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COUPLED MECHANICAL-REACTIVE TRANSPORT MODELING OF DAMAGE OF CEMENTITIOUS MATERIALS DUE TO ACCELERATED DECALCIFICATION

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ABSTRACT

A numerical simulation framework is presented in this paper for assessing degradation of cementitious materials exposed to aggressive ammonium nitrate solution. The coupled mechanical-reactive transport model consists of three parts – (1) transport of species, (2) chemical reactions, and (3) changes in hydraulic and mechanical properties due to changes in mineralogical composition. A geochemical speciation code in conjunction with the pH dependent test data for a Type I/II cement is used to obtain a mineral set that best describes the trends in the test data for the major species. The diffusion profiles of the species are calculated using the concentration gradients of the species and then the equilibrium composition of the material is calculated using the geochemical speciation code. Two homogenization schemes combined with Eshelby's equivalent inclusion method are used to estimate the mechanical properties of the structure due to changes in the mineralogical compositions. The model is then calibrated and validated using accelerated decalcification test data performed on a similar material. The test comprised of immersing a Portland cement paste sample in 6M ammonium nitrate solution (accelerated decalcification) for 7, 14, 28, and 125 days. The test data consisted of changes in pH and leachate concentrations as a function of exposure duration, profiles of species in the cement matrix, and strengths of degraded and undegraded samples.