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Characterization of concrete by calibrating thermo-hydraulic multiphase flow models

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Abstract Evaporation tests in concrete columns have been analysed by numerical models to characterize the thermo-hydraulic properties and the processes in concrete. Two evaporation tests were performed; a column heated by a lamp and a column kept in room conditions. The conceptual model considers unsaturated liquid flow and transport of vapour and energy. We also calculated models that take into account the dissolved salts to study its effect on vapour pressure and evaporation. A retention curve has been obtained from relative humidity and gravimetric water content measured after dismantling the tests. The models have been calibrated by adjusting the model's results to the measured data of water loss, relative humidity and temperature inside the concrete. The parameters obtained with the calibration are the permeability, thermal conductivity, boundary conditions and a tortuosity factor for vapour diffusion. Results show that the vapour diffusion is the dominant water transport process above an evaporation front, and liquid advection is dominant below it.

Keywords drying · retention curve · permeability · concrete · modelling

1 List of symbols

A	constant for relative permeability
a_w	activity of water
D	parameter for diffusion
D_m	molecular diffusion coefficient (m^2s^{-1})

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D'_α	mechanical dispersion coefficient (m^2s^{-1})
d_l	longitudinal dispersivity (m)
E_α	internal energy per unit of mass for each phase (J kg^{-1})
E_α^i	specific internal energy (J kg^{-1})
f	external supply of component
g	gravity (m s^{-2})
HR	relative humidity
i	(superscript) component index, w water, a dry air and h salt
i_α	diffusive or dispersive flux ($\text{J s}^{-1} \text{m}^{-2}$)
i_c	heat conductive flux ($\text{J s}^{-1} \text{m}^{-2}$)
j_α^i	mass flux of component in each phase ($\text{J s}^{-1} \text{m}^{-2}$)
j_g^w	vapour flux ($\text{kg s}^{-1} \text{m}^{-2}$)
j_e	energy flux ($\text{J s}^{-1} \text{m}^{-2}$)
j_e^0	radiation ($\text{J s}^{-1} \text{m}^{-2}$)
k_i	intrinsic permeability (m^2)
k_r	relative permeability
M^i	molecular weight of component i (kg mol^{-1})
m	shape parameter for retention curve
n	parameter for relative permeability
P_α	pressure of phase α (MPa)
P_α^i	partial pressure of component i in phase α (MPa)
$P_{g,sat}^w$	saturated vapour pressure (MPa)
P_0	entry pressure (MPa)
P_{l0}	reference pressure (MPa)
q_α	flow rate (ms^{-1})
R	ideal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
S_α	saturation of phase α
S_e	effective water saturation
T	temperature ($^\circ\text{C}$)
T	gravimetric humidity
α	(subscript) phase index, l liquid, s solid and g gas
β	compressibility (MPa^{-1})
β_g	boundary vapour exchange coefficient (ms^{-1})
γ	solute variation coefficient
γ_g	boundary gas exchange coefficient ($\text{kg s}^{-1}\text{m}^{-2}\text{MPa}^{-1}$)
γ_e	boundary heat exchange coefficient ($\text{J s}^{-1}\text{m}^{-2} \text{ }^\circ\text{C}^{-1}$)
ϵ	volumetric thermal expansion coefficient for liquid ($^\circ\text{C}^{-1}$)
λ	thermal conductivity (W m K^{-1})
μ_α	viscosity of phase α (MPa s)
θ_α	volumetric phase content of α
ρ_α	density of phase α (kg m^{-3})
ρ_{l0}	reference density of the liquid (kg m^{-3})
σ_{l0}	Surface tension at temperature T (N m^{-1})
τ	tortuosity
ϕ	porosity
ω_α^i	mass fraction of solute i in phase α (kg kg^{-1})

1 Introduction

Concrete allows building a large number of architecture and engineering structures. The majority of them are exposed to alternating dry and wet conditions affecting their durability. Thermo-hydraulic processes such as flow of liquid and gas in unsaturated conditions, transport of heat, vapour and dissolved salts, and evaporation and condensation of water are known to play an important role in concrete (Baroghel-Bouny 2007; Carlier and Burlion 2011; Poyet 2013).

Therefore, it is necessary to measure thermo-hydraulic parameters, such as retention curve, thermal conductivity and diffusion coefficients, in order to predict the processes taking place inside the concrete and affecting its durability. Various methods for determining these parameters can be found in the literature. For instance, Leech et al (2006) estimated retention curves from mercury intrusion and water sorption isotherms. Baroghel-Bouny (2007) studied the relation between the pore structure and the retention curve by using water vapour desorption-adsorption experiments. Carlier and Burlion (2011) carried out evaporation tests in concrete under isothermal conditions, so as to obtain its retention curve and relative permeability parameters improving the van Genuchten-Mualem's equations. Brue et al (2012) estimated desorption isotherms experimentally at different temperatures, by using a model based on Kelvin-Laplace's capillary law. Chen et al (2012) obtained water retention properties and a relative gas permeability curve in concrete by studying the effect of water saturation on gas relative permeability. Poyet (2013) used alternative mathematical functions to characterize the retention curve to obtain the intrinsic permeability of concrete, by means of experimental tests in concrete columns at isothermal conditions.

Most of these experiments consist of small samples and all of them were performed in isothermal conditions. In this work we analyse evaporation tests of 20 cm long concrete columns performed in non-isothermal conditions, monitoring the temperature and relative humidity outside and inside the concrete. Such experiments involve various interacting processes and require the simultaneous calibration of several parameters. Of course, this makes obtaining parameters more complex and difficult than for the experiments mentioned in the previous paragraph. Despite of this difficulty, for soils, methods have been reported for modelling evaporation tests and calibrating parameters to experimental data. Pintado et al (2002) calibrated models of experimental tests in bentonite using an algorithm based in the least squares method. Acero et al (2009) modelled evaporation tests at high temperatures of vadose tailings and Gran et al (2011) modelled and calibrated a saline soil using multiphase models coupled to reactive transport. Although evaporation tests in concrete and their models have been reported (Šelih et al 1996), the method of calibration for obtaining thermo-hydraulic parameters has not been applied yet. We feel calibration of these tests can be useful for obtaining parameters for concrete too.

The objective of this work was to obtain thermo-hydraulic parameters of concrete by modelling evaporation tests in concrete columns in non-isothermal conditions. We used a low permeability concrete employed at a radioactive waste disposal facility in El Cabril (Spain). To do so we applied the following methodology:

- Two evaporation tests in concrete columns were carried out. One of them in room conditions and another one heated with a lamp. The relative humidity and temperature were motorized by sensors inside and above the columns.

- The drying retention curve of this concrete was estimated from relative humidity and gravimetric water content measured at the end of the tests.
- Simulations of the evaporation tests and the subsequent calibration by adjusting the model results to the experimental data have allowed finding the relative permeability, the tortuosity factor, the thermal conductivity and the boundary conditions parameters.
- These thermo-hydraulic multiphase flow models were used to better understand the processes inside concrete.

We first give a description of the evaporation test in section 2. Then, in section 3, we explain the processes taken into account by the model and the mathematical equations that describe them. In section 4 we discuss the calibration and the results of the model. Finally, in section 5 we give some conclusions.

2 Experimental tests

2.1 Material

The concrete of the Radioactive Waste Disposal Facility at El Cabril (Spain) is a low permeability concrete with a water-cement ratio (w/c) of 0.44. The specimens of concrete used for the evaporation tests were manufactured at El Cabril, using the same receipt and procedures used to manufacture the concrete of the disposal cells. Its composition is shown in table 1 (Villar et al 2009; Villar and Romero 2014).

Table 1 Concrete composition.

Component	Quantity
Aggregates (4/16)	1023 kg/m ³
Sand (0/4)	634 kg/m ³
Sand (0/2)	203 kg/m ³
Cement I-42.5 R/SR	400 kg/m ³
Melcret-222 additive	6.5 kg/m ³
Water	175 L/m ³

2.2 Hydraulic properties

Besides the evaporation tests, several other hydraulic tests were conducted (Villar et al 2009, 2012; Villar and Romero 2014). The grain density of the concrete (mass of solid per volume of solid) was 2.68 g/cm³, obtained by the picnometer method with water. The porosities calculated from this value are between 0.17 and 0.19. An intrinsic permeability of $4.2 \cdot 10^{-18}$ m² was calculated from hydraulic conductivity,

which was measured using a constant-head permeameter with water. Water retention curves were also determined experimentally by controlling relative humidity in desiccators (Villar and Romero 2014), which are compared with the one obtained from the evaporation test (see section 3.3, Figure 2).

2.3 Evaporation tests

The evaporation tests were conducted in PVC moulds of 8.5 cm in diameter and 20 cm in height (Villar et al 2009). Five 0.8 cm diameter perforations had been previously drilled at different levels, and plastic dummy cylinders had been placed in them. The moulds were filled with liquid concrete. The columns were cured for two months at room temperature and then placed in a room with relative humidity between 70 and 100%, where the non-heated column (C) remained for 11 months and the heated column (D) for 25 months. Just before the evaporation tests, the cylinders were replaced by sensors (Figure 1). The temperature and relative humidity were monitored by Sensirion SHT75 sensors, whose error is approximately 2% but rises to approximately 4% when the relative humidity is close to 0% or 100% at 25 °C. Moreover, the error increases with temperature. A sixth sensor was placed above the column to measure the laboratory conditions. One test was performed in room conditions, while the other column was heated with a lamp, situated 35 cm above the column surface. The latter was wrapped in an insulating wool whose temperature was monitored by two additional sensors, one of them placed between the column and the wool and the other at the outside of the wool. Rather than insulating, its purpose was to quantify heat loss by the difference in temperature of both sensors and the thermal conductivity of the wool ($0.032 \text{ W m}^{-1} \text{ K}^{-1}$). In both cases evaporation took place only through the upper surface of the columns. The columns were placed on a scale to measure the loss of weight. The amount of evaporation can be calculated from this loss. After nearly one year the tests were dismantled when the upper part of the columns did not show important changes in relative humidity. Then, they were cut in 5 horizontal sections and their water content was measured gravimetrically by oven drying at 110 °C.

Fig. 1 Set up for evaporation tests (Villar et al 2009); left: schematic cross section of the test; middle: non heated test; right: heated test.

3 Conceptual model and governing equations

3.1 Conceptual model

The evaporation tests were analysed by a comprehensive model that takes into account all relevant processes taking place. It considers the column as an unsaturated medium, composed of three phases: liquid, solid and gas. The solid phase has concrete as component. The liquid phase is composed of water, solutes and dissolved air. The gas phase is formed by a mixture of water vapour and dry air. Transport of vapour and heat was also considered through advection of the liquid and gas phases, diffusion and dispersion of vapour and heat convection. The gas pressure was not considered constant. In order to study the effect of the dissolved salts on vapour pressure and evaporation two models have been carried out for each test (heated and non-heated column): one model that did and another one that did not consider dissolved salts, leading to four models in total. The models with dissolved salts do not take into account mineral precipitation. Hence, they overestimate the concentration of dissolved salts and its effect on evaporation. Therefore, these two assumptions can be seen as extreme cases between which reality is likely to occur.

3.2 Governing equations

The simulations were carried out with CODE_BRIGHT (Olivella et al 1996), a finite element computer code that can handle multiphase flow, heat transfer and mass transport. It solves the balance equations for water (Eq. 1), air (Eq. 2), energy (Eq. 3) and/or salt (Eq. 4) (Olivella et al 1994).

$$\frac{\partial}{\partial t} (\theta_l \omega_l^w \rho_l + \theta_g \omega_g^w \rho_g) + \nabla \cdot (j_l^w + j_g^w) = f^w \quad (1)$$

$$\frac{\partial}{\partial t} (\theta_l \omega_l^a \rho_l + \theta_g \omega_g^a \rho_g) + \nabla \cdot (j_l^a + j_g^a) = f^a \quad (2)$$

$$\frac{\partial}{\partial t} (E_s \rho_s (1 - \phi) + E_l \rho_l S_l \phi + E_g \rho_g S_g \phi) + \nabla \cdot (i_c + j_{Es} + j_{El} + j_{Eg}) = f^Q \quad (3)$$

$$\frac{\partial}{\partial t} (\theta_l \omega_l^h \rho_l) + \nabla \cdot j_l^h = f^h \quad (4)$$

Constitutive laws are used to express these balance equations as a function of the state variables liquid pressure, P_l , gas pressure, P_g , temperature, T and/or mass fraction of dissolved salt, ω_l^h . In this way we can account for all the relevant processes and properties, such as, relative humidity, retention curve, Darcy's law for an unsaturated medium, vapour diffusion and heat conduction. Also properties such as surface tension, viscosity and density depend on temperature and/or salinity. Appendix A gives a full list of all constitutive laws. For details on each equation we refer to Olivella et al (1994).

3.3 Thermo-hydraulic parameters

The porosity and intrinsic permeability were taken from the experimental tests of Villar et al (2009). We assumed the intrinsic permeability of the model to be constant and equal to the average of the values obtained from all experimental tests. Parameters which were not known or which were more sensitive to the model (relative permeability, tortuosity, thermal conductivity and boundary conditions parameters) were calibrated manually by fitting model results to data measured by the sensors. The retention curve was obtained from the relative humidity measured by the sensors inside the columns at the end of the experiments and from the gravimetric water contents measured in the same positions after dismantling the columns. The results were fitted to the van Genuchten model (Appendix A, Eq.20; Van Genuchten 1980). An air entry pressure (P_0) of 7.7 MPa and shape parameter m of 0.34 were obtained (Figure 2). This high entry pressure reflects a very retentive material due to its small pores. We used the same air entry pressure (P_0) and shape parameter (m) for the heated and non heated column. Following Wu et al (2014), our retention curve takes into account the effect of temperature and dissolved salts on the surface tension (Eq.20 and Eq.25). This simplifies the model reducing the number of parameters to calibrate. However, there is disagreement on the effect of temperature on the retention curve. For instance Poyet (2009) found an important effect of temperature, which was attributed to thermodynamic properties of the adsorbed water. The retention curve obtained by fitting the results of the evaporation tests is compared to the ones determined in desiccators measured by Villar and Romero (2014) (Figure 2). Results show that the latter never reach a saturation of 1. The most probable reason is that the samples had suffered drying during preparation. Before measuring the drying curve (i.e., the retention curve from wet to dry) in the desiccators, the sample had to be re-saturated. However, this may entrap air in the pores giving a maximum saturation lower than 1. On the other hand, the evaporation test started after concrete had hardened without any previous drying, so it is assumed that the retention curve starts when the degree of saturation is 1.

Fig. 2 Fitted retention curve and measured data. The data from the non heated and heated column were measured at the end of each evaporation test. The wetting and drying data were obtained controlling the relative humidity in desiccators by Villar and Romero (2014).

3.4 Geometry and mesh

A one-dimensional domain of 20 cm length was assumed. The column was represented by a finite element mesh of 50 nodes and 49 elements with element sizes ranging from 2 cm at the bottom to 0.05 cm at the top.

3.5 Boundary conditions

Boundary conditions must be applied to take into account the exchange of vapour and heat between the column and its surroundings. For this, daily averaged temperature and relative humidity were used, measured by the sensor situated above the columns (Figure 3). A summary of the parameters used in the boundary conditions is shown in Table 2. For vapour flux at the top of the columns a mixed boundary condition was applied (Eq. 5).

$$\begin{aligned} j_g^w &= (\omega_g^w)^0 \gamma_g (P_g^0 - P_g) + \beta_g \left[(\rho_g \omega_g^w)^0 - (\rho_g \omega_g^w) \right] & \text{if } P_g^0 < P_g \\ j_g^w &= (\omega_g^w) \gamma_g (P_g^0 - P_g) + \beta_g \left[(\rho_g \omega_g^w)^0 - (\rho_g \omega_g^w) \right] & \text{if } P_g^0 > P_g \end{aligned} \quad (5)$$

Where super index 0 refers to external values. The first term of the right hand side represents the advective vapour flux in gas flowing due to gas pressure difference between atmosphere and column. The parameter controlling this flow, γ_g , is high enough to nullify this gas pressure difference, so that it practically prescribes the gas pressure at the top of the column to the atmospheric pressure of 0.1 MPa. The second term of the right hand side represents a vapour flux due to the difference of vapour density ($\rho_g \omega_g^w$) between the atmosphere and the top of the column. Parameter β_g is a vapour exchange coefficient which depends on air movements and turbulent mixing between atmosphere and column. As it is difficult to assess a value to this parameter, it has been calibrated. For the air flux, similarly to the vapour flux, a mixed boundary condition was applied at the top of the column.

$$\begin{aligned} j_g^a &= (1 - \omega_g^w)^0 \gamma_g (P_g^0 - P_g) + \beta_g \left[(\rho_g (1 - \omega_g^w))^0 - (\rho_g (1 - \omega_g^w)) \right] \\ &\quad \text{if } P_g^0 < P_g \\ j_g^a &= (1 - \omega_g^w) \gamma_g (P_g^0 - P_g) + \beta_g \left[(\rho_g (1 - \omega_g^w))^0 - (\rho_g (1 - \omega_g^w)) \right] \\ &\quad \text{if } P_g^0 > P_g \end{aligned} \quad (6)$$

For the non-heated column no temperature gradient was observed by the sensors. Therefore, the temperature was prescribed in the entire column by means of a mixed boundary condition for energy applied to the whole domain with a sufficiently high value for parameter γ_e (in the same way as γ_g). Note, however, that this prescribed temperature varies with time (Figure 3). For the heated column, another mixed boundary condition at the top of the column was applied in order to simulate energy flux (Eq. 7).

$$\begin{aligned}
j_e &= j_e^0 + \gamma_e (T^0 - T) + E_g^w j_g^w \\
&\quad \text{with } \gamma_e = \rho_g^a c_a \beta_g \\
E_g^w &= E_g^w(T) \quad \text{if } T > T^0 \\
E_g^w &= E_g^w(T^0) \quad \text{if } T \leq T^0
\end{aligned} \tag{7}$$

In this case, γ_e was calculated from β_g assuming that energy and heat fluxes are controlled by the same turbulence mechanisms (Arya 2001). For lateral heat exchange and that at the bottom the same mixed boundary condition was applied, but the parameter γ_e was calculated from thermal conductivity and thickness of the insulating wool and the radius of the column. No flow boundary conditions for salt and liquid were assumed ($j_l^w = 0$ and $j^h = 0$). External temperature T^0 , vapour density, $(\rho_g \omega_g^w)^0$, and vapour mass fraction $(\omega_g^w)^0$ varies in time and were obtained from the sensor above the column (Figure 3).

3.6 Initial conditions

Initial conditions must be specified for each node and for all state variables (temperature, liquid pressure, gas pressure and (for the models considering dissolved salts) mass fraction of dissolved salt). Initial liquid pressure was calculated by the psychrometric law (Appendix A, Eq. 14 and 17) from initial values of temperature and relative humidity measured by sensors and then linearly interpolated. Initial gas pressure was assumed to be equal to an atmospheric pressure of 0.1 MPa. Also initial temperature was interpolated from initial measured temperature. For the models considering dissolved salts (a sum of K, Na, Li, Ca, Sr, Ba, Cr, Mo, Fe, Al, Si, S and OH^-), an initial concentration was considered of $0.03 \text{ kg}_s \text{ kg}_l^{-1}$ which was obtained from data from an ordinary Portland cement hardened after 317 days, published by Lothenbach and Winnefeld (2006).

4 Results and discussion

4.1 Calibration

The parameters relative permeability (k_r , Eq. 21 and 22), tortuosity (τ , Eq. 31), thermal conductivity (λ , Eq. 37) and boundary exchange coefficient (β_g , Eq. 5 and Table 2) were calibrated in order to fit the experimental data to the model results. The calibration consists of changing these parameters and comparing the modelled results to the measured data by trial and error in order to obtain the best fit. Mathematically this could give rise to non-unique solutions, that is, various sets of parameters could give equally well fits. To avoid this, we required the parameters to be close to values from literature or the ones measured experimentally. This restriction allows us to find a unique set of values.

The relative permeability for both liquid and gas are functions of saturation through parameters A and n (Eq. 21 and 22). We also tried the van Genuchten-Mualem expression but the fitting was less satisfactory (not shown). Figure 4 shows liquid and gas relative permeability with the calibrated parameters. Theoretically A should

Fig. 3 Boundary conditions. Evolution of temperature and vapour density in both experiments. Vapour density was calculated from temperature and relative humidity data measured by sensor situated above the columns (Eq. 15,17 and 27).

have a value of 1 and for soils n normally has a value of 3. However, for liquid relative permeability we found values of 0.01 for A and 7 for n , which means that at saturation the relative permeability is not equal to 1. In comparison to granular media (soils and sand) the liquid relative permeability drops very fast with saturation. This behaviour in cement materials has also been found in other studies (Monlouis-Bonnaire et al 2004; Wardeh and Perrin 2006).

The tortuosity factor for vapour diffusion (Eq. 31) had to be higher for the heated than for the non-heated column in order to achieve acceptable fits. This discrepancy reflects an often made observation that temperature gradients enhance vapour diffusion more than predicted by Fick's law of Eq. 31. The mechanism may consist of the fact that at the pore scale vapour diffusion is linked to heat flux. Heat flux across a meniscus of water can transport vapour by condensing at one site and evaporating at the other side of the meniscus. This heat flux is larger than vapour diffusion. This phenomenon is called enhanced-vapour diffusion. Ho and Webb (1998) discuss this topic in more detail.

For the heated column, the dry and saturated thermal conductivity were calibrated. First, we used the experimental values measured by Villar et al (2009) (λ between 2.2 and 3). However, using these values not enough gradient of temperature was simulated. So we reduce them in order to fit the model results to the experimental data of temperature. The values obtained ($\lambda_{sat}=1.14 \text{ W m K}^{-1}$ and $\lambda_{dry}=0.66 \text{ W m K}^{-1}$, Eq. 38) are low in comparison to those measured by Villar et al (2009) but they are comparable with the ones reported by Kim et al (2003). It is known that

Table 2 Parameters of the boundary conditions used in the models.

Position	column	
	non-heated	heated
top	$\beta_g = 10^{-3} \text{ms}^{-1}$ $\gamma_g = 1 \text{ kg s}^{-1} \text{m}^{-2} \text{MPa}^{-1}$ $(P_g)^0 = 0.1 \text{ Mpa}$ $j_e^0 = 0$ $\gamma_e = 5 \text{ J s}^{-1} \text{m}^{-2} \text{ }^\circ\text{C}^{-1}$	$\beta_g = 3.7 \cdot 10^{-2} \text{ms}^{-1}$ $\gamma_g = 0.5 \text{ kg s}^{-1} \text{m}^{-2} \text{MPa}^{-1}$ $(P_g)^0 = 0.1 \text{ Mpa}$ $j_e^0 = 1100 \text{ J s}^{-1} \text{m}^{-2}$ $\gamma_e = 41.61 \text{ J s}^{-1} \text{m}^{-2} \text{ }^\circ\text{C}^{-1}$
lateral	$j_e^0 = 0$ $\gamma_e = 5 \text{ J s}^{-1} \text{m}^{-2} \text{ }^\circ\text{C}^{-1}$	$j_e^0 = 0$ $\gamma_e = 18.96 \text{ J s}^{-1} \text{m}^{-2} \text{ }^\circ\text{C}^{-1}$
bottom	$j_e^0 = 0$ $\gamma_e = 5 \text{ J s}^{-1} \text{m}^{-2} \text{ }^\circ\text{C}^{-1}$	$j_e^0 = 0$ $\gamma_e = 0.64 \text{ J s}^{-1} \text{m}^{-2} \text{ }^\circ\text{C}^{-1}$

thermal conductivity is influenced by the type of aggregates, their volume fraction, temperature and porosity (Marshall 1972; Khan 2002; Kim et al 2003). The type of aggregates for the thermal conductivity experiments is probably different from the one used in the evaporation test. So do the volume fractions of these aggregates. Temperature is also different. The experimental thermal conductivity was measured at room conditions, while the evaporation test reach a temperature of 65°C. Moreover, despite of the same chemical composition of the cement, porosity could be slightly different for different samples maybe due to concrete manufacturing (for instance vibration process during manufacturing of the concrete sample). For the non-heated column the calibrated value for the vapour exchange coefficient, β_g (Eq. 5 and Table 2) was high enough to practically fix the vapour density at the top of the column. Hence this value has little physical meaning. For the heated column the calibration of vapour exchange coefficient β_g is linked to that of heat exchange coefficient, γ_e , (Eq. 7). The value obtained is similar to values found in other studies (Pintado et al 2002; Gran et al 2011).

4.2 Temperature

The temperature in the non-heated column is not particularly interesting. As explained in section 3, measured temperatures did not show any temperature gradient in the column and therefore we just fixed the temperature of the model to that measured by the sensor above the column (Figure 3a).

Figure 5 compares the evolution of temperature of the heated column measured by each sensor and calculated by the model without dissolved salts (the model with dissolved salts has practically the same calculated temperature, as it is not shown). There is a good agreement between the data and the model results. However, from day 189 the model overestimates the temperature. This could be because of the fact that the column was moved to another laboratory with more constant temperature.

Fig. 4 Relative permeability for liquid and gas phases.

Moreover, the conditions in the two laboratories (temperature and relative humidity) could lead to different values of boundary exchange coefficient (β_g and γ_e , Eq. 7 and Table 2). However, the models assume them to be constant. Note that there are only experimental data of sensor s5 at the beginning of the test. From the fifteenth day on, it stopped working because it was damaged.

Fig. 5 Evolution of temperature for each sensor in the heated column. Points are experimental data and continuous lines model results (no dissolved salts). The position of sensors is displayed in figure 1. After 189 days the column was moved to another room where temperature was more constant.

4.3 Concentration of dissolved salts

The concentration of dissolved salts, calculated for each column is displayed in Figure 6 (obviously, these results only correspond to the models which take into account the dissolved salts). In the non-heated column the dissolved salts do not have an important effect because the evaporation is low and, therefore, salt concentration

does not increase much. However, in the heated column the concentration is higher due to the higher evaporation. The concentration is highest at the top of the column and this zone of maximum concentration extends downwards with time. This reflects a downward moving front where evaporation takes place and, as a result, concentration increases. Note that at the top of the column the final concentration of dissolved salts is slightly lower than at earlier times. This is due to fluctuations in temperature and relative humidity and, hence, in evaporation rate.

Fig. 6 Dissolved salt concentration along the column at different times and for each test (0 is the top of the column).

4.4 Relative Humidity

Figure 7 compares the relative humidity (Eq. 17) measured by the sensors to the results calculated by the models, for each column (non-heated and heated column) and each model (with and without dissolved salts). In the non-heated column, the model with dissolved salts and the model without have similar results. So dissolved salts do not seem to have an important effect on relative humidity, because only less than 20% of water initially present was evaporated. There is a good agreement between experimental data and the results of the model at sensor s2, s3 and s5. At sensor s1, situated at the top of the column, the model underestimates the relative humidity during the first half of the test and overestimates it during the second half. This could be related to some parameter which in reality may depend on temperature but which the model assumes to be constant (see Figure 3a). The behaviour of sensor s4 is difficult to reproduce by the conceptual model used, because the relative humidity

should be lower than sensor s5 according to its position in the column (see Figure 1). It is possible that this sensor was placed in an area in which the characteristics of concrete were slightly different, since due to the presence of coarse aggregates, the material is quite heterogeneous. As can be observed sensors s3, s4 and s5 have changes in the slope at the beginning of the test. This could be because the sensors are not perfectly sealed to the concrete. During the first 60 days the temperature rises (see figure 3a), which tends to decrease the relative humidity. In a porous medium this decrease is counteracted by evaporating water, retained in the pores. A small gap between concrete and sensor, however, may impede this counteracting. The relative humidity in the heated column is displayed in Figure 7b. The model starts at the same initial relative humidity measured by the sensors. However, sensors s3, s4 and s5 measured an increase of the relative humidity from the first day, which hardly can be appreciated at the figure because of the scale used. This behaviour cannot be reproduced by the numerical model. Relative humidity should decrease because of evaporation. Probably it is due to measurement errors of the sensors. In this test the effect of dissolved salts gains importance because the evaporation is higher, around 40%. The difference between the models with and without dissolved salts is due to two effects. The first one is the fact that dissolved salts reduce evaporation and, as a consequence, increase the saturation. The second effect is the fact that with the same capillary pressure (and saturation) the relative humidity is lower because the salinity is higher (Eq. 14 and 17). At the upper part of the column (sensors s1 and s2), the relative humidity is lower for the model with dissolved salts than for the one without, because the second effect dominates. From mid column downwards (sensors s3, s4 and s5), the model with dissolved salts has a higher relative humidity, because the first effect dominates. However, the effect of dissolved salts seems not to be very important.

Fig. 7 Evolution of relative humidity measured by each sensor for each column. The experimental data and results of the model with salinity and without it are compared. Points correspond to experimental data, continuous lines are model without dissolved salts results and broken lines are dissolved salts model results. The positions of each sensor are displayed in Figure 1

4.5 Loss of mass

The experimental and modelled evolution of loss of mass for each test is displayed in Figure 8. In the non-heated column, both models slightly overestimate the loss of mass during the first 170 days and slightly underestimate it afterwards. This error is related to the relative humidity observed for sensor s1. The relative humidity calculated by the model is lower at the beginning when evaporation is higher, and is higher at the end when there is less evaporation. In the heated column, from day 189 the experimental data show an increase in mass provably because the sample was moved to another laboratory with different conditions leading to different boundary exchange coefficients. In addition, the measurements could have lost precision due to this change. As this was not taken into account by the models, they show a continuous weight loss. As a consequence we obtained a worse fit than for the heated column. In both columns, the loss of mass is higher for the model without dissolved salts than for the model with them. It means that, as expected, dissolved salts reduce the evaporation. However, in the non-heated column the differences between the two models are small. So the reduction of evaporation is higher when the evaporation is also higher.

Fig. 8 Loss of mass during evaporation test and concentration of dissolved salts effect. Both columns are displayed.

4.6 Saturation

The saturation at the end of the test is shown in figure 9 for each column. The saturation of experimental data was calculated from the gravimetric humidity in each section (Eq. 10 and 12). In the non-heated column there is no difference between the model with and without salinity. The saturation calculated numerically is lower at the top of the column and higher at the bottom and fits well to the measured data. For heated column, there are some differences between the models from mid column downwards. The model with dissolved salts has higher saturation because salinity increases the saturation. The fitting for this column is not so good. In the numerical model the saturation increases with depth and the model overestimates the saturation. This error is related to the fact that our retention curve overestimates the saturation from mid column to downwards (figure 2). And the model underestimates the relative humidity (s4 and s5 figure 7).

Fig. 9 Saturation at the end of the test for each column (0 is the top of the column).

4.7 Flux

Figure 10 shows the evaporation rate for both tests. In both columns, there is a front where most evaporation takes place. In the non-heated column this front reduces with time and is near the top of the columns. In the heated column, however, the front moves downwards. There is a slight difference between the models with and without dissolved salts. In order to study the relative importance of the various processes, figure 11 displays advective fluxes of liquid and gas phases and diffusive flux of vapour along the column calculated by the models at the end of the tests. For

the non heated column, above the evaporation front vapour diffusion is the dominant water transport process, which has also been found in soils by Grifoll et al (2005) and Gran et al (2011). Below this front advection of liquid water is the dominant process. Although, gas advection appears negligible above the evaporation front, it has an important effect and the model had to include it in order to obtain an acceptable fit. This confirms the work of Mainguy et al (2001) who studied the role of air pressure and advective vapour fluxes in the gas phase.

The heated column shows a higher vapour diffusion than the non-heated column. The energy from the lamp increases the evaporation and, therefore, lowers the liquid saturation, leading to a higher diffusion according to Fick's law (Eq. 31). In addition, the lamp produces a gradient of temperature and, consequently, a gradient in vapour density. From mid column downwards of the heated column, salinity slightly reduces the vapour diffusion because the evaporation is lower and increases the liquid advection because the saturation increases (Figure 11b).

Fig. 10 Evaporation rate along each column. Initial and final times are displayed.

5 Conclusions

Evaporation tests were performed in concrete columns, one column in room conditions and another one heated by a lamp. The calibration of models made it possible to obtain thermo-hydraulic parameters. We obtained the same values of most parameters for both the heated and the non-heated columns, which strengthens the validation of the calibrated parameter values. An exception was the tortuosity factor, which affects vapour diffusion. The difference in the estimated value of this parameter indicates enhanced vapour diffusion as discussed by Ho and Webb (1998). The retention curve obtained by fitting the results of the evaporation tests agrees with that determined by controlling the relative humidity in desiccators by Villar and Romero (2014), and shows that this concrete is a very retentive material reflected by the high entry pressure obtained. The liquid relative permeability drops

Fig. 11 Advective flux of liquid (j_l) and gas (j_g) phase and diffusive flux (i) along each column at the end of the test.

considerably with saturation in comparison to granular media.

An advantage of the used method of calibrating models may be that it is not necessary to wait several years for the system to reach a steady state, which is required for classical analyses of experiments for retention curves and relative permeabilities. This is particularly interesting for low permeability materials, such as this kind of concrete. We assume a homogeneous medium. Thus only the upper part of the column is needed to reach the steady state in order to calibrate the model.

The thermo-hydraulic multiphase flow models of these evaporation tests help to understand processes in concrete. According to our study the concentration of dissolved salts reduces evaporation to a maximum of 5%. This reduction gains importance when evaporation from the column is higher. However, it could be neglected. According to the calibrated model, in both columns, vapour diffusion is the dominant water transport above the evaporation front where water is mainly in gas phase and gas advection is negligible. Below this front advection of liquid water is the dominant process.

A Constitutive laws

A.1 Definition constraints

Mass fractions

$$\omega_l^w + \omega_l^a + \omega_l^h = 1 \quad (8)$$

$$\omega_g^w + \omega_g^a = 1 \quad (9)$$

Volumetric content

$$\theta_l = \frac{V_l}{V_t} = \frac{1}{\rho_l} w \rho_s (1 - \phi) \quad (10)$$

412 Saturations

$$S_l + S_g = 1 \quad (11)$$

$$S_l = \frac{V_l}{V_p} = \frac{\theta_l}{\phi} \quad (12)$$

413 Partial pressures

$$P_g^a + P_g^w = P_g \quad (13)$$

414 A.2 Equilibrium constraints

415

416 Vapour-liquid water (psychrometric law)

$$P_g^w = a_w P_{g,sat}^w \exp \left(\frac{-(P_g - P_l) M^w}{R \rho_l (273.15 + T)} \right) \quad (14)$$

$$P_{g,sat}^w = 136075 \exp \left(\frac{-5239.7}{273.15 + T} \right) \quad (15)$$

$$a_w = 1 - \left(\left(\omega_l^h \frac{1000}{M^h - 3} \right) 1.9775 \cdot 10^{-5} T + 0.035 \right) \omega_l^h \frac{1000}{M^h - 3} \quad (16)$$

417 where $M^h = 49.37 \text{ g mol}^{-1}$

$$HR = \frac{P_g^w}{P_{g,sat}^w} \quad (17)$$

$$\omega_g^w = \frac{P_g^w M^w}{R \rho_g (273.15 + T)} \quad (18)$$

418 Dissolved-gaseous air (Henry's law)

$$\omega_l^a = \frac{P_g^a M^a}{H M^w} \quad (19)$$

A.3 Phase and interphase properties

Retention curve (van Genuchten law)

$$S_e = \left(1 + \left(\frac{P_g - P_l}{P_0 \frac{\sigma_T}{\sigma_0}} \right)^{\frac{1}{1-m}} \right)^{-m} \quad (20)$$

where $P_0=7.7$ Mpa, $m=0.34$, σ_T is the surface tension at temperature T and $\sigma_0=0.072$ N/m at 20°C

Relative permeability

$$k_{rl} = AS_{el}^n \quad (21)$$

where $A=0.01$ and $n=7$

$$k_{rg} = AS_{eg}^n \quad (22)$$

where $A=1$ and $n=3$

Properties of liquid

$$\rho_l = \rho_{l0} \exp(\beta(P_l - P_{l0}) + \epsilon T + \gamma \omega_l^h) \quad (23)$$

where $\rho_{l0}=1002.6$ kg m⁻³, $P_{l0}=0.1$ MPa, $\beta=4.5 \cdot 10^{-4}$ MPa⁻¹, $\gamma=0.6923$ and $\epsilon=3.4 \cdot 10^{-4}$ °C⁻¹

$$\mu_l = 2.1 \cdot 10^{-12} \left(\frac{1808.5}{273.15 + T} \right) \quad (24)$$

$$\sigma_T = \left(1 - 0.625 \left(\frac{273.15 + T}{647.3} \right) \right) \left(0.2358 \left(\frac{273.15 + T}{647.3} \right)^{1.256} \right) + 0.04055 \omega_l^h \quad (25)$$

$$E_l = E_l^w \omega_l^w + E_l^a \omega_l^a \quad (26)$$

where $E_l^w=4184T$ J kg⁻¹ and $E_l^a=1000T$ J kg⁻¹

Properties of gas

$$\rho_g = \frac{P_g^w M^w}{R(273.15 + T)} + \frac{P_g^a M^a}{R(273.15 + T)} \quad (27)$$

where $M_g^a=0.02895$ kg mol⁻¹ and $H=10000$ MPa

$$\mu_g = \frac{1.48 \cdot 10^{-12} \sqrt{273.15 + T}}{1 + \frac{119.4}{T + 273.15}} \frac{1}{1 + \frac{0.14 - 1.2 \cdot 10^{15} k_i}{P_g}} \quad (28)$$

$$E_g = E_g^w \omega_g^w + E_g^a \omega_g^a \quad (29)$$

where $E_g^w=2.5 \cdot 10^6 + 1900T$ J kg⁻¹ and $E_g^a=1000T$ J kg⁻¹

Properties of solid

The density of the solid phase (ρ_s) is 2360 kg m^{-3} and $E_s = 780T \text{ J kg}^{-1}$

A.4 Fluxes

Darcy's flux

$$q_\alpha = -\frac{k_i k_{r\alpha}}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha g) \quad (30)$$

where $k_i = 4.2 \cdot 10^{-18} \text{ m}^2$

Diffusive flux (Fick's law)

$$i_{\alpha, dif}^i = -(\tau \phi \rho_\alpha S_\alpha D_m^i) \nabla \omega_\alpha^i \quad (31)$$

where $\tau_{non-heated} = 0.08$ and $\tau_{heated} = 0.3$

$$D_m^{vapor} = D \left(\frac{(273.15 + T)^n}{P_g} \right) \quad (32)$$

where $D = 5.9 \cdot 10^{-6} \text{ m s}^{-1} \text{ K}^{-n} \text{ Pa}$ and $n = 2.3$

$$D_m^{solute} = D \exp \left(\frac{-24530}{R(273.15 + T)} \right) \quad (33)$$

where $D = 1.1 \cdot 10^{-4} \text{ m}^2 \text{ s}^{-1}$

Dispersive flux (Fick's law)

$$i_{\alpha, dis}^i = -(\rho_\alpha D_\alpha') \nabla \omega_\alpha^i \quad (34)$$

$$D_\alpha' = d_l q_\alpha \quad (35)$$

where $d_l = 0.015 \text{ m}$

Mass flux

$$j_\alpha^i = q_\alpha \rho_\alpha \omega_\alpha^i + i_{\alpha, dis}^i + i_{\alpha, dif}^i \quad (36)$$

Conductive flux of heat (Fourier's law)

$$i_c = -\lambda \nabla T \quad (37)$$

$$\lambda = \lambda_{sat}^{S_l} \lambda_{dry}^{1-S_l} \quad (38)$$

where $\lambda_{sat} = 1.14 \text{ W m K}^{-1}$ and $\lambda_{dry} = 0.66 \text{ W m K}^{-1}$

Advective flux of heat

$$j_{E\alpha} = q_{\alpha} E_{\alpha} \quad (39)$$

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