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## **MODELLING STRATEGIES FOR THE STUDY OF CRACK SELF-SEALING IN MORTAR WITH SUPERABSORBENT POLYMERS**

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### **Abstract**

In this work, a numerical model is presented to predict the self-sealing effect provided by superabsorbent polymers (SAP) admixtures in mortar. Firstly, the use of a law of absorption kinetics for SAP embedded in a cementitious matrix was validated with experimental results available in literature. Secondly, two extreme strategies are considered for the swelling of SAP in the crack regarding the variation in its deformation capacity under constraint. The results show the appropriateness of the SAP absorption law and explain the mechanisms of water absorption of mortar with such admixtures. Furthermore, the influence of the deformation capacity of SAP on the water penetration in cracks is studied parametrically.

### **INTRODUCTION**

Experiments performed on cement-based composites with superabsorbent polymers (SAP) have shown the potential of these admixtures to provide short-term and long-term self-sealing and self-healing effects, respectively [1-3]. Some analytical formulations have been also proposed for the prediction of the self-sealing effect. In [4] the authors attempted to estimate the reduction of flow rates during permeation tests in mortar with spherical SAP. In the proposed formulation a fitting parameter was proposed to match modelled and experimental flow curves as the SAP dosage was increased in the material. Nevertheless, the authors could not assign a physical meaning to it and therefore, the use of the model remains limited to the type and percentages of SAP tested. Lee et al. (2016) [5] used stereology to estimate the crack volume reduction due to SAP swelling and used it to predict this as crack width and dosage, size and nominal swelling ratio of SAP are changed. Yet, the evaluated reduction cannot be directly correlated to the water blocking effect.

The inability of the described analytical formulations to predict the effects of crack self-sealing in cementitious materials with SAP admixtures highlights the need for more rigorous modelling procedures that can take into account the many involved parameters and that can serve as a departure point for the study of the influence of SAP on autogenous self-healing. In this paper, a numerical model is presented to predict the water penetration perpendicular to the crack of mortar with SAP admixtures. The model is the continuation of a previous work [6]. Firstly, the use of a law of absorption kinetics for SAP embedded in a cementitious matrix was validated with experimental results available in literature. Secondly, two extreme strategies are considered for the swelling of SAP in the crack regarding the variation in its deformation capacity under constraint. The results show the appropriateness of the SAP absorption law and explain the mechanisms of water absorption of mortar with such admixtures. Furthermore, the influence of the deformation capacity under constraint of SAP on the water penetration in cracks is studied parametrically.

## 2. METHODS

### 2.1 Equations

The problem of capillary absorption of water in a porous medium with randomly distributed sinks is considered in this study, as described in a previous work [6]. In this study, the Richards equation is used to describe the water saturation  $\theta(t)$  in the mortar together with the exponential law for mechanical dispersivity  $D(\theta)$ . The sink term  $s(\theta, t)$  is modelled with an absorption kinetics diffusion-like law modified from [7], with rate  $k$  as a function of the SAP surface area and equilibrium absorption considering the availability of upcoming water. The capillary absorption in the cracked domain is modelled as if being in the mortar, but the mechanical dispersivity  $D_{cr}(\theta)$  is estimated using Equation 1 as proposed by [8]:

$$D_{cr}(\theta) = \frac{K_{cr}(\theta)}{C(\theta)} = -K_{cr}(\theta) \frac{dp_c}{d\theta} = \frac{w_{cr}^3}{12\mu l} k_{cr}(\theta) \frac{dp_c}{d\theta} \quad (1)$$

Where  $K_{cr}(\theta)$  is the permeability function which can be decomposed by two factors: the permeability at saturation and the relative permeability  $k_{cr}(\theta)$ . The permeability at saturation is modelled with the cubic law on the crack width  $w_{cr}$  with  $l$  local crack length and  $\mu$  dynamic viscosity of water.  $C(\theta)$  is a capacity function defined as the derivative of the saturation on the capillary pressure  $p_c(\theta)$ . Last,  $k_{cr}(\theta)$  and  $p_c(\theta)$  are estimated with Mualem and van Genuchten curves [9, 10], respectively and their parameter  $\alpha$  is calibrated for narrow cracks from [8].

### 2.2 Numerical implementation

For the discretization of the domain, a lattice network approach [12] was employed to model the problem of water transport in mortar with randomly distributed discrete sinks. In this work, the transport was considered as occurring along the beam elements in the lattice mesh [12, 13] in opposition to other works in which the transport occurs along the facets of the Voronoi polygons (in 2D) [14]. For a more detailed description of the discretization procedure, the reader is redirected to other works [6, 13, 15]. In this work mortar, regarded as homogeneous, and SAP phases are explicitly implemented in the mesh of the SAP mortar, as well as their interface (Figure 1a). The Anm model [16] was used for parking irregular-shaped SAPs into a 5 mm<sup>3</sup> cube with fully periodic boundaries. The cube was later used as primary cell in the creation of a specimen with larger dimensions. Such a procedure reduced drastically the computational time. The simulated SAP particles had the dimensions of the macropores left by the desorption of the SAP after hardening of the mortar.

The Ritz-Galerkin method was employed for the weak formulation of the Richards equation and the Crank-Nicholson non-implicit procedure was used for the time discretization. Regarding the sink term, this was formulated in terms of total water absorption of the individual SAP since transport inside the particle was beyond the scope of this study [6].

A typical sorptivity test with sealed boundaries was simulated in this work for sound and cracked mortars with and without SAP. For the sake of reducing computational costs a mortar bar was simulated with dimensions 5x5x20 mm<sup>3</sup>. This also limited the duration of the time-dependent analysis shown in this study. A scheme of the virtual cracked mortar bar and orientation axes are shown in Figure 1b for future reference.

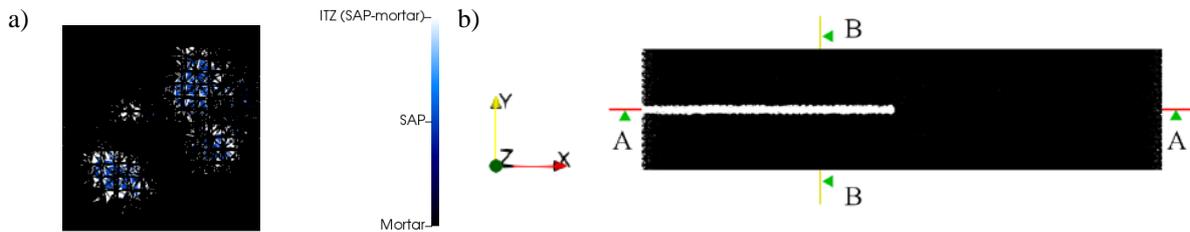


Figure 1: Heterogeneities in the mesh a) and cracked mortar mesh b).

### 2.3 Experimental input parameters

Results from capillary absorption tests from [17, 18] were used here for validation of the sound absorption of mortars with SAP. From this experiment the results from the following samples were simulated: sound mortar with SAP (SAP dosage of 1% by weight of cement - B1.0-) and without (References -R- with two different water-to-cement ratios -0.50, 0.41-). Two data sets were available, corresponding to the age of the samples at the beginning of the preconditioning prior to the test: 7 and 28 days.

The necessary input parameters were available from [18] for the mortars with 28 days of moist curing, while for the other batch, the experimental procedure was repeated by the authors of this study on samples cured for only 7 days in moist conditions. The input parameters for all the simulations in this work are displayed in Table 1. For the simulations, R0.41 and B1.0 are assigned the same input parameters. The experimental methods are described in [18].

Table 1: Input parameters for the mortar phase.

Mixture	Age [days]	Transport properties		Physical Properties	
		Sorptivity [ $mm/min^{1/2}$ ]	Initial Dispersivity ( $D_0$ ) [ $mm^2/min$ ]	Apparent Porosity [-]	$\theta_0$ [-]
R0.50	7	0.0938	0.0037	0.21	0.15
	28	0.03721	0.0027	0.077	0.16
R0.41	7	0.0462	0.001	0.16	0.25
	28	0.01458	0.0017	0.044	0.277
B1.0	7	0.0462	0.001	0.163	0.19
	28	0.01458	0.00064	0.064	0.19

Regarding the SAPs, the input parameters needed for the model were taken from [19] relative to SAP type B.

- PSD at mixing:  $921 \pm 102 \mu m$
- PSD at the dry state:  $477 \pm 53 \mu m$
- Absorption during mixing:  $8.9 \frac{g_{water}}{g_{SAP}}$

- Absorption in Demineralized Water:  $283.2 \frac{g_{water}}{g_{SAP}}$
- Dry density:  $700 \frac{kg}{m^3}$
- Swelling kinetics parameters in Demineralized Water :  $r_1 = 112075.26 \mu m^{1.828} /min$  and  $r_2 = 1.828$

### 3. MODELLING STRATEGIES AND DISCUSSION

#### 3.1 Validation in sound mortar

In this section the capillary absorption of water is simulated for undamaged mortars with SAP admixtures. Also the reference mortars without SAP are simulated. In Figure 2 a comparison is shown between experimental and simulated results for the selected mixtures (R0.50, R0.41 and B1.0) for 7 days (left) and 28 days (right) of moist curing prior to preconditioning.. The plotted absorption results are calculated via Equation 2:

$$Absorption(t) = \frac{m_{wat}(t)}{A * \rho_{wat}} \quad (2)$$

Where  $m_{wat}(t)$  is the uptaken mass of water at time  $t$ ,  $A$  is the area exposed to water and  $\rho_{wat}$  is the density of water.

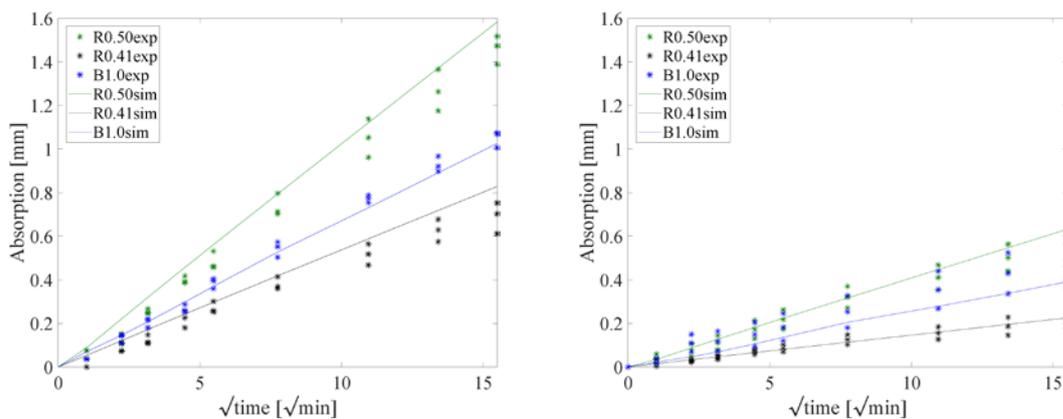


Figure 2: Simulated and experimental capillary water uptake in the mortars R0.50, R0.41 and B1.0, cured for 7 days (left) and 28 days (right).

Overall, the simulation results are in very good agreement with the experimental ones, for all the studied mixtures. As expected, different water-to-cement ratios resulted in marked differences in the bulk water absorption of the mortar samples as can be seen from the graph relative to samples cured for 7 days. R0.50, with higher values of  $D_0$  and apparent porosity, absorbed water faster compared to its counterpart R0.41. On the other hand, B1.0, with transport properties of the matrix corresponding to those of R0.41, presented considerably higher values of absorption with respect to its reference mixture R0.41 following both types of curing regimes, but these differences were more evident after 28 days of moist curing. The same was observed by [20].

In experimental setups, initial fast uptakes of water during sorptivity tests are commonly found and attributed to the presence of macropores presenting higher rates of water uptake than the matrix [21].

### 3.2 Crack Self-sealing: Two modelling strategies

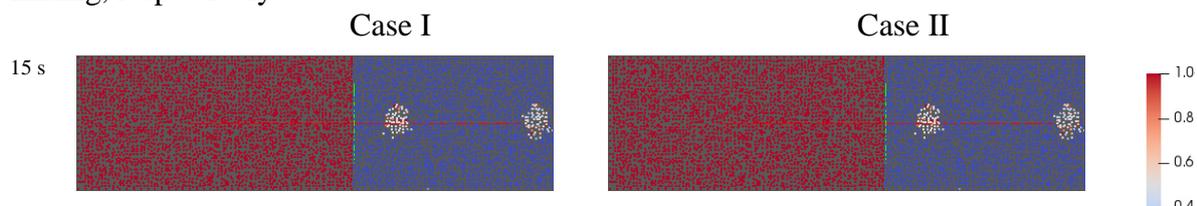
Three main mechanisms are responsible in the model for the blockage of water absorption in the crack. In the first place, the SAP absorbs the upcoming water without instant release, provided that water is available at all times. Secondly, the dispersivity value of the SAP particle is reduced when approaching the swelling equilibrium, which results in the conversion of the SAP particle into a less pervious inclusion. These two mechanisms are implicit consequences of the implementation of the model, as analysed in [6] and applied in the previous section. Lastly, the swelling of the SAP results in an extension of the previous two phenomena into other zones of the crack space, eventually reducing the initially cracked volume.

When the individual SAP is totally confined in the macropore, the absorption capacity at equilibrium is the same as the one during mixing. For SAP in the crack, the elastic properties of the polymeric chains, as well as the level of crosslinking determine the absorption capacity at equilibrium [22]. Two extreme cases were then examined in this work:

- I. The single SAP swells to fill the macropore containing it and the crack within (which is not considered as additional volume in the mesh) and the interface elements in the crack space in order to compensate for the latter.
- II. The single SAP swells to fill the macropore containing it and keeps engaging the adjacent elements in the crack as SAP elements until the maximum absorption has occurred.

For a better understanding of the swelling mechanisms used in the model, in Figure 2 the relative dispersivity values in the section A-A (Figure 1b) are mapped after 15, 45, 60 and 120 seconds of water absorption for cases I and II described above. Relative dispersivity values are obtained by normalizing  $D(\theta(t))$  to its maximum value  $D(\theta = 1)$  for each phase. Section A-A intersects the cracked volume along its mid XZ plane. In the maps, the red colour denotes the highest possible dispersivity value for each specific phase, while dark blue represents the minimum one. Any lighter shades of blue and red denote intermediate relative values.

Until which extent the swelling beyond the macropore occurs depends on the type of SAP and needs to be checked case by case. Nevertheless, herein different intermediate cases between the two extreme strategies are compared in terms of the resulting water penetration perpendicular to the crack in the first 10 minutes of absorption. In Figure 4, the averaged water contents along the Y direction in section B-B are plotted. In the graph, only half of the width is shown because of the symmetry of the results with respect to the crack. The different levels of self-sealing (b, c, d, e, f) are evaluated for increasing values of the ratio  $\frac{S_{crack}}{S_{mixing}}$ . Where  $S_{crack}$  and  $S_{mixing}$  are the water absorptions of SAP B in the crack and during mixing, respectively.



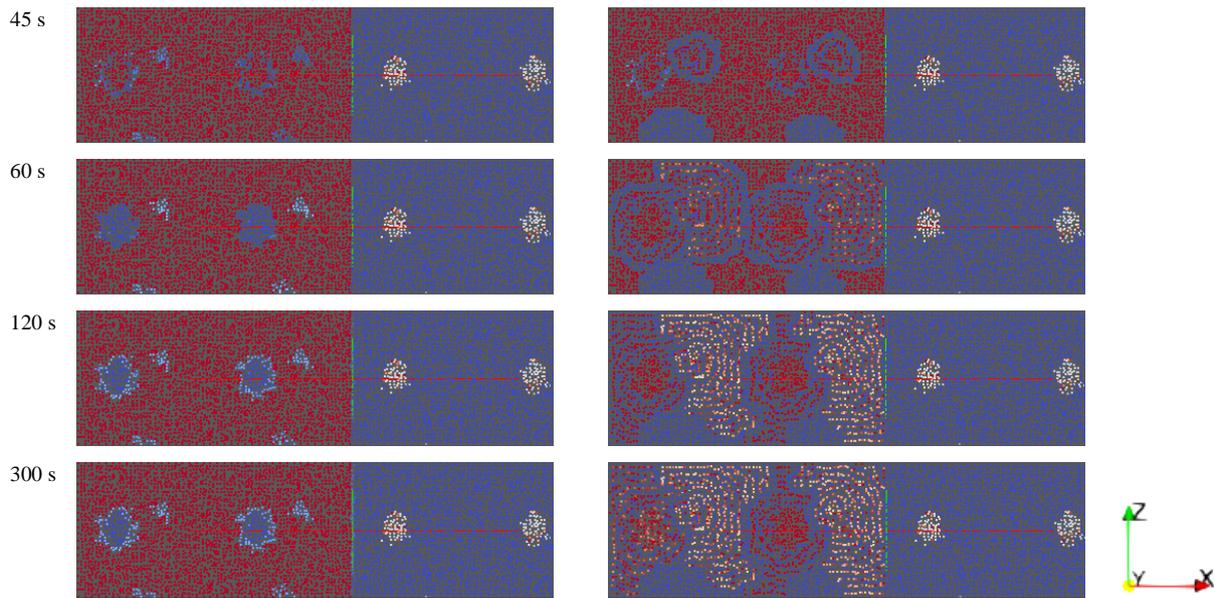


Figure 3: Maps of relative dispersivity in the crack after 15, 45, 60, 120 and 300 s of capillary water absorption for swelling in macropore (left) and unlimited swelling (right).

When only the volume of the macropore is filled and not the crack within (b), the water penetration through the crack walls proceeds very similar to R0.41 with only minor decrements in the degree of saturation along the horizontal direction, while the position of the water front is the same for mortar with and without SAP. The blocking effect when the swelling is limited to the cracked space within the macropore can already be noticed in c) when compared to R0.41. The SAP hinders the water flow in the crack in localized zones and inhibits the water penetration into the matrix through the macropore walls thus slowing the water front down. For increasing swelling degree beyond the macropore (Figure 3d, 3e, 3f) the degree of water saturation progressively diminishes in the crack as in the matrix surrounding it, as more zones of the crack surfaces become covered with hydrogel. An increase on the horizontal penetration depth of the water front is obtained since the water cannot eventually migrate in the crack. Similar findings were described qualitatively in an experimental work [17], where the authors monitored the water penetration through crack surfaces of mortar with SAP.

The potential of this model lies on the wide range of parameters that can be studied, from optimal SAP characteristics for eventual design of such admixtures to composition of the cementitious matrix and dosage of SAP. Furthermore, implementation of such model within a multispecies transport modelling framework could help on the evaluation of the influence of such admixtures on the durability of cementitious materials and autogenous self-healing.

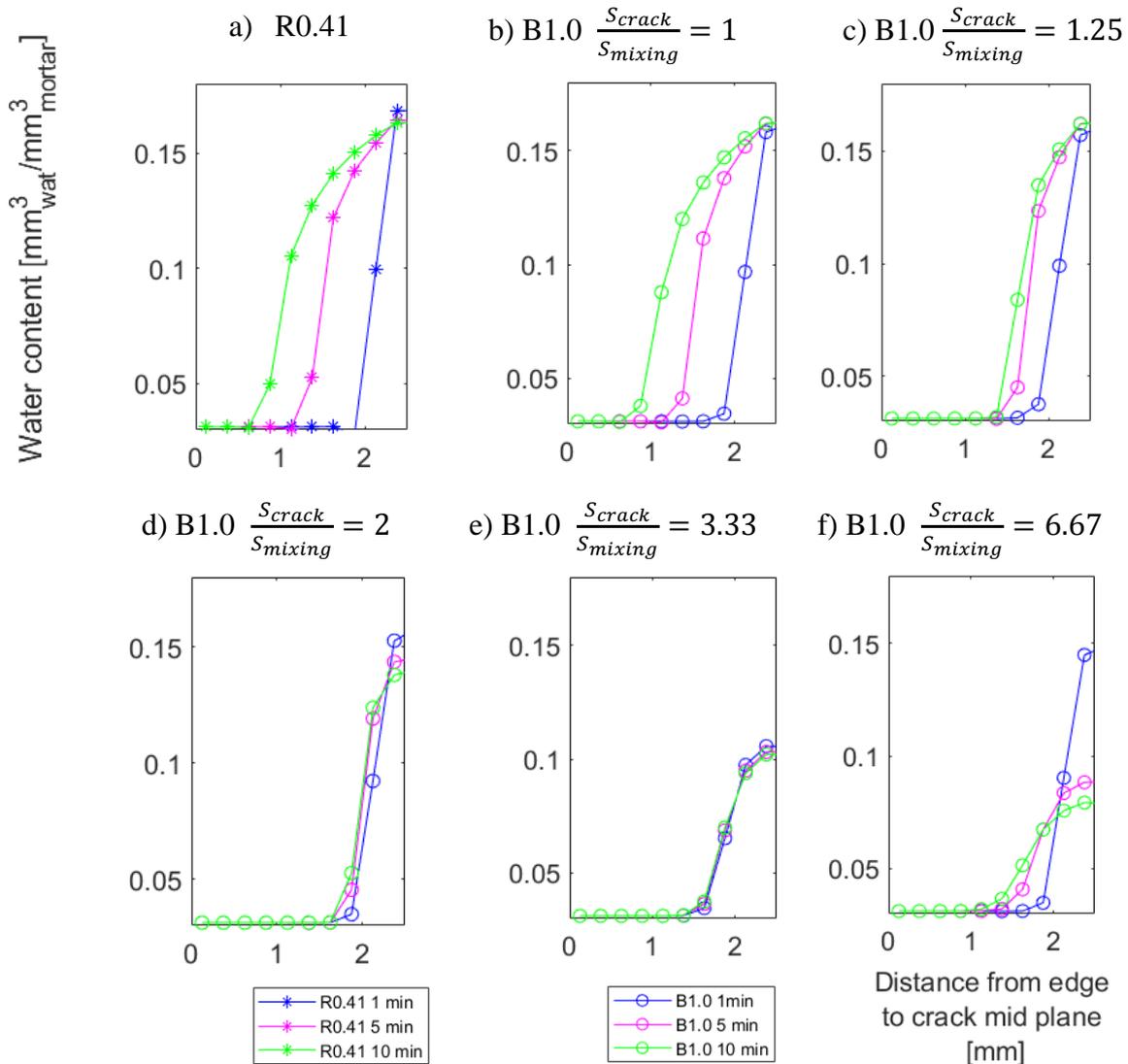


Figure 4: Water content distribution along a horizontal profile for R0.41 a) and for different ratios between the absorption in the crack and during mixing: 1 b), 1.25 (filling macropore+crack) c), 2 d), 3.33 e) and 6.67 (crack totally filled with hydrogel) f).

#### 4. CONCLUSIONS

The following conclusions can be drawn from the results discussed in this study:

- The use of a modified law for the prediction of water absorption of SAP embedded in mortar seems to yield precise results as observed from excellent match with experimental results.
- The presence of large pores and/or SAP in mortar leads to a slight non linearity at the beginning of capillary absorption curve, more or less marked depending on the transport properties of the matrix.
- Different SAP deformation capacities under constraint result in different efficiencies of the self-sealing effect and eventual self-healing effect as seen from the different water penetrations into the matrix from the crack surfaces.

## ACKNOWLEDGEMENTS

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