [12] demonstrated PCA as an unsupervised learning step within NDE acoustic signal processing pipelines. Lotfi et al. [9] directly applied PCA to ultrasonic backscattered signals from mortar at three temperatures, retaining more than 93% of information in 2D projection. Toufigh and Ranjbar [20] developed an unsupervised deep learning framework achieving 95% prediction accuracy for damage detection. Mukhti et al. [21] applied deep learning techniques, Recurrent Neural Networks to ultrasonic pulse wave data for early detection of concrete damage due to rebar corrosion. Aregbesola et al. [10] applied CNN, Inception Time, and Rocket models to classify 16 cementitious mixtures, achieving accuracy greater than 0.98.

Many studies related to cement mortar are generally limited to laboratory conditions whereas studies in real field surroundings are limited to validation. Moreover the application of PCA at different temperature ranges of multi parameter ultrasonic data of mortar are not systematically explored [9]. Additionally, combination of multiple signal processing approaches and PCA enhances the approach of characterisation of complex material systems. The key research gap lies in the lack of energetic, temperature-resolved frameworks capable of capturing transient instabilities and non-linear hydration behaviour in ultrasonic monitoring of cementitious materials.

## III. METHODOLOGY

In this study a hybrid data-driven framework for ultrasonic characterization of cement mortar was proposed by integrating signal processing, PCA analysis, and machine learning techniques. The dataset included backscattered ultrasonic measurements obtained from mortar samples treated at 25C, 32C, and 42C, where four key parameters, acoustic impedance, attenuation, amplitude, and ultrasonic velocity were measured as functions of hydration time [9]. Furthermore, prime mechanical properties, such as density (ρ) and elastic constant (E), were calculatedfrom the relations

$$z = \rho v \qquad (1)$$

$$v = \sqrt{\frac{E}{\rho}} \qquad (2)$$

The dataset was temporally aligned and normalized using standard scaling, followed by an 80:20 train–test split before analysis. Hydration behaviour was examined using time-series, comparative methods, and Principal Component Analysis. This allows ultrasonic responses to be linked with microstructural changes associated with calcium-Silicate-Hydrate development. A localized temporal dynamics was studied using a Sliding Window PCA (SW-PCA) method with a 6-hour window. In each window, standardized variables were reduced to two principal components, and the angular relationship between the loading vectors, attenuation (A) and impedance (B) was evaluated using the relation

$$\theta(t) = \cos^{-1}\left(\frac{\boldsymbol{A}.\boldsymbol{B}}{\|A\|\|B\|}\right) \qquad (3)$$

Additionally, the measurement of angular volatility was introduced to calculatetransient shiftsby computing the rolling standard deviation of θ(t) over a 3-hour window, thereby enabling the identification of accelerated transformation and solidification phases during hydration.

$$\sigma(t) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\theta_i - \bar{\theta})^2} \qquad (4)$$

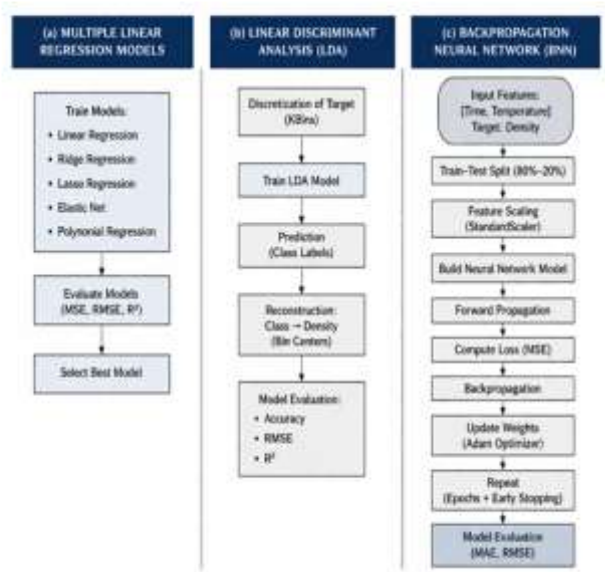


Fig.1: Flowchart illustrating all three ML model approaches for characterization of mortar using density and angular volatility as parameters

Where $\theta_i$ representsliding window angles and $\bar{\theta}$ is their mean. Equation (4) quantifieshydration dynamics; higher value of volatility indicates rapid microstructural transitions whereas lower volatility value corresponds to stabilized phases.

Based on these features, ML models were designed to analyse the calculated density and angular volatility parameters on the extrapolated temperature range in characterizing hydration stages as shown in Fig. 1. The ultrasonic backscattering dataset at three temperatures were organized into parameter wise individual sheet which carries all three temperatures. Overall four parameter data sheets constructed, which include the data sheet of amplitude, attenuation, impedance, velocity. And for validation density data sheet were constructed. These spreadsheets were then subject to machine learning model to expand the impact of temperature on the ultrasonic backscattering parameters.

The machine learning models employed in the study were linear regression model; linear discriminant analysis model; and basic neural network model. Linear regression model utilized third degree polynomial regression for temperature based expansion of dataset while incorporating the constraints of best fit among linear regression, Ridge regression, Lasso regression, Elastic Net, and Polynomial regression.

Linear Discriminant Analysis (LDA) employed the classification approach by discretizing of target into K-bins, which then mapped into training and predicted class. Obtained dataset were then undergoes bin centre based reconstruction to project the influence temperature expansion on the parameter dataset. Basic neural network used Back propagation model. It split input dataset into train set (80%) and test set (20%) data. From train data, feature scaling obtained applied to build neural network model. The neural network model was designed with fully connected layers and ReLU activation, and trained using the Adam optimizer to minimize mean squared error. For regularization, output data were subjected to dropout, batch normalization, and early stopping, to ensure robustness and prevent any chances of over fitting. The performance of model in projection of parameter dataset with temperature expansion largely depends on number of Epochs applied and MSE.

The performance of each of above models were evaluated using statistical metrics such as mean squared error (MSE), root mean square error (RMSE), coefficient of determination (R2), and the classification accuracy. Further the output of the model were correlated with physical parameters, specifically hydration, microstructure, and possible ultrasonic response upon expansion of temperature.

## IV. RESULTS AND DISCUSSION

### Key Findings from Preliminary Analysis

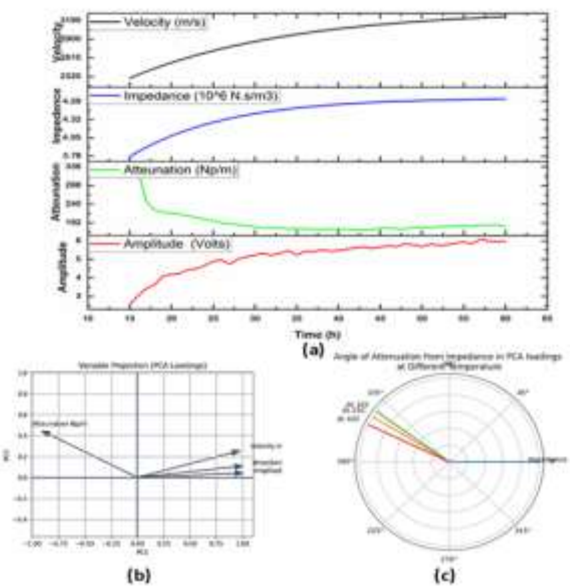


Fig. 2: (a) Stack Plot of Ultrasonic Backscattering Parameters at 25C for mortar, (b) Corresponding PCA Variable Projection (c) PCA Vector Angle between attenuation-Impedance at 25C, 32C, and 42C.

The unprocessed ultrasonic signal backscattering dataset at three different temperatures: 25C, 32C, and 42C on saturating cement mortar specimenswere recorded. The collection of data happened over a period ranging from 15 to 60 hours following the moulding of the cement mortar [9].

Each dataset comprises time-series data of ultrasonic backscattering parameters, including amplitude, attenuation, impedance, and velocity (Fig. 2a).

The principal component analysis (PCA) verified the initial findings of variable projection, with PC1 accounting for 92.8% of the variance at 25C, 92.9% at 32C, and 96.5% at 42C (Fig. 2b, Table 1). These results show the impact of temperature on the primary hydration process of cement mortar saturations. Elevated temperatures resulted in more uniform transitions in mechanical properties, which are directly linked with a singular chemical transformation.

Table 1: PCA Rolling Window Analysis and StructuralImpact

| Feature | 25C (Control) | 32C (Intermediate) | 42C (Accelerated) |
|---|---|---|---|
| PCA Baseline (Fig 3a) | Lower & Stable | Mid-range | Highest Baseline |
| Peak Volatility (Fig 3c) | Controlled (~45h) | Sustained (~58h) | Early (~43h) |
| Global Volatility (Fig 3b) | Moderate (22°) | Maximum (32°) | Minimum (16.5°) |
| Microstructure | Homogeneous | High Heterogeneity | Non-uniform "Shell" |
| Physical Outcome | Highest Durability | Transition Zone | Reduced Long-term Strength |

**Attenuation-Impedance Vector Angles**

The PCA loadings showed that all measured parameters - velocity, attenuation, impedance and amplitude - are physically connected to a single underlying physicochemical process, such as the formation of C-S-H gels [9]. As the temperature increased from 25C to 42C, the vectors for velocity, impedance, and amplitude in the variable projection plot converged and aligned more closely with the PC1 axis (Figure 2c), signifying more synchronized and uniform relationships at higher temperatures.

The PCA angle between vectors of impedance and attenuation shows a strong temperature-dependent transitions between 35–50 hours (Fig 3a), marking critical microstructural reorganization. Stable convergence at 25C indicates uniform densification, while 32C exhibits fluctuations and 42C shows persistent decoupling with irregular trends.

The full-scale volatility analysis of above PCA angle showed a threshold temperature around 32oC (Fig 3b), beyond which large degradation of saturated cement mortar uniformity. The rolling window analysis further evident the status of cement mortar uniformity with the kinetic transition occurred around the 40-hour mark (Fig 3c).

Distinct PCA angular baselines confirm strong thermal stratification, indicating that each curing temperature follows a unique microstructural evolution pathway. A sharp rise in angular volatility after ~40 hours mark, the critical transition from fluid-like paste to rigid, percolated solid matrix. The 25C condition exhibits lower and more stable volatility, reflecting a uniform and controlled hydration process.

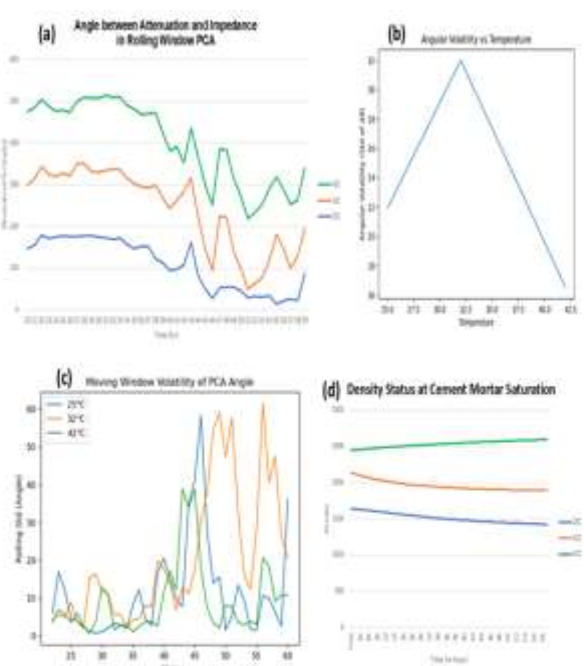


Fig. 3: (a) Rolling Window PCA of acoustic data during Cement Mortar Hydration (b) Full period Volatility (c) Moving Window Volatility of PCA angle, (d) Density Status at Cement Mortar Saturation

Higher temperatures (32C and 42C) show increased instability and rapid early setting, as captured through acoustic feature variations. Table 2 provides rolling window analysis of Attenuation-Impedance Vector Angles and the corresponding implications. In comparison, the density time-series plot (Fig 3d) at different temperatures showed the cement mortar have higher density at higher temperature.

**Thermal Baseline Projection by Linear Regression Model**

The integration of third-degree polynomial regression and 3D surface mapping creates a robust predictive framework for analyzing the thermo-temporal maturation of cement mortar. The full-scale volatility analysis on Attenuation-Impedance vector PCA angles (Fig. 4a) showed high stochastic microstructural reorganization and accurately predicting density trajectories at unmeasured 20C and 45C, with the threshold temperature around 30C. Further the model predicted a non-linear density evolution (Fig 4b).

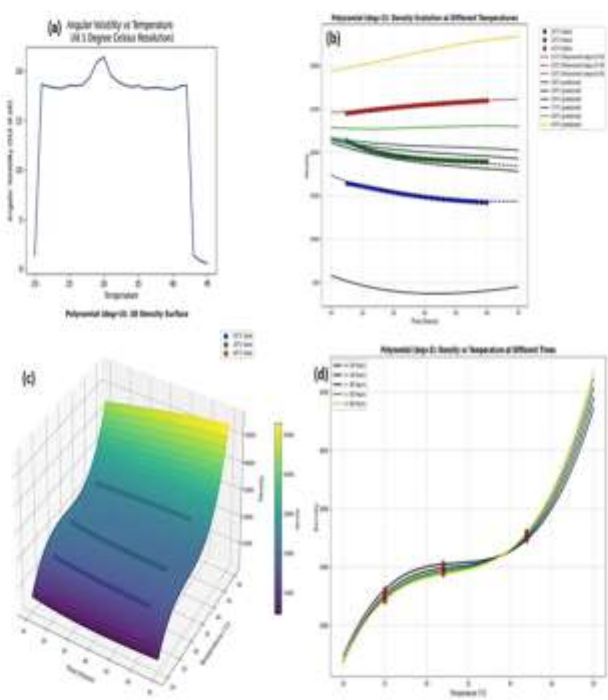

Fig. 4: Third-Degree Polynomial Regression Analysis of Mortar Density and Maturation. a) Full Scale Attenuation-Impedance PCA Angle Volatility (b) Density parameter data fitting (c) 3D density plot (d) Temporal analysis of density parameter

The generated 3D density surface (Fig. 4c)projected as smooth surface representing continuous microstructural reorganization within the mortar matrix. The 3D temporal analysis (Fig 4d) reveals that temperatures above 40C trigger a crossover effect, accelerating initial densification but causing premature tapering via shell formation, resulting in high early strength at the cost of long-term structural integrity and increased porosity. Conversely, 25C ensures gradual, uniform maturation. Overall efficiency of the model to characterize complex hydration kinetics and balancing rapid kinetics with long-term stability is noise free and based on linear extrapolation.

**Thermal Baseline Projection by Linear Discriminant Analysis Model**

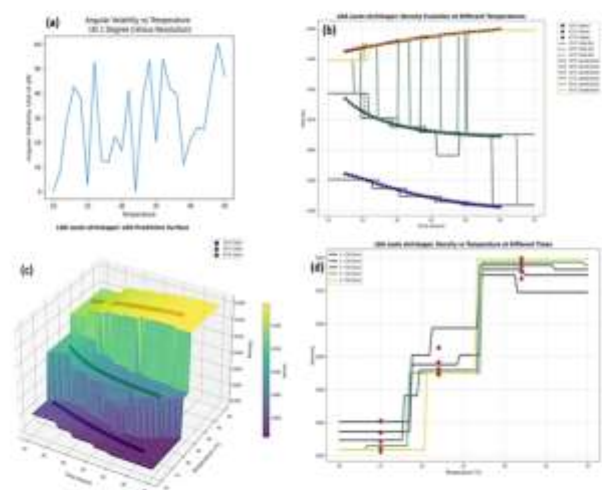

Fig. 5: Linear Discriminant Analysis (LDA) with Auto-Shrinkage for Mortar Density Classification. a) Full Scale Attenuation-Impedance PCA Angle Volatility (b) Density evolution data fitting (c ) 3D density plot (d) Temporal analysis of density evolution

The Linear Discriminant Analysis (LDA) with auto-shrinkage analysis identifies discrete density "plateaus," characterizing mortar maturation as a series of distinct structural phases rather than a continuous transition. The full-scale analysis on Attenuation-Impedance vector PCA angles generated (Fig 5a) highly irregular angular volatility map, indicating increased sensitivity to microstructural fluctuations. Further LDA captures abrupt density jumps in density evolution plot (Fig

5b). As a result, discrete density plateaus during temperature data expansion observed (Fig 5c).

The time evolution plot (Fig 5d) also showed the step-wise transitions highlighting phase-wise transformation. It clusters the mortar into low, medium, and high-density regimes based on thermal history. Overall, the non-linear classification, combined with higher angular volatility, effectively maps the "structural signatures" of the crossover effect, proving the model's ability to cluster experimental data into specific maturation states.

**Thermal Baseline Projection by Back Propagation Neural Network Model**

The Neural Network analysis provides a highly dynamic and realistic representation of the hydration process by capturing complex. The full-scale analysis on Attenuation-Impedance vector PCA angles generated highly irregular angular volatility map (Fig 6a), indicated the model retained the sensitivity to microstructural fluctuations.

Further it effectively identifies multiple kinetic transition zones, including a primary volatility peak around 31C, indicating intensified hydration activity. The density evolution plot (Fig 6b) showed the model projected the saturation period of cement mortar around 40 hours. It was further the projected in 3D density surface (Fig. 6c), which displayed an undulating, wavy topography, reflecting non-uniform densification and continuous microstructural reorganization within the mortar matrix.

This model, built on extrapolated data, produces a fluid and continuous landscape that is highly sensitive to microstructural variations, particularly across the temperature range of 21C to 42C. Additionally, the sigmoidal (S-shaped) maturation (Fig. 6d) trend highlights the role of temperature as a kinetic catalyst, accelerating hydration and promoting the formation of a dense and homogeneous C-S-H gel network. The convergence behaviour observed between 25C and 40C further defines an optimal thermal "sweet spot" for rapid strength development and material stabilization.

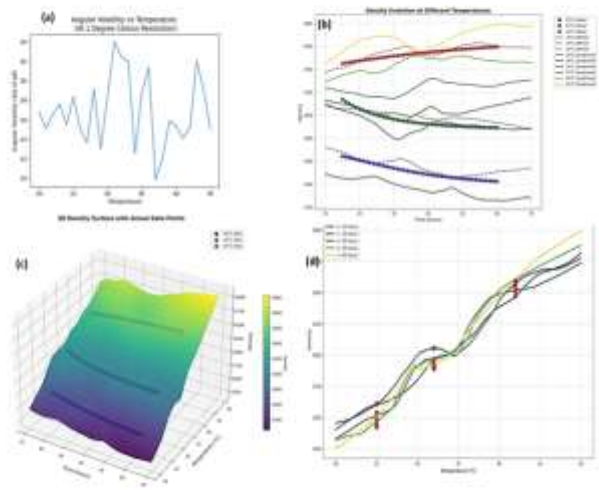

Fig. 6: Neural Network (NN) Analysis of Stochastic Mortar Maturation and Density Evolution a) Full Scale Attenuation-Impedance PCA Angle Volatility (b) Density evolution data fitting (c ) 3D density plot (d) Temporal analysis of density evolution.

**Performance of Machine Learning Models**

The machine learning based thermal baseline expansion was conducted over ultrasonic backscattering parameters individually. Therefore, the performance toward temperature effect on ultrasonic parameters was largely depended of ML models ability to train itself from recorded dataset. As seen in the PCA angle volatility diagram, the outcome of strong perturbations showed higher sensitivity of machine learning model. However, it also reduces the interpretability of cement matrix maturity status. In comparison this, the density data projected by machine learning model for temperature expansion provide more interpretable features.

This includes the transition of cement maturity status after 31oC. Further the density data expansion provided details of temperature as well as time-based evolution of hydration system (structural hydration >90%) during cement matrix stabilization, strength development, and material stabilization. Table 3 provided a detailed interpretation of three modelling approaches generated during the cement mortar characterization by temperature data expansion.

Table 2: Comparison of Predictive Models for Mortar Maturation

| Feature | Polynomial Regression (3rd degree) | LDA (Auto-Shrinkage) | Back-propagation Neural Network (NN) |
|---|---|---|---|
| Model Nature | Continuous & Smooth | Categorical & Discrete | Stochastic & Nonlinear |
| Primary Strength | Captures overall kinetic trends and long-term gradients. | Identifies sharp "jumps" and structural phase boundaries. | Captures "organic" fluctuations and complex micro-strains. |
| Volatility Peak | 30C (Single, broad threshold) | High/Erratic (Sensitive to transition noise) | 31C (Primary) with multiple secondary peaks. |
| Maturation Style | Uniform densification curves. | Step-function "plateaus" (High/Med/Low). | Undulating, "wavy" trajectories. |
| Best Use Case | Quantifying the Crossover Effect magnitude. | Classifying material quality and hydration states. | Modelling real-world variability and "sweet spots." |
| Global Volatility | Moderate (22degree) | Maximum (32 degree) | Minimum (16.5 degree) |
| Microstructure | Homogeneous | High Heterogeneity | Non-uniform "Shell" |
| Physical Outcome | Highest Durability | Transition Zone | Reduced Long-term Strength |

## V. CONCLUSION

Present study explores the thermo-temporal maturation of cement mortar through a predictive framework, integrating Linear Discriminant Analysis (LDA), Polynomial Regression and Neural Networks (NN) to compute the Crossover Effect. While the LDA reveals discrete density "plateaus" that categorize hydration into distinct structural phases third-degree polynomial modelling successfully identifies a broad structural instability peak at 30C. The Neural Network come up with the most refined "acoustic fingerprint," expressing stochastic microstructural fluctuations and a primary volatility peak at 31C. Collectively, the results reveal that while temperatures exceeding 40C accelerate early-stage densification, they trigger a "shell formation" technique that leads to increased porosity and substantially lower ultimate strength compared to the consistency, high-durability matrix developed at 25C.

Ultimately, the NN effectively balances experimental accuracy with the fundamental "noise" of non-ideal hydration, providing the most realistic "acoustic fingerprint" for long-term mortar durability. The model's ability to follow the experimental data points while maintaining predictive "noise" validate that neural networks are superior for representing the real-world, non-ideal behaviour of cementitious materials. Angular volatility was found useful only during early stages (10-20 hours) to capture initial reaction dynamics, while density remained a consistent measure of final material quality. The results demonstrate that standard linear regression is insufficient for capturing the complex thresholds of hydration, necessitating physics-informed approaches that include acoustic angular volatility as a key feature.

**Future Scope**

This research work highlights on various ML models which interpreted the kinetic transition of mortar at different temperature which purely extracted from the given dataset. This work can be extended by incorporating Physics informed neural network (PINNS) framework along with Arrhenius and the Vogel-Fulcher-Tammann (VFT) equations to produce a more strong predictive method for construction materials. PINNs utilize optimization algorithms to iteratively update neural network parameters by minimizing a physics-informed loss function.

This process guides the model toward solutions that satisfy both experimental data and underlying physical laws. As a result, the framework enhances predictive accuracy, generalization, and interpretability for material behaviour analysis. While the three models employed (3rd-degree Polynomial, LDA, and Basic Neural Network) offer significant insights, they each possess inherent mathematical "blind spots" that necessitate the transition to a Physics-Informed Neural Network (PINN).

**Declaration of AI Usage:**
Python codes for Machine Learning Models were generated from DeepSeek using structured prompts. The generated Python codes are debugged and verified by authors, and further modified as per requirement of the study. The initial manuscript was constructed by authors and subjected to ChatGPT for language corrections.

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