

MODELLING OF DRYING-WETTING EFFECTS ON MOISTURE TRANSPORT WITHIN CEMENTITIOUS MATERIALS

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Introduction

The durability of reinforced concrete structures and their service span are closely related to the moisture properties of the material. Therefore, to deal with durability issues, it requires the study of the movement of liquid-water and gas diffusion. For the modelling of moisture behavior during the frequent external humidity changes conditions, the water vapour sorption isotherms (WVSIs) [1], describing the relationship between relative humidity RH (or capillary pressure P_c) and water content θ (or degree of saturation S), should be investigated carefully because of the existing hysteresis between WVSIs. However, the earlier modelling normally neglected hysteresis and used the same sorption isotherm for both drying and wetting processes [2], which might be due to lack of experimental verification and premature computation technique.

Recently, modelling of moisture transport taking into account of hysteresis becomes a more interesting topic. Johannesson *et al.* [3] adopted an empirical model, which considered that each scanning isotherm can be expressed as a cubic polynomial. An independent domain theory model, called PM model (Preisach-Mayergoyz [4, 5]) that was developed initially for the physical mechanisms of magnetization, has been employed by Derluyn *et al.* [6]. Both researches emphasised the necessity of considering the hysteresis for modelling of moisture transport. But the conclusion has been not verified by supportive experimental data.

Modelling of hysteresis

In previous studies [8], the hysteresis models, including conceptual and empirical models, have been compared. The conclusions revealed that empirical models provide better results against the experimental data thanks to additional parameters. However, “pumping effects”, referring to the non-closed form scanning loops, are still critical. In contrast, the conceptual models, mainly Mualem’s models, can avoid this unreal behavior inherently. So in this paper, two kinds of hysteresis models are implemented and compared.

Conceptual hysteresis model – Mualem Model II

Mualem Model II [9] was developed based on the independent domain theory. Two basic pore water distribution functions H and L are used to calculate a scanning curve.

$$L = S_w; \quad H = \frac{S_d - S_w}{1 - S_w} \quad (1)$$

where $S_w = S_w(P_c)$ is the water saturation of the main adsorption curve and $S_d = S_d(P_c)$ is for the main desorption curve. According to Mualem’s diagram [9], for the case of the first scanning is wetting, the expression for the wetting scanning curve of order N (odd number) is deduced as:

$$S_{N,w}(P_c) = S(P_{c,N}) + [L(P_c) - L(P_{c,N})][1 - H(P_{c,N})], \quad L(P_c) \leq L(P_{c,N-1}) \quad (2)$$

where $S(P_{c,N})$ is the saturation at the starting point of current scanning curve. If $L(P_c) \geq L(P_{c,N-1})$, Mualem’s diagram indicates that $L(P_{c,N-3})$ will be used instead of $L(P_{c,N-1})$ for calculation until the scanning curve reduces to the main curve (order $N = 0$). In the same manner, the expression for the drying scanning curve of order N (even number) is written as:

$$S_{N,d}(P_c) = S(P_{c,N}) + [L(P_{c,N}) - L(P_c)][1 - H(P_c)], \quad L(P_c) \geq L(P_{c,N-1}) \quad (3)$$

If $L(P_c) \leq L(P_{c,N-1})$, $L(P_{c,N-3})$ will be used instead of $L(P_{c,N-1})$.

Empirical hysteresis model – Improved Rubin’s model

Rubin [10] proposed a formula to calculate the drying scanning curve, while this formula does not take into account the position of the starting point. Thus, it is not able to simulate scanning loops. An improvement was introduced in [8]. The expression is given for the drying scanning curve:

$$P_c(S_{N,d}) = P_{c,d}(S) + [P_{c,d}(S) - P_c(S_1)] \exp[\gamma_d(S - S_1)] \quad (4)$$

The expression for the wetting scanning curve is written as:

$$P_c(S_{N,w}) = P_{c,w}(S) + [P_c(S_1) - P_{c,w}(S)] \exp[\gamma_w(S_1 - S)] \quad (5)$$

where two material constant γ_d and γ_w are used to regulate the shape of the scanning curves.

One simulation result performed by two hysteresis models is shown in Fig. 1.

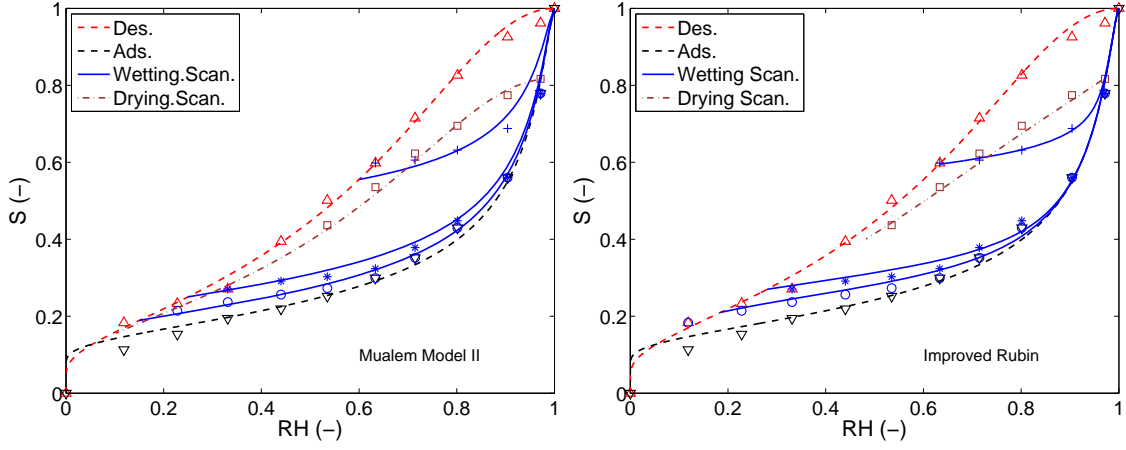


Fig. 1: The first drying and wetting scanning curves simulated by Mualem Model II (left) and Improved Rubin's model (right) for OPC cement paste with $w/c=0.35$. Experimental curves are taken from [1].

Continuum approach to model moisture transport at isothermal conditions

In the research of Mainguy *et al.* [11], an isothermal drying model was proposed, which considered that the mass transport includes liquid phase and gas phase (vapour + dry air). But that research and the following research [12] reported that if only considering the mass transport and using the constant gas pressure, the mass balance can be simplified as a single equation:

$$\frac{\partial S}{\partial t} = \text{div } w = \text{div}(w_l + w_v) = \text{div}\left(\frac{\rho_l K_0 k_{rl}(S)}{\phi \eta} \text{grad } P_l + \frac{D_{v0} f(S, \phi)}{\phi} \text{grad } \rho_v\right) \quad (6)$$

where w is the moisture flux, which contains the contribution from both liquid water and vapour; ρ_l = liquid water density; ϕ = porosity; K_0 = intrinsic permeability; k_{rl} = relative permeability; η = liquid water dynamic viscosity; P_l = liquid water pressure; D_{v0} = free vapour diffusion coefficient in the air; f = resistive factor related to the pore network; ρ_v = vapour density.

The functions for main sorption curves, k_{rl} and f are [13, 14]:

$$S(P_c) = \left[1 + (P_c/a)^{1/(1-m)}\right]^{-m} \quad (7)$$

$$k_{rl}(S) = S^{0.5} \left[1 - (1 - S^{1/m})^m\right]^2 \quad (8)$$

$$f(S, \phi) = \phi^{x_D} (1 - S)^{x_D+2} \quad (9)$$

where parameters a and m are determined by fitting experimental sorption curves. x_D has been validated as 2.74 in research of Thiéry [15] by using the experimental data based on CO₂ gas.

Drying-wetting modelling results and discussion

Non-hysteretic effect modelling

Non-hysteretic effect modelling can be easily achieved by using the same sorption isotherm for drying and wetting processes. In the literature, normally the main desorption curve is used [2, 3, 6], while this might be due to lack of experimental adsorption curve and has been proved that the simulation result does not agree the experimental data for the wetting process. Hence, a new calculation for a sorption curve is proposed here on the basis of the measured main desorption and main adsorption curves, involving in a weight factor ω .

$$S = \omega S_d + (1 - \omega) S_w \quad (10)$$

Hysteretic effect modelling

For the implementation of a hysteresis model into simulating drying-wetting cycles, two issues need to be solved: how to check whether the mesh is going to change state and how to keep the mesh on current state. Following the method proposed by Gillham *et al.* [16], this research introduces two retardation factors, each of which is used to deal with one above issue.

Either for conceptual models or empirical models, they need the reverse points (the starting points) of each scanning curve for each mesh. So the programme only needs to store these reverse points combining with two retardation factors to simulate drying-wetting cycles. This method is applicable for most hysteresis models.

Experimental data verification

One numerical simulation result is shown here. The experimental data is collected from literature [1] and [17]. Before the experiments, the cement paste with $w/c=0.35$ was sealed curing for 200 days. Specimens were exposed to $RH=53\%$ and 63.2% for around five months in desiccators, and then the relative humidity was changed to 97% for wetting process. K_0 in Eq. (6) is validated by the drying process, and it also used for the wetting process. So the simulations of drying and wetting processes use the same parameters, except the boundary conditions and WVSIs. Two parameter involved in improved Rubin's model are determined by experimental scanning curves (see Fig. 1).

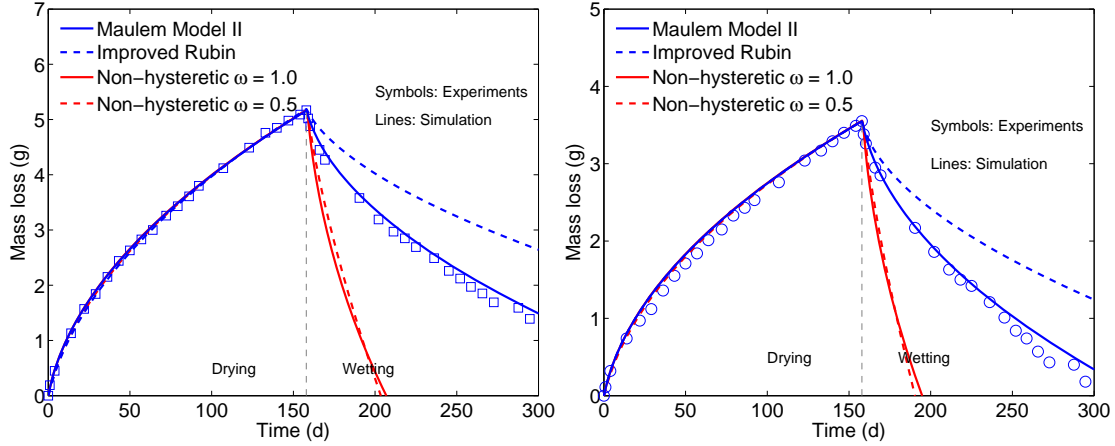


Fig. 2: Comparison of mass change simulated by non-hysteretic and hysteretic effect modelling with experimental results. Two cases of drying at $RH=53\%$ (left) and at 63.2% (right) are included.

It is clear that Maulem Model II reveals the best simulation results; meanwhile, improved Rubin's model overestimates the mass change during the wetting process. Even though ω can be used to adjust the sorption curve, the non-hysteretic effect modelling provides the result which is far away from the experimental data.

“Pumping effects” analysis

The “pumping effects” is the main difference between conceptual and empirical hysteresis models [8]. To analyse the “pumping effects” quantitatively, the simulations were carried out on the same material as the last section by using the initial $RH=83\%$, drying boundary $RH=63\%$ and wetting boundary $RH=83\%$. Firstly, the material is submitted to drying, and then changed to wetting. Each process uses the same duration (20 days). Totally, two cycles were simulated.

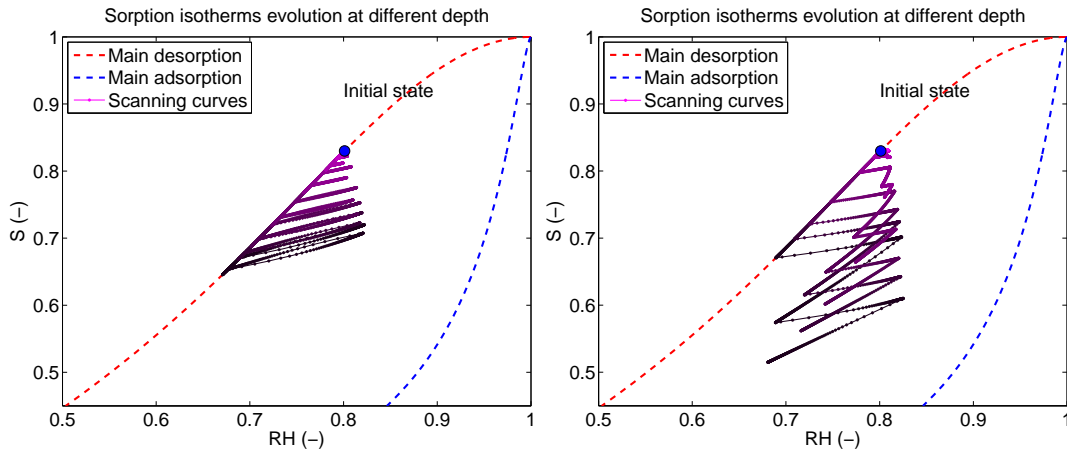


Fig. 3: WVSIs simulated by Maulem Model II (left) and Improved Rubin's model (right)

Fig. 3 clearly shows that “pumping effects” simulated by the improved Rubin's model reveal the largest errors during the first cycle. The effects on the mass changes are provided in Fig. 4. The difference of two curves at 40 days is due to that the drying scanning curves simulated by two models have different shapes, while the difference in later cycles (at 60, 80 and 100 days) is mainly from the “pumping effects”. One should notice that the errors increase with the number of cycles, such as from 3.6% at 60 days to 6.1% at 100 days and from 5.3% at 40 days to 17.1% at 80 days. The comparison results demonstrate that if the empirical model fails to eliminate “pumping effects”, the cumulative errors associated with oscillations of hysteresis loops are probably significant and lead to unrealistically simulated results.

Conclusions

In this research, a method taking into account of the hysteretic effect to simulate moisture transport under drying-wetting cyclic changes conditions has been proposed. It can be used for most hysteresis models, either conceptual or empirical models. Simulations in cases of non-hysteretic and hysteretic effects have been performed. Results show that non-hysteretic effect modeling does not provide a good result against to experimental data. Among the hysteresis models, the mass change curve simulated by Mualem Model II matches the experimental curve very well, that could be the model recommended for modeling of moisture transport.

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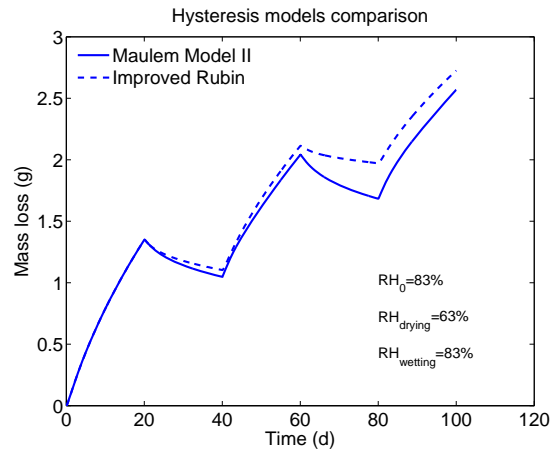


Fig. 4: Comparison of mass change simulated by Mualem Model II (solid line) and Improved Rubin's model (dashed line)