Development and Performance Evaluation of a Stacking Ensemble-Based Prediction Model for Carbonation Depth of Cementitious Materials

Introduction

Carbonation is a major durability mechanism in cementitious materials and an important process for estimating long-term service performance and CO_2 uptake in construction materials [1–4]. The progression of carbonation is governed by coupled material and environmental factors, including binder-related parameters, supplementary cementitious materials, relative humidity, CO_2 concentration, and exposure duration [1–4]. Although mathematical formulations and single machine-learning models have improved carbonation-depth prediction, their performance can deteriorate when heterogeneous literature data and complex nonlinear interactions must be handled simultaneously [1,4,6,7].

Recent studies have shown that artificial neural network (ANN), random forest (RF), support vector regression (SVR), extreme gradient boosting (XGBoost), and hybrid ensemble models can provide more accurate carbonation-related predictions than conventional empirical or curve-based approaches [2–7]. Nevertheless, there remains a need for a robust stacking framework capable of integrating complementary learners while preserving prediction stability across varied cementitious systems. Therefore, this study develops a stacking ensemble-based meta-model to improve the predictive accuracy of carbonation depth and to provide a practical data-driven tool for carbon mineralization assessment and CO_2 uptake quantification in the construction sector.

Method and/or Theory

A literature-derived database containing 300 data points was assembled from previous carbonation studies on cementitious materials. Six primary mixture and exposure variables were used to define the input space. To preserve the diffusion-controlled time dependence of carbonation, exposure time was handled in $\sqrt{t}$ form during feature engineering, and additional nonlinear interaction terms were introduced to better represent coupled effects among the governing variables [1]. The dataset was randomly divided into training and test subsets in a 70:30 ratio.

The proposed framework consisted of two stages In the first stage, ten base learners were trained, comprising linear regression, ridge regression, lasso regression, support vector regression (SVR), random forest (RF), gradient boosting regression (GBR), and several tuned variants of SVR, RF, and GBR. Out-of-fold predictions were generated using five-fold cross-validation to minimize training–inference mismatch and to construct meta-features with improved generalization. In the second stage, five meta-learners—XGBoost regressor, LightGBM regressor, random forest regressor, ridge regression, and multilayer perceptron (MLP) regressor—were comparatively evaluated. Furthermore, inverse-variance weighting based on the base-learner prediction errors was applied so that more reliable learners contributed more strongly to the final prediction. This weighted stacking strategy was designed to reduce individual model bias and improve the robustness of carbonation-depth estimation under heterogeneous data conditions.

The developed stacking ensemble model showed strong predictive capability for carbonation depth. Among the evaluated meta-learners, the RF-based meta-model achieved the best performance, with $R^2 = 0.9809$ and RMSE = 1.6188 on the test set. The other meta-learners also performed competitively, but their agreement with the observed data was slightly lower. These results indicate that the weighted stacking strategy successfully combined the complementary strengths of multiple base models and improved the representation of complex nonlinear relationships between material composition, exposure conditions, and carbonation response.

The observed performance trend is consistent with previous studies reporting the advantages of ensemble and hybrid approaches over single learners in carbonation-related prediction problems [4–7]. Earlier work on fly-ash concrete and hybrid ensemble models showed that carbonation depth is particularly sensitive to time, CO_2 concentration, humidity, and binder-related parameters [2–4], while recent studies also emphasized the benefits of interpretable and ensemble machine-learning frameworks for complex carbonation systems [5,7]. In this study, the meta-model structure effectively leveraged diverse prediction patterns from the base learners, leading to a more accurate and stable estimate of carbonation depth than could be expected from an isolated model.

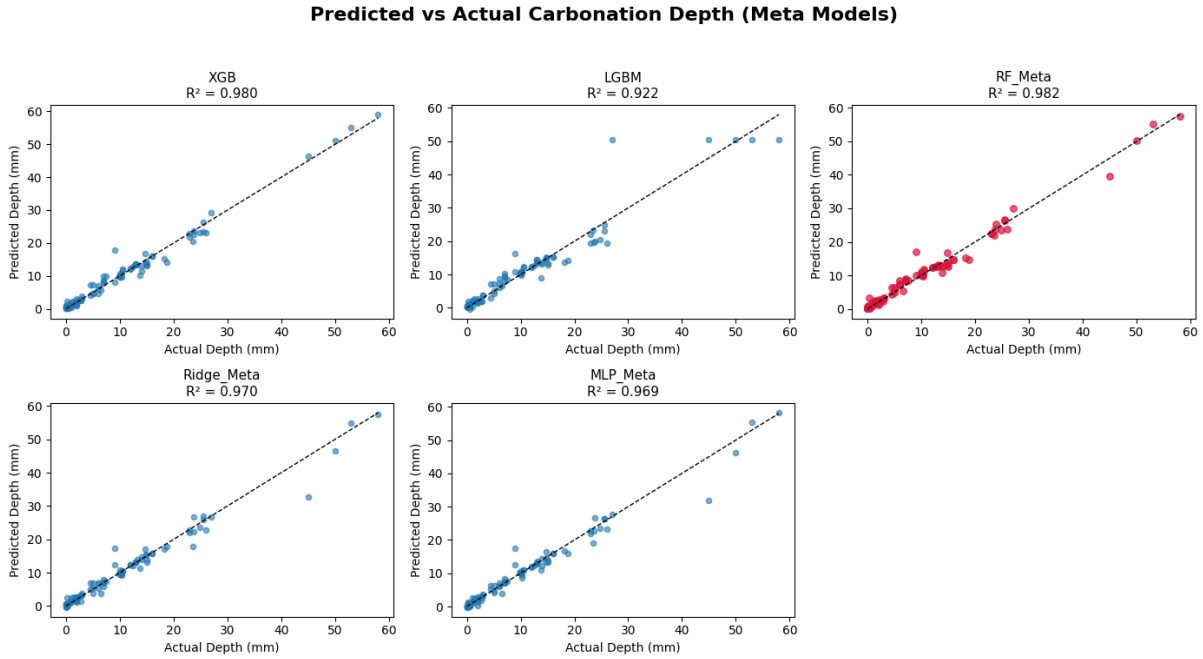

Figure 1 *Predicted versus actual carbonation depth for the evaluated meta-learners. The RF-based meta-model shows the closest agreement with the observed data.*

The practical implication of this work is that a stacking-based ensemble framework can support faster and more reliable carbonation-depth assessment for cementitious materials, which is relevant to both durability evaluation and carbon mineralization analysis. At the same time, the current model was trained using literature-derived data, and its performance under previously unseen input boundaries should be further verified. Because engineering prediction problems frequently involve extrapolation beyond the training domain, future work should incorporate boundary-aware validation and external datasets to strengthen the reliability of the model in real applications [8].

Conclusions

This study developed a weighted stacking ensemble-based meta-model for predicting the carbonatio n depth of cementitious materials using a literature-derived database of 300 cases. By combining ten b ase learners and five meta-learners through out-of-fold prediction and inverse-variance weighting, the proposed framework achieved high predictive accuracy, with the RF-based meta-model providing the best overall performance. The results demonstrate that stacking ensemble learning is an effective strat egy for capturing the complex nonlinear interactions governing carbonation depth. The proposed fram ework can serve as a useful scientific basis for future studies on CO_2 uptake quantification, carbon mi neralization assessment, and data-driven optimization of cementitious materials.

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