High Resolution Solid State NMR Structural Study of a Ternary Hydraulic Mixture

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Abstract : The chemical phenomena occurring during cement hydration are complex and interdependent, and even after almost two centuries of studies, they are still difficult to solve for complex mixtures combining different hydraulic binders. Powder-XRD has been widely used for characterizing the crystalline phases in both anhydrous and hydrated cement, but only limited information is obtained in the case of strongly disordered and amorphous phases. In contrast, local spectroscopies like solid-state NMR can provide a quantitative description of noncrystalline phases. In this work, the structural modifications occurring during hydration of a fast-setting ternary binder based on white Portland cement, white calcium aluminate cement, and calcium sulfate were investigated using advanced solid-state NMR methods. We particularly focused on the early stage of the hydration up to 28 days, working with samples whose hydration was controlled and stopped. ²⁷Al MQ-MAS as well as {¹H}-²⁹Si Cross- Polarization MAS NMR techniques were combined to distinguish all of the aluminum and silicon species formed during the hydration. The NMR quantification of the different phases was conducted in parallel with the XRD analyses. The consumption of initial products, as well as the precipitation of hydraulic phases (ettringite, monosulfate, strätlingite, CSH, and CASH), were unambiguously quantified. Finally, the drawing of the consumption and formation of phases was correlated with mechanical strength measurements.

Keywords : cement, hydration, hydrates structure, mechanical strength, NMR

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