Applicability of DEM - Rate Process Theory approach for rock creep simulation

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ABSTRACT: One main long-term strength and safety concern in many geotechnical designs is rock creep response. Creep is the progressive deformation with time that many materials (soil, rocks, etc.) exhibit under an approximately constant stress. Based on laboratory and numerical results, several creep models (e.g., the Burgers Model) have been proposed; however, their main limitation is that the tertiary creep stage is often not well captured. To overcome this limitation, some progress has been made and new viscoelastic-viscoplastic creep models have been formulated. As an alternative, the Rate Process Theory (RPT) has recently been employed to successfully simulate all creep stages of rock samples. In this work, the Authors' recent advances in this topic are used to illustrate the applicability of Discrete Element Method (DEM) modeling plus RPT to simulate rock creep, with particular attention to modelling of laboratory tests and rock creep in tunnels.

Keywords: Discrete Element Method (DEM), Rate Process Theory (RPT), Rock creep, Tertiary creep.

1 INTRODUCTION

Extended reports in the literature demonstrate that rock creep is a key aspect in many rock engineering projects, especially when rocks are exposed to high stresses over time. For instance, significant strains associated with rock creep occurred during construction of the Yacambu–Quibor tunnel in Venezuela (Hoek & Guevara 2009). Also, Horvath & Chae (1989) reported up to an 245% increase in settlements due to creep for piles socketed in a soft rock. Furthermore, Xu et al. (2013) suggested that most of the rock slope failure that occurs at Yunjiang road in China is due to rock shear creep within discontinuities of the rock mass.

The study of factors affecting the rock creep behavior is still receiving considerable attention in recent years. As an example, Yu et al. (2019) and Tang et al. (2022) carried out uniaxial compressive creep tests (UCCTs) on sandstone and granite samples and indicated that water conditions affect their short and long-term strength. Also, Wang et al. (2021) –based on direct shear tests performed on pseudo-rock samples with different Joint Roughness Coefficients values– suggested that creep deformation and creep rate decreased with increasing pre-peak shear stress in the loading section.

More recently, Dong et al. (2023) conducted triaxial creep tests on rock salt under multi-stage temperatures and observed that an increase of temperature decreases the duration of the primary creep stage, and increases duration of the secondary creep rate.

Some efforts have been done to improve the rock creep constitutive models, and to capture the three stages of rock creep: primary creep, secondary creep, and tertiary creep (see e.g., Kabwe et al. 2020 and Yin et al. 2022); however, they are complex rheological formulations involving many parameters. Alternatively, the Rate Process Theory (RPT) and its implementation through the Discrete Element Method (DEM) has been recently employed to successfully reproduce all stages of rock creep including rock creep failure (Gutiérrez-Ch et al. 2021, 2022, 2023). In this work, several examples are employed to illustrate the applicability of DEM + RPT approach to simulate all stages of rock creep; in particular, to model (i) laboratory creep tests –Uniaxial Compression Multistage Creep Tests (UCMCTs) and Direct Shear Creep Tests (DSCTs)– and (ii) deformations of deep tunnels excavated in soft rock.

2 BACKGROUND OF DEM-RPT APPROACH

2.1 Rate Process Theory (RPT)

The RPT formulated by Eyring (1936) describes the motions of particles (at molecular level) as a function of potential-energy barriers, which restrict the movements of particles in the system. Following Gutiérrez-Ch et al. (2021), the equation of the RPT can be simplified as:

$$\dot{s} \cong \frac{\alpha}{2} e^{\beta \mu} \tag{1}$$

with:

$$\alpha = \lambda \frac{2kT}{h} e^{\frac{-\Delta F}{RT}}$$
(2)

$$\beta = \frac{\lambda}{2kT} \frac{1}{n_1} \tag{3}$$

where \dot{s} represents the sliding velocity at each contact between particles, λ is the flow unit (in meter), k is Boltzmann's constant (1.381 × 10⁻²³ J/K), T is the temperature (in Kelvin), h is Planck's constant (6.626 × 10⁻³⁴ Js), ΔF is the activation energy (kJ/mol), R is the universal gas constant (8.314 × 10⁻³ kJ/(Kmol)), n_1 is the number of bonds per unit of normal contact force (bonds/N), and μ is the friction coefficient at each contact between particles (Additional details about these parameters are available in Mitchell & Soga 2005 and Gutiérrez-Ch et al. 2021, 2022).

2.2 DEM modelling with PFC

Particle Flow Code (PFC) is a particle-based DEM code that provides several contact models –such as Linear Model (LM), Flat-Joint Contact Model (FJCM), etc.– to model the macroscopic response of bonded or unbonded materials (Itasca Consulting Group Inc 2014). To model rock creep under different conditions, the Authors have used a hybrid model composed of particles interacting with the LM and the FJCM (see Gutiérrez-Ch et al. 2021, 2022, 2023). The LM-to-FJCM contact ratio employed in the hybrid model depends on the rock creep response of the material involved in the problem.

3 NUMERICAL MODELLING OF ROCK CREEP WITH DEM-RPT APPROACH

The DEM–RPT methodology is composed of the following aspects (Gutiérrez-Ch et al. 2021, 2022, 2023):

3.1 RPT implementation into DEM models

The RPT is implemented into the LM and the FJCM by using the flowchart in Figure 1, that modifies μ at each contact between particles during the time-stepping of DEM simulation. The values of parameters used for RPT implementation (see Table 1; and Equations 1-3) are chosen to reproduce the problem conditions (see Section 4) within the range recommended by Kuhn and Mitchell (1993).



Figure 1. Flowchart of RPT implementation (modified from Gutiérrez-Ch et al. 2023).

Table 1. Parameters used for RPT implementation.

Parameter		Data for slate rock, from	Data for pseudo-rock, from
		Gutiérrez-Ch et al. (2021; 2022)	Gutiérrez-Ch et al. (2023)
ΔF	[kJ/mol]	100	170
Т	[K]	293	293
λ	[m]	3×10^{-10}	2.8×10^{-10}
n_1	[bonds/N]	1×10^{9}	1×10^{9}

3.2 DEM model calibration

The DEM model calibration is composed of the following three steps:

- a) Calibration of DEM micro-parameters: First, the "trial-and-error" calibration of microproperties employed for the LM and the FJCM is conducted; by comparing the macroscopic response of laboratory tests against DEM tests. As an illustration, Figure 2 shows a comparison of the axial stress-axial strain curves –and the maximum stress value (σ_{peak})– obtained in a laboratory UCMCT and a DEM UCMCT.
- b) Selection of the LM-to-FJCM contact ratio: Next, the selection of the LM-to-FJCM contact ratio is conducted iteratively to match the rock creep response (e.g., the deformation obtained during primary and secondary creep stages). As an example, Figure 3 shows the sensitivity analysis conducted to select the LM-to-FJCM contact ratio of DEM models needed to reproduce the creep deformation recorded during a DSCT and a UCCT.
- c) Calibration of DEM simulation time (t_{DEM}) : Finally, since the real time of the analyzed problem is different to t_{DEM} , their relationship needs to be matched. To do that, the total strain obtained during a creep loading stage is used a benchmark. For instance, note that when $t_{DEM} = 12$ s and $t_{lab} = 24$ h, the shear displacement of the DEM test is equivalent to the laboratory test for the case shown in Figure 3a; thus, its specific t_{DEM}/t_{lab} relationship can be defined.



Figure 2. Comparison between DEM and laboratory UCMCT tests on a slate (Gutiérrez-Ch et al. 2021).



Figure 3. Sensitivity analysis conducted to select the LM-to-FJCM ratio and to calibrate the t_{DEM} and t_{lab} relationship: (a) DSCT (Gutiérrez-Ch et al. 2023), (b) UCCT (Gutiérrez-Ch et al. 2021).

4 DEM MODELS SET-UP

Figure 4 shows the general view of three models where the DEM–RPT methodology has been employed by the Authors; in particular, to analyze the rock creep behavior of (1) UCMCTs, (2) DSCTs, and (3) deep tunnels excavated in a soft rock. (For additional details about their set-up, see Gutiérrez-Ch et al. 2021, 2022, 2023).



Figure 4. General view of DEM models: (a) UCMCT (Gutiérrez-Ch et al. 2021), (b) DSCT (Gutiérrez-Ch et al. 2023), (c) circular tunnel (Gutiérrez-Ch et al. 2022).

5 RESULTS

Results obtained for each model with the DEM–RPT approach are presented next. Figure 5 shows the shear strain and shear stress (vs t_{DEM}) obtained during a DSCT conducted on a pseudo-rock sample; and Figure 6a shows the creep deformations computed with "gauge particles" (denoted as array 2-2') located along the radial direction for DEM tunnel simulations with different depths; Figure 6b illustrates all phases of creep behavior of the model at 4000 m depth. Figures 5 and 6 demonstrate that the DEM–RPT methodology is able to reproduce all stages of rock creep response including tertiary creep stage and creep failure.



Figure 5. (a) Evolution of shear strain and shear stress vs t_{DEM} for a DSCT conducted on a pseudo-rock under Constant Normal Load (CNL) with $\sigma_n = 1.4$ MPa, (b) zoom-in view of all stages of rock shear creep (Gutiérrez-Ch et al. 2023).



Figure 6. (a) Evolution of tunnel strains vs computational steps, (b) illustration of all phases of creep behavior of the model at 4000 m depth (Gutiérrez-Ch et al. 2022).

6 CONCLUDING REMARKS

In this work, the Authors have presented recent advances by Gutiérrez-Ch et al. (2021, 2022, 2023) on the applicability of the DEM–RPT approach to simulate rock creep response in laboratory tests, and during tunnel construction. Some key aspects of the DEM–RPT approach are:

- Results suggest that the DEM–RPT approach is suitable to reproduce rock creep under the different scenarios considered, successfully reproducing all creep stages, including tertiary creep and creep failure.
- To apply the DEM–RPT methodology, a hybrid model composed of the LM and FJCM can be used, but with a significant preponderance of FJCM with respect to the LM.

- A key finding is that the RPT implementation, and the DEM model calibration, are relatively easy to be conducted using only one laboratory test (e.g., a single stage direct shear creep test under CNL conditions or a single stage uniaxial compression creep test), which facilitates the applicability of the new approach.

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