

Numerical simulations of the hydrogeological behavior of an experimental waste rock pile with a flow control layer: calibration using an automated approach.

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Abstract

Mining operations produce large volumes of waste rock to access economically valuable mineralized zones. Waste rock is usually stored in surface piles, which construction and reclamation often represent a challenge for the industry. A flow control layer (FCL), made of crushed waste rock or sand, could contribute to control infiltration of water, thus improving waste rock pile stability and limiting contamination. An experimental waste rock pile was built and instrumented at the Tio mine (Rio Tinto Fer et Titane) to evaluate the performance of an FCL in field conditions. Large infiltration tests and rainfall monitoring were carried out, and measured outflow and water contents were used to calibrate numerical simulations. However, data were noisy and sometimes incomplete, and the models were difficult to calibrate. A new approach based on parameters describing the hydrogeological response to water infiltration was therefore proposed. An algorithm was developed to automate the data processing for inverse problems in groundwater flow. To do so, a black-box optimization approach minimizes the error between simulated and measured data. The proposed method reduces the bias induced by a manual calibration and allows for a multivariable calibration.

RESUMÉ

L'exploitation minière génère d'importants volumes de roches stériles généralement entreposées dans des haldes, dont la construction et la restauration représentent un défi pour l'industrie. Une couche de contrôle des écoulements constituée de roches stériles concassées ou de sable pourrait permettre de contrôler l'infiltration d'eau, améliorant ainsi la stabilité des haldes et limitant les risques de contamination. Une halde expérimentale a été construite et instrumentée à la mine Tio (Rio Tinto Fer et Titane). Des essais d'infiltration à grande échelle et un suivi des précipitations ont été réalisés afin d'évaluer la performance de la méthode in situ. Les débits et les teneurs en eau mesurés ont été utilisés pour calibrer des simulations numériques. Cependant, les données étaient bruitées, parfois incomplètes, et les modèles étaient par conséquent difficiles à calibrer. Une nouvelle approche basée sur des paramètres décrivant la réponse hydrogéologique de l'infiltration d'eau a donc été proposée. Un algorithme a été développé afin d'automatiser le processus de calibration, en utilisant une méthode d'optimisation par boîte noire afin de minimiser l'erreur entre les données simulées et mesurées. La méthode proposée contribue à réduire le biais induit par un ajustement manuel et permet une calibration multivariable.

1 Introduction

Mining operations produce large volumes of waste rock to access economically valuable mineralized zones. Waste rock is characterized by a wide range of particle sizes, from metric blocs to clay size particles. It is usually stored in surface piles, which height can exceed several dozen of meters and which surface can cover dozen of hectares (McCarter 1990, Hawley and Cunning 2017). Waste rock piles are usually built on the surface and therefore exposed to atmospheric conditions.

The exposition of materials containing sulfide minerals to water and oxygen can result in acid mine drainage (AMD), or contaminated neutral drainage (CND). AMD is characterized by low pH and high concentrations of sulfates, and dissolved metals (Aubertin et al., 2002; Molson et al., 2005). Some sulfide minerals may also oxidize without producing acid, or acidity may be neutralized by carbonate minerals. Resulting CND can contribute to the release of metals and metalloids such as As, Co, Ni, and Zn in the environment (Plante et al. 2010, Benzaazoua et al. 2013). However, reclamation of waste rock piles is often challenging, because of the size of the structures, the steep slopes (close to waste rock repose angle) and the deep water table (Aubertin et al., 2013).

A new method was therefore proposed to improve geochemical and geotechnical stability of the waste rock pile during construction and after closure (Aubertin et al. 2002a, 2013, Fala et al. 2005). This approach consists in building a flow control layer (FCL) on top of each bench of the pile (Figure 1). This FCL is usually made of compacted finegrained materials, such as sand or crushed waste rock, and is inclined by around 5% towards the exterior of the waste rock pile. Fine grained materials create a capillary barrier effect with the underlying coarse waste rock, therefore preventing infiltration downwards. FCL slope enhances lateral diversion of water, thus preventing contacts with potential AMD/CND generating waste rock. More details about the FCL concept can be found in Aubertin et al. (2002b) and Broda et al. (2014). because they simulated large precipitation events over a short period, thus inducing stronger responses in terms of water content variations. During these tests, 28 m₃ and 16.8 m₃, respectively, were sprayed with a water truck at the surface of the experimental waste rock pile over a period of 10 h (Dubuc et al., 2017; Martin et al., 2019). An impermeable plastic membrane was also installed on top of the experimental waste rock pile after the large infiltration test I-D to simulate a drought (Dubuc 2018). The membrane was removed after two months. The data recorded in situ were then used to calibrate numerical simulations. The objective of the simulations was to extrapolate and optimize the FCL





An experimental pile was built and instrumented at the Tio mine (Rio Tinto Fer et Titane, Québec, Canada) to evaluate the performance of an FCL at a large scale and in real field conditions (Martin et al., 2017, 2019). The FCL was made of a 0.6 m compacted layer of sand covered by a 0.3 m layer made of crushed anorthosite. The experimental waste rock pile was 70 m long, and between 10 and 12 m wide. The maximal height was 7 m and the surface of the pile was inclined with a 5 % slope. The core of the experimental waste rock pile was made of CND-generating waste rock (Figure 1). Non-reactive anorthosite waste rock was placed in the last ten meters (x = 60-70 m, where water infiltrates).

Suction probes and water pressure sensors were installed in the FCL and the waste rock to monitor water flow in the experimental pile (Broda et al., 2017; Martin et al., 2017, 2019). Six lysimeters were also built at the bottom of the pile to collect and measure water outflow and characterize water quality. Material hydrogeological properties (including hydraulic conductivity and water retention curves) were measured in situ and in the laboratory (Bréard Lanoix 2017; Bréard Lanoix et al., 2020). Large scale infiltration tests were conducted in 2016 and 2017 to evaluate the pile hydrogeological response under controlled conditions. A total of six large scale infiltration tests were carried out. Tests I-C and I-D were selected in this study design for other climatic conditions and materials at other mine sites.

However, numerical simulations of waste rock piles can be complex, mainly because of the heterogeneity of the structure, the wide particle size distribution, and the scale effects (Nichol et al. 2005). Also, the quality of field measurements can often be affected by noise, and sometimes by missing data, thus complicating calibration. In general, numerical simulations are calibrated by varying each parameter individually (Gao 2011). Such an approach is, however, time-consuming and does not always guarantee that the best set of parameters is determined.

In this paper, a new approach based on parameters describing the hydrogeological response to water infiltration was proposed. An algorithm was developed to automate the numerical simulation calibration, using a black-box optimization method to minimize the error between simulated and measured data. The automatization of data processing can provide a finer resolution of the observed phenomena and a more robust calibration of the numerical simulations.

2 METHODOLOGY

2.1 Model geometry and properties

In this study, numerical simulations used the equivalent porous method to simulate water flow in waste rock. The numerical simulations were carried out using the software HydroGeoSphere (HGS, Aquanty). HGS resolves the 3D Richards equation for subsurface flow using the control volume finite element approach (Brunner and Simmons 2012).

Material properties included the saturated hydraulic conductivity and van Genuchten parameters for the water retention curve (van Genuchten, 1980) (Table 1). Initial properties were obtained based on laboratory or field measurements and preliminary models carried out with Seep/W (Dubuc, 2018). The geometry of the waste rock pile was simulated as a trapezoid of 60 m by 10m, with a maximal height of 7m and a surface slope of 5%. The mesh was of hexahedral structured formed blocks of 0.25 m x 0.25 m x 0.20 m. Mesh refined was to 0.25 m x 0.25 m x 0.06 m for the FCL.

Lysimeters were simulated as seepage faces. At x = 60 m (Figure 1), a (vertical) seepage face simulated a Neumann boundary to ensure the continuity of the water flow towards the exterior of the waste rock pile. Infiltration tests and precipitations were simulated by applying a unit flux condition on the top boundary (constant infiltration flux over the test period). Initial conditions were defined by applying a suction equal to the water entry value (WEV) for each material. Snowmelt was not simulated.

2.2 Calibration approach

The waste rock pile hydrogeological response to large scale infiltration tests I-C and I-D were used to calibrate the simulations. Validation of the calibrated models was then achieved by comparing simulated volumetric water contents to measured values between May 1, 2017, and August 31, 2017.

Calibration was carried out based on the variation of volumetric water content measured at a depth of 0.80 m (i.e. in the FCL) and at 6 different positions along the FCL (red points in Figure 1). Water contents were initially relatively small (test I-C was carried out after a few days without precipitation) but rapidly increased after the infiltration test started. After water content reached a peak, it decreased again, but more slowly, towards its initial value. Hydrogeological response was similar for tests I-C and I-D, but the amplitude of the peak for test I-C was applied at the surface.

The FCL and waste rock hydrogeological response (i.e. the curve showing the variation of volumetric water content with time) was characterized by three parameters in this study:

- in the FCL: t1, the time corresponding to 50% of the increase of the volumetric water content induced by the wetting front, and t2, the time corresponding to 50% of the decrease of volumetric water content during drainage at a depth of 0.80m.
- in the waste rock: ta, the arrival time of the wetting front at a depth of 1.30m

Measured and simulated water contents were compared at the center of each of the six instrumented zones (Figure 1). A low pass filter removed the small variations of volumetric water content to reduce the noise and facilitate the detection of local extrema by the moving average method and thus to automate the calculation of the parameters defined above.

An algorithm was then coded to link the hydraulic conductivity and the parameters α_{VG} and n the fitting parameters of the Van Genuchten equation (van Genuchten 1980) of the 3 materials with the error between the numerical simulation and measured data (Figure 2). A black-box function, a function for which the analytic form is not known. For example, it could be a numerical code involving results of a numerical simulation. The calibration was considered achieved when the objective of the black box function (esum) converged to zero.



Figure 2: Schematic of the calibration algorithm: Black-box functions are represented in black.

3 RESULTS

3.1 Calibration results

The Black Box algorithm typically iterates an important number of possible hydrogeologic properties until it converges (Figure 2). In this case, the algorithm reached a stable solution after 86 iterations (Table 1).

The calibrated saturated hydraulic conductivities for the sand of the FCL and the reactive waste rock were somewhat greater than measured (Table 1). Differences were, however, limited and smaller than one order of magnitude. The calibrated hydraulic conductivity of the crushed anorthosite was around one order of magnitude smaller than the measured value. This difference could be explained (in part) by the high density observed in situ (Dubuc, 2018). Calibrated properties were deemed realistic for those types of materials (e.g. Bussière, 2007).

Table 1: Initial and calibrated material properties used in the simulations. k_{sat} : saturated hydraulic conductivity, $\alpha_{VG} n$: Van Genuchten parameters

		ksat	αvg	n
	MATERIALS	(m.s-1)	(m-1)	(-)
Initial	Crushed anorthosite	5×10-4	3.98	2.16
	FCL sand (2)	9×10-5	1.25	6.00
	Waste rock	5×10 -з	7.75	2.34
Calibrated (Iteration = 86)	Crushed anorthosite	9.×10-6	13.79	2.34
	FCL sand	1×10-4	2.44	3.89
	Waste rock	2×10-2	6.16	4.13

(1) Dubuc, 2018 (2) Bréard-Lanoix, 2017

The calibrated water retention curves for the sand and the waste rock were relatively similar to initial properties (Figure 3). The calibrated water retention curve for waste rock was slightly steeper (indicating a material with a somewhat smaller coefficient of uniformity) but the air entry values

remained similar around 1 kPa. The difference between initial and calibrated curves for crushed anorthosite was more marked and could be related to the lack of information for that material.



Figure 3: Measured and calibrated water retention curves of the materials of the experimental waste rock pile. Initial water retention curves are shown with dashed lines. Calibrated water retention curves are shown with solid line.

Volumetric water contents were monitored at two positions in the FCL and two positions in the waste rock during the two large infiltration tests I-C and I-D. Here, only results at 0.8 m depth (bottom of the FCL) are presented (Figure 4). The volumetric water content increased between 5.9 and 15 hours after the beginning of the infiltration test. Maximal volumetric water content was reached when the wetting front passed the sensors. The volumetric water content then decreased and tended to an equilibrium water



Figure 4: Measured (orange curve) and simulated (blue curve) volumetric water content 0.80 m below the surface after large scale infiltration tests I-C (day = 0) and I-D (day = 7).

content (θ =0.09). The same trend was observed for both tests IC and ID.

The wetting front arrived 5.89 h after the beginning of test I-C (Figure 4), and 4.75 h after the beginning of test I-D. Maximum volumetric water content increase was 0.05 for test I-C and 0.03 for test I-D. However, large variations were observed between sensors. For example, the increase of water content for P1 and P6 was more important for measured. The time required to reach the maximal volumetric water content was similar for measured and simulated results. The difference was slightly greater for P6 but remained limited (0.4 days maximum difference for test I-D).

The trend during the drainage was also similar between measured and simulated curves (less for P4). For P1, P2 and P3, the simulated volumetric water content decreased faster than the measured curve. The numerical simulations tended to an equilibrium water content of 0.09 at the end of the drainage for test I-C and test I-D. These results were similar to measured water contents which were around 0.10 for test I-C and test I-D.



Figure 5: Measured (orange curve) and simulated (blue curve) cumulative water flux in lysimeters 2, 4 and 6.

The cumulative water volume or flow was simulated for each of the six lysimeters and compared to measured results. The cumulative water flow in the experimental was rock pile increased when the wetting front reached the lysimeters boundary at the bottom of the experimental waste rock pile. Arrival times in the field were comprised between 12 h and 108 h. The total outflow was around 10.9 m₃ after test I-C which corresponded to 39 % of the infiltration.

The simulated cumulative water volume was three to four times greater than field measurements (Figure 5). The arrival time was smaller than measured. For example, the water front arrived in Lysimeter 4 between 48 h and 62 h after the beginning of the infiltration test I-C, but simulations indicated an arrival time around 36 h. These difference could be explained by the water retention inside the lysimeters (Howell 2005)

3.2 Validation for the 2016-2017 period

The calibrated hydrogeological properties were used to simulate the hydrogeological response of the experimental waste rock pile for a period of approximately 17 months, including two summers (April 4th, 2016 to September 13th, 2017). Some precipitation was not recorded in the study area in 2017, just as the snow melted in 2016 and 2017. Thus, the precipitations of 2017 were adjusted with a weather station from Environment Canada located at 100km from the mine. This station did not record all the precipitation happened in the study area.

During winter (days 245 to 390), there was no infiltration, and the volumetric water content decreased slowly towards residual saturation. Measured volumetric water contents during winter were significantly lower than simulated ones (Figure 5) because most of the water was frozen in the field (water content probes only measure liquid water; (Guo et al. 2018)).

During snowmelt (around day 400), the measured volumetric water content increased significantly and exceeded the simulated results. This is mainly because snow cover was not simulated in the models. However, this did not have an impact on following events occurring afterward.

During the summer of 2016 and 2017 (days 59 and 181, and days 418 to 470), the numerical simulations reproduced relatively well the trends of the water content variations (Figure 6). To illustrate, the wetting fronts at 59 d and 83 d were recorded by the probes. The numerical simulation displayed the same arrival time for P1, P2, P3, and P6. More, the simulation results for P1 and P3 were in good agreement with the general trends of the volumetric water content between day 80 and 181 (Figure 6).

The calibration of the numerical simulations based on large scale infiltration tests I-C and I-D was therefore sufficient to reproduce well the hydrogeological behavior of the experimental pile. Calibrated models could then be used to optimize the FCL design and/or evaluate the effect of extreme climate events.

4 RESULTS ANALYSIS AND DISCUSSION

Waste rock pile numerical simulation calibration was carried out manually in previous research (Dubuc 2018). After recording the large infiltration test, the water content probes were adjusted with different offset and correction methods. This approach can give good results but is time consuming and subject to bias. In this study, the calibration focused on raw hydrogeological response of tests I-C and I-D (Figure 4). The algorithm based the calibration on a few characteristic values only (2 values per probes in the FCL and one value per probe in the top of waste rock).

Optimization using Black Box accelerates the process and a wide range of hydrogeological properties can be tested, thus improving the chances to obtain the best set of input



Figure 6: Volumetric water content at the depth of 0.80m. The graphic starts on April 4th, 2016. The simulation results (blue curve) and the GS3 measurement (orange curve) are shown.

parameters. This large number of trials were independent of field observations that generally are used in manual calibration (Carrera et al. 2005).

In general, calibration and inverse problems are frequent for saturated hydrogeological models (Carrera et al. 2005). Geostatistic tools is often used to adjust the spatial distribution of hydraulic conductivity to satisfy the measures in situ (Carrera et al. 2005). The calibration complexity increases with the number of properties reproducing the hydrogeological behavior of soil for unsatured models (Hollenbeck and Jensen 1998). In this study, the mesh adaptive direct search (MADS) (Audet and Dennis 2006) method used in the Software Nomad allows solving multivariable calibration problems in a black-box function (Audet and Kokkolaras 2016). The black box enabled to gather data processing and numerical simulation with a fully automated. Also, the black box optimization has many computational options that were not used in this study. Since, the hydraulic conductivity has dependency on the air entry value and water entry value (Hollenbeck and Jensen 1998, Aubertin et al. 2003). Thus, a bi-objective algorithm with a black-box function may be used to reproduce the correlation between those properties. A similar approach was used in civil engineering to optimize dampers for adjacent buildings under seismic excitations(Bigdeli et al. 2012).

5 CONCLUSION

An experimental waste rock pile was built with the support of Rio Tinto Fer et Titane at the Tio mine site to validate a new management approach which aims to control water infiltration and limit drainage contamination in piles using an inclined FCL. Experimental results were used to calibrate numerical simulations. A black box algorithm was proposed to automate the calibration of the hydrogeological properties. The algorithm could reduce bias induced by manual calibration. The calibrated models were validated using a 523 d numerical simulation. Simulations tended to reproduce the volumetric water content well at a depth of 0.80 m. However, the calibrated simulations were not very precise regarding the evaluation of the volume of leachate.

This calibration method could be applied to other calibrations to study climate change, geotechnical stability or capillary barriers.

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