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Reactive transport modeling of cementitious materials exposed to aggressive environment

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Reactive transport models have received a lot of attention from geochemists to simulate transport of contaminants in soils and natural environments. In most cases, these models are based on dispersion/advection transport coupled, using different approaches, to chemical reaction relationships. The authors propose here a variation on these models to simulate reactive transport in cementitious materials. The proposed model takes into account core characteristics of these materials such as highly concentrated pore solution, strong pH, very soluble solid matrix, and time-dependent pore structure. The model incorporates the effect of chemical activity gradients, electrodiffusion coupling, moisture and thermal coupling, and feedback effect. It also takes into account the effect of pore solution viscosity on species diffusion rate. Since concrete structures are commonly exposed to rapidly-changing boundary conditions such as deicing salt applications and seawater in tidal zones, time-dependent boundary conditions are a key feature of the model. Examples of common civil engineering structures such as bridges and quay walls are discussed. The use of the model in the context of long-term nuclear waste storage is also presented. Validation of exposure to chloride and low-pH sulfate-laden environments are presented by comparing model results with data collected on cementitious materials in controlled laboratory environment. Experimental characterization was performed using microprobe analysis, XRD, and acid dissolution of thin layers.