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Determining hydraulic properties of concrete and mortar by inverse modelling

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ABSTRACT

This paper presents a methodology and results on estimating hydraulic properties of the concrete and mortar considered for the near surface disposal facility in Dessel, Belgium, currently in development by ONDRAF/NIRAS. In a first part, we estimated the van parameters for the water retention curve for concrete and mortar obtained by calibration (i.e. inverse modelling) of the van Genuchten model [1] to experimental water retention data [2]. Data consisted of the degree of saturation measured at different values of relative humidity. In the second part, water retention data and data from a capillary suction experiment on concrete and mortar cores was used jointly to successfully determine the van Genuchten retention parameters and the Mualem hydraulic conductivity parameters (including saturated hydraulic conductivity) by inverse modelling.

WATER RETENTION CURVES OF CONCRETE AND MORTAR

Concrete constitutes one of the main materials used in engineered barriers limiting radionuclide leaching to the environment, especially in case of near surface disposal of low-level radioactive waste. It is then crucial to accurately determine the (unsaturated) flow and transport properties of the envisaged concrete components, as such properties have an effect on the long-term performance of engineered barriers, including limiting water flow and providing for retardation of contaminant migration. Also, the coupling between flow and transport properties is important to develop defensible models of physical and chemical degradation of concrete. In this paper methodology and results on estimating hydraulic properties of the concrete and mortar considered for the near surface disposal facility in Dessel, Belgium, are presented.

Experimental water retention data

Water retention curves have been estimated for the concrete and mortar samples referenced, respectively, as C-15-A and M1 [2]. The concrete C-15-A is a mix of CEM I, calcium carbonate, calcareous aggregates and superplasticizer, whereas the mortar M1 is a mix of CEM III, silica fume, limestone and superplasticizer. Absorption and desorption isotherms have been determined by letting 50-mm diameter and 5-mm thick concrete samples equilibrate in a closed chamber until constant weight (different humidity levels were controlled by different saturated aqueous solutions). In total 11 different controlled atmospheres have been imposed by using saturated aqueous solutions covering a relative humidity range from 11.3% to 97.6%. All equilibria were reached in rooms having a controlled temperature fixed to 21°C. In order to determine the water retention curves, relative humidity conditions were changed into matric potential P_c [Pa] in a capillary tube using the Kelvin-Laplace relationship:

$$P_c = -RT\rho_w \ln HR/M \quad (1)$$

where M is the atomic mass of water (0.018 kg mol^{-1}), R is the universal gas constant (8.314 J K^{-1} mol^{-1}), T is the absolute temperature (K), ρ_w is the density of water (998 kg m^{-3} at 20°C), and HR (%) is the relative humidity of condensation. Retention curve data obtained from [2], originally expressed as degree of saturation S_e (dimensionless) versus relative humidity (%), were converted in volumetric water content θ (cm^3 cm^{-3}) versus pressure head h (m) data, using $\theta = \phi \times S_e$ with the porosity ϕ (cm^3 cm^{-3}) measured independently from weight loss of saturated samples, and $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ is degree of saturation (-). The mean porosity ϕ was 0.109 and 0.185 cm^3 cm^{-3} for concrete (type C-15-A) and mortar (type M1) (3 samples), respectively.

van Genuchten – Mualem hydraulic function

The van Genuchten – Mualem expression for the water retention curve $\theta(h)$ is [1]:

$$\theta(h) = \theta_r + (\theta_s - \theta_r)\Big/\left(1 + (\alpha h)^n\right)^m \quad (2)$$

where θ_r is the residual water content (cm^3 cm^{-3}), θ_s is the saturated water content (cm^3 cm^{-3}), and α (m^{-1}), n, and m are empirical parameters. When fitting $\theta(h)$ data independently, the assumption $m = 1-1/n$ is used for Eq. (2). The following van Genuchten parameters were optimized with the RETC software [5] when using the water content - pressure head data: θ_r, θ_s, α, and n (m was related to n). Independent values for m and n are fitted in this study for the Mualem hydraulic conductivity relationship $K(h)$ by linking HYDRUS-1D with a global genetic search algorithm:

$$K(h) = K_s Se^l \left[1 - \left(1 - Se^{1/m}\right)^m\right]^2 \quad (3)$$

where K_s is the saturated hydraulic conductivity (m s^{-1}), l (-) is a factor that accounts for the pore connectivity and tortuosity estimated by *Mualem* [3] to be 0.5 as an average of many soils.

Table I. Fitted van Genuchten parameters based on RETC [5]. Parameter n (dimension-less) was optimized separately for adsorption/desorption data (case 1), or a single n was optimized for both adsorption/desorption data (case 2). R^2 = coefficient of determination.

Data	Concrete C-15-A					Mortar M-1				
	θ_r (cm^3 cm^{-3})	θ_s (cm^3 cm^{-3})	α (m^{-1})	n (-)	R^2	θ_r (cm^3 cm^{-3})	θ_s (cm^3 cm^{-3})	α (m^{-1})	n (-)	R^2
Absorption-1	0.000	0.078	7.12E-4	1.521	0.969	0.000	0.100	2.91E-4	1.554	0.953
Desorption-1	0.000	0.080	1.46E-4	2.201	0.989	0.008	0.101	1.02E-4	2.592	0.988
Absorption-2	0.000	0.090	2.48E-4	1.917	0.969	0.000	0.162	1.64E-4	1.937	0.954
Desorption-2	0.000	0.107	1.83E-4			0.000	0.179	1.29E-4		

DETERMINING VAN GENUCHTEN PARAMETERS BY INVERSE MODELLING

Absorption and desorption water retention curves display hysteresis: the water desorption branch is different from the water absorption branch. The retention curves were first fitted using a separate *n* parameter for each branch (case 1). Because HYDRUS-1D will be used in the fitting of the capillary suction data, with the restriction that its hysteresis model uses one *n*-parameter for both branches, the retention curve was also fitted using a single *n*-parameter for desorption and adsorption branches. **Figure 1** and **Table I** present the optimized water retention curves and the hydraulic parameter values, respectively. The hysteresis model shows a good fit between data and model with differences between predictions and data which never exceed 0.01 $cm^3\ cm^{-3}$.

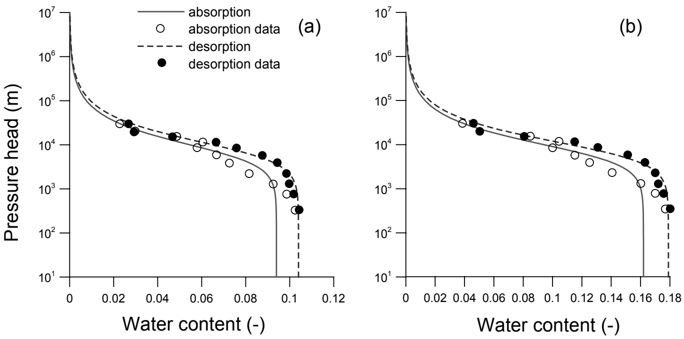

Figure 1. Water retention curves for concrete C-15-A (a) and mortar M1 (b). A single-*n* parameter is used (case 2).

DETERMINING HYDRAULIC PROPERTIES BY INVERSE MODELLING AND ABSORPTION EXPERIMENTS

Experimental setup and data

A capillary suction experiment has been performed on three circular specimens (15-cm diameter and 5-cm thickness) for both concrete C-15-A and mortar M1. Details of experimental conditions are given in [2]. Prior to the suction test, specimens had been equilibrated with an atmosphere having 54% of relative humidity. The bottom part of the specimen has been put in contact with the water level reaching until 0.005 m above the specimens' bottom surface, whereas the other surfaces of the specimens have been covered with plastic to make them impermeable. By measuring the weight of the samples at different times, the evolution of water absorbed by capillary suction was recorded. After 35 days, the experiment has been stopped. The samples were not fully saturated at the end of the experiment as was evident from the shape of the absorption curve.

Modelling approach

The numerical modelling approach aims at mimicking the experimental results obtained during the capillary suction test. The goal is to numerically reproduce the cumulative water flux, which corresponds to the water that penetrates in the sample by capillary suction. In the meanwhile, parameters should also describe correctly the independently obtained retention curves (wetting curve). Therefore an inverse procedure will be implemented in order to optimize both the retention curve and the capillary suction test data. The previously fitted van Genuchten parameters for the wetting curve will be used to define parameter ranges for use in genetic algorithm-based inverse modelling.

The HYDRUS-1D software package [7] was used for simulating the one-dimensional unsaturated water flow experiment. The main characteristics of the conceptual model are summarized as follows: as lower boundary condition a constant pressure head equal to +0.005 m. This boundary condition reflects the fact that the sample has been immersed in water by 5 mm. As upper boundary condition a zero flux (specimen covered with plastic). Furthermore, a spatially uniform initial pressure head condition in the entire sample was considered. It was calculated in two steps: (1) by determining the initial saturation degree according to the quantity of water infiltrated in the sample at the end of the absorption experiment (measured by differences of final and initial weight) and the knowledge of the porosity, (2) by calculating the initial pressure head according to the initial saturation degree obtained from step (1) and the VGM parameters from **Table I**.

Hydraulic parameters were estimated using an inverse modelling approach in which hydraulic parameters that describe the $K(h)$ relationship are optimized (eq. (4)). We chose to optimize θ_r, α, n, m, K_s, and l, while keeping θ_s fixed and equal to the independently measured total porosity. Note that parameter m has also been optimized as this provides larger flexibility in the description of the $\theta(h)$ and $K(h)$ relationships. Because two types of data (i.e. flux and water content) are jointly taken into account in this optimization process, the following formulation of the objective function, OF, was used:

$$OF = \sum_{i=1}^{M} w\left(q_{i^*} - q_i\right)^2 + \sum_{j=1}^{N} \frac{1}{w}\left(\theta_{j^*} - \theta_j\right)^2 \tag{4}$$

where M and N represent the number of measurements of cumulative flux and water retention data (i.e. water content) respectively, q_{i^*} and q_i are the ith measured and predicted cumulative flux, respectively, θ_{j^*} and θ_j are the jth measured and predicted water content, respectively, and w is a weighting factor introduced in order to give both data sets a similar weight, which is defined as:

$$w = \sum_{j=1}^{N} \theta_{j^*} \Big/ \sum_{i=1}^{M} q_{i^*} \tag{5}$$

To cope with the limitations of local search algorithms such as gradient-based methods (e.g. the Levenberg-Marquardt method), we performed the optimization by linking HYDRUS-1D with a global search algorithm, i.e. a genetic algorithm [8, 9]. This allows to determine the actual minimum of complex non-linear optimisation problems.

MODELLING RESULTS

Calculated cumulative water fluxes based on inverse modelling are displayed in **Figure 2**. Whereas at the end of the experiment (day 35) full saturation is not reached in the sample, numerical simulations predict that saturation is reached for the concrete after 12 days and after

4.5 days for the mortar. The observation that the simulated equilibrium is much quicker reached than the measured one (provided that the measurements are in equilibrium, which is very unlikely to be true as we discussed later) is in line with similar observations reported by *Hall* [10], i.e. that long-term (days+) water transfer by unsaturated flow is likely to be slower than predicted from material property values obtained in short term experiments. For such long-term tests additional processes other than water absorption by diffusion may be at work, including chemomechanical processes modifying the pore structure of the concrete.

Table II. van Genuchten-Mualem parameter values estimated by inverse modelling using HYDRUS-1D. θ_s fixed at measured porosity, i.e. 0.109 and 0.185 cm^3 cm^{-3} for concrete C-15-A and mortar M1, respectively. Parameter *m* was optimized independently from *n*. Lower and upper bound are bounds imposed during optimization.

	van Genuchten-Mualem hydraulic parameters						
	θ_r (cm^3 cm^{-3})	θ_s (cm^3 cm^{-3})	α (m^{-1})	n (-)	m (-)	K_s (m s^{-1})	l (-)
	Concrete (R^2 =0.971 for water retention data; R^2 =0.983 for cumulative flux data)						
Best fit	0.000	<u>0.109</u>	7.65E-4	1.307	0.404	5.67E-13	35.2
Lower bound	0.000	-	1.00E-4	1.050	0.200	1.00E-13	-3.0
Upper bound	0.070	-	1.00E-3	2.000	0.500	1.00E-11	50.0
	Mortar (R^2 =0.956 for water retention data; R^2 =0.977 for cumulative flux data						
Best fit	0.000	<u>0.185</u>	3.23E-4	1.217	0.435	5.87E-14	-3.0
Lower bound	0.000	-	1.00E-4	1.050	0.200	1.00E-14	-3.0
Upper bound	0.070	-	1.00E-3	2.000	0.500	1.00E-14	50.0

Optimized VGM parameter values are provided in **Table II**, and the corresponding water retention curve for concrete is plotted in **Figure 2**. It appears that parameter *l* is estimated to have values close to or equal to the parameter bounds: for the concrete *l* is equal to 35.2 which is very high. For soils *l* values significantly different from 0.5 have also been reported [11], although a different functional form of the Mualem model is used here (Eq. (3)). High values of *l* indicate that the unsaturated hydraulic conductivity decreases very strongly when moving away from saturation. For the mortar *l* is equal to -3.0, i.e. the imposed parameter bound. The estimated saturated hydraulic conductivity K_s is 5.67×10^{-13} m/s and 5.87×10^{-14} m/s for the concrete C-15-A and the mortar M1, respectively. These are consistent with values found in the literature for similar types of concrete and mortar (e.g. [12]).

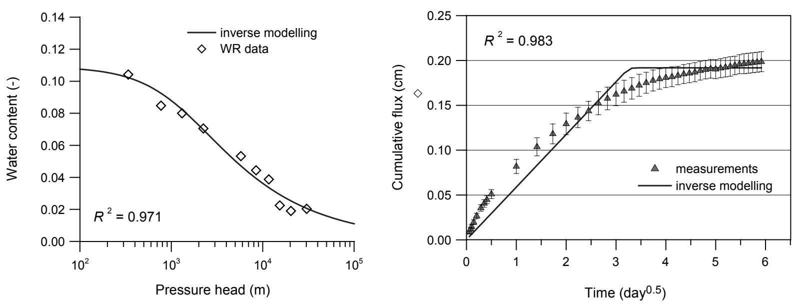

Figure 2. (a) Measured and simulated water retention, (b) cumulative measured and simulated fluxes by inverse modelling (vertical error bars = one standard deviation) for concrete C-15-A.

As concerns the initial condition, it is interesting to notice that the initial pressure head, which was derived from the optimized hydraulic parameters and the estimated saturation degree of 0.646 for concrete C-15-A is equal to 2100 m. The latter value is far from the one derived from Eq. (2) when applying a relative humidity of 54% (as in the capillary absorption test), i.e. h = 8500 m. This is an indication that the samples did not yet reach an equilibrium moisture content nor a capillary pressure commensurate with the imposed vapour pressure boundary condition, and hence that a much longer equilibration time is needed.

CONCLUSIONS

Of significant importance to long-term prediction of water and radionuclide migration in concrete is the choice of a suitable hydraulic model and the determination of accurate unsaturated hydraulic parameters. In a first part, we estimated the van Genuchten retention curve parameters using experimental moisture retention data encompassing both the wetting and drying branch. In a second part, numerical simulations of a capillary absorption experiment were performed. Results showed a satisfactorily agreement between model and data when the van Genuchten-Mualem parameters (α, n, m, θ_r, K_s, l) were fitted simultaneously to both water retention data and capillary absorption data. Because optimized K_s values resulted in a good description of the capillary absorption test and are in agreement with literature values for similar concrete and mortar, the K_s values (5.67×10^{-13} m/s and 5.87×10^{-14} m/s for concrete and mortar, respectively) are considered appropriate for use in saturated-unsaturated flow calculations.

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