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Phosphate Additives for Tailoring Magnesium Silicate Hydrate Formation

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Mg-silicate cements are a sustainable alternative to Portland cement with reduced carbon emissions [1], but slow kinetics and high water demand limit their application [2]. These binders form through reactions between reactive magnesia (MgO) and silicate sources, producing magnesium silicate hydrate (M-S-H) via dissolution-precipitation, with $Mg(OH)_2$ as an intermediate [3]. The main challenge is that $Mg(OH)_2$ forms passivating layers on MgO surfaces, restricting Mg^{2+} release and slowing hydration. Phosphate-based additives are promising candidates to overcome this by complexing Mg^{2+}, preventing premature $Mg(OH)_2$ precipitation, and promoting M-S-H development [4], though their molecular-level influence remained poorly understood.

This study investigates M-S-H and brucite formation using titration and batch experiments with real-time pH, transmittance, and conductivity monitoring, complemented by FTIR, XRD, TGA, NMR, SEM, and TEM characterization, building on crystallization scenarios developed in our group [5]. Three structurally distinct phosphate additives were compared: phytic acid (organic cyclic), sodium hexametaphosphate (SHMP, inorganic cyclic), and sodium tripolyphosphate (TriP, linear).

Each additive showed distinct concentration-dependent behavior. Phytic acid produced the strongest nucleation delay, shifting the process from one-step to two-step nucleation at ≥50 mg/L through concurrent formation of magnesium-phytate precipitates alongside M-S-H. SHMP and TriP promoted magnesium-silicate-phosphate glass phases at higher concentrations (≥100 and ≥500 mg/L, respectively), significantly delaying nucleation and growth.

Long-term hydration studies (1–28 days) confirmed that all additives accelerate brucite and silica dissolution, altering the M-S-H formation pathway. Low concentrations promoted earlier ordered M-S-H structures, while high concentrations initially hindered but ultimately accelerated structural maturation. Nanoindentation confirmed enhanced mechanical properties at intermediate concentrations, with FTIR wavenumber shifts correlating directly with mechanical modulus.

These findings demonstrate that phosphate additives tailor M-S-H formation through competitive precipitation (phytic acid), glass phase formation (SHMP/TriP), and enhanced dissolution kinetics, providing a framework for optimizing sustainable Mg-silicate binders.

References

[1] E. Gartner & T. Sui, *Cem. Concr. Res.* 114, 27–39 (2018). [2] E. Bernard et al., *Phys. Chem. Earth* 99, 142–157 (2017). [3] Z. Li et al., *Constr. Build. Mater.* 61, 252–259 (2014). [4] M. Tonelli et al., *J. Therm. Anal. Calorim.* 138, 3311–3321 (2019). [5] A. Bastian et al., *J. Chem. Phys.* 162, 064704 (2025).