Cement and Concrete Research 68 (2015) 10–23

Contents lists available at ScienceDirect

Cement and Concrete Research

journal homepage: http://ees.elsevier.com/CEMCON/default.asp

Numerical modelling of moisture transfers with hysteresis within cementitious materials: Verification and investigation of the effects of repeated wetting–drying boundary conditions

Zhidong Zhang [a,b], Mickaël Thiery [b,c,*], Véronique Baroghel-Bouny [b]

[a] Department of Civil and Environmental Engineering, Princeton University, Princeton, NJ 08544, USA
[b] Paris-Est University, IFSTTAR, MaSt/FM^{2}D, F-77447 Marne-la-Vallée, France
[c] DGAC, STAC, F-94385 Bonneuil-sur-Marne, France

ARTICLE INFO

Article history:
Received 16 January 2014
Accepted 24 October 2014
Available online 14 November 2014

Keywords:
Cementitious materials (E)
Moisture transport (C)
Hysteresis (C)
Drying–wetting cycles (A)
Moisture penetration depth (B)

ABSTRACT

In natural environment, the cover layer of reinforced concrete structures is affected by periodic variations of external relative humidity (RH). However, most moisture transport models in the literature only focus on drying of materials. In this study, a method coupling a moisture transport model with any kind of hysteresis modelling is presented. Two hysteresis models (conceptual and empirical) have been implemented and compared. The scope of the study is limited to cyclic variations of RH with no direct contact with liquid water during the wetting steps. Experimental data verifications show that the conceptual approach yields better results than the empirical one. Comparisons of non-hysteresis and hysteresis modellings have been carried out for different cycle durations, RH amplitudes and initial moisture states. All comparisons and investigations enhance the necessity of considering hysteresis to quantify moisture transport under repeated drying–wetting boundary conditions.

1. Introduction

The durability of reinforced concrete structures is closely related to environmental conditions. External conditions are various, including drying action of wind and sun, wetting from rain-water and spray, freezing and thawing actions, *etc.* The movement of liquid-water and the diffusion of gas or ions are the essential transport phenomena which govern durability of concrete. Most of the mechanisms of degradation (chloride ingress, carbonation, corrosion, *etc.*) are highly influenced by the moisture state of the material. To evaluate the durability of concrete structures, it is hence extremely useful to study moisture interactions between the cementitious materials and the environment.

In the literature, modelling of moisture transport in cementitious materials generally focuses on the drying process caused by low ambient RH (*e.g.*, [1]). However, the natural environment does not only correspond to drying conditions. Drying and wetting appear alternatively in natural conditions. This is considered as the most unfavourable environmental situation for concrete structures exposed to high ion content surroundings, because drying and wetting cycles can accelerate the penetration of ions (*e.g.*, chlorides [2]). Therefore, to understand durability issues, there is a need to model moisture behaviour under drying and wetting cycles. Let's bear in mind that the terms "drying" and "wetting" used here refer to moisture transport occurring in the hygroscopic range. In other words, the present study only considers the material exposed to the humid air with no direct contact with liquid-water.

For modelling of moisture transport using a continuum model [3], the water vapour sorption isotherms (WVSIs) [4], describing the relationship between RH (or capillary pressure P_c) and water content θ (or degree of saturation S), are generally used. Modelling of drying process normally employs the main desorption curve [1] while modelling of wetting or re-drying processes is more complicated because of sorption hysteresis. Sorption hysteresis is illustrated as a difference in water content for a same RH value (see the saturation differences for the same RH in Fig. 1). Previous models generally neglect hysteresis and use the main desorption isotherm to model moisture transport for both drying and wetting processes (*e.g.*, [5]); it might be due to the lack of experimental data for verification and premature computation techniques.

More recently, modelling considering hysteresis has become a topic of interest. Johannesson and Nyman [6,7] and Johannesson and Janz [8] have adopted empirical hysteresis models in which each scanning isotherm is expressed by a polynomial function. The independent domain theory model (Preisach–Mayergoyz PM model [9,10]), which was initially developed for modelling of physical mechanisms of magnetization, has been employed in the research performed by Derluyn et al. [11]. These studies have emphasised the necessity of considering hysteresis for predicting moisture behaviour in cementitious materials.

* Corresponding author at: Paris-Est University, IFSTTAR, MaSt/FM^2, F-77447 Marne-la-Vallée, France. Tel.: +33 1 80 68 80 00.
E-mail address: mickael.thiery@aviation-civile.gouv.fr (M. Thiery).

http://dx.doi.org/10.1016/j.cemconres.2014.10.012
0008-8846/

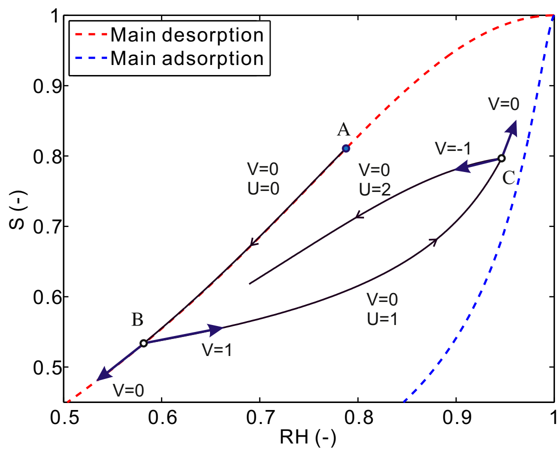

Fig. 1. Implementation of the hysteresis models.

Derluyn et al. [11] concluded "durability risks may be underestimated when omitting moisture hysteresis". Johannesson et al. [7] even argued that "the error in determining the water content may be as high as 30–35%" for the non-hysteresis modelling.

Nonetheless these conclusions have been only verified thanks to limited supporting experimental data which generally correspond to sorption measurements carried out on thin samples and for small RH steps. According to the authors, there are no real comparisons in the literature between simulations and mass loss kinetics and/or moisture content profiles showing the effects of repeated drying and wetting boundary conditions on specimens whose size are representative of the concrete cover thickness. The present study provides experimental data (desorption and adsorption isotherms, mass loss curves and liquid-water saturation profiles) for three materials to verify and compare the proposed models. Moreover empirical and conceptual hysteresis models are separately used in studies provided by Johannesson and Nyman [6,7], Johannesson and Janz [8] and Derluyn et al. [11]. Thus a comparison of these two kinds of models with the same set of experimental data is needed to investigate the differences between them.

One important factor to evaluate the durability of concrete structures under repeated drying–wetting corresponds to the moisture penetration depth x_p which is of major importance for engineers. This factor is used to quantify how deep moisture variations can influence the material; it represents the depth that ions can reach into the material under drying–wetting cycles and is thus particularly important for the description of ion penetration. Previous researches have concluded that x_p is dependent on the material properties (porosity, diffusivity coefficient, *etc.*), the cycle duration and the external RH amplitude [12]. Nevertheless, this conclusion was based on non-hysteresis modelling. Results in the case of hysteresis modelling have not been studied yet. The present paper is going to provide such investigations.

The purpose of this paper is to find an appropriate modelling of moisture transfers which can be used to simulate various ambient humidity loads and which is enough flexible to be performed with any kind of hysteresis description. Different approaches of modelling will be studied through comparisons with experimental data for verification. In the first part, commonly-used hysteresis models will be briefly introduced, and then a continuum moisture transport model will be described. A method to incorporate hysteresis models within a moisture transport model will be proposed. Experimental data, including mass loss curves and saturation profiles, will be used to verify the proposed method. Modelling results based on non-hysteresis and hysteresis modellings (empirical and conceptual) will also be compared. Then, effects of the drying and wetting cycle duration, RH amplitude and initial state will be discussed. The last part will investigate the moisture penetration depth performed with non-hysteresis and hysteresis modellings.

2. Modelling of hysteresis

The response of a concrete to repeated cyclic wetting–drying boundary conditions depends on its sorption behaviour represented by the de- or adsorption isotherms which are defined as the mass of physically bound water held in a material with respect to RH at a specific temperature. The desorption isotherm relates the water saturation state to the relative humidity if RH is decreasing. If RH is increasing, the evolution of the water content of the material is related to surface adsorption of water molecules and capillary condensation. When RH increases from a low value, surface adsorption occurs first since water vapour molecules begin to adsorb on the pore walls; it corresponds to one-layer adsorption followed by multi-layers adsorption. Beyond 60% RH in the case of cement-based materials, the increase of RH is followed by capillary condensation [4].

Whereas the process of drying of a porous material leads to an equilibrium curve commonly called desorption isotherm, there is not a real consensus about the way to name the process of liquid-water uptake in a cement-based material. Some authors use the term "adsorption" by generalizing the IUPAC nomenclature (International Union of Pure and Applied Chemistry) [13–15] and by including surface adsorption and capillary condensation together in the same definition [16,4,17–19]. Other authors prefer using the term "sorption" to represent the uptake of water molecules [20,21]. Finally, there are authors who opt for "absorption" to refer exactly to the same definition [22–24]. These latter make this choice to avoid any confusion between surface adsorption and capillary condensation, especially if models (for instance BJH, Barret, Joyner and Halenda, [25]) are used to investigate the pore size distribution of a porous material thanks to a distinction between surface adsorption and capillary condensation phenomena. In the present research, we made the choice of using "adsorption" in compliance with previous works performed by the authors of the present research. Moreover water vapour sorption data are not used here to investigate microstructure properties.

According to previous studies [26], hysteresis models of the sorption behaviour are roughly divided into two groups: conceptual and empirical models. The conceptual models were developed on the basis of domain theories, such as dependent and independent domain theories [9,27–29]. The empirical models were based on fitting the shapes of experimental scanning curves to determine the parameters of these models [7,8,30,31,6]. Our comparisons [26] showed that empirical models provide better results for the prediction of the first scanning curves thanks to additional parameters. However, the non-physical "pumping effect", generally related to the use of empirical models and referring to the non-closed form of the scanning loops, remains problematic [32,33]. On the contrary, conceptual models can inherently avoid this non-physical behaviour. In this study, both conceptual and empirical hysteresis models will be implemented to compare their effects on moisture transport.

2.1. The conceptual hysteresis model—Mualem Model II [34]

Mualem Model II [34] is one of the typical independent domain models. It was developed based on the "similarity hypothesis" proposed by Philip [35]. According to Mualem's diagram [34], two basic pore water distribution functions L and H are used to calculate a scanning curve:

$$L(P_c) = S_w \qquad H(P_c) = \frac{S_d - S_w}{1 - S_w} \tag{1}$$

where $S_w = S_w\,(P_c)$ is the saturation of the main adsorption curve and $S_d = S_d\,(P_c)$ is the saturation of the main desorption curve. After a