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Modeling and simulation of cement hydration kinetics and microstructure development

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ABSTRACT

Efforts to model and simulate the highly complex cement hydration process over the past 40 years are reviewed, covering different modeling approaches such as single particle models, mathematical nucleation and growth models, and vector and lattice-based approaches to simulating microstructure development. Particular attention is given to promising developments that have taken place in the past few years. Recent applications of molecular-scale simulation methods to understanding the structure and formation of calcium–silicate–hydrate phases, and to understanding the process of dissolution of cement minerals in water are also discussed, as these topics are highly relevant to the future development of more complete and fundamental hydration models.

Contents

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