Numerical modelling of the resaturation of swelling clay with gas injection

P. Gerard & J.-P. Radu

Université de Liège, Département ArGEnCo, Liège, Belgique

J. Talandier & R. de La Vaissière

Agence nationale pour la gestion des déchets radioactifs (ANDRA), Chatenay-Malabry, France

R. Charlier & F. Collin

Université de Liège, Département ArGEnCo, Liège, Belgique

ABSTRACT: During long-term storage of radioactive waste, steel containers are corroded and this process leads to hydrogen production. An in-situ experiment has been designed by Andra, in order to analyze the influence of gas migration on the dynamics of resaturation of the bentonite plug. The competition between liquid water coming from argillite and a gas injection at both ends of the plug is studied. Predictive numerical modelling of the experiment is performed in order to support the design, with a special emphasis on the coupling between the water and gas transfers and the mechanical behaviour.

1 INTRODUCTION

In the frame of nuclear waste disposal, the numerical modelling of the underground facilities construction is used to simulate the different physical processes occurring during the live-time of the nuclear waste. The final objective of the design is the following: the host formation and the engineered barrier systems must be as impervious as possible in order to preserve the biosphere from the radionuclides migration. The thermo-hydromechanical modelling needs numerical codes able to tackle this highly coupled problem. In most cases, these numerical computations are achieved under the assumption of constant gas pressure. However, after the introduction of the waste canisters, different potential gas sources exist in the storage gallery (Volckaert et al. 1994, Ortiz et al. 2002). The main origin of the gas is the corrosion of canister steel component. In this latter case, hydrogen is mainly produced and it is thus important to study how the gas will diffuse in the host formation and in the bentonite plugs. Indeed gas overpressure can maybe have a negative impact on the design. Experimental tests showed that gas entry and breakthrough are often accompanied by the development of preferential pathways, which propagate through the samples (Horseman et al. 1999, Delahaye & Alonso 2002, Olivella & Alonso 2008). Moreover the gas migration into the bentonite can delay the resaturation of the plug, which reduces the swelling pressure of the bentonite and

can alter the good confinement between the canisters and the access gallery.

The paper deals with an in-situ experiment that is currently performed by Andra in its underground laboratory at Bure. The objective of the PGZ experiment is the analysis of the dynamic of the bentonite plug resaturation, studying the competition between the liquid water coming from the host formation and a gas injection at both ends of the plug. In order to support the design of the experiment, predictive numerical simulations of the gas migration in both the host formation and the swelling clay plug are achieved, with a special emphasis on coupling between the gas transfers and the mechanical strains and stresses. The influence of damage or plasticity on the fluid transfer parameters, which can explained the preferential pathways, are not taken into account in the modelling of the experiment.

In this paper, the concept of the experiment and the boundary value problem of the simulations are described in section 2. The hydro-mechanical model is then defined in section 3. In section 4 the results of the modelling are presented and analyzed, before the conclusions (section 5).

2 BOUNDARY VALUE PROBLEM

The general concept of the PGZ experiment is presented on Figure 1. A 25 m long horizontal borehole is drilled in the callovo-oxfordian argillite,

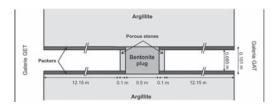


Figure 1. Schematic view of PGZ experiment.

between two existing galleries in the underground research laboratory at Bure. The diameter of the drilling is 101 mm. A plug of MX-80 bentonite is set therein. The plug is 50 cm long and the contact with the borehole is assumed perfect. The gas injection is achieved through two porous stones (with a radius of 85 mm) located at both ends of the plug, imposing a gas pressure higher than the initial water pressure.

An axisymetrical modelling of the experiment is performed with the finite element code Lagamine. Lateral boundaries are defined by the symmetry axis of the experiment (Figure 2). The packers and the porous stones are not simulated. The initial water pressure in argillite is 4.5 MPa. The stress state is assumed isotropic and the initial total stress in argillite is equal to 12.3 MPa.

Different phases are considered for the modelling. First the borehole drilling is modelled for 1 hour, decreasing the relative humidity at the borehole wall down to 70% and the radial stresses down to the atmospheric pressure. Then a 2 days open-drift period is imposed, during which water pressures remains constant at the wall. During the second step, the MX-80 bentonite plug is set, with an initial water saturation of 70%. A 5 days resaturation phase of the plug is then modelled, during which the displacements are fixed at the plug ends and at the borehole wall (due to the porous stones and the packers). During these two first steps, the gas flow problem is not solved and gas pressure remains constant. Finally, during the third step, a nitrogen gas pressure of 7 MPa is imposed at the end of the plug (gas pressure is increased in 4 days and then maintained constant). The other hydraulic and mechanical boundary conditions remain the same as the ones imposed during the second step.

3 BIPHASIC FLOW MODEL AND MECHANICAL BEHAVIOURS

To reproduce water and nitrogen flows in porous media, a biphasic flow model is used. The developed model manages explicitly liquid water and dissolved nitrogen in the liquid phase and a mixture of vapour water and gaseous nitrogen in the gaseous

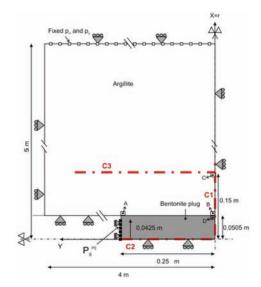


Figure 2. Boundary conditions during the gas injection phase and cross sections and elements definition for the results

phase. The advection of each phase is modelled by a Darcy's flow for unsaturated cases. The diffusion of the components is taken into account in each phase by the Fick's law. The quantity of dissolved nitrogen is proportional to the quantity of gaseous nitrogen, controlled by Henri's law. Details about the exact formulation of the biphasic flow model and the value of the water and nitrogen properties used in the modelling are available in (Gerard et al. 2008).

The retention curves of the different materials are given by the van Genuchten's relationship:

$$S_{r,w} = S_{res} + \frac{S_{max} - S_{res}}{\left[1 + \left(\frac{p_c}{P_r}\right)^{\frac{1}{1-m}}\right]^{-m}} \quad \text{and}$$

$$S_{r,w} = 1 \text{ if } p_s < 0$$

with $S_{r,w}$ the water relative saturation, S_{max} the maximal saturation, S_{res} the residual saturation, p_c the capillary pressure and P_r and m two parameters of the van Genuchten's law. Cubic relations of the effective saturations are adopted for the water and gas relative permeability functions:

$$k_{r,w} = \left(\frac{S_{r,w} - S_{res}}{S_{\text{max}} - S_{res}}\right)^3 \quad k_{r,g} = A \cdot \left(\frac{1 - S_{r,w}}{S_{\text{max}} - S_{res}}\right)^3 \quad (2)$$

A coefficient A is introduced in the gas relative permeability function in order to distinguish the intrinsic permeability according to the considered fluid (water or gas). However such experimental data are available neither for the MX-80 bentonite nor for the callovo-oxfordian argillite. The values of this parameter for the modelling are based on experimental results on Boom clay and FEBEX swelling clay (Volckaert et al. 1994, Villar 1998), that show a high gas intrinsic permeability for the swelling clay. All the hydraulic parameters of argillite and bentonite are presented in Table 1.

For the considered materials and stress levels, the solid grain deformability is no more negligible and the general Biot framework is used to model the hydro mechanical coupled terms (Biot 1941).

The proposed mechanical model for the bentonite is a simplified version of the BBM model (Alonso et al. 1990), expressed in terms of the net stress and the suction and considering only the nonlinear elastic behaviour described by the following relationship:

$$d\varepsilon_{\nu}^{\ell} = d\varepsilon_{\nu}^{\ell-m} + d\varepsilon_{\nu}^{\ell-s} = \frac{d\tilde{\sigma}_{m}}{K} + \frac{ds}{K}.$$
 (3)

where $\tilde{\sigma}_m$ is the mean net stress, s is the suction, K is the bulk modulus and K_s is the bulk modulus related to suction changes. Details about the evolution of K_s with suction and the value of these coefficients for bentonite can be found in (Gerard et al. 2008).

The mechanical law for the argillaceous rocks is an associated elastoplastic perfectly plastic model, defined by a Drucker-Prager yield surface. This constitutive mechanical model is written in terms of the Bishop's definition of effective stress (Nuth & Laloui 2008):

$$\sigma_{ij} = \sigma'_{ij} + b \left(S_{r,w} P_w + \left(1 - S_{r,w} \right) p_g \right) \delta_{ij} \tag{4}$$

Table 1. Hydraulic parameters for the different materials.

		Argillite	Bentonite
$k_{ m int}^{sat}$	Intrinsic permeability (m²)	4.8×10^{-20}	9.6×10^{-20}
Φ	Porosity (-)	0.18	0.35
m	van Genuchten coefficient (-)	0.3289	0.3789
P_r	van Genuchten parameter (MPa)	15	18
S_{max}	Maximal saturation (-)	1	1
S_{res}	Residual saturation	0.01	0.4
A	Gas permeability parameter (-)	100	10^{7}
au	Tortuosity (-)	0.25	0.0494

Table 2. Mechanical parameters for the different materials.

		Argillite	Bentonite
E_0	Young modulus (MPa)	4000	150
$v_{\scriptscriptstyle 0}$	Poisson coefficient (-)	0.30	0.2
c	Cohesion (MPa)	3	-
ϕ	Friction angle (°)	20	-
b	Biot coefficient (-)	0.6	1.0

with σ_{ij} the effective stress, b the Biot coefficient, δ_{ii} the Kronecker symbol.

The mechanical parameters for the different materials are presented in Table 2.

4 NUMERICAL RESULTS

A first modelling without gas injection shows a time resaturation at the centre of the bentonite plug about 30 days (Figure 3–Node 2). For the gas injection modelling, nitrogen pressure is imposed at both ends of the plug the 7th day. The swelling clay is not totally saturated at the beginning of the injection, what makes easier the nitrogen migration into the gaseous phase. The high gas permeability of the bentonite ensures a quasi instantaneous homogeneous gas pressure of 7 MPa into the plug, as observed on the gas pressures profiles along a section through the plug (Figure 4). The water relative saturation becomes also quickly homogeneous in the plug (Figure 3). Moreover nitrogen injection avoids the long-term total resaturation of the swelling clay, related to the imposed gas pressure higher than the initial water pressure.

A low coupling between the gas migration and the water transfers is observed, evidenced by the water overpressures obtained at the centre of the plug end when gas is injected (Figure 5). Nevertheless, these water overpressures disappear after 30 days and no water pressure higher than the initial water pressure is observed, which decreases the risk of hydro-fracturation.

The gas pressure profiles along a section through the bentonite and argillite (at the centre of the plug) are presented on Figure 6. The vertical dotted line indicates the transition between the swelling clay and the argillaceous rock. Gas pressures are homogeneous in the plug. Then nitrogen migrates in argillite and argillite is desaturated on 25 cm long after 1 month. The slope change in the gas profiles corresponds to the transition between the saturated domain (where the diffusion of dissolved nitrogen is the predominant transfer mechanism) and the unsaturated domain (where the advection of gaseous nitrogen prevails), as explained in (Gerard et al. 2008).

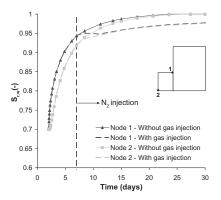


Figure 3. Time evolution of water relative saturation in the bentonite plug with and without gas injection.

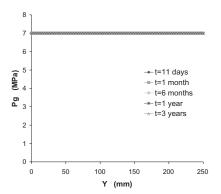


Figure 4. Gas pressures profiles along section C2.

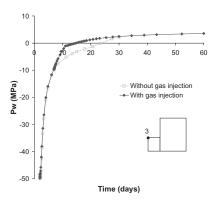


Figure 5. Time evolution of water pressure with and without gas injection at the center of the plug end.

The nitrogen migration is also illustrated on Figure 7, where the gas pressures distribution is drawn after 1 year. The nitrogen moves in argillite, developing an elliptic gaseous front around the plug.

The desaturation observed in the bentonite plug and in argillite is low (Figure 8). The influence

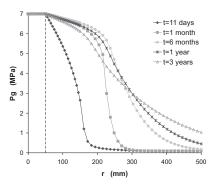


Figure 6. Gas pressure profiles along section C1.

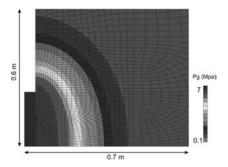


Figure 7. Gas pressures distribution after 1 year.

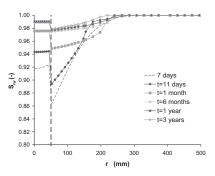


Figure 8. Relative water saturation profiles along section C1.

of the gas injection on the coupling between the mechanical behaviour and the fluids transfers is thus reduced, according to the Bishop's effective stress definition (equation 4). For instance, the axial swelling behaviour in bentonite is weakly influenced by the gas injection and a swelling pressure about 4.5 MPa is recovered (Figure 9), which should ensure a sufficient confinement of radioactive waste for practical applications of long-term storage.

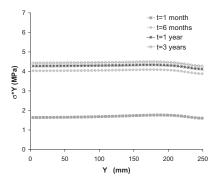


Figure 9. Axial net stress profiles along section C2.

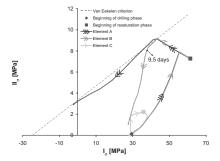


Figure 10. Stress paths at different points of argillite without gas injection.

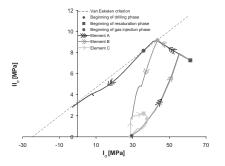


Figure 11. Stress paths at different points of argillite with gas injection.

The Figures 10 and 11 show the stress paths without and with gas injection at different integration points of argillite (defined on Figure 2). The different modelling steps are evidenced on the stress paths. For the problem without gas injection (Figure 10), a small zone of argillite around the borehole becomes plastic during the resaturation phase (elements A and B). At the contact with the plug end (element A), argillite remains plastic during the resaturation phase, mainly due to the stress concentration at the corner between the swelling

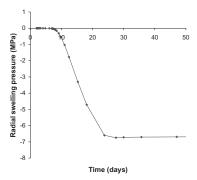


Figure 12. Time evolution of radial swelling pressure in element D without gas injection.

clay and the argillaceous rock. At the middle of the bentonite plug (element B), argillite remains plastic until the development of swelling pressures in the bentonite (from 9,5 days—Figure 12). The radial swelling of the plug affects the stresses in argillite. Radial stresses in argillite increase and orthoradial stresses decrease, which implies a reduction of the deviatoric stress and an elastic behaviour. In element C located 10 cm behind the borehole wall, the behaviour remains elastic during all the resaturation phase, which shows the small damage zone developed around the cavity.

With a gas injection phase, the stress paths at the three elements remain mostly similar (Figure 11). It shows the low coupling of the gas transfers on the mechanical behaviour. The main difference is observed at the borehole wall, at the middle of plug (element B). At the beginning of the gas injection, the behaviour becomes immediately elastic, whereas a plastic zone subsists without gas injection. It can be explained by the bentonite behaviour during the first injection days. Gas pressure is increased to 7 MPa at the plug end in 4 days. At the same time, the net stresses at the middle of the plug remain negligible, because the water relative saturation is still too low to develop swelling pressures in the bentonite (Figure 13—element D). During the first injection days, it implies an increase of the total stress imposed by the bentonite to argillite, which is mainly controlled by the gas pressures increase (Figure 13—element D). At the same time, the water pressures in argillite (element B) don't rise so fast as the gas pressure in the bentonite. Moreover, the contribution of the gas pressure into the Bishop's effective stress is negligible, because the desaturation is low (Figure 13—element B). As a consequence, in spite of the absence of swelling pressure in bentonite during the first 4 injection days, a radial confinement of argillite is observed, which involves a decrease of the deviatoric stresses. The argillite behaviour becomes elastic faster than without gas injection.

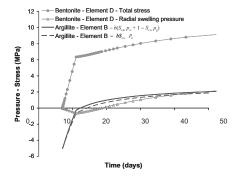


Figure 13. Time evolution of total stress in bentonite and hydraulic contribution to Bishop's effective stress in argillite with gas injection.

Then radial swelling pressures appear, which induces a new decrease of the deviatoric stress.

5 CONCLUSIONS

An in-situ experiment in its underground laboratory at Bure is proposed by Andra in order to study the influence of gas production on the dynamic of resaturation of the bentonite plugs. Predictive numerical modelling is performed to support the design of the experiment. The modelled in-situ test consists of a borehole drilled, inside which a plug of MX-80 bentonite is set. The bentonite is naturally resaturated by water coming from the argillaceous rock. At the same time a gas pressure, higher than the initial water pressure in the host rock, is imposed at both ends of the plug. The developed model takes into account mechanical equilibrium, water and gas transfers in partially saturated conditions. It manages explicitly liquid and vapour water, gaseous and dissolved nitrogen. Elastoplastic and non linear elastic model are used, respectively for the argillite and for the swelling clay.

The numerical results show the instantaneous gas migration in the plug, explained by the high gas permeability of the bentonite. Gas pressures in the swelling clay are thus homogenous and equal to the imposed gas pressure. Then nitrogen migrates in argillite and a 25 cm long zone is partially desaturated. Water overpressures are observed in the bentonite, due to the fast migration of the gas. Nevertheless, these water overpressures are not higher than the initial water pressures in the host rock and disappear quickly, which reduce the risk of hydrofracturing. Numerical results highlight the low coupling between the mechanical behaviour and the gas transfers. It can be explained by the Bishop's effective stress definition and the low water relative saturation observed in argillite, which reduces the influence of the gas pressures on the mechanical stresses and strains. The analysis of the argillite stress path at the borehole wall (at the middle of the plug) shows that the gas injection implies a decrease of the deviatoric stress and an elastic behaviour, whereas argillite remains longer plastic without gas injection.

The gas pressures distribution is mainly influenced by the highly gas permeability of bentonite. It is based on experimental data on FEBEX bentonite (Villar 1998). Experimental data on the fluid transfers in the MX-80 bentonite and in the callovo-oxfordian rocks in the quasi-saturated domain are needed in order to define with precision retention curves and gas and water relative permeability functions, especially in the quasi-saturated domain.

Other coupling effects could be taken into account, as the development of an excavated damage zone around the borehole and its influence on the argillite transfer parameters (for instance the permeability). Such coupling could evidence the development of preferential pathways for the gas migration.

The PGZ experiment is presently performed in the underground laboratory at Bure. The comparison between experimental data and the predictive numerical results will follow in order to improve our models.

REFERENCES

Alonso, E.E., Gens, A., Josa, A. 1990. A constitutive model for partially saturated soils. *Géotechnique* 40:405–430.

Biot, M.A. 1941. A general theory of three-dimensional consolidation. *Journal of Applied physics* 12:155–164.

Delahaye, C.H. & Alonso, E.E. 2002. Soil Heterogeneity and Preferential Paths for Gas Migration. *Engineering Geology* 64: 251–271.

Gerard, P., Charlier, R., Barnichon, J.-D., Su, K., Shao, J.-F., Duveau, G., Giot, R., Chavant, C. & Collin, F. 2008. Numerical modelling of coupled mechanics and gas transfer around radioactive waste in long-term storage. *Journal of theoretical and applied mechanics* 38(1–2): 25–44.

Horseman, S.T., Harrington J.F. & Sellin, P. 1999. Gas Migration in Clay Barriers. *Engineering Geology* 54: 139–149.

Nuth, M. & Laloui, L. 2008. Effective stress concept in unsaturated soils: clarification and validation of a unified framework. *International Journal of Analytical* and Numerical Methods in Geomechanics 32:771–801.

Olivella S. & Alonso E.E. 2008. Gas flow through clay barriers. *Géotechnique* 58(3): 157–176.

Ortiz, L., Volckaert, G. & Mallants, D. 2002. Gas Penetration and Migration in Boom Clay, a Potential Host Rock Formation for Nuclear Waste Storage. *Engineering Geology*, 64: 287–296.

Villar, M.V. 1998. Ensayos para el proyecto FEBEX. CIE-MAT-report 70-IMA-L-5-51, prepared for ENRESA.

Volkaert, G, Ortiz, L., De Canniere, P., Put, M., Horseman, S.T., Harrington, J.F., Fioravante, V. & Impey, M. 1994. Modelling and experiments on gas migration in repository host rocks. MEGAS Project, Final Report, Phase 1.