Modelling of isothermal coupled moisture–ion transport in cementitious materials

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A B S T R A C T

A numerical model has been developed to predict isothermal coupled moisture–ion transport in cementitious materials. Ionic transport is described by the extended *Nernst–Planck* equation, which accounts for advection of the liquid phase. Moisture transport includes Fickian water-vapour relative diffusion and Darcian liquid-phase movement. The ion effect on liquid/vapour water equilibrium is taken into account. The variations of the transport properties *vs* the degree of saturation are described by integral functions or analytical formulas. A *Freundlich's* type description along with instantaneous *Friedel's* salt formation is considered for chloride binding at equilibrium. A kinetic equation is added in the cases of non-instantaneous binding processes. The governing equations, as well as the methods of assessment of the material properties required as input data, are described in the paper. Moreover, examples of application of the model in lab conditions are provided, which highlight its capability of predicting moisture/ionic concentration profiles even in complex configurations.

1. Introduction

Chloride-induced reinforcement corrosion is the major cause of premature damage in reinforced concrete (RC) structures located in marine, coastal or road environments [1,2]. Various mechanisms may occur simultaneously depending on the environmental conditions and on the material. In saturated conditions (*e.g.* permanent immersion in seawater), chlorides from the environment penetrate into the covercrete by a coupled diffusion-binding process. In coastal areas, in tidal zones or in the presence of deicing salts, wetting–drying cycles coupled with the effect of wind induce a non-saturated state and an inhomogeneous spatial distribution of moisture in the structure. In such non-saturated conditions, ionic transport relies on advection, in addition to diffusion. This induces a significant higher rate of chloride ingress and of reinforcement corrosion, in particular in the case of wetting–drying cycles, compared to the case of diffusion (in saturated conditions) [3–5,13]. Only in some cases (*e.g.* high-performance concretes), the impact of these cycles will be limited to the surface zone of RC elements and will have no significant effect on the chloride concentration distribution deeper in the element [24]. Besides, research works [6–8,34,35] have shown that the presence of salts in the pore system yields a decrease in the drying rate. Moreover, when a salt-contaminated concrete structure is drying, ions are transported towards the evaporation front, where they accumulate and where salts can crystallise, generating for example unaesthetic efflorescences [13].

Therefore, ionic transport in non-saturated cementitious materials involves complex chemical and physical mechanisms. A detailed knowledge of these mechanisms and a relevant implementation of the associated laws in a numerical model are essential to understand the phenomena and hence to predict accurately RC structure service life.

A lot of works have contributed to clarify the fundamental aspects of ionic transport in non-saturated concrete and numerous models have been developed, in order to predict chloride ingress in RC structures (see *e.g.* [12,14,15,26,36,37,39,47,48] and the literature reviews in Refs. [2,16]). The difficulties linked to the description of transport processes in non-saturated concrete can be related to the intrinsic complexity of the material and to the intricate nature of the phenomena. Some of these difficulties also rely on the fact that the various researchers have used different approaches to study these processes: for example differences in the state variables, in the driving forces of moisture or ionic transport or in the physical–chemical binding description can be found. In addition, even if some of the authors account for the advection process, most of them do not take into account all of the other mechanisms/processes. Moreover, movements of liquid water (involved in the advection process) and of water vapour are usually not separated. This may induce inaccuracies in the predictions for low-permeability cementitious materials when the total gas pressure cannot be considered as a constant (*i.e.* when gas pressure variations are not sufficiently rapidly dissipated) [67].

This paper deals with the analysis and simulation of coupled moisture–ion transport in isothermal conditions in cementitious materials on the basis of well-identified physical mechanisms. A multispecies transport model, which combines liquid-water, water-

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