EXPLORATORY ADVANCED RESEARCH

Physically Informed Data-Driven Methods for Greatly Enhancing the Use of Heterogeneous Supplementary Cementitious Materials in Transportation Infrastructure

INSTITUTION: University of California, Los Angeles

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OBJECTIVE: To enhance the use of fly ash for producing more sustainable concrete.

RESULTS: Concrete is the dominant material used in the construction of buildings and infrastructure.[1] However, the production of ordinary portland cement (OPC) is associated with substantial carbon dioxide (CO_2) emissions, estimated at nearly 9 percent of the global carbon emissions.[2] To counteract the CO_2 impact of OPC production and use, the industry has sought to replace OPC in concrete with supplementary cementitious materials (SCMs). Fly ash, a residue from the combustion of coal, is currently the only SCM available in sufficient abundance to replace OPC in concrete.[3] However, fly ash's diverse chemical composition and the presence of crystalline (i.e., ordered) and noncrystalline (i.e., disordered) phases can make it difficult to use in concrete production. Although it is defined as either Class C or F, the specific composition of a certain fly ash can greatly affect the performance of the concrete with which it is mixed. Even similar fly ashes can result in vastly different concrete behavior. As a result, over the past decades, fly ash has had limited success as a high-volume substitute, replacing a limited amount of OPC in concrete (e.g., ≤25 percent by mass).[3]

With an unprecedented massive concrete and fly ash dataset collection of 40,000 data records, a research team conducted a series of experiments that used advanced material characterizations, machine-learning (ML) techniques, and numerical simulations to uncover the fundamental attributes governing the reactivity of fly ash and its suitability as an OPC replacement. This work aimed to enhance the use of fly ash for producing more sustainable concrete.

Using topological constraint theory and classical molecular dynamics simulations, the researchers developed an analytical model to predict the atomic topology of calcium aluminosilicate (CAS) glasses that make up the essential components of fly ash's noncrystalline (i.e., glassy) phase, that is, the most reactive phase of fly ashes (which contribute to increasing concrete's strength). This model could be used to accurately estimate the state of rigidity (flexible, isostatic, or stressed-rigid) of CAS glasses based on their chemical composition and temperature. The results revealed that the glass-forming ability of CAS glasses (which is closely related to the reactivity of fly ash) is encoded in its network topology (molecular structure), which is captured by the number of constraints per atom (n_c). Importantly, this finding indicates that the n_c of the amorphous phase of a fly ash can serve as a reliable structural proxy for its reactivity. The researchers then used an ML-based methodology to predict fly ash's rigidity (i.e., n_c) based on the sole knowledge of its bulk chemical composition. This approach can enable the rapid screening of reactive fly ashes via fast, inexpensive bulk characterization techniques (e.g., x-ray fluorescence). The team's predictive model can be used to maximize the beneficial use of fly ashes obtained from routine power plant production and enhance the reclamation of reactive fly ashes that are presently stored in impoundments.

The researchers developed a generic theoretical framework that can produce reliable predictions of binder properties that bring together portland cement and fly ash [PC + FA] to create concrete. This framework relied on a deep forest (DF) model, which consists of an ensemble of decision trees. Each tree offers a distinct prediction, which depends on whether or not the condition attached to each of its branches are satisfied. The DF model is trained with a collection of experimental data on the strength development of binders containing various fractions of cement being replaced by fly ash. Furthermore, theoretical knowledge of fly ash's composition-structure correlations and cement's hydration mechanism (i.e., which is governed dimensionally by the number of constraints per atom n_c previously mentioned) are infused into the DF model to boost its prediction performance. As a result, the DF model can accurately predict composition- and time-dependent hydration kinetics (i.e., the rate at which the reactive solids dissolve and react to form a cement paste) and compressive strength (the capacity of concrete to withstand loads before failure) of [PC + FA] binders. More importantly, the study derived a simple, closed-form analytical model that can robustly map the compositional attributions of cement and fly ash to the compressive strength of the binders.

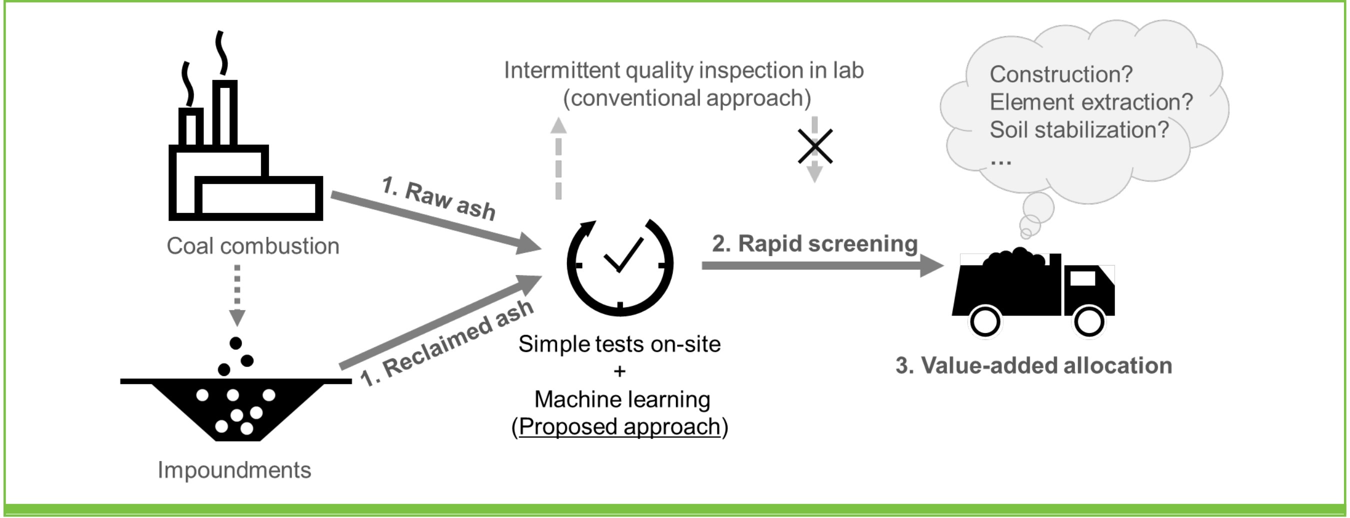

Figure 1. Schematic. Proposed ML-based screening approach.

This analytical model can offer important insights into the interactive effects of cement and fly ash on the strength development of [PC + FA] binders.

Due to the complex chemical reactions involved with cement hydration (the reaction between water and cement during the mixing process) and the interactions between different phases in concrete, reliable predictions of the strength of fly-ash-containing concrete materials (and many other key properties) remain unavailable through conventional approaches. As an alternative, ML offers a new pathway to developing powerful predictive models for concrete materials. After curating a collection of large-scale concrete datasets based on raw data obtained from actual concrete production, the research team demonstrated the potential of using different ML models to accurately predict the strength development of concrete.

The researchers first compared the performance of several prevailing ML algorithms in predicting the 28-d compressive strength (the strength of concrete 28 d after being cast) based on the knowledge of the mixture proportion, where the tradeoff between model accuracy, simplicity, and interpretability across those ML algorithms was specifically studied. The research team also investigated the influence of the training dataset's size on the accuracy of the team's ML models—as high-quality concrete strength data is limited. In that regard, several techniques were studied that could be used to improve the efficiency of ML methods when applied to small concrete datasets.

To enable the use of high-volume fly ash in concrete, the researchers also looked into using ML to infer the strength activity index (SAI) (an indicator of the quality of additional materials mixed into cement) of fly ashes based on the knowledge of their key material attributes. Based on a large fly ash dataset curated from the team's testing records, the researchers trained an ML model that offered accurate predictions of the 28-d SAI based on the sole knowledge of the fly ash's ASTM C618 attributes.(4) These models allowed the researchers to clarify how each of the chemical and physical attributes of fly ash affects their ability to replace cement in concrete.

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