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学　位　論　文　内　容　の　要　旨

博士の専攻分野の名称　　博士（工学）　　氏名　Kong Yukun

学　位　論　文　題　名

Optimization of sustainable mix design for alkali-activated materials using machine learning methods
(機械学習を用いたアルカリ活性材料のサステイナブル材料設計)

The rapid increase in greenhouse gas emissions, primarily due to human activities, has become a significant environmental concern in the 21st century. The manufacturing of ordinary Portland cement (OPC) contributes significantly to these emissions, accounting for 6%–8% of total anthropogenic carbon dioxide (CO_2) emissions worldwide. Alkali-activated material (AAM) is a promising replacement to OPC, which is generally produced by low carbon-footprint supplementary cementitious materials mixed with alkali solution. The superior performance of AAM in strength to OPC is strongly dependent on the dense pore structures which is closely related to the mix design. However, the commercial use of AAMs faces three main challenges. First, current prediction models for AAM properties are often limited by narrow experimental datasets, lacking generality and practicality. Second, while forward analysis models predict properties based on mix design parameters, there's a rising demand for inverse analysis to determine optimal mix designs for specific construction needs. However, methods capable of predicting all mix design parameters based on desired properties are lacking. Third, balancing performance and sustainability is a challenge in optimizing AAM mix designs, requiring careful consideration to achieve desired properties while minimizing environmental impacts. For fulfilling this research gap, the presented research incorporates three main areas that are (i) Identifying the key factors of mix design and constructing mathematical models for predicting the workability, compressive strength and drying shrinkage of AAM; (ii) Inverse analysis for determining the mix design of AAMs; and (iii) Life cycle assessment of the optimized AAM mixtures considering the key factors. Overall, the above research systematically investigated the AAM and provided a practical guidance for the mix design of AAM. It is believed that an optimized mix design of AAM with high performance and sustainability can be drawn out.

Chapter 1 sets the stage by providing the research background, articulating the problems addressed across the three main research areas investigated in this thesis, and outlining the primary objectives and contributions of this study.

Chapter 2 offers an extensive literature review covering alkali-activated materials (AAMs), the impact of mix design on both fresh and hardened properties, the utilization of machine learning technology, and the environmental implications associated with AAMs.

In the next three chapters, forward predictive models for fresh and hardened properties of AAMs are given using three machine learning methods, i.e., artificial neural network (ANN), LightGBM (LGBM) and XGBoost (XGB). Chapter 3 gives a prediction model for workability of AAMs based on 402 individual mixtures collected from 26 existing papers. For constructing the prediction model for AAMs, a typical workflow including data collection, data processing, data analysis and modelling is used.

This workflow is as well adopted for constructing the models for predicting compressive strength and drying shrinkage. Eight key factors influencing the workability performance of AAMs are recognized, including the activity moduli and specific surface area of precursors (SSA), Silicate modulus (Ms) of the alkali activator, NaOH concentration, Liquid to binder ratio (L/B ratio), Geopolymer paste content (GPC), and aggregate ratio. The qualitative results show that workability increases with the Ms and GPC but decreases with the NaOH concentration and aggregate content. In the proposed models, the above eight factors are set as input data, while the flowability results are set as output data. Three machine learning-based models demonstrate notable robustness and accuracy in forecasting the workability of AAMs, achieving coefficient of determination (R^2) values of 0.81, 0.96 and 0.95 for ANN, LGBM and XGB, respectively.

Chapter 4 offers the prediction model for 28-day compressive strength of AAMs utilizing a total of 301 AAM mixture from 23 previous papers.The selection of key factors for strength is the same as workability. The data analysis results reveal that higher activity of precursor, Ms and NaOH concentration may favor the strength development of AAMs, while L/B ratio and GPC usually hinder the strength development. In this machine learning-based model, the abovementioned key factors were inserted as the input data and the compressive strength is set as the output data. ANN, LGBM and XGB models all achieve significantly high R^2 values of 0.85, 0.96 and 0.97, respectively, in which XGB display the highest performance.

Chapter 5 introduces machine learning models for predicting drying shrinkage in AAMs. The database includes 438 AAM mixes from 43 papers, incorporating factors such as curing temperature, relative humidity (RH), and volume/surface (V/S) ratio. Qualitative analysis reveals that drying shrinkage resistance typically increases with higher NaOH concentrations, aggregate ratios, curing temperature, RH, and V/S ratios, while decreasing with higher GPC, L/B ratio, and Ms. ANN, LGBM, and XGB models demonstrate high accuracy and robustness, with R^2 values of 0.94, 0.99, and 0.99, respectively.

Chapter 6 outlines an inverse analysis method for predicting optimal mix designs of AAMs based on desired properties. The method comprises data generation using a Gaussian mixture model, property prediction using the XGB algorithm, and mix design filtration. Data generation is based on a pre-collected database, aligning well with existing AAM mixes. The XGB algorithm is employed for predicting mechanical properties due to its high performance in both fresh and hardened states. Additionally, a life-cycle assessment evaluates environmental impacts across five categories, i.e., Global warming, Ozone depletion, Acidification, Eutrophication, and Ecotoxicity, using the CML 2002 approach. The integration of mechanical properties and environmental impacts offers decision-makers a workflow for selecting suitable AAM mixes.

Finally, Chapter 7 serves as the conclusion, summarizing the key findings of the thesis. It also delves into discussions concerning the challenges and potential of utilizing machine learning techniques in civil engineering. Additionally, it proposes potential directions for future research endeavors.