Modelling AECL's Isothermal Test using a porosity dependent permeability (kwn) model and an elastoplastic model

D. G. Priyanto
Atomic Energy of Canada Limited, Pinawa, Manitoba, Canada
J. A. Blatz
Department of Civil Engineering – University of Manitoba, Winnipeg, Manitoba, Canada

ABSTRACT
This paper summarizes the numerical modelling of AECL's full-scale Isothermal Test (ITT) using a porosity dependent permeability (kwn) model and an elasto-plastic model of Blatz and Graham (2003). The results of this numerical simulation compared to the measurement of the full-scale ITT (Dixon et al. 2002) show that the application of the kwn model can be used in the simulation of the HM behaviour of the unsaturated swelling clay to match field measurements.

RÉSUMÉ
Cette communication résume la modélisation numérique du test isothermique à échelle réelle d'EACL, à l'aide d'un modèle de perméabilité selon la porosité (kwn) et d'un modèle élastoplastique de Blatz et Graham (2003). La comparaison des résultats de cette simulation numérique, aux mesures du test isothermique à échelle réelle (Dixon et coll. 2002) montre que le recours au modèle kwn améliore la simulation du comportement hydromécanique de l'argile gonflante non saturée et la rend plus conforme aux mesures sur le terrain.

1 INTRODUCTION

The concept for management of used nuclear fuel adopted by Canada's Nuclear Waste Management Organization (NWMO) includes Deep Geologic Repository (DGR) that utilizes a multiple barrier sealing-system (Gierszewski et al. 2004, Russell and Simmons 2003). One of the possible sealing materials in this system is Bentonite-Sand Buffer (BSB), which is composed of a 50:50 mixture (by dry mass) of bentonite clay and sand.

The large-scale Isothermal Test (ITT) (Dixon et al. 2002) was conducted at the Underground Research Laboratory (URL) in Lac du Bonnet, Manitoba, by Atomic Energy of Canada Limited (AECL) to assess the behaviour of the BSB when subjected to water infiltration. The borehole for the ITT had a diameter of 1.24 m and a depth of 5 m. This test was instrumented to allow monitoring of water uptake by the BSB from the surrounding host rock for approximately 6.5 years. The BSB in the ITT was in unsaturated condition for the entire duration of the test. Simulation of the ITT requires hydraulic (H), and mechanical (M) constitutive models, and coupled HM software.

This paper discusses the numerical simulation of the ITT using a 2D-finite-difference code, FLAC (Fast Lagrangian of Continua) (Itasca 2001). An elastoplastic mechanical constitutive model (BGM) (Blatz and Graham 2003) and porosity-dependent permeability model (kwn) (Priyanto 2007) are used in the simulation. The results of this numerical simulation are compared to the measurement of the full-scale ITT (Dixon et al. 2002).

2 LARGE-SCALE ISOTHERMAL TEST

The ITT was located in room 205 on the 240 m Level of AECL's URL. The configuration of the ITT (Dixon et al. 2002) is illustrated in Figure 1.

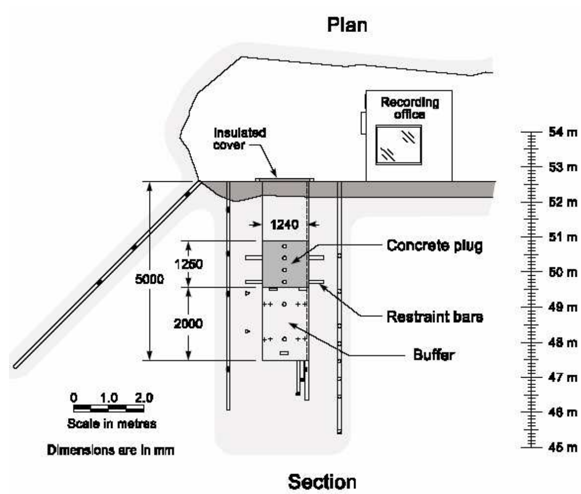


Figure 1. Configuration of the isothermal test (Dixon et al. 2002)

The ITT consisted of three types of solid materials: rock, buffer, and concrete. The focus of this paper is on the HM behaviour of the BSB. The BSB used was composed of 50% sodium bentonite and 50% silica sand by dry weight. It was compacted in situ to a dry density of 1.73 Mg/m^3 and gravimetric water content of 17.5%. For ease of comparison with previous papers describing the

ITT, the BSB material in this paper will be referred to as buffer.

The buffer was installed within a 5-m-deep by 1.24-m-diameter borehole in the unfractured, homogeneous, grey granite on the 240 level of the AECL's URL. The buffer material was compacted in situ into the bottom 2 m of the borehole. A 1.25m-thick concrete plug overlaid the compacted buffer to provide a vertical restraint against swelling (Figure 1). This assembly was then allowed to passively take on water from the adjacent rock.

At the completion of the experiment, intensive sampling of the gravimetric water content and dry density of the buffer was conducted with up to 107 gravimetric water content samples and 33 density samples being taken at eight elevations (Dixon and Chandler 2000).

A number of psychrometers were installed inside the buffer to monitor the changes of the relative humidity (RH) values during the test (Dixon et al. 2002). The RH measurements were related to the suction and gravimetric water contents within the buffer. The spatial measurements of the total stress in the buffer and the displacements at the top of the concrete were also measured during the test.

The groundwater pressure contours in a fracture zone just below the 240 level of the URL before the start of the ITT were measured to be approximately 1600 kPa and this value is used to define the boundary conditions for the numerical modelling.

3 CONSTITUTIVE MODELS

3.1 Mechanical Constitutive Model

An elasto-plastic mechanical constitutive model considered in this paper is the Blatz-Graham Model (BGM) (Blatz and Graham 2003). The BGM was developed based on the results of triaxial tests conducted with controlled suction and suction measurements at the University of Manitoba (Blatz and Graham 2000). The BGM employs three stress-state variables: mean stress (p), deviatoric stress (q), and suction (s) to describe the state of stress in a three-phase soil material. The yield surface and critical state surface for the BGM is illustrated in Figure 2.

Figure 3 shows the yield loci in p-s space for the isotropic condition defined in the BGM. Collapse due to suction increase has not been observed in laboratory tests on the BSB material even for high values of suction (12 MPa) (Blatz and Graham 2003) or 80 MPa (Anderson 2003). Yielding due to suction increase is therefore not considered in the BGM, although it is still postulated to exist under some as-yet undetermined condition.

The yield loci and critical state lines at constant suction in p-q space of the BGM are shown in Figure 4. The critical state slope (N) for the BGM increases when suction (s) increases with the relationship shown in Figure 5.

Figures 6a and 6b illustrate the stress-volume relationship of the BGM showing v-ln(p) and v-ln(s) relationships. Parameters κ and λ control deformation due to changes in mean stress (p). The parameters κ and λ are constants. The parameter κ_s controls the deformation due to change in suction (s) and it is independent of suction.

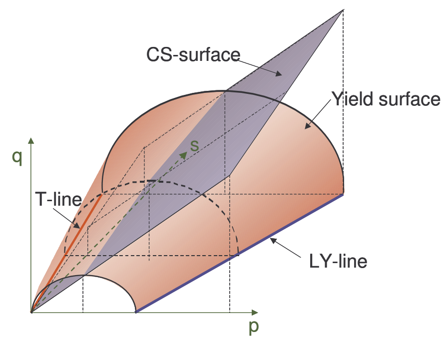


Figure 2. Yield surface and critical state surface for the BGM (after Blatz and Graham 2003)

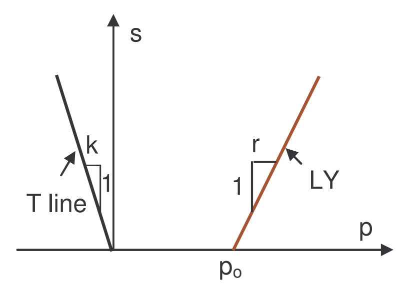


Figure 3. Yield loci in p-s space of the BGM (after Blatz and Graham 2003)

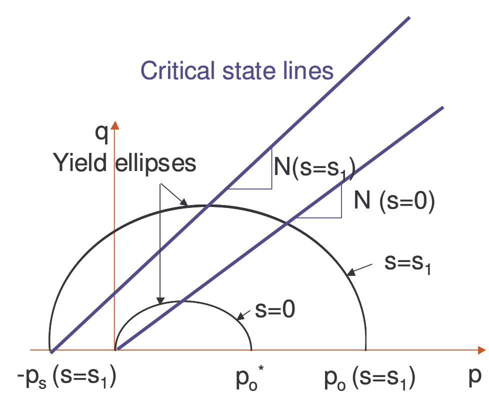


Figure 4. Yield loci in p-q space of the BGM (after Blatz and Graham 2003)

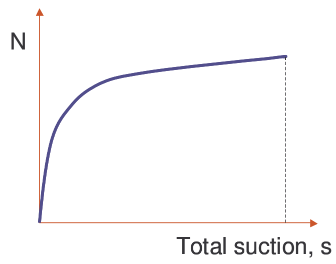
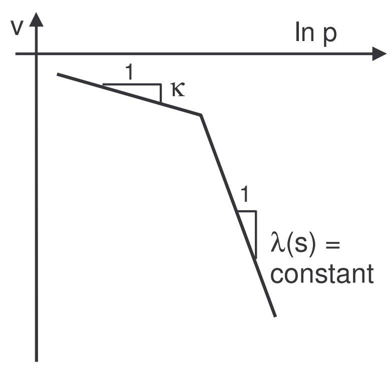
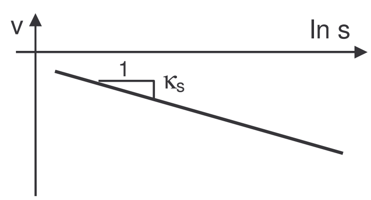


Figure 5. Critical state slope as a function of suction in the BGM (after Blatz and Graham 2003)



(a) v-ln(p) relationship



(b) v-ln(s) relationship

Figure 6. Stress-strain relationship of the BGM (after Blatz and Graham 2003)

3.2 Permeability Surface (kwn) Model

An attempt to model the ITT tests by Thomas et al. (2003) used an 'exponential relationship' to define the relationship of water permeability (k_w) and degree of water saturation (S_w). This 'exponential relationship' demonstrates a decrease of water permeability (k_w) with an increase in the degree of water saturation (S_w) for Sw>90%. This is contradictory to the conventional water permeability functions (e.g. Brooks and Corey 1964, van Genuchten 1980, Fredlund and Xing 1994).

This need for an 'exponential relationship' indicates the need for a 3D permeability surface such as the example illustrated in Figure 7. In this 3D permeability surface, the water permeability (k_w) is dependent on the degree of water saturation (S_w) and the total porosity (n). This 3D permeability surface in Figure 7 maintains the original characteristic of the conventional water permeability function (e.g. Brooks and Corey 1964, van Genuchten 1980, Fredlund and Xing 1994). In this formulation water permeability (k_w) increases with an increase in the degree of water saturation (S_w), and water permeability (k_w) increases due to an increase in total porosity (n) for a constant degree of water saturation (S_w).

The 'exponential relationship' (Thomas et al. 2003) can then be drawn on this 3D permeability surface as illustrated in Figure 7. This 3D permeability surface will be referred to as the kwn model in this paper. This model is used in to simulate the hydraulic behaviour of the buffer.

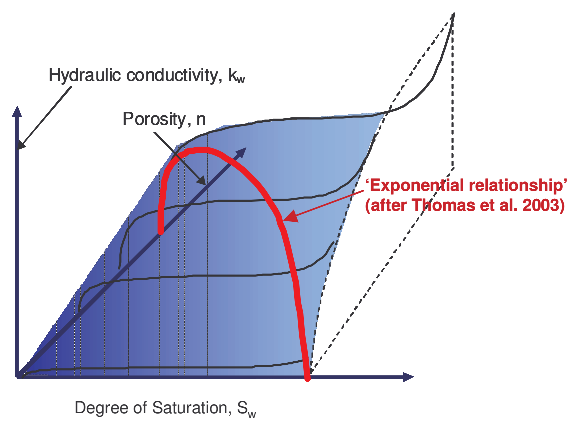


Figure 7. Permeability surface in S_w-n-k_w space

The permeability surface shown in Figure 7 can be generated using:

$$k_w = f\,(S_w, n) \qquad (1)$$

where k_w is the water permeability; S_w is the degree of water saturation; and n is the total porosity.

The water permeability follows the van Genuchten (1980) model for constant porosity (n), such as:

$$k_w = k_{sat}(n).\ \kappa_{rw} \qquad (2)$$

$$\kappa_{rw} = S_e^{\,b}\,[\,1 - (\,1 - S_e^{1/a})^a]^2 \qquad (3)$$

where κ_{rw} is the relative water permeability; a is the fitting parameter, S_e is the effective degree of water saturation, which is defined as:

$$S_e = \frac{S_w - S_{res}}{S_{max} - S_{res}} \qquad (4)$$

The saturated water permeability (k_{sat}) is a function of total porosity (n). The relationship of the saturated water permeability (k_{sat}) as a function of the porosity (n) is described as:

$$\kappa_r^{sat}(n) = n_e^{nb}\left[1-\left(1-n_e^{1/na}\right)^{na}\right]^2 \tag{5}$$

where κ_r^{sat} is the relative water permeability at saturated condition, n_e is the porosity factor that has value of 0 to 1, na and nb are the fitting parameters. The porosity factor (n_e) is defined as:

$$n_e = \frac{n - n_{min}}{n_{max} - n_{min}} = \frac{n_{eff}}{n_{max} - n_{min}} \tag{6}$$

where n is total porosity, n_{min} and n_{max} are the minimum and maximum porosities that define the limits where change in total porosity (n) resulting a change in water permeability. The effective porosity ($n_{eff} = n - n_{min}$) is defined as the porosity available for water to flow. If the total porosity (n) is less than n_{min}, the porosity factor (n_e) is approximately zero. If the total porosity (n) is greater than n_{max}, the porosity factor (n_e) is equal to one.

The relationship of the saturated water permeability and porosity can be described as:

$$k_{sat}(n) = k_{max} \cdot \kappa_r^{sat}(n) \tag{7}$$

where k_{max} is the maximum water permeability correlated with the maximum porosity (n_{max}).

Considering the relationship of effective porosity and water permeability from laboratory testing (Dixon et al. 1999), Equation (5) can be simplified by substitution of na=1 to reduce the number of parameters required for this model, but still allow to fit the experimental data as shown as:

$$\kappa_r^{sat}(n) = n_e^{nb+2} \tag{8}$$

Thus, only two more additional parameters are required to define the kwn model illustrated in Figure 7.

Parameters of the permeability surface for the buffer material were calibrated using permeability measurements (Graham et al. 1997, Dixon et al. 1999) and end-of-test measurements from infiltration tests using controlled suction and suction measurements (Siemens 2006).

3.3 Water Retention Curve

The van Genuchten (1980) model is used to define the water retention curve defining the relationship of suction (s) and degree of water saturation (S_w). The reader is referred to the original reference for the equation.

3.4 Constitutive Model Parameters

The mechanical behaviour of the buffer is simulated using an elastoplastic model of BGM, while the hydraulic behaviour of the buffer is simulated using the kwn permeability model and the van Genuchten (1980) water retention curve. The rock was simulated using a linear elastic model and permeability and water retention curve of van Genuchten (1980) to simulate the mechanical and hydraulic behaviour, respectively. The parameters used in this numerical modelling are discussed further by Priyanto (2007).

4 HM NUMERICAL MODELLING

The HM numerical modelling of the ITT in this paper is conducted using FLAC (Itasca 2001). The HM analysis with the two-phase flow option is used to consider the unsaturated state of the materials. User-defined functions are created in the FISH language (Itasca 2001) to implement the BGM elasto-plastic model (Blatz and Graham 2003) and permeability surface model (kwn). FISH is an embedded programming language in FLAC that enables users to create user-defined functions (Itasca 2001).

The numerical analysis in this paper considers buffer-rock interaction behaviour. Axisymmetric models are used in the analysis. Due to the symmetrical geometry and boundary conditions, only half of the system is considered in the numerical analysis.

An axisymmetric domain of 20x30 m^2 was used for the analysis (Figure 8). The far-field pore water pressure at the URL 240 level, where the isothermal test is located, was approximately 1600 kPa (Chandler 2000). A pore water pressure with a linear variation of 1450 kPa to 1750 kPa was applied at the perimeter to give an average pore water pressure of 1600 kPa (Thomas et al. 2003). The top and the bottom of the buffer have pore water pressures of 1450 kPa and 1750 kPa respectively. Impermeable hydraulic and fixed mechanical boundaries are applied at the buffer-concrete and concrete-rock interfaces. A zero pore water pressure boundary condition is applied at the location of the ITT for the whole test (as shown in Figure 8)

The analysis consists of two stages: stage 1, seepage into an empty borehole; and stage 2, seepage from the rock to the buffer material. The analysis of stage 1 only considers the rock components and it was run for 3 years following the duration of the ITT (Dixon et al. 2002). The-end-of analysis of stage 1 is used as the initial condition of the analysis in stage 2. The finite difference grid used in stage 1 is shown in Figure 9.

The buffer component is added to the model at the start of stage 2. The hydraulic and mechanical constitutive models described in section 3 were used to simulate the HM behaviour of the buffer. The analysis is run to cover the 6.5 years duration of the second stage of the ITT.

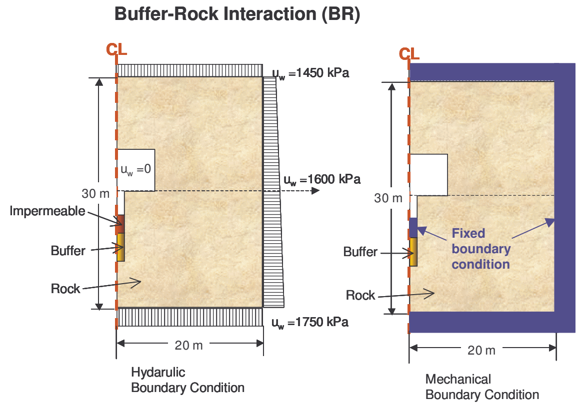


Figure 8. Hydraulic and mechanical boundary Conditions.

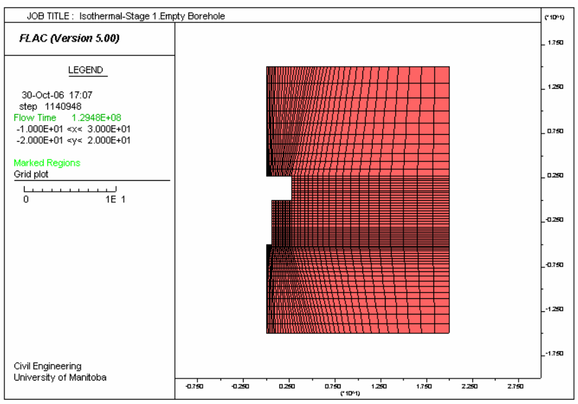


Figure 9. Finite difference grids used to model stage 1 of the isothermal test (ITT)

5 RESULTS

Some of the results of the HM numerical analysis are stress, displacement, and degree of saturation distribution within the buffer and the surrounding rock. The displacement and the degree of saturation are used to define the gravimetric water content. This paper presents the results of total stress and gravimetric water content. The complete results of the HM analysis can be found in Priyanto (2007).

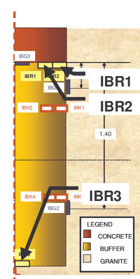
Figure 10b compares total pressure determined by the HM numerical analysis to the field measurement at three selected locations (Figure 10a). The total pressures at these locations of the HM numerical analysis and the field measurement have relatively similar magnitudes. The maximum total pressure is approximately 1400 kPa and 1200 kPa for the field measurement and the HM numerical analysis, respectively. For both the HM numerical analysis and field measurement, the total pressure at these locations increases with time. As expected, the total pressure at IBR2 is the greatest, followed by IBR3 and IBR1.

Figure 11 shows end-of-test gravimetric water content contours from the FLAC analysis and the field measurements. At the end-of-test, the buffer was not saturated. The gravimetric water content around the perimeter and the bottom of the buffer was greater than that close to the centre line for both field measurements and HM analysis.

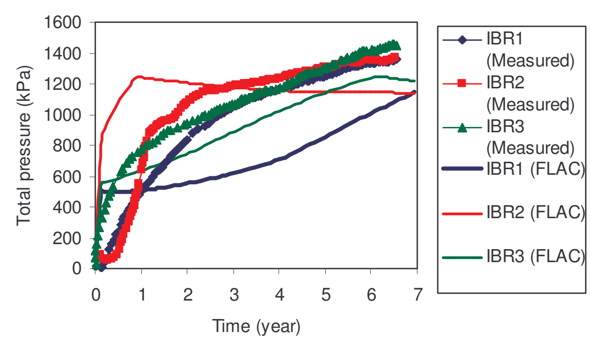
The range of the gravimetric water content of both the measurement and the HM numerical analysis are comparable with a gravimetric water content range of 17 to 22% for the field measurement and 16 to 21% for the HM numerical analysis. The results show that the application of the kwn model and the BGM can be used in the simulation of the HM behaviour of the unsaturated swelling clay to produce a reasonable match field measurement.

6 CONCLUDING REMARKS

This paper has demonstrated the application of HM numerical analysis using FLAC with new constitutive models (i.e., the kwn model and the BGM) to simulate AECL's full-scale Isothermal Test (ITT). The results of this numerical simulation are compared to the measurement of the full-scale ITT (Dixon et al. 2002) and show that the application of the kwn model can be used in the simulation of the HM behaviour of the unsaturated swelling clay to produce a better match field measurement.

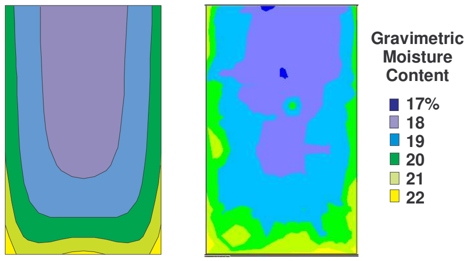


(a) Selected locations of field measurements

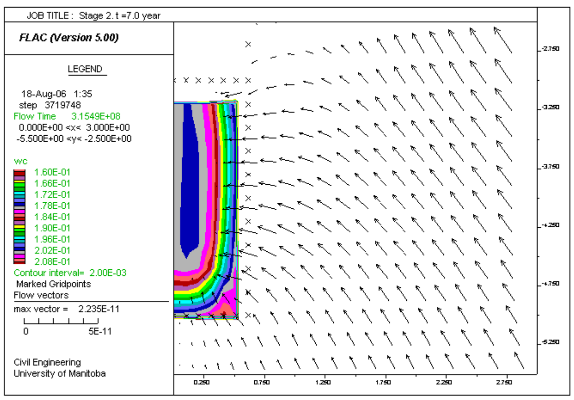


(b) HM numerical analysis (using the BGM and kwn model) versus field measurements

Figure 10. Total pressure at selected location in the buffer



(a) Measurements (Dixon et al. 2001)



(b) HM numerical analysis (using the BGM and kwn model)

Figure 11. End-of-Test Gravimetric Water Content Measurements Compared to the HM Analysis

ACKNOWLEDGEMENTS

The authors would like to acknowledge the financial support provided by Atomic Energy of Canada Limited (AECL), Nuclear Waste Management Organization (NWMO), Natural Sciences and Engineering Research Council (NSERC) of Canada, the friends and colleagues of Neil Burgess, Ontario Power Generation (OPG), and the Department of Civil Engineering at the University of Manitoba, Canada.

REFERENCES

Anderson, D. E. S. 2003. *Evaluation and comparison of mechanical and hydraulic behaviour of two engineered clay sealing material.* M.Sc Thesis, Dept. Civil Engineering, University of Manitoba, Winnipeg, Manitoba.

Blatz, J. A., and Graham, J. 2000. A system for controlled suction in triaxial tests. *Géotechnique*, 50(4): 465-478.

Blatz, J. A., and Graham, J. 2003. Elastic plastic modelling of unsaturated high-plastic clay using results from a new triaxial test with controlled suction. Géotechnique, 53(1): 113-122.

Brooks, R. H., and Corey, A. T. 1964. *Hydraulic properties of porous media.* Hydrology paper number 3, Colorado State University, Fort Collins.

Chandler, N. A. 2000. *Water inflow calculations for the isothermal buffer-rock-concrete plug interaction test.* Ontario Power Generation Report No: 06819-REP-01200-10046-R0, Toronto, Canada.

Dixon, D. A., Graham, J., and Gray, M. N. 1999. Hydraulic conductivity of clays in confined tests under low hydraulic gradients. *Can. Geotech. J.*, 36: 815-825.

Dixon, D., Chandler, N., Graham, J., and Gray, M. N. 2002. Two large-scale sealing tests conducted at Atomic Energy of Canada's underground research laboratory: the buffer-container experiment and the isothermal test. *Can. Geotech. J.*, 39: 503-518.

Dixon, D. A., and Chandler, N. A. 2000. *Physical properties of the materials recovered from the isothermal buffer-rock-concrete plug interaction test conducted at the URL*. Used Fuel Disposal Program Supporting Technical Report 06819-REP-01300-10003-R00. Ontario Power Generation, Toronto, Canada.

Fredlund, D. G., and Xing, A. 1994. Equations for the Soil-Water Characteristic Curve. *Can. Geotech. J*, 31(3): 521-532.

Gierszewski, P., J. Avis, N. Calder, A. D'Andrea, F. Garisto, C. Kitson, T. Melnyk, K. Wei and L. Wojciechowski. 2004. *Third case study – Postclosure safety assessment.* Ontario Power Generation, Nuclear Waste Management Division Report 06819-REP-01200-10109-R00. Toronto, Ontario, Canada.

Graham, J., Chandler, N. A., Dixon, D. A., Roach, P. J., To, T., and Wan, A. W. L. 1997. *The Buffer/Container Experiment: Results, synthesis, issue.* Report AECL-11746, COG-97-46-I. Atomic Energy Canada Limited, Ontario.

Itasca Consulting Group, Inc. 2001. *FLAC Fast Lagrangian Analysis of Continua, Fluid-Mechanical Interaction*. Minneapolis, Minnesota: Itasca Consulting Group, Inc.

Priyanto, D. G. 2007. *The Development and Application of New Constitutive Models to Simulate the Hydraulic-Mechanical Behaviour of Unsaturated Swelling Clay*. Ph.D Thesis. University of Manitoba, Winnipeg, Canada.

Russell, S.B. and G.R. Simmons. 2003. Engineered barrier system for a deep geologic repository. *Presented at the 2003 International High-Level Radioactive Waste Management Conference*. 2003 March 30-April 2, Las Vegas, NV.

Siemens, G. A. 2006. *Influence of boundary conditions on the hydraulic-mechanical behaviour of an unsaturated swelling soil*. Ph.D Thesis, Dept. Civil Engineering, University of Manitoba, Winnipeg, Manitoba.

Thomas, H. R., Cleall, P. J., Chandler, N., Dixon, D., and Mitchell, H. P. 2003. Water infiltration into a large-scale in-situ experiment in an underground research laboratory. *Géotechnique*, 53(2): 207-224.

van Genuchten, M. Th. (1980). A Closed Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. *Soil Sc. Soc. Am. J.*, 44: 892-898.