Simulating Hydration of Lime-cement Binders with HYMOSTRUCT Model

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ABSTRACT

Despite their superiorities in carbon sequestration ability and gas permeability, pure lime mortars are weak and fragile in early ages, as they usually gain strengths through long-term carbonation. Therefore, mixtures of slaked lime and Portland cement are preferred in masonry structures to balance sustainability and early-age mechanical performances. However, due to the lack of understanding in reaction kinetics, there is no reliable microstructure formation models for lime-cement binders, and the material design can only be carried out in an empirical approach. To bridge this gap, this research focuses on hydration, the dominant hardening mechanism in early ages, and empirically determines the hydration kinetics through the combined use of X-ray diffraction (XRD), thermogravimetric analyses (TG), and calorimetry. Based on experiment results, the HYMOSTRUCT model, which was originally developed for cement hydration, is further extended to lime-cement binders. In the extended model, spherical lime and cement clinker particles were firstly generated with laser diffraction test results of raw materials. Then the hydrations of four major phases (i.e., C_3S, C_2S, C_3A and C_4AF) were separately considered with basic hydration factors obtained through quantitative analyses of XRD results, and the hydration product was calculated as a uniformly distributed shell outside of cement clinker particles. The influence of slaked lime is interpreted in two aspects – increase in basic hydration rates and the change in cement clinker distribution. The model was finally compared with pore size distribution data obtained with mercury intrusion porosimetry (MIP) and could be used as the input for further carbonation simulation.

KEYWORDS: *Slaked lime, Portland cement, hydration simulation, extended HYMOSTRUCT model*

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