Modification and application of the TOUGH2 code for modeling of water flow through swelling unsaturated sealing constructions

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Abstract

Making use of the TOUGH2 capabilities to model two-phase flow driven by capillary forces fluid movement through a sealing construction can be analyzed. The original version of the TOUGH2 code does not simulate the arise of a swelling pressure which is partly time-dependent and the corresponding reduction of the permeability. Based on publications and laboratory results during the project, in this paper a validated modification of the code is proposed to study the influence of an increasing swelling pressure as a function of saturation on the fluid movement through a sealing construction.

1. Introduction

Sealing of underground cavities are main topics during and after the operational period of a final disposal of radioactive and/or toxic waste. The penetration of water into unsaturated clay plugs, which seems to be the favorite material, is characterized by a swelling of the clay which is a function of the kind of the clay, i.e. the chemical composition and the dry density of the material. Many investigations can be found in the literature mainly focused on the hydraulic behavior of saturated clays. The installation of a clay plug for sealing of underground cavities is feasible by using clay which is dry and highly compacted. After an open or backfilled cavity is filled up with groundwater, the fluid penetrates into the plug and the material begins to swell. Due to this behavior a swelling pressure will arise which, among other things, results in a reduction of the permeability of the material and the sealing requirements can be met.

To convert this knowledge into practical application the Federal Ministry for Education, Science, Research and Technology in Germany launched a R&D project to demonstrate feasibility and to investigate engineered barriers for safe shaft closure for hazardous waste repositories. One of the DBE tasks is to perform model calculations to analyze the fluid movement through the sealing yielding in predictive calculations of the tightness of the plug.

2. Modification of TOUGH2

The original version of TOUGH2 (Pruess, 1991+1987) assumes a constant permeability and does not allow to use a time dependent decrease of permeability. Due to this reason, a permeability function is introduced based on constitutive laws obtained from laboratory measurements.

2.1 Constitutive Laws

Laboratory measurements on Calcium- and Sodium-bentonite performed by Börgesson et al. (1995) yield relationships between swelling pressure and void fraction as well as hydraulic conductivity and void fraction. In figure 1 a,b the values are plotted in a double logarithmic scale together with the corresponding fitting curves.

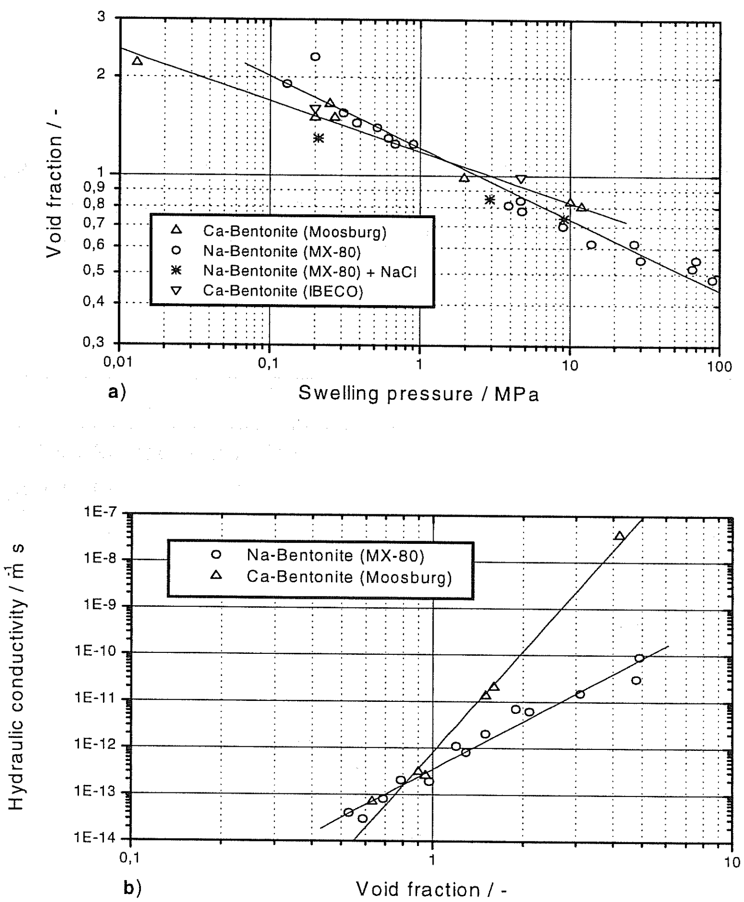

Fig. 1: a) Void fraction versus swelling pressure and b) Hydraulic conductivity versus void fraction for Ca- and Na-bentonite after Börgesson et al. (1995).

In the double logarithmic scale the relationship in figure 1 are characterized by a linear functions according to equation (1) and (2)

$$e = e_o \cdot \left(\frac{P}{P_o} \right)^{\beta} \tag{1}$$

$$K_f = K_{fo}\left(\frac{e}{e_o}\right)^{\eta} \qquad (2)$$

where e is the void fraction, P the swelling pressure, k_f the hydraulic conductivity, $\beta = \Delta(\ln e)/\Delta(\ln P)$ and $\eta = \Delta(\ln k_f)/\Delta(\ln e)$. The index 0 indicate reference parameters.

With regard to the above mentioned problem of modelling the effect of swelling on the hydraulic behavior of the clay the void fraction can be eliminated by insertion of equation (1) in (2). Using the relation between permeability and hydraulic conductivity, the permeability of the bentonite can be expressed as a function of the swelling pressure (3).

$$k(P) = k_{fo} \cdot \left(\frac{P}{P_o}\right)^{\beta\cdot\eta} \cdot \frac{\mu}{\rho \cdot g} \qquad (3)$$

where k(P) is the permeability, μ and ρ are the dynamic viscosity and the density of the fluid and g is the gravitational acceleration. A graph of this function is plotted in figure 2 for Calcium and Sodium bentonite.

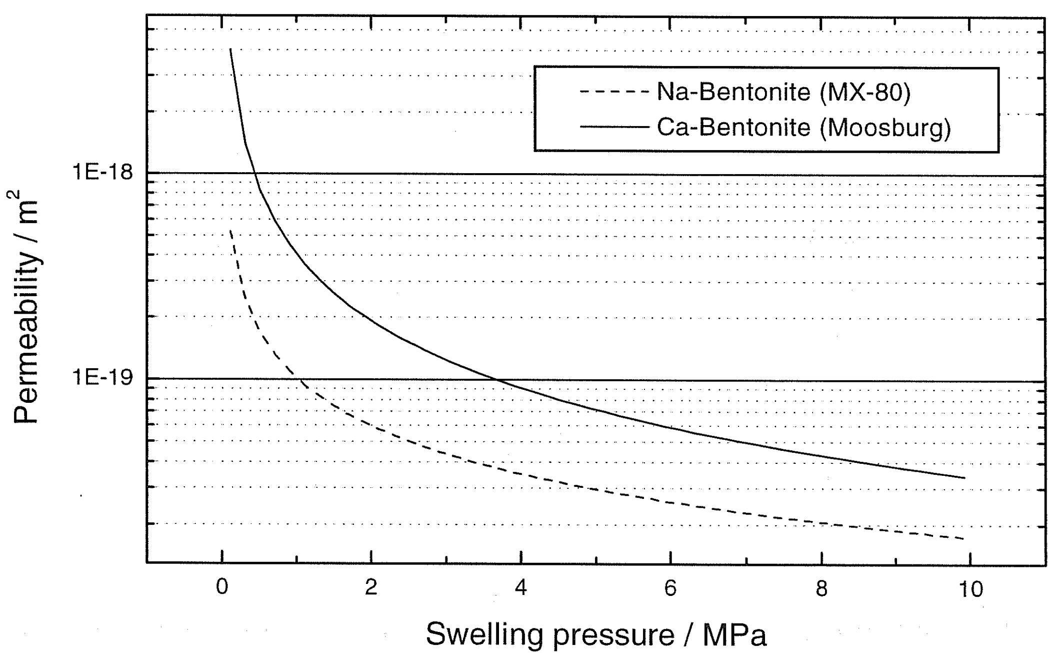

Fig. 2: Permeability as a function of swelling pressure according to equation (3).

To implement this dependency of the permeability in the TOUGH2 code, another relationship is necessary to combine the swelling pressure with one of the parameters modeled in TOUGH2. This relation can be found by Studer et al. (1984) and Börgesson (1984).

Figure 3 shows the result of tests on samples with dry densities of 1760 kg m^{-3} and 1570 kg m^{-3}. The swelling pressure seems to be direct proportional to the degree of saturation according to equation (4).

$$P = S_l * P_s \tag{4}$$

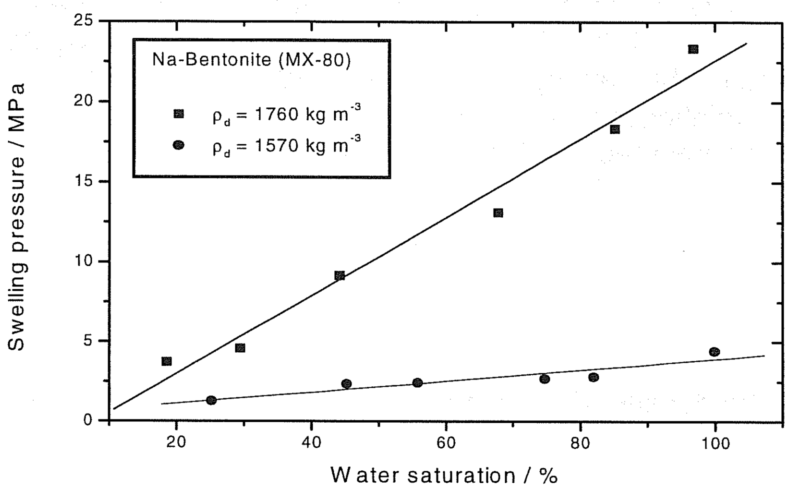

Fig. 3: Swelling pressure as a function of the degree of water saturation for Na-Bentonite with different dry densities after Studer et al. (1984) and Börgesson (1984).

P_s is the swelling pressure at saturation and S_l is the degree of liquid saturation. The maximum swelling pressure which could be reached depends on the initial dry density. Based on oedometer tests Villar & Rivas (1994), for example, proposed the following expression for montmorillonitic clay:

$$\ln (P) = 5.9 * \rho_d - 7.9 \tag{5}$$

with ρ_d being the dry density of the clay. As a result, the determination of the initial clay dry density allows the calculation of the swelling pressure development during the water infiltration into the bentonite. The time (saturation) dependent increase of the swelling pressure simultaneously decreases the permeability according to equation (3).

2.2 Implementation in TOUGH2

To implement the modification concerning the time dependence of the permeability as mentioned above, a slightly extension of the two subroutines CONVER and MULTI was necessary. The extended calculation of the permeability according to equation (3) yields an effective permeability expressed by equation (6)

$$k = k_{rel} * k(P) \tag{6}$$

where k_{rel} ist the relative permeability.

3. Validation

To check, whether the explained modification yields reliable calculations, a validation to measured values was performed. Börgesson (1984) performed several tests on samples consisting of pure bentonite and bentonite-sand mixtures. During these oedometer tests the water uptake of the samples was measured at different distances to the water inlet and at two different times. Hence, the calculated results could be compared to the real spatial distribution of the water content and simultaneously to the time dependence at several distances. In figure 4 the laboratory values are plotted together with the calculated results obtained by using equation (3). For the „relative permeability - saturation" relationship the linear function was used. The degree of saturation was converted into the water content w using the equation (Studer et al. (1984):

$$w = S_l \cdot \rho_w \cdot \left(\frac{1}{\rho_d} - \frac{1}{\rho_s} \right) \tag{7}$$

where ρ_w is the density of the water and ρ_s the density of the clay particles.

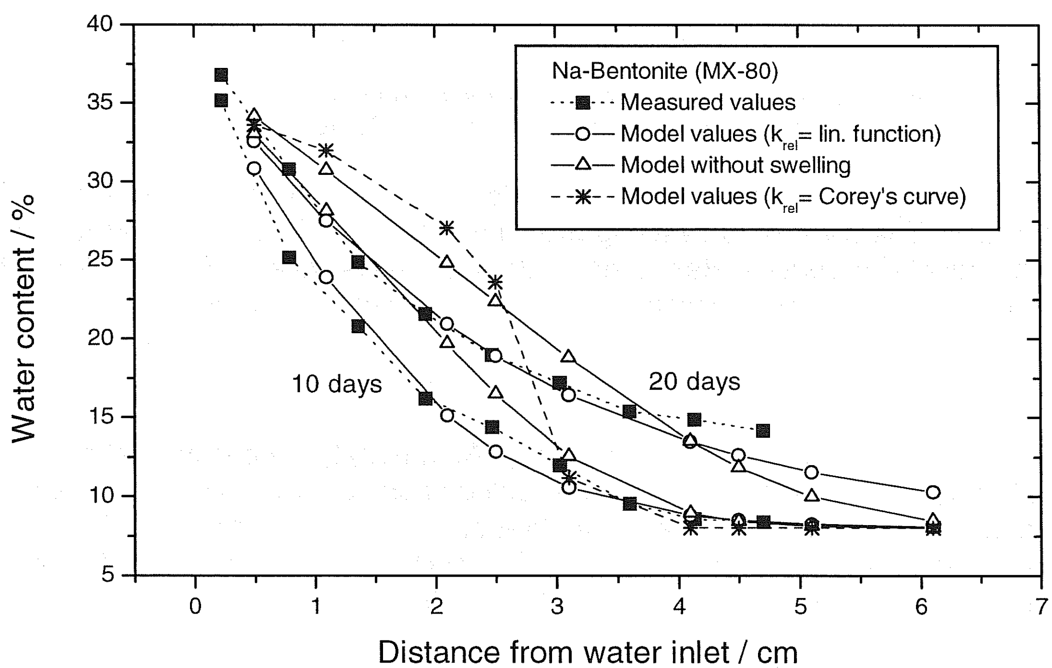

Fig. 4: Measured and calculated values of the water content distribution for two different times.

Additionally, results obtained by using a constant permeability and another „relative permeability - saturation" relationship (Corey's curve) are plotted. A good correspondence of the measured and the calculated values, especially regarding the curvature of the functions, could be reached with the new permeability function.

4. Application

As mentioned above, within a running research project DBE's tasks is to perform measurements and model calculations to analyze the fluid movement through a prepared sealing in a shaft. The modified TOUGH2 code will be applied to this sealing construction accompanying the in situ investigations. Recurrent comparison with in situ measurement of water flow into the plug will be used for validation of the model, respectively the used constitutive laws. The last step will be the performance of predictive calculations for evaluation of the tightness of the complete sealing.

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