A DUAL CONTINUUM COUPLED MULTIPHASE FLOW MODEL WITH MIXED SECOND ORDER WATER TRANSFER TERM FOR STRUCTURED SOILS: PART II. TESTING WITH SYNTHETIC CASES AND APPLICATION TO A REAL EXPERIMENT

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ABSTRACT. The dual porosity model presented in part I (Zheng and Samper, 2005) of this series of two papers is tested here. Numerical solutions of the second order term are compared with reference results obtained with both 1-D and 2-D single domain models. The dual domain model reproduces accurately the transfer term when the scaling term is properly estimated. Estimated value is around 0.8 for bentonite. The water transfer term by chemical osmosis is significant when there is a large geochemical non-equilibrium betweenn macro and micro domains. A dual-domain model is used to interpret the FEBEX 'mock-up' test, a long-term full-scale thermal hydration test of the compacted bentonite barrier. Optimum values of scaling term and weighting factor for bentonite are estimated by an inverse algorithm based on measured inflow data. Agreement between computed and measured water inflows improves when the dual continuum model is used.

RESUMEN. El modelo de doble porosidad presentado por Zheng y Samper (2005) en la primera parte de esta serie de dos trabajos se contrasta aquí con datos sintéticos y datos reales. Los parámetros del término de transferencia de agua entre los dominios macro y micro del modelo de doble porosidad se obtienen a partir de la comparación con los resultados de un modelo de referencia para dos casos de flujo uni- y bi- dimensional. La estimación automática de los factores de escala y de ponderación mediante la solución de un problema inverso conduce a ajustes excelentes. Un factor de escala de 0.8 para la bentonita permite reproducir adecuadamente el flujo de agua entre ambos dominios. El análisis numérico indica que la ósmosis química puede producir un flujo considerable entre los dos dominios cuando existe un fuerte desequilibrio geoquímico entre ellos. El modelo de doble porosidad se ha aplicado también a la interpretación del ensayo en maqueta del proyecto FEBEX, un ensayo a largo plazo de hidratación y calentamiento realizado sobre bentonita compactada. El modelo de doble porosidad mejora los resultados de los modelos anteriores de porosidad simple mediante la estimación automática de los factores de escala y de ponderación a partir de los datos de entrada de agua.

1. Evaluation of the water transfer term

1.1. Water transfer caused by a hydraulic pressure gradient

A DCM can be implemented in two ways. The first method consists of solving two or more equations for each node/element and computing a water transfer term which accounts for the water exchange. It is assumed that two or more different domains coexist in a given element each of which occupies different volumes and obbeys different equations. The drawback of this method is the inaccuracy of the water transfer term. The second method requires the spatial discretization of both domains (Dai, 2000; Lichtner, 2000; Dai & Samper, 2004). For example, a 1-D DCM is solved using a 2-D mesh in which different material zones (i.e. different sets of elements) represent different domains. Samper et al. (2005b) present an example of such approach. This method not only requires more CPU time, but it is also harder to implement in 2 and 3 dimensions. However, the second method has been widely used to verify the water transfer term of the first method (Gerke and van Genuchten, 1993b; Köhne et al., 2004). In this paper, we also use the second method to evaluate the second order water transfer term for compacted bentonite.

1.1.1. Results for horizontal flow with transient boundary conditions

Fig. 1 illustrates the concept of a DCM. Since in most DCMs, the water transfer between macro-porous and micro-porous domains is assumed to be perpendicular to the flow direction, horizontal flow of an elementary unit of a dual continuum system (shown in Fig. 1) has been used to evaluate the water transfer term (Gerke and van Genuchten, 1993b; Köhne et al., 2004)

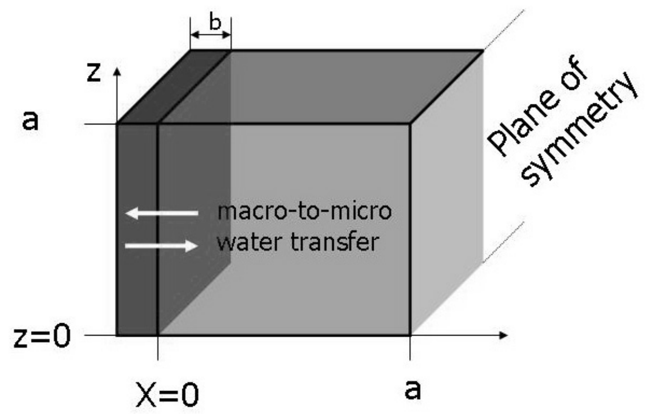

Fig. 1. Schematic representation of an elementary unit of a DCM consisting of parallel rectangular aggregate blocks of half width *a* separated by a macro-porous domain of half width b (Köhne et al., 2004).

The water transfer between macro and micro domains in Figure 1 is obtained by solving a 1-D single porosity model with INVERSE-FADES-CORE (Samper et al. 2005c). A variable liquid pressure boundary condition is used. The time function *P(t)* for the boundary liquid pressure is shown in Figure 2 Initial and boundary conditions for liquid pressure P_L and flux Q are given by:

$$P_L(x=0, t\geq 0) = P(t) \quad (1)$$

$$P_L(0\leq x\leq a, t=0) = P_L^i = -125000 \quad kPa \quad (2)$$

$$Q(x=a, t\geq 0) = 0 \quad (3)$$

Flow parameters used in the 1-D single porosity model are listed in Table 1.

Table 1. Parameters used in the 1-D single porosity model. Ψ is suction which is equal to $P_g - P_L$,and S_L is saturation degree.

Parameter	values
Porosity	0.41
Intrinsic permeability	$2.75\cdot10^{-21}$ m^2
Relative permeability	$K_{rL} = (S_L)^3$
Retention curve	$S_L = \left((1-\psi/1100000)^{1.1}\right) \Big/ \left(\left(1+(5\cdot10^{-5}\psi)^{1/0.82}\right)^{0.18}\right)$

In order to evaluate the second order water transfer term, synthetic case shown in Figure 1 has been solved with a DCM using a 1-D mesh. The time function shown in Figure 2 is used for the time evolution of liquid pressure in the macro-porous domain. Initial and boundary conditions are:

$$P_L^{ma}(0\leq z\leq a, t=0) = -125000 \quad kPa \quad (4)$$

$$P_L^{mi}(0\leq z\leq a, t=0) = -125000 \quad kPa \quad (5)$$

$$Q(z=0, z=a, t\geq 0) = 0 \quad (6)$$

In order to make the evaluation of the second order water transfer term comparable with published values (Köhne et al., 2004), the intrinsic permeability of the macro-porous domain is assumed in this case to equal to that of the micro-porous domain, i.e. $2.75\cdot10^{-21}$ m^2. The volume fraction for the macro-porous domain is 5%. The local porosities for the two domains are 0.41. The shape factor β in the water transfer term is equal to 3 (Gerke and van Genuchten, 1993a;b) and the half width of the micro-porous domain α is equal to 0.05 m. The scaling term γ_w and the weighting factor *w* are estimated simultaneously. Figure 3 shows the cumulative water transfer obtained with a single porosity horizontal model (reference) and a DCM. Estimated values of the scaling term γ_w and the weighting factor w are listed in Table 2. With γ_w=0.887 and w=8.34, agreement between the results obtained with single porosity horizontal flow model and the DCM is archived during the entire time. According to Gerke and van Genuchten(1993a; 1993b) a scaling factor γ_w of 0.4 should give the best fit for the first-order water transfer term. Köhne (2004) used a value of γ_w of 0.5 for the second order term. It should be noticed that the scaling term estimated here differs from those two values because, as pointed out by Gerke and van Genuchten (1993b), the scaling term depends on the initial condition and varies up to 5 times for initial heads ranging from -0.3 to -30 m. In the DCM for bentonite, the initial pressure head is -125000 kPa which is much smaller than that used by Gerke and van Genuchten (1993b) (-30 m) and Köhne (2004) (from -1 to -10 m). Therefore, a scaling factor γ_w of 0.887 is plausible for bentonite.

Köhne (2004) indicated that the weighting factor for the evaluation of the effective conductivity varies between 8 for a sandy loam to 59 for silty clay. The finer the texture, the larger the weighting factor. In our case, w is equal to 8.34 for bentonite. Actually, the weighting factor depends on the contrast between the conductivities of the macro-porous (fracture) and micro-porous (matrix) domains. In our model, the hydraulic conductivity of the micro-porous domain is about one fifth of that of the macro-porous domain. It should be noticed that the relative conductivity of macropores is 1 while that of micropores is $(S_L)^3 = 0.185$. This explains the small weighting factor for bentonite. Köhne (2004) did not report the conductivities of macro- and micro-pores.

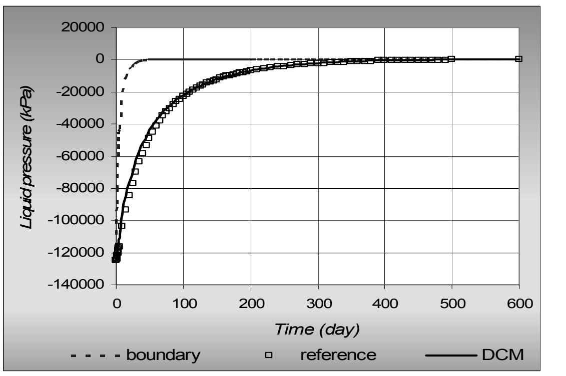

Fig. 2. Liquid pressure obtained with a single porosity horizontal flow model ('reference') and a DCM.

Table 2. Estimated scaling term γ_w and weighting factor w .

Parameter	Estimated value	Variance	Confidence interval (95%)
γ_w	0.887	$5.21\cdot10^{-5}$	(0.869, 0.904)
w	8.34	0.48	(6.63, 10.04)

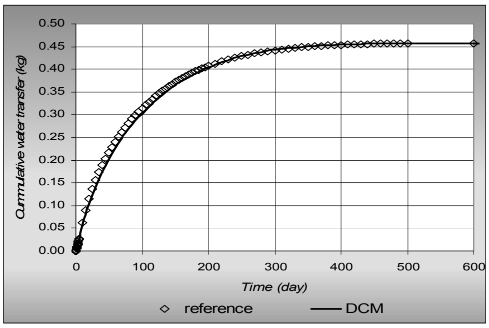

Fig. 3. Comparison of cumulative water transfer obtained with a single porosity horizontal flow model ('reference') and a DCM.

1.1.2. Evaluation of DCCM model for a 2-D single porosity model

Case II addresses preferential flow through macropores in a 0.05 m × 0.1 m bentonite block. This case is simulated with both a 2-D single porosity model (reference model, Figure 4 left) and a 1-D DCCM (Figure 4 right). Material 1 in the reference model represents the macro-porous domain while material 2 is used for the micro-porous domain. According to García-Gutiérrez et al. (2002) bentonite free water may account for 2.3%. Fernández et al. (2004) report a value of 8.5% of the total volume. Here we assume that Material 1 (macro-porous) accounts for 5% of the total volume. Therefore, in the DCCM the volumetric weighting factor W^{ma} is 5%. Parameters for each domain are listed in Table 3. The rest of parameters are those of Table 1. Equivalent physical values are calculated by:

$$P = W^{ma} \cdot P^{ma} + (1 - W^{ma}) \cdot P^{mi} \quad (7)$$

where P is the equivalent physical value of a given parameter (for example porosity or thermo-osmosis coefficient), W^{ma} is the volumetric weighting factor of the macro-porous domain, and p^{ma} and p^{mi} are parameters used for macro and micro domains, respectively. It should be noticed that equation (1) only holds for permeability during steady state unsaturated flow or when the system is completely saturated (Gerke and van Genuchten, 1993a). In the hydration of unsaturated bentonite, equation (7) does not hold for intrinsic permeability.

Table 3. Parameters used in the 2-D single porosity reference model.

Parameter	Macropores	Micropores	Equivalent physical values
Intrinsic permeability	$2.075 \cdot 10^{-20}$ m/s	$2.75 \cdot 10^{-22}$ m/s	
Porosity	1	0.378	0.41

Table 4. Estimated scaling term γ_w and weighting factor w.

Parameter	Estimated value	Variance	Confidence interval (95%)
γ_w	0.887	1.12E-07	(0.8869, 08871)
w	63.4	0.067	(63.26, 63.45)

Initial and boundary conditions for the reference model are:

$$P_L(z = 0.1, \ \ 0 \le x \le 0.05, \ \ t \ge 0) = 100 \ \ kPa \quad (8)$$

$$P_L(0 \le z < 0.1, \ \ 0 \le x \le 0.05, \ \ t = 0) = -125000 \ \ kPa \quad (9)$$

$$Q(z = 0, \ \ t \ge 0) = 0 \quad (10)$$

while the conditions for DCCM are:

$$P_L^{ma}(z = 0.1, \ \ t \ge 0) = 100 \ \ kPa \quad (11)$$

$$P_L^{mi}(z = 0.1, \ \ t \ge 0) = 100 \ \ kPa \quad (12)$$

$$P_L^{ini}(0 \le z < 0.1, \ \ t = 0) = -125000 \ \ kPa \quad (13)$$

$$Q(z = 0, \ \ t \ge 0) = 0 \quad (14)$$

The scaling term γ_w and the weighting factor w are estimated based on the results of the reference model. Estimated parameters are shown in Table 4. It should be noticed that the weighting factor w in case II is much larger than that obtained in Case I because in case II the permeability of the macro domain is 2 orders of magnitude larger than that of the micro domain (in Case I, the ratio of permeabilities is only 5). The estimated scaling term γ_w is consistent with that estimated in Case I.

Figure 5 shows the total water transfer across the interface of macro-porous and micro-porous domains obtained with the 'reference' model and DCM. The excellent agreement between both models indicates that the second order water transfer term can correctly calculate the water transfer between the two domains. Figure 7 shows the spatial distribution of the flux across the interface of the two domains at different times. Although the DCCM model catches the total water transfer (Figure 6), it underestimates the results of the 'reference' model at the upper part and overestimates the flux at the lower part at early times. It should be noticed that the second order water transfer term is derived using the Vermeulen (1953) approximation to an analytical solution of the pressure response in a cube (Crank, 1975). The difference between the Vermeulen approximation and the analytical solution at early times (Zimmerman, 1993) results in the lack of accuracy at early times.

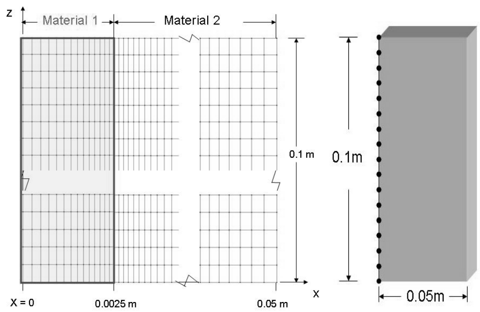

Fig. 4. Finite element mesh used in the 2-D single porosity reference model (left) and the 1-D grid for DCCM (right).

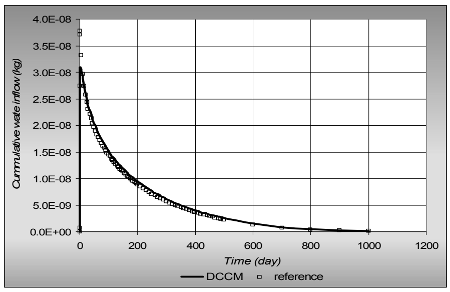

Fig. 5. Comparison of the total water transfer across the interface of macro and micro domains computed with 2-D single porosity model and DCCM.

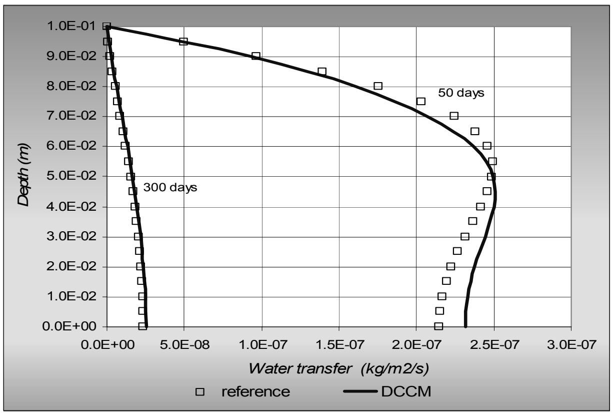

Fig. 6. Comparison of the water transfer rate across the interface of macro- and micro- domains obtained with 2-D single porosity model ('reference') and a DCCM at t = 50 and 300 days.

1.2. Evaluation of water transfer caused by a osmotic pressure gradient

The same example of bentonite hydration of the previous case is used here to analyze teh role of chemical osmosis using the 'reference' model and a DCCM. The reflection coefficient σ is assumed to be 0.1 for macropores and 0.9 for micropores. Although the reflection coefficient σ ranges from 0.001 to 0.27 (Keijzer et al., 1999), a reflection coefficient σ of 0.9 for micropores is plausible because, when bentonite is divided into macro- and micro-porous domains, the micro-porous domain can be as efficient as a membrane. Initial and boundary conditions for transport are:

$$C^{mi}(0.0025 \le x \le 0.05,\ \ 0 \le z \le 0.1\ \ t \ge 0) = 0.001\ \ mol/L \quad (15)$$

$$C^{ma}(0 \le x \le 0.0025,\ \ 0 \le z \le 0.1\ \ t = 0) = 0.001\ \ mol/L \quad (16)$$

$$C^{ma}(0 \le x \le 0.0025,\ \ 0 \le z \le 0.1\ \ t > 0) = 5\ \ mol/L \quad (17)$$

Figure 7 shows the time evolution of total water content in the micropores (material 2 for reference model) obtained in Case II (without chemical osmosis) and Case III (with chemical osmosis). Water transfer from micro- to macro-porous domains is induced by a gradient in osmotic pressure, which in turn slows down the hydration of the micro-porous domain. The scaling term γ_w and the weighting factor w for liquid pressure transfer term are the same as those of Case II. The weighting factor w for σ is the same as that for permeability. The scaling term γ_w for osmotic 0.95 flux is slightly larger than that of hydraulic flux.

2. Application of DCCM to the FEBEX mock-up test

2.1. Description of the test and previous models

The 'mock-up' test is one of the two main tests performed in the FEBEX project (ENRESA, 2000). In this test, the bentonite barrier is hydrated from the outer ring at a constant and controlled pressure. The hydration process is well controlled and the boundary conditions are well defined. A coupled thermo-hydro-geochemical (THG) model was set up by UDC (ENRESA, 2000). Discrepancies between measured and computed cumulative water inflow were observed. After that, modelling results were improved by incorporating a constitutive law of variable permeability depending on ionic strength of pore water (Samper et al., 2005a) and by considering chemical and thermal osmosis (Samper et al., 2005c). However, none of these processes can reproduce the measured water inflow data at all times. In this paper, a dual-domain THG model is adopted to interpret the 'mock-up' test. The scale term and weighting factor of the second order water transfer term for bentonite are estimated.

2.2. THG DCCM model

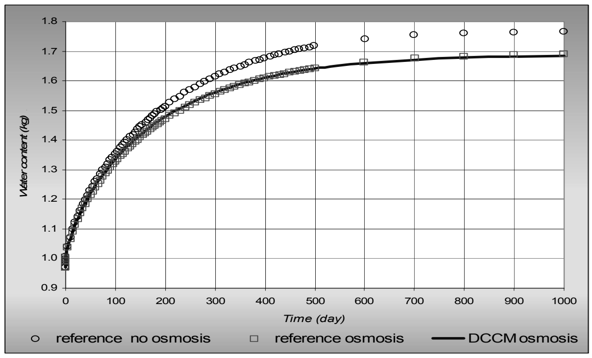

Fig. 7. Comparison of total water content in material 2 (micro-porous domain) obtained with a 2-D single porosity model with and without osmosis and a DCCM with osmosis.

The following assumptions are used to define the volume fraction of the macro-porous domain for FEBEX bentonite:

1) The macro-porous domain is composed of the porous space accessible for free water and the non-smectite minerals.
2) The porosity for free water deduced from geochemical studies ranges from 3% (García-Gutiérrez et al., 2002) to 8.5% (Fernández et al., 2004). On the other hand, Sánchez (2004) adopted a value of porosity of macro-porous domain from 11.8 to 12.8% in a double porosity THM model. Since the volume of free water accessible for chloride transport may not represent the total mobile water due to anion exclusion, it is reasonable to assume that the porosity of macropores is larger than 8.5%. Here we assume a avalue of 12.8% of the total volume.
3) The non-smectite minerals in FEBEX bentonite accounts for around 4.72% of the total volume. In FEBEX bentonite, non-smectite minerals are approximately 8% of total mineral by weight (Fernández et al., 2004). Assuming that all minerals have the same density, the volume fraction of non-smectite mineral is $8\% \times (1\text{-}\phi)$ = 4.72%, where ϕ = 0.41. Therefore, the volumetric weighting factor is 0.175.

In order to account for chemical osmosis, geochemical processes have to be considered. It is assumed that:

1) The initial pore water composition is that of previous THG models of the 'mock up' test (see Samper et al., 2005c), recalculated with an accessible porosity of 12.8%.

2) The pore water chemical composition in micropores is assumed to be initially in equilibrium with that in macropores.

In order to simplify the calculation, a fictitious conservative species is used instead of all cations and anions.

Due to the swelling of bentonite, the porosity of both macro-porous and micro-porous domains changes during the hydration . Therefore, in this paper the intrinsic permeability is calculated by Kozeny's law:

$$K = K_0 \frac{\phi^3}{(1-\phi)^2} \frac{(1-\phi_0)^2}{\phi_0^3} \qquad (18)$$

where ϕ is porosity (ϕ_0 is the reference value for ϕ), and K is intrinsic permeability (K_0 is the reference value for K). In the DCCM, K_0=1.8·10^{-20} m^2 and ϕ_0=0.118 for the macro porous domain (Sánchez, 2004) while it is assumed that K_0=2.75·10^{-22} m^2 and ϕ_0=0.292 for the micro-porous domain. Time functions for the changes in the porosity of macro-porous domain are taken from Sánchez (2004).

A 1-D mesh with axial symmetry is used for the dual-domain THG model. Model parameters are listed in Table 5. Other parameters related to multiphase flow are the same as previous single porosity models. A complete list of these parameters is given by Samper et al. (2005c). A prescribed water pressure head of 550 kPa was applied to the outer ring of the bentonite barrier.

Table 5. Parameters used in the DCCM of the 'mock up' test.

Parameter	Macropores	Micropores	Equivalent physical values
Initial porosity	0.73	0.34	0.41
Vol. weighting factor	0.175	0.825	
Reflection coef. σ	0.2	0.9	
Tthermo-osmosis coefficient m^2/K/s	4.1·10^{-12}	5·10^{-15}	7.58·10^{-13}

In the verification cases presented in previous sections, we considered β, α and scaling term γ_w (Equation 14 in Part I) as separate parameters. However, in practical calibration it is better to consider a_w^* as one empirical. Parameters a_w^* and the weighting factor for the second order water transfer term are estimated based on measured cumulative water inflow data. Estimated values are listed in Table 6. Model results reproduce measured cumulative water inflow data (Figure 8). Figures 8 to 10 show the sensitivity analysis of computed cumulative water inflow to thermo-osmotic permeability, a_w^* and the weighting factor, respectively. Model results are sensitive to thermo-osmotic permeability (Figure 8). They are also sensitive to a decrease of a_w^* but not sensitive to its increase. The reason is that the water transfer is limited by the differences in liquid pressures between the two domains which have already attained their maximum in the optimum run, therefore, an increase of a_w^* can increase slightly the water inflow. For the same reason, model results are not sensitive to a decrease of the weighing factor. Since an increase of the weighting factor only causes a little decrease of the effective permeability in the water transfer term when weighting factor is larger than 61.7, model results are not sensitive to a decrease of weighting factor. It should be mentioned that model results are not sensitive to chemical osmosis (results are not shown here). The reason is that the chemical osmosis pressure gradient is so small that the water transfer by chemical osmosis contributes only a small portion to the total water transfer. For example, at 100 days, the water transfer due to chemical osmosis is 3 to 4 orders of magnitude smaller than that caused by hydraulic gradients. The results of the THG DCCM of 'mock up' indicate that: 1) A dual domain model can help the interpretation of the hydrodynamic behavior of the bentonite barrier; 2) Thermal osmosis is a key process especially when large temperature gradients exist; and 3) Swelling of bentonite has to be considered in order to simulate correctly its hydration either by resorting to a THMG model or by considering time-varying permeability and porosity.

Table 6. Estimated empirical parameter a_w^* and weighting factor w.

Parameter	Estimated value	Variance	Confidence interval (95%)
a_w^*	324.39	8.42·10^{-3}	(262, 393)
w	61.7	0.17	(61.3, 62.1)

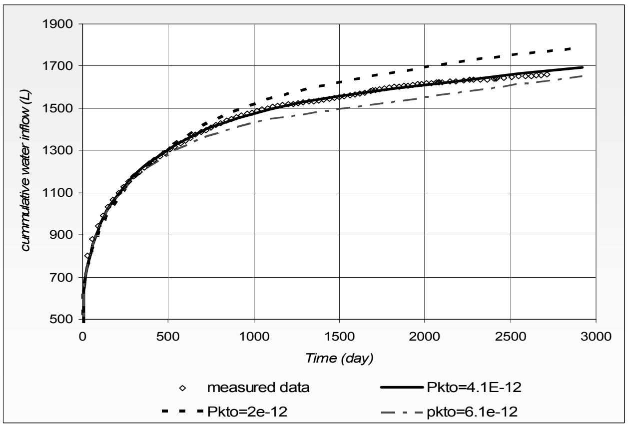

Fig. 8. Comparison of measured cumulative water inflow with computed results and sensitivity analysis to thermo-osmotic permeability.

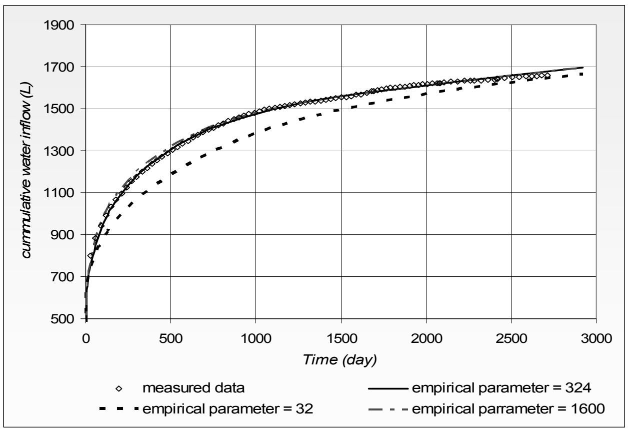

Fig. 9. Sensitivity analysis of computed cumulative water inflow to the empirical parameter a_w^*.

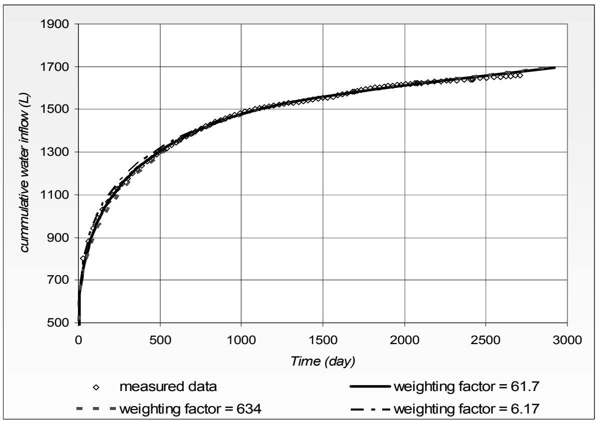

Fig. 10. Sensitivity analysis of computed cumulative water inflow to the weighting factor.

3. Conclusions

Experimental evidence indicates that bentonite exhibits different types of porosity which calls for the need of using dual-domain models. A second order water transfer term which accounts for water transfer caused by both hydraulic and osmotic pressure gradients has been implemented in a dual-domain non-isothermal multiphase flow model. The water transfer term caused by hydraulic gradients have been evaluated in two cases: a horizontal 1-D single porosity model (case I) and 2-D single porosity model for the hydration of a bentonite block (case II). The water transfer term caused by a osmotic pressure gradient has been tested with a synthetic case in which a significant geochemical non-equilibrium is imposed between macro- and micro-porous domains. Taking advantage of an inverse algorithm, optimum values of the scale term and the weighting factor in the water transfer term are estimated. A scale term around 0.8-0.9 leads to the correct calculation of water transfer between the two domains for bentonite. The optimum weighting factor ranges from 8 to 73.4 depending on the difference between permeability for macro-porous and micro-porous domains. The use of dual-domain models is limited by the difficulty of identifying the empirical parameter a_w^* and the weighting factor. However, this problem can be overcome by the application of dual-domain models to well-controlled experiments. A DCCM has been used to interpret the FEBEX 'mock-up' test. Computed cumulative water inflows reproduce the measured data. Optimum values of a_w^* and the weighting factor are estimated based on measured data. The THG DCCM for the 'mock up' test reveals also that thermal osmosis and porosity changes caused by swelling are two key processes. Based on the parameters estimated from the 'mock-up' test, a dual-domain model can be extended to fully coupled THG models for bentonite.

Acknowledgementss. This work has been carried out within the FEBEX Project funded by ENRESA and the European Commission (contract FIKW-CT-2000-00016 of the Nuclear Fission Program). The first author was awarded a reaserch scholarship from the Univeristy of Coruña.

References

Crank, J., 1975. The Mathematics of Diffusion. clarendon, Oxford.

Dai, Z., 2000. Inverse Problem of Water Flow and Reactive Solute Transport in Variably Saturated Porous Media. Ph.D. Thesis, University of La Coruña, La Coruña, Spain, 334 pp.

Dai Z y J. Samper. 2004. Inverse problem of multicomponent reactive chemical transport in porous media: Formulation and Applications Water Resour. Res., Vol 40, W07407, doi:10.1029/2004WR003248.

ENRESA, 2000. Full-scale engineered barriers experiment for a deep geological repository in crystalline host rock FEBEX Project. EUR 19147 EN, European Commission.

Fernández, A.M., Baeyens, B., Bradbury, M. and Rivas, P., 2004. Analysis of the pore water chemical composition of a Spanish compacted bentonite used in an engineered barrier. Physics and Chemistry of the Earth, 29(1): 105-118.

García-Gutiérrez, M., Missana, T. and Cormenzana, J.L., 2002. Diffusion coefficients and accessible porosity for HTO and 36Cl in compacted bentonite, International Meeting at REIMS Clay in natural and engineered barriers for radioactive waste confinement, pp. 331-332.

Gerke, H.H. and van Genuchten, M.T., 1993a. A dual porosity model for simulating the preferential movement of water and solutes in structured porous media. Water Resour. Res., 29: 305-319.

Gerke, H.H. and van Genuchten, M.T., 1993b. Evaluation of a first order water transfer term for variably saturated dual porosity flow models. Water Resour. Res., 29: 1225-1238.

Keijzer, T.J.S., Kleingeld, P.J. and J.P.G., L., 1999. Chemical osmosis in compacted clayey material and the prediction of water transport. Engineering geology, 53: 151-159.

Keijzer, T.J.S. and Loch, J.P.G., 2001. Chemical osmosis in compacted dredging sludge. Soil Sci. Soc. Am. J., 65: 1045-1055.

Köhne, J.M., Mohanty, B.P., Simunek, J. and Gerke, H.H., 2004. Numerical evaluation of a second-order water transfer term for variably saturated dual-permeability models. Water Resour. Res., 40: W07409.

Lichtner, P.C., 2000. Critique of dual continuum formulation of multicomponent reactive transport in fractrued porous media. Geophysical Monograph, 122: 281-298.

Samper, J., Zheng, L., Molinero, J., Montenegro, L., Fernández, A.Mª and Rivas, P. 2005a. Reactive solute transport mechanisms in nonisothermal unsaturated compacted clays, Proc. Of Int. Symp. On Large Scale Field Tests in Granite. Advances in Understanding Engineered Clay Barriers, Sitges, Barcelona, Spain, pp. 525-533.

Samper, J., Zheng, L., Montenegro, L., Fernández, A.Mª and Rivas, P., 2005b. Direct and inverse modelling of multicomponent reactive transport in single and dual porosity media., Proc. Of Int. Symp. On Large Scale Field Tests in Granite. Advances in Understanding Engineered Clay Barriers, Sitges, Barcelona, Spain, pp. 493-503.

Samper, J., Zheng, L. and Montenegro, L., 2005c. Final THG modelling report (Deliverable D25). Techn Report 70-UDC-M-6-20, E.T.S Ingenieros de Caminos, Universdad de La Coruña, A Coruña.

Sánchez, M., 2004. Thermo-hydro-mechanical coupled analyses in low permeability media. Ph.D Thesis, Universitat Politècnica de Catalunya, Barcelona, Spain.

Vermeulen, T., 1953. Theory of irreversible and constant-pattern solid diffusion. Ind. Eng. Chem., 45: 1664-1670.

Zimmerman, R.W., Chen, G., Hadgu, T. and Bodvarsson, G.S., 1993. A numerical dual-porosity model with semianalytical treatment of fracture/matrix flow. Water Resour. Res., 29: 2127-2137.

Zheng, L. and Samper, J., 2005. The dual continuum coupled multiphase flow model with mixed second order water transfer term for structured soil: I. Theory, en este mismo volumen.