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# Journal of Rock Mechanics and Geotechnical Engineering

journal homepage: www.rockgeotech.org



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# Workflow to numerically reproduce laboratory ultrasonic datasets

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#### ARTICLE INFO

Article history: Received 10 September 2014 Received in revised form 9 October 2014 Accepted 10 October 2014 Available online 29 October 2014

Keywords: Numerical methods Calibration Velocity model Bentonite Viscoelastic wave propagation

#### ABSTRACT

The risks and uncertainties related to the storage of high-level radioactive waste (HLRW) can be reduced thanks to focused studies and investigations. HLRWs are going to be placed in deep geological repositories, enveloped in an engineered bentonite barrier, whose physical conditions are subjected to change throughout the lifespan of the infrastructure. Seismic tomography can be employed to monitor its physical state and integrity. The design of the seismic monitoring system can be optimized via conducting and analyzing numerical simulations of wave propagation in representative repository geometry. However, the quality of the numerical results relies on their initial calibration. The main aim of this paper is to provide a workflow to calibrate numerical tools employing laboratory ultrasonic datasets. The finite difference code SOFI2D was employed to model ultrasonic waves propagating through a laboratory sample. Specifically, the input velocity model was calibrated to achieve a best match between experimental and numerical ultrasonic traces. Likely due to the imperfections of the contact surfaces, the resultant velocities of P- and S-wave propagation tend to be noticeably lower than those a priori assigned. Then, the calibrated model was employed to estimate the attenuation in a montmorillonite sample. The obtained low quality factors (Q) suggest that pronounced inelastic behavior of the clay has to be taken into account in geophysical modeling and analysis. Consequently, this contribution should be considered as a first step towards the creation of a numerical tool to evaluate wave propagation in nuclear waste repositories.

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## 1. Introduction

Isolation of high-level radioactive waste (HLRW) is an important issue which must be thoroughly addressed. HLRW is generally enveloped in multiple engineered and natural barriers and placed in deep geological repositories. Such a technique is currently considered as a viable and reliable option to safely isolate HLRW from the aquifers and the biosphere (Chapman and McCombie, 2003; Alexander and McKinley, 2007). Montmorillonite is a swelling clay that is extensively used as the base material for those engineered barriers as it acts as an impermeable (hydraulic conductivity  $k \approx 10^{-14}$  m/s) seal between the HLRW and the host rock as it saturates (Lajudie et al., 1994).

In the vicinity of the HLRW containers, the temperature, pressure, and water content of the barrier are expected to increase dramatically over few years after completion. The reasons for that are (a) radioactive decay of HLRW, (b) swelling of the clay and (c)

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Peer review under responsibility of Institute of Rock and Soil Mechanics, Chinese Academy of Sciences. imbibition from the surrounding aquifer, respectively (Villar et al., 2005; Alonso et al., 2008). Therefore, the sealing material will change the physical state and its integrity can be also jeopardized. This might lead to harmful leakage of noxious condensate into host rock and surrounding aquifers.

The aforementioned physical changes affect the elastic and viscoelastic properties of the montmorillonite, such as longitudinal and shear wave velocities ( $V_P$  and  $V_S$ , respectively), density ( $\rho$ ), and seismic attenuation. Tisato and Marelli (2013) showed that a variation in confining pressure ( $p_c$ ) ranging between 0 MPa and 20 MPa induces the increases in  $V_P$  and  $V_S$  up to 90% approximately. Similarly, the increase of water saturation ( $w_c$ ) from 10% to 52% at  $p_c < 10$  MPa causes increases in  $V_P$  and  $V_S$  up to 50%. These changes in velocities will result in a variation of the seismic signal transmitted through the montmorillonite barrier. Therefore, once the variation of the elastic parameters due to the changes in physical conditions is known, seismic monitoring may be used as a non-intrusive tool to track the condition of the plug.

The equipment employed in seismic monitoring consists of a set of emitters and receivers, installed in the proximity of the bentonite barrier (Manukyan et al., 2012). The input signal is periodically sent by the emitters, propagates through the barrier, and is recorded by the receivers. First-arrival times are evaluated based on the recorded waveforms for each cycle. If  $p_c$  or  $w_c$  of montmorillonite changes between any two cycles, the corresponding change in the

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elastic parameters will be illustrated by a first-arrival time shift. As soon as changes in first arrivals are detectable, full waveform analysis may be applied to locate the areas of anomalous pressure or water saturation (Manukyan et al., 2012). However, high-quality and well-calibrated data acquisition systems and experimental repeatability are required to correctly reflect the variation in water saturation or pressure in the barrier. Therefore, the numerical simulation of the procedure in complex repository geometry should be conducted and thoroughly analyzed to aid in design and optimization of the monitoring system (Marelli et al., 2010).

Numerical tools provide accurate results if calibrated with rigorous laboratory investigation. To the best of our knowledge, only Saenger et al. (2014) incorporated the calibration of numerical tools to support laboratory experiments (and vice versa) and to simplify the interpretation of the obtained results. Often, the analytical prediction of the recorded waveform across the geometry of the experiment investigating elastic properties of a certain material is cumbersome. Saenger et al. (2014) simulated the ultrasonic wave propagation velocity measurements in the rock samples tested in a Paterson gas-medium apparatus. It is shown that dispersive and wave conversion effects caused by the presence of assemble items (e.g. jackets or buffer rods) may hinder the firstarrival time. As a result, the estimated values of  $V_{\rm P}$  and  $V_{\rm S}$  will be erroneous and deviate from values a priori assigned in the numerical model. Thus, numerical modeling of the commonly used experimental techniques is of paramount importance for accurate interpretation of the results.

The purpose of this particular contribution is twofold: (a) to propose a methodology to calibrate 2D (two-dimensional) numerical tools to yield synthetic traces, accurately reproducing the experimental results of ultrasonic wave propagation in the material of interest; (b) to use the calibrated framework and employ the iterative optimization technique as an attempt to evaluate the variation of attenuation in bentonite caused by the water saturation. The results of the calibration are validated by the comparison of the synthetic seismograms of shear wave propagating in bentonite with the experimental dataset reported in Tisato and Marelli (2013). Eventually, the long-term scope of our research is to create a numerical tool to simulate the seismic monitoring of physical changes in a generic HLRW barrier.

## 2. Methods

In this section we explain the strategy that allows us to numerically reproduce the experimental ultrasonic traces in montmorillonite samples collected in the laboratory by Tisato and Marelli (2013).

#### 2.1. Laboratory setup

Tisato and Marelli (2013) determined the longitudinal and transverse ultrasonic wave propagation velocities in montmorillonite, employing an axially loaded assembly comprising two aluminum caps that enclose the sample and two ultrasonic piezoceramic transducers (ultrasonic facility). The facility allowed the recording of ultrasonic signals transmitted through the sample at set temperatures while measuring the sample length (Fig. 1). The setup was designed to reproduce those conditions expected at a HLRW waste repository throughout its lifespan as well as to simulate anomalous conditions outside the predicted range.

Longitudinal and transverse vibrations with a fundamental frequency of 100 kHz (Fig. 1d) were generated by means of 1 MHz corner frequency compression and planar shear piezoceramic transducers, respectively.

## 2.2. Numerical setup

We performed simulations on a 2D numerical model representing the laboratory setup to compare numerical results with laboratory data. The mesh was produced following a schematic



**Fig. 1.** (a) Schematic diagram of the ultrasonic facility employed in the experiments to measure  $V_P$  and  $V_S$ ; (b) a subdomain used for iterative calibration; (c) a photo of the ultrasonic facility in a fully assembled state; and (d) normalized signal sent to the emitter.

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