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NUMERICAL MODELLING OF CHEMICAL REACTIONS IN CEMENTITIUOS MATERIALS

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ABSTRACT

The paper is concerned with chemo-mechanical models describing the interaction of highly non-linear transport processes, chemical reactions and mechanical damage in cemetitious materials. Chemically caused phenomena which have a major influence on the durability of concrete structures are explained, modelled by the theory of porous media and simulated by spatial and temporal finite element methods. For the purpose of reproducing the local chemical reaction and the additional diffusion exactly on the microlevel, a dissolution-diffusion model is developed. In particular, the Onsager & Fuoss model of electrolyte diffusion [1] in chemically inert porous materials based on the theory of ionic clouds by Debye & Hückel [2] is presented. This electrolyte diffusion model is able to represent the electric charged mass transport and covers the ion-ion interaction. Furthermore a reaction kinetics model for portlandite dissociation due to carbonated water attack $Ca(OH)_2 \rightleftharpoons Ca^{2+} + 2\,OH^-$ is investigated. This equation indicates the relevance of the amount of calcium ions within the pore space with regards to the state of chemical equilibrium. The Arrhenius equation provides the quantitative basis of the relationship between the activation energy and the rate at which the reaction of this dissolution process takes place. The material degradation due to chemical matrix dissolution and mechanical induced damage is captured by an isotropic scalar damage model with an equivalent strain damage criterion.

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