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MATHEMATICAL MODELLING OF WATER MOVEMENT IN AUTOCLAVED CONCRETE

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Abstract. The paper presents a mathematical model developed for the description of water movement in selected construction materials. In the creation of the model the Richards equation was employed that was introduced in 1931 for a homogeneous and isotropic soil medium. The equation was solved with the method of finite differences, using an explicit scheme. The experiment was conducted on a sample made of autoclaved cellular concrete in which TDR probes were placed for moisture measurement. Water movement in the sample was caused by capillary rise. Results from computer simulation were compared with those obtained in the experiment. It was demonstrated that the Richards equation can be used for the description of the dynamics of air-water conditions in cellular concrete. It was also found that differences between results obtained from the simulation and those obtained from the experiment could have been caused by the lack of calibration of the TDR apparatus that should be made individually for every medium.

Keywords: autoclaved cellular concrete, TDR technique, Richards equation

INTRODUCTION

Application of the TDR technique for the study of moisture in construction materials is the subject of studies at numerous research centres, including in particular the Institute of Agrophysics PAS in Lublin, the Universities of Technology in Dresden, Prague, Łódź and Lublin, and recently also at the Institute of Environment Conservation and Management of the University of Life Sciences in Wrocław (Janik 2009, Janik *et al*. 2006, Jiřičková 2003, Pavlik 2005a, Pavlik 2005b, Plagge *et al.* 2003, Sobczuk et al. 2004). Moisture is one of the more important parameters of construction materials. Among other things, it affects their bulk density, and that in turn is important in the technology of realization of construction works, e.g. during the transport of construction materials, and has also a structural significance by causing changes in loads. Moisture can be determined in a classic way, e.g. with the thermo-gravimetric method. That, however, has the disadvantage of the material tested being destroyed, rendering the replication of the determination at the same point impossible. It is also possible to apply for that purpose an apparatus based on time domain reflectometry, e.g. the TDR apparatus designed and made at the Institute of Agrophysics PAS in Lublin (Malicki 1999, Skierucha 2005, Skierucha *et al*. 2008). In such a case, the measurement is virtually non-invasive and can be conducted in a continuous manner. This permits accurate determination of the dynamics of moisture changes in a given medium.

Moisture conditions in porous media can also be determined through mathematical modelling. To build such a model, one needs to adopt equations used for the description of water movement in soil. The objective of this study was to test the applicability of the Richards equation for modelling water movement in construction materials.

METHOD

The applicability of the Richards equation for the description of water movement in porous construction materials was analysed on the basis of a study performed in September 2005 at the locality of Sucha Rzeczka in the Province of Warmia and Mazury (Janik *et al*. 2006). The experiment was conducted on a sample block made of autoclaved cellular concrete with porous structure developed through the formation of gas bubbles in the material mixture. In the dry state the bulk density of the concrete was 573 $kg \cdot m^{-3}$. TDR probes were placed in the sample prepared as above, at 5 cm spacing. The dimensions of the sample block and a schematic of the experiment are given in Figure 1. Moisture was measured with the TDR apparatus at 1 hour intervals for a period of 7 days. Water movement within the sample was caused by capillary rise.

The Richards equation was applied for the description of water movement in the sample block under analysis, on the grounds that water movement in cellular concrete follows the same laws of physics as that in a capillary-porous medium. The lateral surfaces of the sample block were isolated from the environment, therefore any water movement within the space analysed could only take place in the vertical direction (the sense of the axes as in Fig. 2). The Richards equation for a mono-dimensional space assumes the following form (Walczak *et al*. 1998, Reinhard 2004):

$$C(h)\,\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial \Phi}{\partial z}\right], \qquad (1)$$

where: $C(h)$ – differential hydraulic capacity , $C = d\theta / dh$, h – matric potential, cm H_2O, θ – moisture, $m^3\ m^{-3}$, Φ – total potential, cm H_2O, $\Phi = h + z$, z – height, z – vertical coordinate, cm, $K(h)$ – hydraulic conductivity, cm min^{-1}.

For the determination of moisture distribution within the sample block the method of finite differences was applied, characterising the space modelled (Fig. 2). The differential form of equation 1 for mono-dimensional space (explicit scheme) can be given as:

$$\frac{C_i^K}{\Delta t}\left(\Phi_i^{k+1} - \Phi_i^k\right) = \frac{1}{\Delta z}\left[K_{i+1/2}^k \frac{\Phi_{i+1}^k - \Phi_i^k}{\Delta z} - K_{i-1/2}^k \frac{\Phi_i^k - \Phi_{i-1}^k}{\Delta z}\right], \quad (2)$$

where: Δt – time step, min, Δz – spatial step, cm, k – index of time, i – index of space.

Moreover, for further calculations it was assumed that:

$$K_{i\pm 1/2} = \sqrt{K_i^k \cdot K_{i\pm 1}^k}\ . \quad (3)$$

For the determination of relation corresponding to the curve of hydraulic conductivity the following formula was employed (Genuchten van 1980):

$$K(h) = \frac{K_s\left\{1 - \left(\alpha|h|\right)^{mn}\left[1 + \left(\alpha|h|\right)^n\right]^{-m}\right\}^2}{\left[1 + \left(\alpha|h|\right)^n\right]^{m/2}}, \quad (4)$$

while the relation corresponding to the pF curve was determined from the formula:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + \left(\alpha|h|^n\right)\right]^m}, \quad (5)$$

where: m, n, α – indices related to the type of soil, $m = 1 - 1/n$, θ_r – content of residual water, $m^3\,m^{-3}$, θ_s – moisture in the fully saturated zone, $m^3\,m^{-3}$, K_s – filtration coefficient, $cm \cdot min^{-1}$.

To solve an equation it is necessary to define the initial and boundary conditions. The adopted initial condition was the distribution of moisture in the modelled space at the moment of start of the experiment. The lower limit condition was the time-variable distribution of moisture in layer 1, and the upper limit – the distribution of moisture in layer 5. Therefore, the modelled space comprised layers 2, 3 and 4 (Fig. 2). The simulation was performed for a time step ΔT = 30 minutes, covering a period of 7 days. The stability and convergence of the numeric solution was validated by means of a numerical experiment.

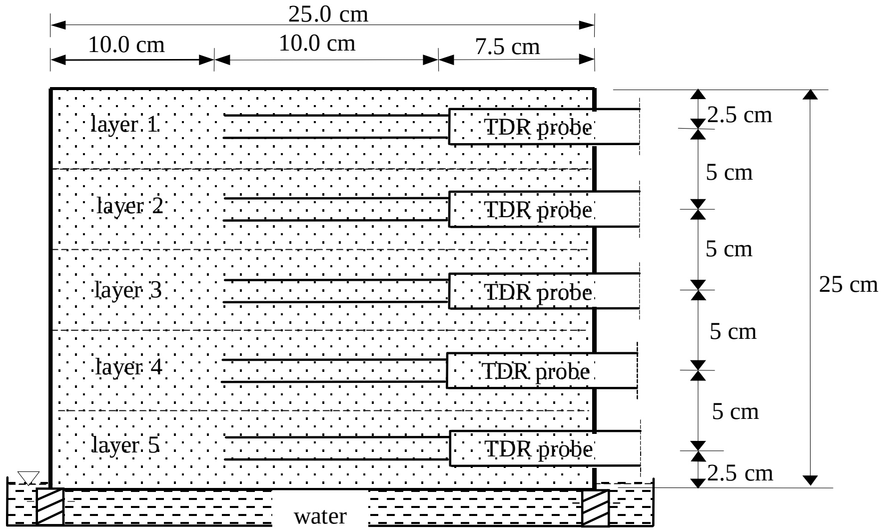

Fig. 1. Schematic of the experiment

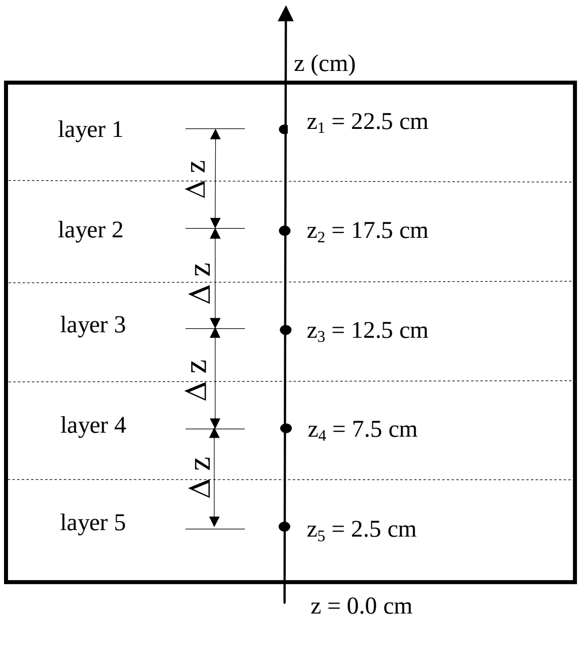

Fig. 2. Area covered by modelling

RESULTS

Figure 3 presents a comparison of moisture values obtained from the computer simulation with those obtained from direct measurements. It was found that the moisture responses caused by capillary rise were correct.

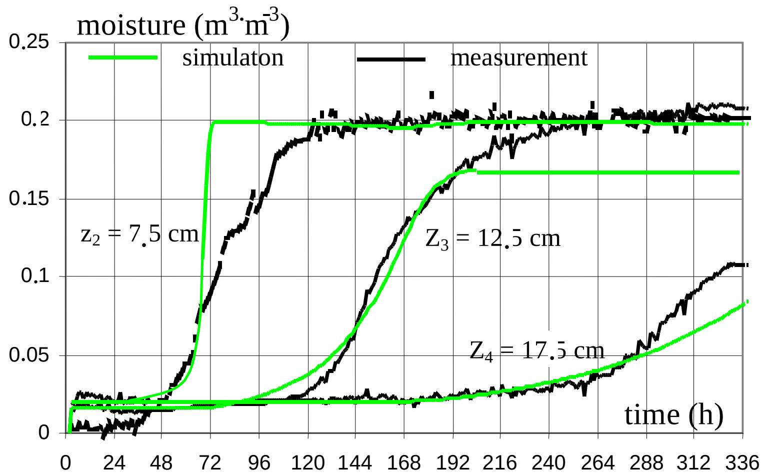

Fig. 3. Dynamics of moisture in cellular concrete block caused by capillary rise

With increase of height z_i the response time increased and the moisture increments decreased. Solid line represents the dynamics of moisture at depths z_i (z_2 = 7.5 cm, z_3 = 12.5 cm, z_4 = 17.5 cm). The indices (θ_r, θ_s, K_s, n, α) affecting the form and the positioning of the lines depending on the physical properties of the modelled space were selected so as to obtain the least possible differences between calculated moisture values and those measured with the TDR apparatus. The procedure consists in minimisation of error, i.e. selection of parameters of van Genuchten equations for the water retention curve and the hydraulic conductivity coefficient. This is the so-called calibration of mono-dimensional model of water movement based on the solution of the Richards equation. The criterion of fitting was adopted to be the sum of average deviations (B_c) calculated for each layer from the formula:

$$B_c = \sum_{i=2}^{4} B_i \, , \qquad (6)$$

where: B_c – sum of average deviations in layers 2, 3 and 4, B_i – average deviation in the i-th layer.

The deviation in the i-th layer (B_i) was calculated from the formula:

$$B_i = \frac{1}{N}\sum_{k=1}^{N}\left|\theta_i^{k\ obl} - \theta_i^{k\ pom}\right|, \tag{7}$$

where: B_i – average deviation for the i-th layer, i – number of layer (index of space), N – number of moisture pairs compared in the course of the experiment (N = 336), $\theta_i^{k\ obl}$ – calculated moisture in i-th layer, at k-th moment, m^3 m^{-3}, $\theta_i^{k\ pom}$ – measured moisture in i-th layer, at k-th moment, m^3 m^{-3}.

The minimum value of B_C was obtained in the following manner. First, the values of B_C were calculated for freely selected parameters θ_r, θ_s, K_s, n, α. Next, equation 2 was solved, increasing or decreasing the value of the first parameter, θ_r. That trial-and-error procedure was continued until the minimum value of B_C was obtained. At that sage the value of θ_r was accepted as a set value. Then, equation 2 was solved, increasing or decreasing the values of the second parameter, θ_s. Again the calculations were continued until the value of B_C achieved a minimum, and parameter θ_s could be accepted as set. Analogous calculations were made for the remaining parameters, changing their values. When the first loop of calculations was completed, the process of optimisation of the first parameter, θ_r , was repeated. Calculations in the particular loops were conducted until the moment when a change in any of the parameters being optimised caused only an increase in the value of $B_{C.}$ As a result of the identification procedure conducted as described above, the total average deviation of B_C decreased from the initial value of B_C = 1.457 to B_{Cmin} = 0.0104. The value of B_{Cmin} was obtained for: θ_r = 0.003 m^3 m^{-3}, θ_s = 0.24 m^3 m^{-3} , K_s = 0.688 cm min^{-1}, n = 1.364, α = 0.238 m^{-1}.

Figure 4 presents an example of the relation between a selected parameter and the total average deviation (B_C) calculated from formula 6. The example values of B_C obtained on the basis of the numeric experiment were determined for $1.3 < n < 1.4$. As follows from the Figure, the lowest value of B_C was obtained for n = 1.364.

The discrepancies between the calculated and measured values (Fig. 3) may result from the lack of calibration of the TDR apparatus that should be made individually for every medium in which measurements are conducted. Moreover, the Richards equation (in the form of equation 1) is true only when the medium is homogeneous, i.e. when its water conductivity $K(h)$ and the hydraulic potential Φ, related to the water content, are constant at every point in the medium (Reinhard 2001). The medium should be isotropic, i.e. its conductivity should not depend on the direction of water movement. In the equation it is also assumed that θ_s is approximately equal to porosity, and that the volume of solid particles is invariable in time. Neither of those assumptions was verified in this study. It should also be kept in mind that the numerical solution of the Richards equation generates errors by its very nature. Ultimately, it can be stated that the Richards equation provides a satisfactory description of water movement in autoclaved cellular concrete under conditions of capillary rise.

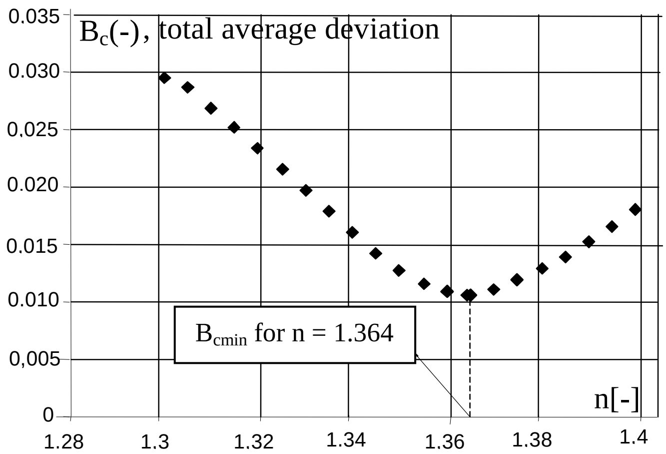

Fig. 4. Total average deviation for moisture values obtained from measurements and from computer simulation

CONCLUSIONS

1. The experiment carried out and the computer simulations allowed to demonstrate that the Richards equation can be applied for the prediction, with satisfactory accuracy, of the dynamics of water movement in autoclaved cellular concrete caused by capillary rise.

2. It was also found that differences between results obtained from the simulation and those obtained from the experiment could have been caused by the lack of calibration of the TDR apparatus that should be made individually for every medium.

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MATEMATYCZNE MODELOWANIE RUCHU WODY W BETONIE AUTOKLAWIZOWANYM

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Streszczenie. W pracy przedstawiono model matematyczny opisujący ruch wody w wybranych materiałach budowlanych. Do budowy modelu zastosowano równanie Richardsa, które wyprowadzono w 1931 r. dla homogenicznego i izotropowego porowatego ośrodka glebowego. Równanie to rozwiązano metodą różnic skończonych, stosując schemat jawny. Eksperyment przeprowadzono na próbce wykonanej z autoklawizowanego betonu komórkowego, w której umieszczono czujniki TDR służące do pomiaru wilgotności. Ruch wody w badanej próbce wywołano podsiąkiem. Wyniki uzyskane z symulacji komputerowej porównano z wynikami eksperymentu. Wykazano przydatność równania Richardsa do opisu dynamiki warunków powietrzno-wodnych w betonie komórkowym. Stwierdzono ponadto, że różnice pomiędzy wynikami uzyskanymi z symulacji i uzyskanymi na podstawie eksperymentu mogą być spowodowane brakiem kalibracji aparatu TDR, która powinna być przeprowadzana indywidualne dla każdego ośrodka.

Słowa kluczowe: beton komórkowy, technika TDR, równanie Richardsa