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学 位 論 文 内 容 の 要 旨

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学 位 論 文 題 名

Performance Enhancement of Cementitious Materials by Nano-additives: An Experimental and Numerical Study

(ナノ添加剤によるセメント系材料の性能向上: 実証実験および数値モデル)

In recent years, nanomaterials like nano-silica, nano-alumina, carbon nanotubes, and graphene oxide have been increasingly used to improve the mechanical and durability properties of cementitious materials. However, determining the optimum dosage and mechanical properties of nano-modified cement-based requires significant time, effort, and cost. However, accurately predicting the dosage and mechanical properties of nano-modified cement-based materials remains challenging. Various techniques, including mathematical and statistical analyses, as well as analytical, numerical, computational, homogenization, and multi-scale models, have been employed to develop prediction models. While earlier analytical models failed to account for the complexity of influencing factors accurately, newer Machine Learning (ML) techniques have shown promise but lack transparency. As the microstructure of hydrated cement paste significantly affects concrete strength, recent models have focused on simulating cementitious material hydration to bridge nano and macro properties. However, existing models often rely on assumptions and cannot directly correlate with concrete's macro properties. Therefore, this research aims to develop a robust model capable of realistically predicting the mechanical properties of nano-silica-modified cementitious materials by incorporating detailed microstructure information, fundamental physics and chemistry, thermodynamic considerations, and particle bonding and packing arrangements.

Nanomaterials such as nano silica and graphene oxide (GO) were investigated for their impact on the mechanical properties of cementitious materials. Experimental studies, including TGA, XRD, XRF, FTIR, SEM, Si NMR, H NMR, and zeta potential analysis, were conducted to understand the effects of these nanomaterials on hydrate formation. Nano silica was found to enhance the mechanical properties of cement paste, especially at early ages (¡ 7 days), through its pozzolanic and nucleation effects. However, an increase in nano silica content led to agglomeration, diminishing its effectiveness.

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A systematic model was then developed to optimize nano silica and graphene oxide (GO) use in cement paste and predict their nonlinear behaviour. The model integrates a hydration model, which calculates the dissolution rate of each clinker mineral, with a thermodynamic model simulating the hydration reaction and interaction between hydrates and nano-silica/GO. For nano-silica, the hydration model was modified to account for its reaction degree, dependent on portlandite availability, and to accurately represent the formation of calcium-silica-hydrate (C-S-H) with a transition from jennite-type to tobermorite C-S-H. Similarly, for GO, only tobermorite C-S-H formation during hydration was considered. The model computed volume fractions of various phases, and a representative volume element (RVE) was formulated for cement pastes with and without nano silica/GO using MATLAB. Finite element analysis with COMSOL Multiphysics was used to evaluate the RVE, allowing computation of homogenized material properties like compressive strength. Predictions aligned well with experimental findings. Additionally, the model was extended to predict mortar mechanical properties, considering fine aggregate content and Interfacial Transition Zone (ITZ) properties, and validated with experimental results.

In summary, this systematic model accurately predicts the nonlinear behaviour of cement pastes with different nano silica/GO replacement levels and can be extended to predict nano-modified mortar, offering the potential for optimizing cement-based composites in various engineering applications.