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Physicochemical evaluation of fly ash utilization in cemented paste backfill (CPB) systems using interpretable causal machine learning

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Abstract: This study investigates the effect of fly ash substitution on compressive strength in cemented paste backfill (CPB) systems using an integrated framework combining predictive machine learning, explainable artificial intelligence, and causal machine learning approaches. A dataset comprising 116 experimental CPB mixtures prepared with mineral processing tailings from a Pb–Zn underground mine and fly ashes from different thermal power plants was analyzed. The maximum compressive strength reached 10.33 MPa at 90 days of curing. The cross-validated XGBoost model achieved an R^2 of 0.58 and successfully predicted strength values up to 9.73 MPa. Causal analysis indicated an average treatment effect of approximately 0.28 MPa per 1% fly ash substitution, although the effect showed substantial heterogeneity across physicochemical conditions. Global and local SHapley Additive exPlanations (SHAP) analyses identified curing time as the dominant factor controlling strength development, emphasizing the importance of late-age performance in fly ash–containing systems. The fly ash ratio itself was not a primary explanatory variable; instead, chemical composition, particle size distribution, and specific gravity played decisive roles. These findings demonstrate that fly ash performance in CPB systems cannot be reliably evaluated using dosage-based approaches alone and should be optimized by considering physicochemical characteristics and curing conditions. The proposed explainable and causal data-driven framework provides a practical decision-support tool for sustainable utilization of mineral processing by-products in cement-based systems.

Keywords: cemented paste backfill, mineral processing tailings, fly ash, compressive strength, causal machine learning

1. Introduction

Cemented paste backfill (CPB) is one of the most widely applied backfilling techniques in underground metal mining operations due to its ability to ensure ground stability while enabling the underground disposal of mine tailings. In CPB systems, cement is used as the primary binder to provide the uniaxial compressive strength required for safe mining operations. However, cement represents the most expensive component of CPB mixtures and is also associated with high energy consumption and carbon emissions (Tuylu, 2022a). Consequently, reducing cement consumption without compromising mechanical performance has become a major research focus in underground mining and mineral processing applications (Sun et al., 2025; Valenzuela-Díaz et al., 2025; Wang et al., 2025).

Mining and mineral processing operations generate large volumes of tailings as a result of ore beneficiation processes, posing significant environmental and geotechnical challenges due to their potential for heavy metal contamination, acid generation, and long-term storage risks. Recent studies emphasize that tailings storage facilities may present serious environmental and disaster risks if improperly managed (Hudson-Edwards et al., 2024). At the same time, coal-fired thermal power plants produce substantial quantities of fly ash, which accumulate in large stockpiles and create long-term land use, air quality, and water contamination problems (Chen et al., 2024; Tenza and Aphane, 2026). The simultaneous utilization of mineral processing tailings and fly ash within CPB systems, therefore, offers a unique opportunity to address two major industrial waste streams through a single underground application while promoting circular economy principles in mining operations.

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In this context, the use of fly ash as a supplementary material in cement-based systems has attracted considerable attention due to its potential to reduce cement consumption and environmental impacts (Malhotra, 2002; Snellings et al., 2012; Scrivener et al., 2018; Quan and Fall, 2025). Numerous studies report that the influence of fly ash substitution on compressive strength is not unidirectional and strongly depends on curing time, chemical composition, and physical characteristics of the system (Thomas, 2013; Hewlett and Liska, 2019; Li et al., 2022). While early-age strength development is often limited, significant strength gains may occur at later ages as pozzolanic reactions progress, particularly in fly ash–containing systems (Hawileh et al., 2025).

Beyond curing conditions, the chemical and physical heterogeneity of fly ash plays a critical role in determining its effectiveness. Variations in oxide composition, particle size distribution, and specific gravity influence hydration kinetics, pozzolanic activity, and microstructural development in cementitious systems (Scrivener et al., 2016; Araujo et al., 2022; Abbadi and Mucsi, 2024; Akbulut et al., 2024). As a result, compressive strength development in CPB mixtures incorporating fly ash is governed by complex and nonlinear interactions between multiple physicochemical parameters, which cannot be adequately captured using conventional univariate or linear evaluation approaches.

Recent advances in machine learning have enabled the prediction of mechanical properties of cement-based materials with high accuracy (Jia et al., 2022; Chi et al., 2023; Zhang et al., 2023; Benaicha, 2024; Li et al., 2024; Palanisamy et al., 2025; Singh et al., 2025). Similar data-driven approaches have also been adopted in mineral processing research for process modeling and optimization (Alsafasfeh et al., 2022; Ozkan, 2023; Pural, 2023). However, most existing studies rely primarily on correlation-based models and provide limited insight into the causal mechanisms governing material performance. In complex systems such as CPB mixtures containing heterogeneous industrial by-products, high predictive accuracy alone is insufficient to determine under which conditions fly ash substitution truly contributes to strength development.

Despite growing interest in data-driven modeling, there remains a critical gap in the literature regarding the causal interpretation of fly ash substitution effects in CPB systems. In particular, few studies have systematically distinguished between variables that explain compressive strength and those that causally modify the effectiveness of fly ash substitution under varying physicochemical and curing conditions (Adiguzel Tuylu et al., 2025).

To address this gap, the present study proposes an integrated framework combining predictive machine learning, explainable artificial intelligence, and causal machine learning techniques to evaluate the utilization of fly ash in cemented paste backfill systems. By jointly analyzing compressive strength prediction, outcome-level explainability, and heterogeneous causal effects, this study aims to identify the physicochemical conditions under which fly ash substitution provides tangible benefits. The proposed approach offers a robust decision-support tool for optimizing the sustainable use of mineral processing by-products in underground mining applications.

2. Materials and methods

2.1. Experimental dataset and material characterization

The dataset used in this study was compiled from experimental uniaxial compressive strength tests performed on cemented paste backfill (CPB) mixtures containing mineral processing tailings and fly ash, as reported by Tuylu (2022b). A total of 116 experimental samples were included in the dataset. A representative subset of the input and output variables is presented in Table 1 to illustrate the structure of the modeling dataset.

Mineral processing tailings were obtained from a Pb–Zn underground mine beneficiation plant in Balya/Balıkesir, while fly ash samples were collected from different coal-fired thermal power plants in Soma/Manisa (TPP_S), Yatagan/Mugla (TPP_Y), Catalagzı/Zonguldak (TPP_C), and Tufanbeyli/ Adana (TPP_T). The selection of fly ash samples from four different thermal power plants was based on the geological diversity of the coal formations supplying these plants. Differences in coal origin result in variations in mineralogical composition and major oxide contents of the produced fly ash. This chemical and physical variability provides a suitable basis for investigating how different fly ash types, exhibiting distinct pozzolanic potentials, influence compressive strength development in CPB systems.

The use of multiple fly ash sources therefore enabled a comparative evaluation of their performance

Table 1. Representative subset of the experimental dataset used for modeling and interpretation

Day	Cement	Tailing	FA	Fe_2O_3	SiO_2	Al_2O_3	CaO	MgO	K_2O	Na_2O	SO_3	≤20μm	>45μm	>90μm	Specific gravity	MPA
28	5.625	88.750	5.625	12.514	35.143	8.573	25.381	2.416	2.448	0.223	7.635	0.423	0.385	0.112	3.166	2.470
28	8.250	86.250	5.500	12.258	34.718	8.471	26.388	2.385	2.405	0.225	7.528	0.428	0.378	0.109	3.164	6.730
28	6.875	86.250	6.875	12.273	34.908	8.678	25.844	2.397	2.414	0.228	7.665	0.424	0.381	0.110	3.159	6.090
56	9.000	88.750	2.250	12.521	35.119	8.208	26.314	2.387	2.482	0.216	7.005	0.440	0.372	0.110	3.178	2.310
56	11.000	86.250	2.750	12.282	34.878	8.233	26.984	2.362	2.455	0.219	6.894	0.445	0.365	0.107	3.173	4.670
90	6.875	86.250	6.875	12.273	34.908	8.678	25.844	2.397	2.414	0.228	7.665	0.424	0.381	0.110	3.159	9.650
90	5.625	88.750	5.625	12.514	35.143	8.573	25.381	2.416	2.448	0.223	7.635	0.423	0.385	0.112	3.166	5.729
200	11.250	88.750	0.000	12.453	34.366	7.729	27.609	2.365	2.409	0.211	7.073	0.440	0.370	0.107	3.189	5.930

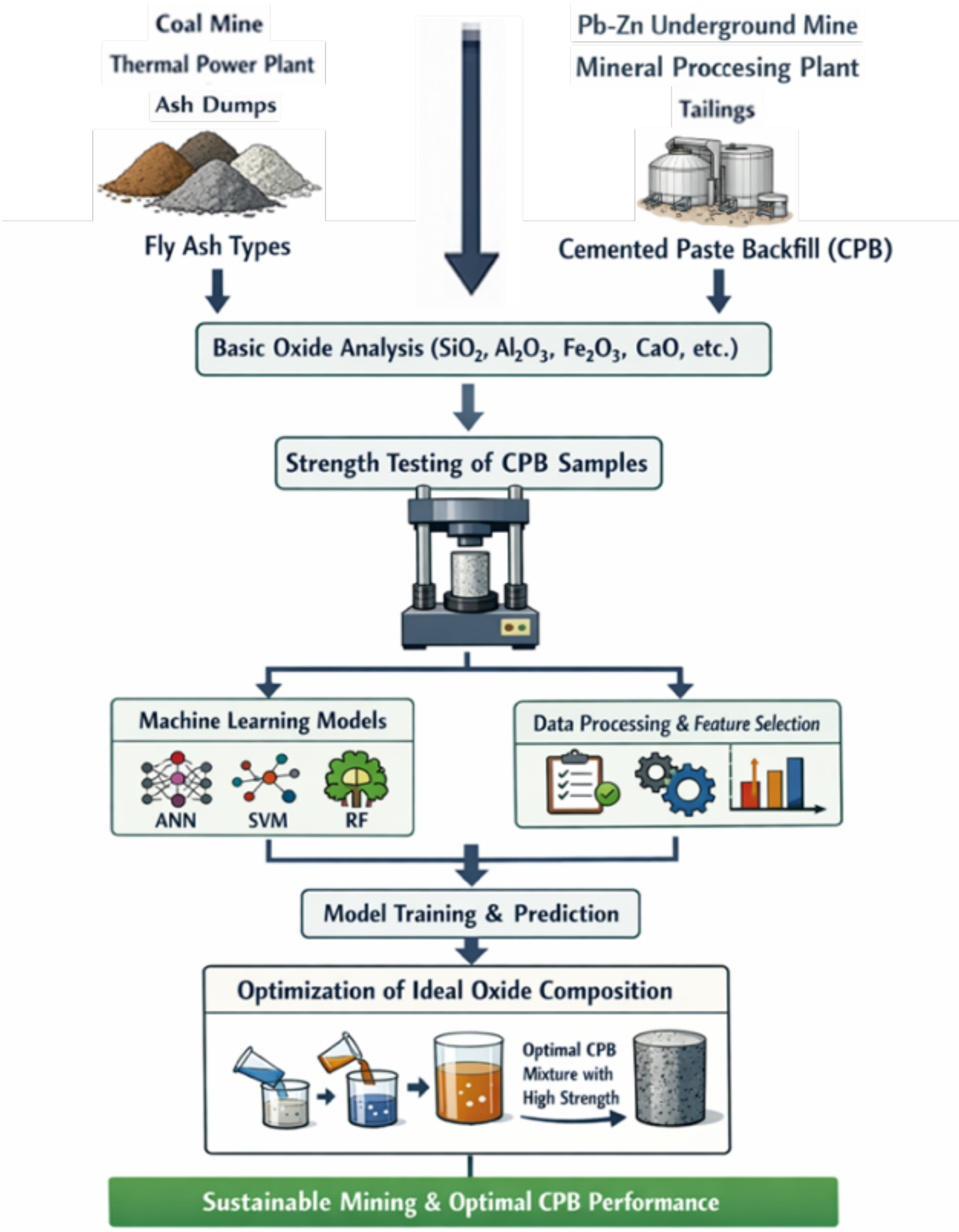

Fig. 1. Sustainable cemented paste backfill design using fly ash and mine tailings through machine learning–based optimization

within a consistent CPB matrix framework.

The chemical composition of the solid materials was characterized in terms of major oxide contents, including CaO, SiO_2, Al_2O_3, Fe_2O_3, MgO, K_2O, Na_2O, and SO_3. Physical properties were represented by particle size distribution parameters (≤ 20 µm, > 45 µm, and > 90 µm) and specific gravity. Curing time was included as a key variable to capture strength development at different ages (28, 56, 90, and 200 days), while compressive strength (MPa) was defined as the output variable.

The experimental dataset analyzed in this study was derived from previously published laboratory investigations on CPB mixtures (Adiguzel Tuylu et al., 2025). In those experiments, CPB samples were prepared with a constant total solid content of 80 wt% and 20 wt% water. The total binder content (cement + fly ash) was varied at 3%, 5%, 7%, 9%, and 11% of the total mixture mass, while fly ash was incorporated as a partial cement replacement at substitution ratios of 0%, 20%, 30%, 40%, and 50%.

Cylindrical specimens (50 mm diameter × 100 mm height) were cured under controlled laboratory conditions (22°C and 80% relative humidity) and tested for uniaxial compressive strength (UCS) at 28, 56, 90, and 200 days in accordance with ASTM C39. Detailed mixture preparation procedures and physicochemical characterizations are comprehensively reported in Adiguzel Tuylu et al. (2025).

A schematic overview of the experimental workflow and data-driven analysis framework adopted in this study is presented in Fig. 1.

As seen from Fig. 1, the proposed methodology integrates material sourcing, physicochemical characterization, experimental strength testing, and data-driven modeling into a unified CPB design framework. The workflow illustrates how mineral processing tailings and fly ash obtained from different thermal power plants are first characterized in terms of their basic oxide composition and physical properties, which are known to govern hydration and pozzolanic reactions. Uniaxial compressive strength testing is subsequently employed to capture the mechanical response of CPB mixtures at different curing ages. These experimental results constitute the input for machine learning–based modeling, which enables the identification of nonlinear relationships between material characteristics and strength development. Finally, the optimized oxide composition derived from the modeling stage provides a basis for designing high-performance and sustainable CPB mixtures, linking experimental observations with practical underground mining applications.

The corresponding chemical and physical properties of the solid materials used in the CPB mixtures are summarized in Table 2, in which, the solid materials used in the CPB mixtures exhibit substantial variability in both chemical composition and physical properties. In particular, the fly ashes obtained from different thermal power plants show notable differences in major oxide contents such as SiO_2, Al_2O_3, CaO, and Fe_2O_3, reflecting their heterogeneous origin. Similarly, variations in particle size distribution and specific gravity indicate differences in packing behavior and reactivity among the materials. Such heterogeneity is expected to influence hydration kinetics, pozzolanic activity, and microstructural development in CPB mixtures, thereby motivating the need for multivariate and data-driven analyses to systematically evaluate their combined effects on compressive strength.

2.2. Prediction models

For the purpose of predicting compressive strength in cemented paste backfill (CPB) systems containing mineral processing tailings and fly ash, tree-based machine learning algorithms were preferred due to their strong capability to model nonlinear relationships and interaction effects among chemical and physical parameters. As discussed in the previous sections, CPB strength development is governed by complex and heterogeneous physicochemical interactions, which cannot be adequately captured using linear or univariate modeling approaches. In this context, Random Forest (RF) and Extreme Gradient Boosting (XGBoost) algorithms, which have been widely applied in cement-based systems and fly ash–containing mixtures, were selected for this study (Chou et al., 2014; Adiguzel Tuylu et al., 2025).

These algorithms are particularly well suited for handling multicollinearity, variable interactions, and threshold-type behaviors commonly observed in systems incorporating heterogeneous industrial by-products. In this study, model performance was evaluated using a 5-fold cross-validation strategy to ensure robustness and generalizability. The model exhibiting higher predictive accuracy was subsequently selected as the base model for the explainability and causal analysis stages.

Table 2. Chemical and physical properties of solid materials used in paste backfill mixtures

Solid materials in the mixing	Properties	Tailings	Cement	TPP_C	TPP_S	TPP_Y	TPP_T
Chemical Properties	Fe_2O_3	13.6	3.4	6.46	3.99	6.43	4.5
	SiO_2	36.2	19.9	53.34	45.04	46.23	33.7
	Al_2O_3	8.1	4.8	26.12	23.36	23.04	19.8
	CaO	23.3	61.6	4.06	19.04	12.98	22
	MgO	2.5	1.3	2.27	1.72	2.81	2.2
	K_2O	2.6	0.9	4.14	1.31	2.36	1.6
	Na_2O	0.2	0.3	0.49	0.43	0.62	0.5
	SO_3	7.5	3.7	0.68	4.88	2.85	13.7
Physical Properties	D_{10}	2.5	2.5	3.5	8	7	5
	D_{30}	11.5	8.7	9	15	15	20
	D_{50}	30	15	15	38	20	37
	D_{60}	45	20	20	55	38	45
	D_{90}	140	50	120	145	155	90
	≤ 20 µm	42%	60%	60%	35%	50%	30%
	> 45 µm	40%	13%	22%	45%	35%	40%
	> 90 µm	12%	0.10%	13%	25%	16%	10%
	Specific gravity	3.2	3.1	2.6	2.4	2.2	2.7

2.3. Outcome level explainability analysis (XAI)

To interpret the decision mechanism of the selected prediction model and to identify the physicochemical factors governing compressive strength development in cemented paste backfill (CPB) systems, the SHapley Additive exPlanations (SHAP) method was employed. SHAP is a model-agnostic, additive explainability approach grounded in cooperative game theory, which enables the quantitative attribution of each input variable's marginal contribution to the model output (Lundberg and Lee, 2017). Owing to its ability to provide both global and local interpretability, SHAP has been increasingly adopted for the analysis of machine learning models in cementitious and binder systems (Li et al., 2024).

In this study, SHAP analysis was used not only to explain the predictive behavior of the machine learning model, but also to gain insights into the relative importance and interaction of chemical composition, physical properties, and curing conditions controlling CPB strength. First, global variable importance was evaluated using SHAP beeswarm plots to identify the most influential parameters across the entire dataset. Subsequently, SHAP dependence plots were analyzed for curing time and selected chemical components to investigate their nonlinear and range-dependent effects on compressive strength. This outcome-level explainability stage provides a critical link between data-driven predictions and physicochemical interpretation, forming the basis for the subsequent causal analysis.

2.4. Causal machine learning approach

To move beyond correlation-based interpretation and to evaluate the actual causal effect of fly ash substitution on compressive strength, a causal machine learning framework was adopted in this study. Fly ash content was treated as a continuous intervention variable, and the Causal Forest Double Machine Learning (DML) approach was employed. This method enables the estimation of causal effects in high-dimensional and nonlinear systems by explicitly controlling for confounding variables and separating treatment effects from spurious correlations (Athey and Imbens, 2016; Chernozhukov et al., 2018).

In the causal analysis, compressive strength was defined as the outcome variable, while chemical composition parameters, physical properties, and curing time were included as confounder variables. Cement content was intentionally excluded from the causal model due to the mixture constraint inherent in CPB design, whereby increases in fly ash content necessarily imply reductions in cement content. Including cement as a covariate would therefore introduce post-treatment bias and distort the estimation of the true causal effect of fly ash substitution. By conditioning on material properties and curing conditions instead, the model isolates the net causal contribution of fly ash to strength development.

Using this framework, both the average treatment effect (ATE) and sample-level conditional average treatment effects (CATE) were estimated, allowing the investigation of heterogeneous causal responses across different mixture compositions and curing regimes. This approach provides a robust basis for causal inference in CPB systems, where complex physicochemical interactions and material heterogeneity limit the applicability of conventional experimental or purely predictive analyses. Consequently, the causal machine learning framework complements the outcome-level explainability analysis and supports more reliable decision-making for the optimization of fly ash utilization in underground mining applications.

2.5. Explaining causal effect heterogeneity

To explain why fly ash substitution exhibits heterogeneous causal effects under different physico-chemical and curing conditions, a second-stage explainability analysis was conducted on the estimated conditional average treatment effects (CATE). While the causal forest framework quantifies how the effect of fly ash varies across samples, it does not directly reveal which material characteristics drive this heterogeneity. Therefore, in this stage, the estimated CATE values were treated as the target variable, and SHAP-based analyses were employed to investigate how chemical composition, physical properties, and curing time modify the causal effect of fly ash on compressive strength.

This approach enables the identification of key moderators that amplify or suppress the effectiveness of fly ash substitution, thereby providing insight into the underlying mechanisms governing heterogeneous treatment responses. A similar methodological framework has previously been proposed for the interpretable analysis of causal effects in complex systems across different application domains (Adiguzel Tuylu, 2025). However, to the authors' knowledge, this is the first study to apply SHAP-based explainability to CATE estimates in cement-based systems incorporating fly ash substitution. By linking causal heterogeneity with physicochemical properties, this stage extends conventional causal analysis and provides actionable guidance for optimizing fly ash utilization in cemented paste backfill systems.

3. Results and discussion

3.1. Prediction performance of machine learning models

In this study, Random Forest (RF) and Extreme Gradient Boosting (XGBoost) algorithms were employed to predict the uniaxial compressive strength of cemented paste backfill mixtures. Model performance was evaluated using a 5-fold cross-validation strategy and assessed in terms of root mean square error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2). The comparative performance results of the two models are summarized in Table 3.

Table 3. Prediction performance of machine learning models for compressive strength.

Model	RMSE	MAE	R^2
XGBoost	1.34	0.97	0.58
Random Forest	1.50	1.10	0.47

The results indicate that both models are capable of predicting compressive strength with acceptable accuracy, despite the high heterogeneity of the dataset arising from variations in chemical composition, physical properties, and curing time. However, the XGBoost model consistently outperformed the Random Forest model, exhibiting lower prediction errors and a higher coefficient of determination. As presented in Table 3, XGBoost achieved an RMSE of 1.34 MPa and an R^2 value of 0.58, compared to 1.50 MPa and 0.47 obtained by the Random Forest model.

The superior performance of XGBoost can be attributed to its gradient boosting framework, which iteratively learns residual patterns and effectively captures complex nonlinear relationships and interaction effects among input variables. This capability is particularly advantageous in CPB systems containing heterogeneous industrial by-products, where strength development is governed by threshold-type behaviors and coupled physicochemical interactions. Although the R^2 values may be considered moderate, they are consistent with the inherent variability of experimental CPB datasets and comparable to those reported in similar studies involving multi-source waste materials.

Based on its improved predictive accuracy and robustness, the XGBoost model was selected as the base model for subsequent explainability and causal analyses. This selection ensures a stable foundation for interpreting variable contributions using SHAP and for estimating causal effects through the causal machine learning framework, thereby strengthening the reliability of the overall analytical pipeline.

3.2. Global explainability of compressive strength

To identify the variables on which the XGBoost model relies most strongly when predicting compressive strength, a global explainability analysis was conducted using the SHapley Additive exPlanations (SHAP) framework. The SHAP beeswarm plot provides a comprehensive visualization of the relative importance of each input variable, as well as the direction and magnitude of their contributions to the model output across the entire dataset (Fig. 2).

The SHAP results clearly indicate that curing time (Day) is by far the most dominant factor governing compressive strength prediction. Higher curing times are predominantly associated with positive SHAP values, reflecting their strong positive contribution to strength development. This observation is fully consistent with the time-dependent nature of hydration and pozzolanic reactions in fly ash–containing CPB systems and highlights the critical role of late-age strength gain in such mixtures.

Among the chemical components, oxides such as Fe_2O_3 and K_2O exhibit a more pronounced influence on model predictions compared to SiO_2 and CaO. The relatively higher SHAP values associated with Fe_2O_3 and K_2O suggest that these oxides play an important role in modifying hydration kinetics and secondary reaction mechanisms, thereby contributing indirectly to strength development. In contrast, the SHAP distributions for SiO_2 and CaO are more concentrated around zero, indicating that while these oxides are essential constituents of cementitious systems, their direct explanatory power for compressive strength variability within the studied dataset is limited.

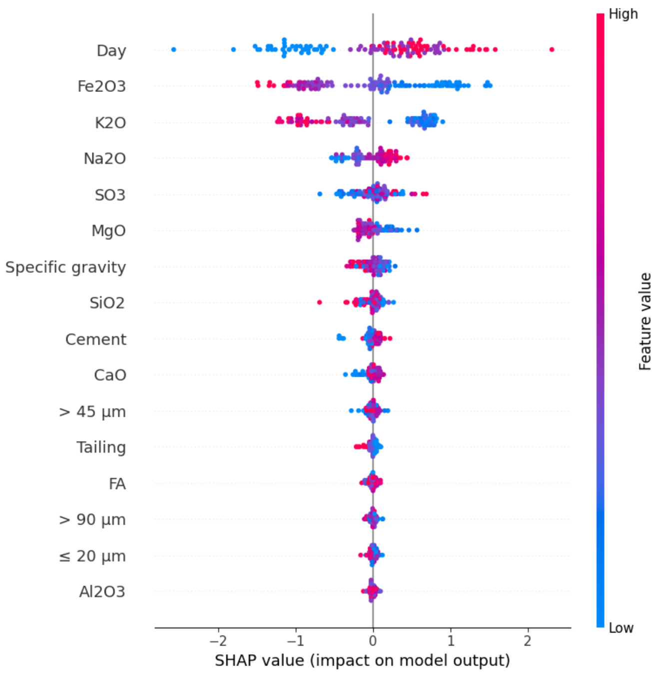

Fig. 2. SHAP summary (beeswarm) plot showing the global importance of input variables for compressive strength prediction

Notably, the SHAP values associated with the fly ash (FA) ratio are clustered within a narrow range close to zero, suggesting that fly ash content alone is not a dominant predictor of compressive strength.

Instead, the influence of fly ash emerges indirectly through its interaction with curing time, chemical composition, and physical properties. This finding implies that the effect of fly ash substitution cannot be fully interpreted using predictive explainability alone and requires a causal framework to distinguish genuine treatment effects from correlation-driven patterns.

Overall, the global explainability analysis demonstrates that compressive strength in CPB systems is primarily driven by curing time and selected chemical components, while the contribution of fly ash is highly conditional and heterogeneous. These insights provide a critical foundation for the causal and CATE-SHAP analyses presented in the subsequent sections, where the conditions under which fly ash substitution becomes effective are examined in greater detail.

3.3. Local effects of physicochemical parameters on compressive strength

Following the global explainability analysis, the local and nonlinear effects of key physicochemical parameters on compressive strength were investigated using SHAP dependence plots. This analysis enables the identification of the value ranges and trends over which curing time and selected oxide components influence strength development in cemented paste backfill (CPB) systems (Fig. 3).

The SHAP dependence results demonstrate that curing time (Day) exerts a strong time-dependent effect on compressive strength. At early ages (28 days), SHAP values are predominantly negative, indicating limited early-age strength development in fly ash–containing mixtures. As the curing period extends to intermediate ages (56 and 90 days), SHAP values shift markedly toward positive values, reflecting significant strength gain associated with the progression of hydration and pozzolanic reactions. At longer curing times (200 days), positive contributions are maintained; however, the rate of increase becomes less pronounced, suggesting a saturation trend as hydration and pozzolanic reactions approach completion. This behavior confirms the long-term performance of fly ash substitution while indicating diminishing marginal strength gains at extended curing durations.

The dependence plot for CaO content reveals a distinctly nonlinear relationship with compressive strength. Negative SHAP values are observed at low CaO levels, while positive contributions are concentrated within an intermediate CaO range, indicating the existence of an optimal calcium content for strength development. At higher CaO levels, the contribution weakens again, suggesting that excessive calcium does not further enhance strength and may adversely affect the binder system.

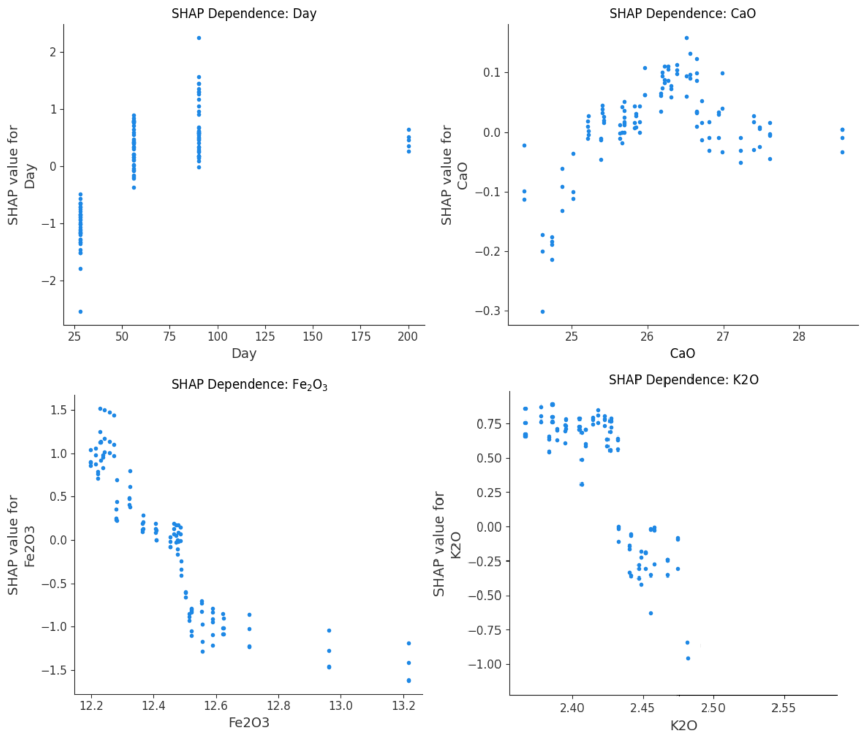

Fig. 3. Combined SHAP dependence plots illustrating the local effects of curing time (day) and selected oxide components (CaO, Fe_2O_3, and K_2O) on compressive strength

For Fe_2O_3, the SHAP results indicate a range-dependent effect on compressive strength. Positive contributions dominate at lower Fe_2O_3 contents, whereas increasing Fe_2O_3 levels are associated with negative SHAP values. This trend suggests that elevated iron oxide content may indirectly hinder binder phase formation or alter hydration pathways, thereby limiting strength development. Similarly, the SHAP dependence for K_2O exhibits a clear threshold behavior: low alkali contents contribute positively to compressive strength, while SHAP values become negative beyond a certain K_2O level, indicating potential adverse effects of excessive alkali content on the cementitious system.

The observed time-dependent strength development trend is consistent with previous studies reporting that fly ash-containing cementitious systems exhibit delayed pozzolanic reactivity and enhanced long-term strength gain (Li et al., 2022; Hawileh et al., 2025). Similarly, the nonlinear contribution of CaO observed in the SHAP dependence plot aligns with literature findings indicating that calcium availability must be maintained within an optimal range to ensure sufficient formation of C-S-H phases without causing adverse microstructural effects (Scrivener et al., 2016; Thomas, 2013).

The negative trend observed at higher Fe_2O_3 contents may be associated with reduced effective binder reactivity, as excessive iron oxides are reported to have limited direct contribution to strength-forming hydration products in cementitious systems (Hewlett and Liska, 2019). Moreover, the threshold behavior identified for K_2O content is compatible with studies suggesting that excessive alkali content can alter hydration kinetics and microstructural stability, thereby influencing long-term strength development (Snellings et al., 2012; Akbulut et al., 2024).

These consistencies with established physicochemical mechanisms support the reliability of the SHAP-based interpretations and indicate that the data-driven findings are not merely statistical artifacts but reflect underlying material behavior.

Overall, the combined local explainability analysis confirms that compressive strength in CPB systems is governed by the joint and nonlinear interaction of curing time and chemical composition, rather than by any single parameter acting independently. A key finding of this study is that fly ash content (FA) does not emerge as a dominant variable directly explaining compressive strength in outcome-level SHAP analyses. Instead, strength development is primarily controlled by the chemical and physical characteristics of the fly ash, including oxide composition, particle size distribution, and specific gravity. This observation further indicates that fly ash should not be treated as a homogeneous substitute material, but rather as a heterogeneous mineral by-product whose performance depends on its physicochemical properties. Consequently, ratio-based evaluation approaches alone are insufficient for assessing fly ash substitution, and detailed material characterization is essential. These insights provide a solid foundation for the causal and CATE-based analyses presented in the subsequent section.

3.4. Causal effect of fly ash substitution on compressive strength

To quantify the effect of fly ash substitution on compressive strength within a causal framework, fly ash content was treated as a continuous treatment variable, and both the average treatment effect (ATE) and conditional average treatment effects (CATE) were estimated. This approach enables the evaluation of not only the mean impact of fly ash substitution, but also how its effect varies across different physicochemical and curing conditions.

The results indicate that the estimated ATE corresponding to a 1% increase in fly ash content is approximately 0.28 MPa, suggesting that fly ash substitution has a positive average effect on compressive strength. When interpreted cumulatively, this value implies that moderate increases in fly ash content may lead to meaningful strength gains under favorable conditions. However, the fact that the 95% confidence interval associated with the ATE includes negative values clearly indicates that this positive effect is not universal and that substantial heterogeneity exists across the dataset.

To further investigate this heterogeneity, the distribution of individual treatment effects was examined using the estimated CATE values (Fig. 4). The CATE distribution reveals a wide range of responses to fly ash substitution, with individual effects spanning from slightly negative values to approximately 0.67 MPa per 1% increase in fly ash content. This finding demonstrates that while fly ash can significantly enhance compressive strength in certain systems, its contribution may be limited or even adverse under specific physicochemical conditions.

These results confirm that the effect of fly ash substitution on compressive strength is highly condition-dependent rather than uniform. When considered together with the SHAP-based global and local explainability analyses presented in the previous sections, it becomes evident that the effectiveness of fly ash is strongly influenced by curing time and chemical composition. In particular, longer curing durations and favorable oxide balances are associated with higher positive causal effects. Consequently, fly ash substitution should not be regarded as a universal solution in cement-based or CPB systems, but rather as a component whose performance must be optimized under well-defined material and curing conditions.

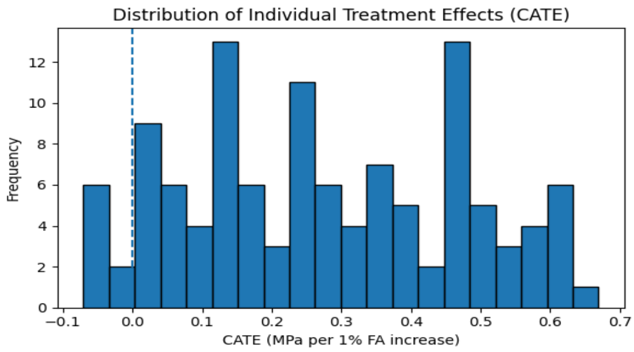

Fig. 4. Distribution of individual treatment effects (CATE) showing the heterogeneous impact of fly ash substitution on compressive strength

3.5. Interpretation of heterogeneous treatment effects using CATE-SHAP

To further investigate the heterogeneous causal effects of fly ash substitution on compressive strength, SHAP-based explainability analyses were applied to the estimated conditional average treatment effects (CATE). This approach enables the identification of the physicochemical conditions under which fly ash substitution becomes more effective or yields limited benefits.

The CATE-SHAP summary (beeswarm) plot highlights that the heterogeneity of fly ash treatment effects is primarily driven by SiO_2 content, curing time (Day), specific gravity, and the fine particle fraction (≤ 20 µm) (Fig. 5). These variables emerge as key moderators controlling the magnitude and direction of the causal effect of fly ash on compressive strength, rather than merely influencing the predicted strength itself.

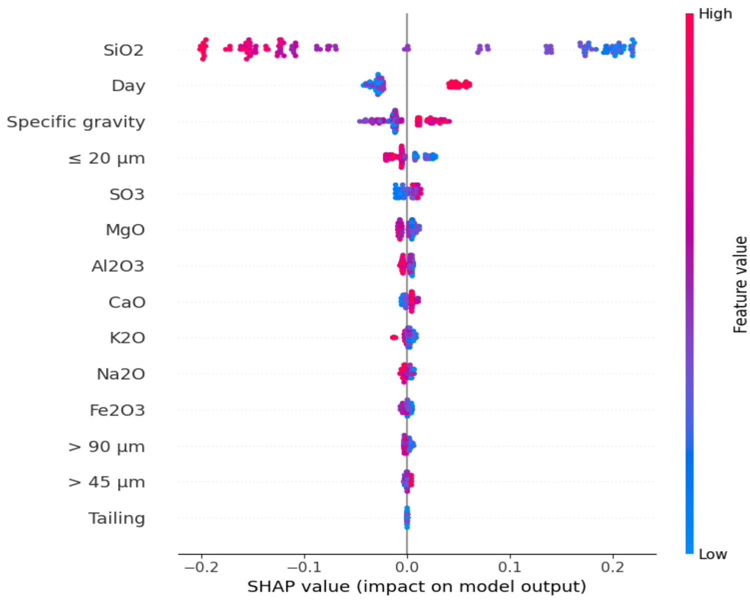

Fig. 5. CATE-SHAP summary (beeswarm) plot highlighting the key variables driving the heterogeneity of fly ash treatment effects on compressive strength

To better understand how these factors condition the fly ash effect, CATE-SHAP dependence plots were evaluated jointly (Fig. 6). The results for curing time demonstrate a pronounced time-dependent behavior: while the causal effect of fly ash remains limited at short curing durations, positive CATE-SHAP values increase substantially at longer curing times (90 and 200 days). This trend confirms that fly ash substitution becomes increasingly effective in the long term as pozzolanic reactions progress.

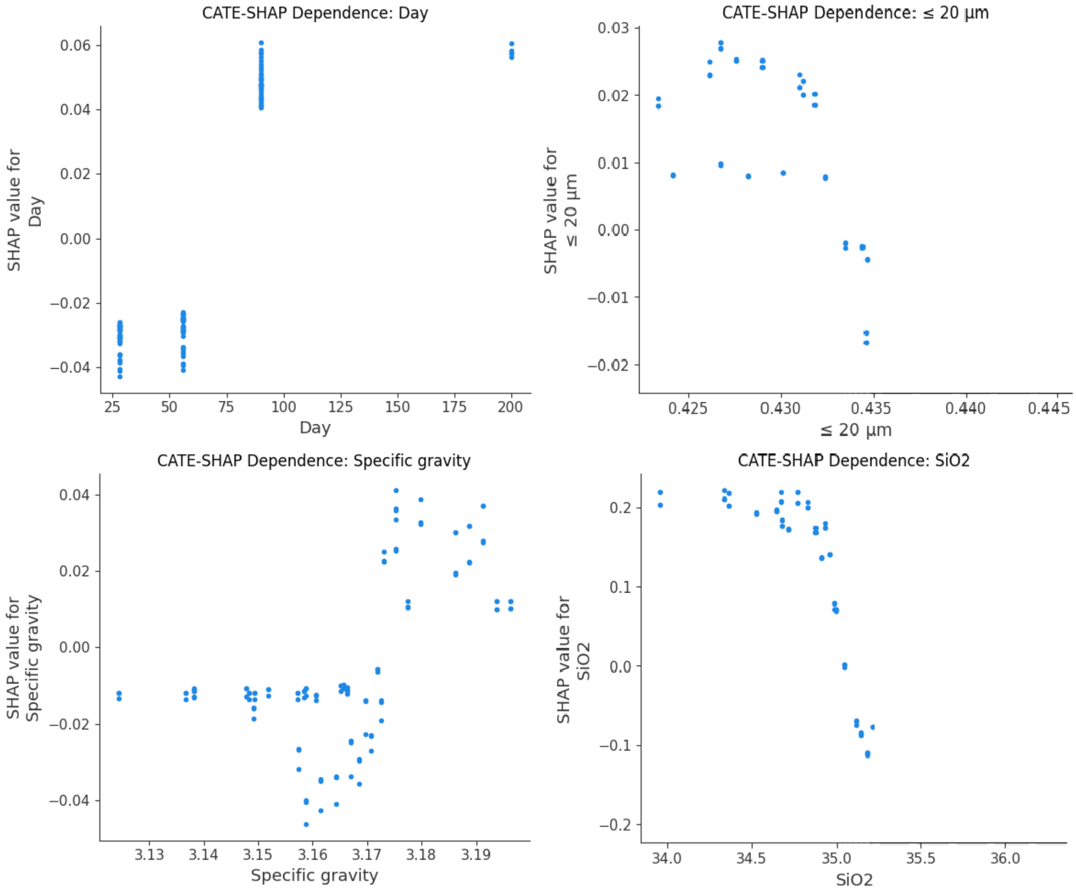

Fig. 6. Combined CATE-SHAP dependence plots illustrating the conditional effects of fly ash substitution with respect to curing time (Day), fine particle fraction (≤ 20 μm), specific gravity, and SiO_2 content

The dependence analysis for the fine particle fraction (≤ 20 μm) reveals a clear interaction between particle size distribution and fly ash effectiveness. Positive causal contributions are concentrated within a specific range of fine particle content, indicating that sufficient fines enhance the binding environment and facilitate the beneficial role of fly ash in the cementitious matrix.

The observed influence of the fine particle fraction is consistent with established cementitious material behavior reported in the literature. Finer particles are known to increase specific surface area, accelerate hydration and pozzolanic reactions, and enhance microstructural densification, thereby contributing to strength development (Scrivener et al., 2016; Thomas, 2013). In CPB systems, optimized particle size distribution improves packing density and reduces pore connectivity, which directly enhances mechanical performance (Wang et al., 2025). However, excessive fineness may increase water demand and negatively affect rheological stability, potentially limiting strength gain (Li et al., 2022). The threshold-like behavior identified in the CATE-SHAP results is therefore physically meaningful and reflects the balance between surface reactivity and mixture workability.

Similarly, the CATE-SHAP dependence for specific gravity indicates that the causal effect of fly ash is sensitive to system density. Fly ash exhibits stronger positive effects in systems with moderate specific gravity, whereas its contribution weakens at very low or very high density levels, suggesting the existence of an optimal packing and pore structure for effective fly ash utilization.

The dependence plot for SiO_2 content further emphasizes the chemical sensitivity of fly ash substitution. Positive causal effects dominate at low to moderate SiO_2 levels, while the effect diminishes or becomes negative at higher SiO_2 contents. This behavior suggests that high silica availability without sufficient calcium may limit the pozzolanic contribution of fly ash, thereby reducing its effectiveness.

Overall, the CATE-SHAP analysis demonstrates that the effect of fly ash substitution on compressive strength is highly condition-dependent, governed by curing time, particle size distribution, specific gravity, and chemical composition. Importantly, when outcome-level SHAP analyses are evaluated together with CATE-SHAP results, it becomes evident that variables explaining compressive strength do not necessarily coincide with those governing the causal effectiveness of fly ash substitution. This distinction highlights that predictive importance and causal relevance represent different conceptual layers. Consequently, interpretations based solely on predictive explainability may fail to capture the true performance conditions of substitute materials. By contrast, CATE-SHAP analyses explicitly reveal under which physicochemical conditions fly ash substitution provides tangible benefits, offering a robust basis for the rational and optimized use of mineral processing by-products in cemented paste backfill systems.

Finally, it should be noted that the present analysis primarily focused on major oxide components and physicochemical parameters directly governing hydration and strength development. The potential direct mechanical influence of residual heavy metals such as Pb and Zn in the tailings was not explicitly evaluated within the scope of this study. Since all tailings were obtained from the same beneficiation plant, their heavy metal content was assumed to represent the typical residue characteristics of the facility. Nevertheless, the proposed machine learning framework is flexible and can readily incorporate additional compositional variables, including trace metal contents, if such data are available. Therefore, the developed predictive and causal modeling approach remains applicable under varying sample conditions, provided that relevant physicochemical parameters are included as model inputs.

4. Conclusions

This study investigated the effect of fly ash substitution on compressive strength in cement-based systems through a holistic framework integrating predictive machine learning, explainable artificial intelligence, and causal machine learning approaches. The results clearly demonstrate that the influence of fly ash on compressive strength is neither unidirectional nor uniform, but is strongly governed by the physicochemical characteristics of the system and curing conditions.

The analyzed CPB mixtures reached compressive strength levels up to 10.33 MPa at 90 days of curing, confirming that optimized binder–tailings combinations can achieve structurally adequate performance. The predictive model successfully represented this high-strength region (R^2 = 0.58), while causal analysis quantified an average strength increase of approximately 0.28 MPa per 1% fly ash substitution under favorable conditions.

Predictive analyses revealed that curing time is the most dominant factor controlling compressive strength development. Extended curing periods significantly enhance late-age strength, particularly in fly ash–containing systems, reflecting the progressive contribution of pozzolanic reactions. Among the chemical components, oxides such as $Fe2O_3$ and K_2O were found to play a more prominent role in explaining strength variability compared to SiO_2 and CaO, highlighting the importance of detailed chemical composition in strength prediction.

A key finding of this study is that fly ash content alone does not emerge as a dominant variable directly explaining compressive strength. Instead, strength development is primarily controlled by the chemical and physical characteristics of fly ash, rather than by its dosage. This observation indicates that fly ash should not be treated as a homogeneous substitute material, but rather as a heterogeneous mineral processing by-product whose performance varies depending on its composition and physical properties.

Causal machine learning analyses further showed that fly ash substitution has a positive effect on compressive strength on average; however, this effect is highly heterogeneous and not valid across all systems. The distribution of conditional average treatment effects (CATE) revealed that fly ash can provide substantial strength gains under favorable conditions, while offering limited or negligible benefits under others. CATE-SHAP analyses identified curing time, SiO_2 content, particle size distribution, and specific gravity as the key moderators governing this heterogeneity.

Overall, the findings of this study demonstrate that the performance of fly ash substitution cannot be reliably evaluated using ratio-based approaches alone. Instead, optimization should be guided by a comprehensive assessment of physicochemical properties and curing conditions. The proposed explainable and causal data-driven framework provides a robust tool for the rational, reliable, and sustainable utilization of mineral processing by-products in cement-based systems, including cemented paste backfill applications.

Although the present framework was developed using a specific experimental dataset and fly ash types, the combined explainable and causal machine learning approach is readily transferable to other mineral processing by-products and binder systems. Future studies incorporating different fly ash classes, activation techniques, multi-substitution strategies, larger datasets, and field-scale applications are expected to further enhance the generalizability and practical relevance of the proposed methodology.

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