## **Predicting Long-Term Performance of Concrete under Sulfate Attack**

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Abstract : Cement-based materials have been using in various reinforced concrete structural components as well as in nuclear waste repositories. The sulfate attack has been an environmental issue for cement-based materials exposed to sulfate bearing groundwater or soils, and it plays an important role in the durability of concrete structures. The reaction between penetrating sulfate ions and cement hydrates can result in swelling, spalling and cracking of cement matrix in concrete. These processes induce a reduction of mechanical properties and a decrease of service life of an affected structure. It has been identified that the precipitation of secondary sulfate bearing phases such as ettringite, gypsum, and thaumasite can cause the damage. Furthermore, crystallization of soluble salts such as sodium sulfate crystals induces degradation due to formation and phase changes. Crystallization of mirabilite (Na<sub>2</sub>SO<sub>4</sub>:10H<sub>2</sub>O) and thenardite (Na<sub>2</sub>SO<sub>4</sub>) or their phase changes (mirabilite to thenardite or vice versa) due to temperature or sodium sulfate concentration do not involve any chemical interaction with cement hydrates. Over the past couple of decades, an intensive work has been carried out on sulfate attack in cement-based materials. However, there are several uncertainties still exist regarding the mechanism for the damage of concrete in sulfate environments. In this study, modelling work has been conducted to investigate the chemical degradation of cementitious materials in various sulfate environments. Both internal and external sulfate attack are considered for the simulation. In the internal sulfate attack, hydrate assemblage and pore solution chemistry of co-hydrating Portland cement (PC) and slag mixing with sodium sulfate solution are calculated to determine the degradation of the PC and slag-blended cementitious materials. Pitzer interactions coefficients were used to calculate the activity coefficients of solution chemistry at high ionic strength. The deterioration mechanism of co-hydrating cementitious materials with 25% of Na<sub>2</sub>SO<sub>4</sub> by weight is the formation of mirabilite crystals and ettringite. Their formation strongly depends on sodium sulfate concentration and temperature. For the external sulfate attack, the deterioration of various types of cementitious materials under external sulfate ingress is simulated through reactive transport model. The reactive transport model is verified with experimental data in terms of phase assemblage of various cementitious materials with spatial distribution for different sulfate solution. Finally, the reactive transport model is used to predict the long-term performance of cementitious materials exposed to 10% of Na<sub>2</sub>SO<sub>4</sub> for 1000 years. The dissolution of cement hydrates and secondary formation of sulfate-bearing products mainly ettringite are the dominant degradation mechanisms, but not the sodium sulfate crystallization.

Keywords : thermodynamic calculations, reactive transport, radioactive waste disposal, PHREEQC

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