AI-guided auto-discovery of low-carbon cost-effective ultra-high performance concrete: data synthesis, semi-supervised learning, and many-objective optimization

Soroush Mahjoubi – Graduate Research Assistant, Stevens Institute of Technology, Department of Civil, Environmental and Ocean Engineering, Hoboken, NJ, USA, Email: smahjoub@stevens.edu

Weina Meng – Assistant Professor, Stevens Institute of Technology, Department of Civil, Environmental and Ocean Engineering, Hoboken, NJ, USA, Email: weina.meng@stevens.edu

Yi Bao (corresponding author) – Assistant Professor, Stevens Institute of Technology, Department of Civil, Environmental and Ocean Engineering, Hoboken, NJ, USA, Email: yi.bao@stevens.edu

Abstract

This study presents an AI-guided approach for designing low-carbon cost-effective ultra-high performance concrete (UHPC). The approach automates the design process for UHPC by integrating data synthesis, automated machine learning, and many-objective optimization techniques. Machine learning models are trained on both experimental and synthesized data obtained by generative modeling and semi-supervised learning to predict UHPC properties including compressive strength, flexural strength, mini-slump spread, and porosity. The approach is demonstrated in two design scenarios: the first maximizes the compressive and flexural strengths and minimizes porosity while retaining self-consolidation, and the second minimizes the life-cycle carbon footprint, embodied energy, and material cost in addition to the objectives of the first scenario. Using a state-of-the art many-objective optimization algorithm, called adaptive geometry estimation-based many-objective evolutionary algorithm (AGE-MOEA), and a decision-making method, namely technique for order of preference by similarity to ideal solution (TOPSIS), two UHPC mixtures are discovered based on the predictive models and specified objectives. The UHPC mixtures generated in the second scenario achieve a reduction of 73% in the life-cycle carbon footprint, 71% in embodied energy, and 80% in material cost compared to those in the first scenario. This research presents a promising solution for achieving low-carbon cost-effective UHPC and advances the development of cementitious composites including UHPC using AI-guided approaches.

Keywords: carbon footprint; embodied energy; machine learning; many-objective optimization; semi-supervised learning; synthetic tabular data; ultra-high performance concrete (UHPC)

1. Introduction

Ultra-high performance concrete (UHPC) is a type of advanced cementitious material that possesses self-consolidation, superior mechanical properties, and long-term durability. UHPC is characterized by a 28-day compressive strength that exceeds 120 MPa under standard curing conditions (Du et al.). This high strength is due to its dense microstructure, which is achieved through a high particle packing density and low porosity. Additionally, the incorporation of chopped fibers dispersed in the cementitious matrix results in high tensile and flexural strengths, with the fibers providing crack-bridging effects (Karim and Shafei). UHPC's exceptional durability is due to its dense microstructure and discontinuous pore network.

Despite its numerous advantages, the high material cost and carbon footprint of UHPC have hindered its wider acceptance in engineering practices. This is largely due to the use of costly and high-carbon raw materials such as steel fibers, chemical admixtures, and cement. Many studies have been conducted to develop low-carbon and cost-effective UHPC mixtures by using alternative materials based on experimental testing. For example, some researchers have developed UHPC mixtures using local river sand, masonry sand, and supplementary cementitious materials (SCMs) such as fly ash and slag (Meng et al.). Test results have shown that the developed UHPC mixtures deliver high mechanical properties and low cost, carbon footprint and embodied energy.

An alternative approach to develop UHPC is to use data-driven machine learning models that are trained to predict UHPC properties based on calibrated relationship between design variables and properties (Fan et al.; Mahjoubi et al.). This study aims to address four limitations in using data-driven models and optimization algorithms for predicting UHPC properties: 1) lack of data for training, addressed by using generative modeling to enlarge datasets; 2) simple machine learning models used to predict high-dimensional relations with many variables, improved through the development of high-fidelity models; 3) difficulty for non-experts in machine learning to develop models with satisfactory performance, addressed through the development of an automated framework; and 4) previous studies focusing on optimizing either mechanical properties or material cost, while this study aims to optimize mechanical properties, cost, and eco-efficiency.

2. Methodology

The proposed framework includes seven steps: (1) Four datasets are established and divided into training and test sets. (2) Automated machine learning generates predictive models. (3) Generative techniques synthesize artificial data to enlarge training datasets. (4) Predictive models are re-trained using the enlarged datasets and compared against eight state-of-the-art methods. (5) Objective functions and design constraints are formulated to optimize mechanical properties, eco-efficiency, and cost-efficiency. (6) An evolutionary many-objective optimization algorithm (AGE-MOEA) is used to solve the optimization problems. (7) A decision-making method (TOPSIS) is applied to select the most preferable optimal solutions.

3. Results and Discussion

To assess the predictive performance of the automated machine learning models for compressive strength, flexural strength, mini-slump spread, and porosity, we calculated two widely-used performance metrics: root mean squared error (RMSE) and coefficient of determination (R^2), as detailed in **Table 1**. Our analysis reveals that the R^2 values of the predictive models evaluated on the test datasets are consistently higher than 0.92, which indicates that these models offer high accuracy and generalizability. These findings demonstrate that the data-driven models have satisfactory accuracy and generalizability and can be utilized to design UHPC mixtures.

Table 1. Performance metrics of the predictive models for UHPC properties

Metric	Compressive strength	Flexural strength	Mini-slump spread	Porosity
RMSE	6.40	1.89	9.62	0.16
R^2	0.95	0.92	0.94	0.97

Table 2 lists two UHPC mixtures discovered using the proposed approach for the two design scenarios and compares the two mixtures with three representative cost-effective UHPC mixtures that were developed through step-by-step experimental tests. The mixture discovered for DS1 (design obtained using design scenario 1) has higher mechanical properties than the mixture discovered for DS2 (design obtained using design scenario 2). The mixture discovered for DS2 has low carbon footprint, embodied energy, and material cost while satisfying the requirements of mechanical properties, workability, and porosity. The carbon footprint, embodied energy, and material cost of the UHPC mixture for DS2 are 73%, 71%, and 80% lower than those of DS1. Compared with existing UHPC mixtures developed through experiments, the discovered UHPC mixture for DS2 has comparable mechanical properties, workability, and porosity while highly reducing the carbon footprint, embodied energy, and material cost.

Table 2. UHPC mixtures discovered for different design scenarios

No.	UHPC property	Unit	DS1*	DS2""	UHPC-2 (Wille and Boisvert-Cotulio)	UHPFRC (Yu et al.)
1	Compressive strength	MPa	171.82	133.3	166	160
2	Flexural strength	MPa	32.24	19.22	18.5	20
3	Mini-slump spread	mm	260.2	271.9	265	283
4	Porosity	%	8.88	12.13	9.64	14
5	Carbon footprint	kg CO_2-eq/m^3	922.5	247.1	652	984
6	Embodied energy	MJ/m^3	9,631	2,750	5,014	9,507
7	Material cost	\$/m^3	1,664	329.1	472	1,203

*DS1: Design obtained using design scenario 1; ""DS2: Design obtained using design scenario 2.

4. References

- Du, Jiang et al. "New Development of Ultra-High-Performance Concrete (UHPC)." *Composites Part B: Engineering*, vol. 224, 2021, p. 109220.
- Fan, Dingqiang et al. "Precise Design and Characteristics Prediction of Ultra-High Performance Concrete (UHPC) Based on Artificial Intelligence Techniques." *Cement and Concrete Composites*, vol. 122, 2021, p. 104171.
- Karim, Rizwan and Behrouz Shafei. "Flexural Response Characteristics of Ultra-High Performance Concrete Made with Steel Microfibers and Macrofibers." *Structural Concrete*, vol. 22, no. 6, 2021, pp. 3476-3490.
- Mahjoubi, Soroush et al. "Auto-Tune Learning Framework for Prediction of Flowability, Mechanical Properties, and Porosity of Ultra-High-Performance Concrete (UHPC)." *Applied Soft Computing*, vol. 115, 2022, p. 108182.
- Meng, Weina et al. "Factorial Design and Optimization of Ultra-High-Performance Concrete with Lightweight Sand." *ACI Materials Journal*, vol. 115, no. 1, 2018.
- Wille, Kay and Christopher Boisvert-Cotulio. "Material Efficiency in the Design of Ultra-High Performance Concrete." *Construction and Building Materials*, vol. 86, 2015, pp. 33-43.
- Yu, Rui et al. "Sustainable Development of Ultra-High Performance Fibre Reinforced Concrete (UHPFRC): Towards to an Optimized Concrete Matrix and Efficient Fibre Application." *Journal of Cleaner Production*, vol. 162, 2017, pp. 220-233.