

Development of a predictive numerical model of water–rock interaction to estimate mine drainage water quality evolution from a waste rock dump located in northern Chile

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Abstract

Waste rock dumps are considered one of the main sources of compromised mine drainage, both due to their geochemical and physical properties, and the large volumes they can reach.

The objective of the study is to evaluate the chemical stability of an extensive waste rock dump located in northern Chile, at a high geographic altitude (over 4,000 m) in extremely arid and high evaporation conditions, and to predict the water quality of its effluents in preparation for the mine closure stage.

The heterogeneous particle size, when considered with the extended geometry of the waste dump, favours water and oxygen circulation through the material. Its internal structure was modelled using a detailed block model and it was characterised by different geoenvironmental units, depending on the area and future growth stages, as determined using detailed geochemical tests. A prediction of effluent water quality was made through numerical modelling carried out with iCP software, which couples unsaturated flow, heat transmission, solute transport and geochemical reactions in the waste dump. Thereafter, the reaction rates of the various minerals were calibrated by performing kinetic geochemical tests.

Reactive materials vary both in location and concentration inside the dump, which leads to a spatially and temporally variable mine drainage generation process. In response, modelling allows for the prediction of mine drainage evolution in time and space, and therefore evaluation of the need for and/or relevance of prevention, control and/or treatment measures. This can be considered according to the risk that they pose as part of an onsite chemical stability management strategy.

Keywords: *acid-base accounting, acid mine drainage, acid rock drainage, block model, effluent chemical quality, geochemical characterisation, geoenvironmental units, kinetic tests, metal leaching, predictive numerical modelling, reactive transport, static tests, unsaturated flow, waste dump, water quality*

1 Introduction

Among other factors, the quality and quantity of acid rock drainage (ARD) produced by a waste rock dump depends on the geochemistry, porosity, weather and rock exposure. Estimating rock exposure for a waste dump is a difficult task.

Waste rock dumps are usually built based on pit progress and the truck-dumping location, with geochemical aspects not always considered in the design.

To make early decisions related to management and possible growth scenarios it is essential to evaluate the chemical stability of the dump during its useful life, as well as to predict the water quality of its future effluents for closure.

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The example case presented represents mining industrial facilities located in northern Chile at an altitude of 4,400 m above sea level in an arid climate (low rainfall and great thermal amplitude), and applies to a waste rock dump that has been in operation for 20 years (Figure 1).

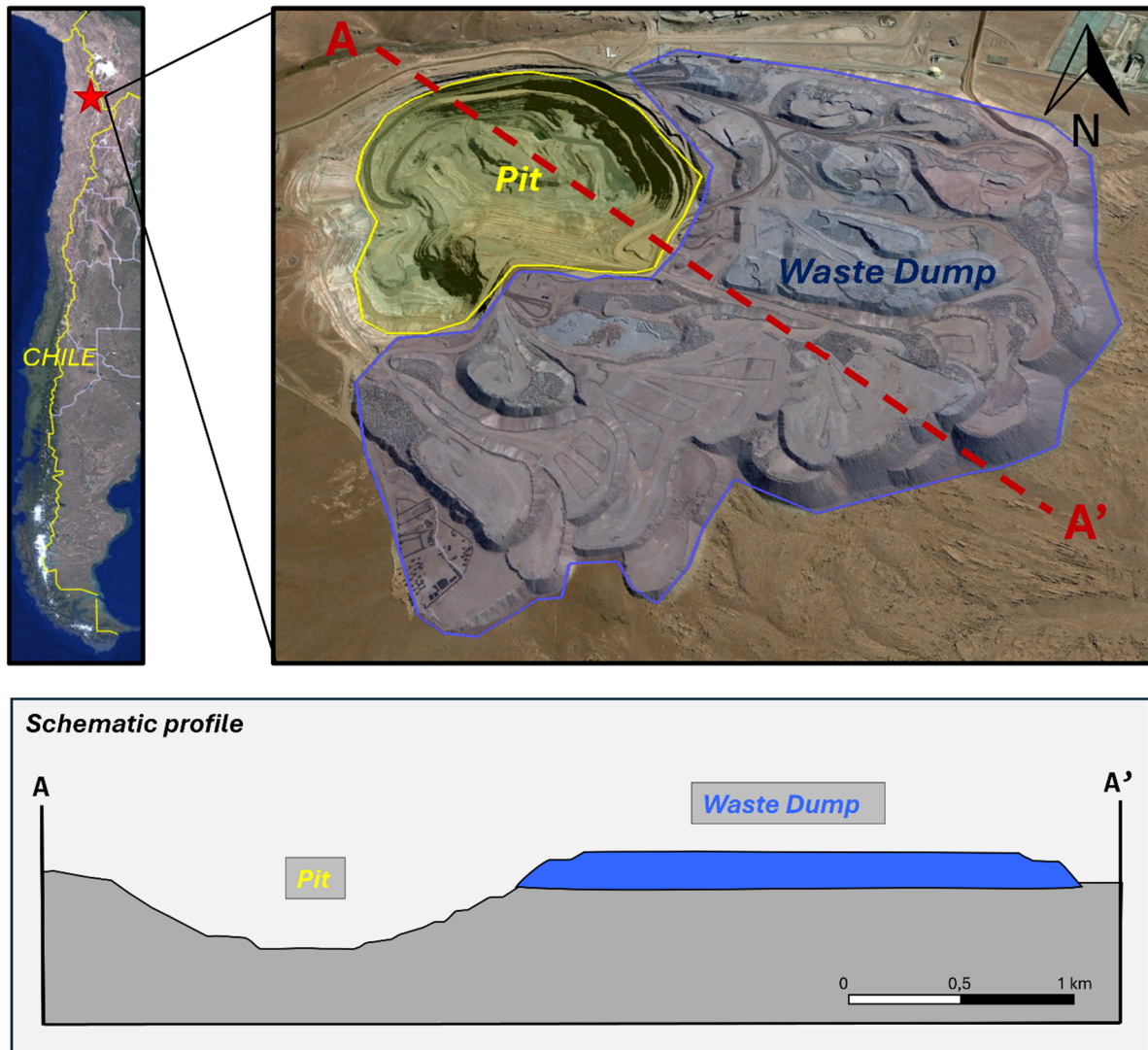


Figure 1 Location of the example case

1.1 Geological context

The geology of the mining district is composed of stratified rocks (rhyolites, andesites, dacites) and intrusive rocks, where volcanic units are intercalated with sandstones and limestones. The spatial distribution of the geological units is strongly controlled by fault systems which are oriented northwest–southeast and north-northwest–south-southeast. The geological faults also exert significant control over both high-grade hypogene copper mineralisation and supergene mineralisation.

The hydrothermal activity led to two types of mineralisation: porphyry-type and high-sulphidation epithermal-type. Of note:

- The low-grade Cu-Mo porphyry mineralisation is developed both in veins and disseminated, and is centred in the vicinity of, and within, the porphyry.
- The high-sulphidation Cu-Ag mineralisation occurs in massive sulphide veins and is located in the Rosario fault system, which cuts through the Cu-Mo porphyry mineralisation in the centre of the porphyry.

In porphyry-type mineralisation, the earliest alteration, apparently sterile, is dominated by disseminated and veinlet magnetite in various proportions. Cu mineralisation in chalcopyrite-bornite is associated with early stages of quartz-biotite-albite and quartz-feldspar veinlets cutting through magnetite veinlets. Some veins are associated with biotite-albite-potassic feldspar alteration. A large proportion of biotite-albite alteration occurs in the surrounding host rock of the porphyry, with only a small amount occurring within the intrusion itself. Molybdenite is observed in transitional veins as scaly aggregates intergrown with quartz and varying amounts of potassic feldspar. Intermediate quartz-pyrite-chalcopyrite veinlets are associated with illite-chlorite alteration (Masterman 2003).

2 Geochemical classification

To characterise the different types of rocks present, geoenvironmental units (UGAs) were defined. These correspond to materials that can be grouped according to different common criteria (lithology, alteration, mineralisation and sulphur content, among others) and that present similar geochemical behaviour. This allows for identification of geological materials with a higher potential for generating ARD leaching of metals while also laying the foundation for the proper management of the chemical stability of the remaining mining deposits after the end of operations (Gascon et al. 2015).

Static and kinetic geochemical analyses were performed on over 152 waste rock samples. Based on those results, the UGAs were defined by considering as the main criterion the mineral zone and the sulphide content as representing the geochemical behaviour of each type of rock in terms of their acid-forming and metal leaching potential (Table 1).

Table 1 Geoenvironmental units (UGAs) classification (Amphos21 2020)

Mineral zone	0–0.1 wt% sulphide	0.1–0.5 wt% sulphide	> 0.5 wt% sulphide
Leached rock		UGA-02	
Oxides and mixed			
Secondary mineralisation	UGA-01		UGA-04
Primary mineralisation		UGA-03	
Primary pyritic			

2.1 Static geochemical analyses

The net potential ratio (NPR) from the acid-base accounting (ABA) procedure is defined by the neutralisation potential (NP) divided by the acid potential (AP). Based on this criterion, a material is defined as non-potentially acid generating (non-PAG) for values higher than three, and PAG for values lower than one (Gascon et al. 2015).

Based on the NPR and on the sulphide sulphur content criterion, the results of the geochemical characterisation show that (Figure 2):

- UGA-01 was non-PAG
- UGA-02 had very low acid-generating potential
- UGA-03 had intermediate acid-generating potential
- UGA-04 had intermediate to high acid-generating potential.

UGA 0 corresponds to a simplified UGA due to the lack of information available to reconstruct the distribution of UGAs in the materials deposited from the start of operations until 2010. This UGA has been established as an average UGA, with its composition determined by the proportion of each of the UGAs (1 to 4) deposited during this period. The calculated proportion of UGAs indicates that it corresponds to 50% UGA 1 and 50% UGA 4.

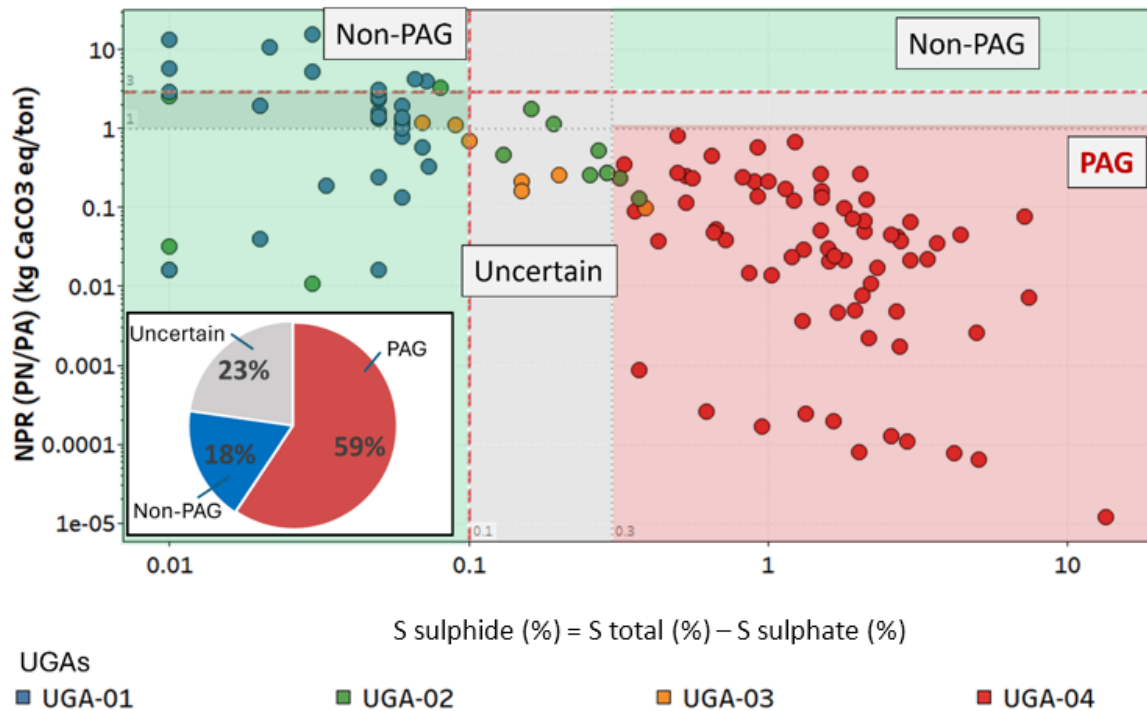


Figure 2 Geoenvironmental units (UGAs) acid-generating potential according to the net potential ratio and sulphur content of the sulphide criterion

Regarding mineralogy, most of the UGAs exhibit a low presence of carbonates, typically below 0.5 wt%, limiting the in situ neutralisation capacity of the materials.

The historical data shows that the classification into UGAs has effectively characterised the materials that will form the waste dump. However, data from the current period indicate an anomaly in the behaviour of a few samples from UGA-01, UGA-02 and UGA-03. Therefore, continued monitoring of mineralogical characteristics is recommended to confirm their behaviour and assess a possible UGA redefinition.

Net acid generation (NAG) leaching tests were also performed, with the results showing that metals and/or leached elements such as aluminium (Al), copper (Cu), cadmium (Cd), iron (Fe), lead (Pb), sulphate (SO₄) and zinc (Zn) tend to be released in effluents and present the highest concentrations at acidic pH levels.

2.2 Kinetic geochemical analyses

Finally, humidity cell tests (HCT) have been conducted on a total of six waste samples. This assay involves subjecting the samples to successive weathering cycles for at least 20 weeks (one cycle = one week) to obtain information on leachate quality and leaching rates.

Since the pH of each cycle reflects the progressive interstitial water interaction and its capacity to generate acidity (or neutralise it), this variable is key to analysing the behaviour of waste rock over time.

At the end of the HCT, the sulphate leaching in the samples was as follows:

- UGA-01 — an average of 1.7 mg/L
- UGA-02 — an average of 1.4 mg/L
- UGA-03 — an average of 4.8 mg/L
- UGA-04 — an average of 16 mg/L (from 9.9 to 46.5 mg/L).

The different samples of UGA-04 trend towards acidification. An inverse correlation between grain size and metal leaching is observed: the fine granulometry fraction of UGA-04 exhibits the highest metal contents, suggesting greater reactivity associated with a larger reactive surface.

3 Distribution and representativeness of the geoenvironmental units in the waste rock dump

Once the UGA definition was completed, the UGAs were implemented into the block model in such a way that, along with the mining plan information, the per cent of each UGA in the waste dump was determined from its inception to the present. The per cent of each UGA until the end of the operation (life of mine, LOM) was determined (Figure 3a) with particular emphasis on the medium term (the next five years).

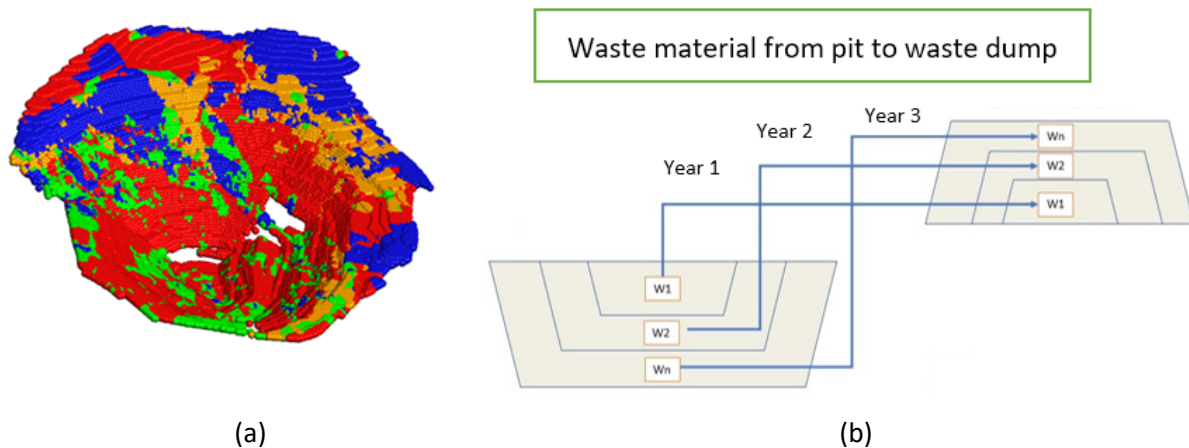


Figure 3 Spatial representation of geoenvironmental units in the open pit and block cubication from the pit to the waste rock dump

To assess the effect of rock exposure and truck-dumping locations on the waste dump's chemical stability, the latter's construction history was rebuilt and its growth projected. The waste blocks (the pit block model) were identified within the intersection volume of the estimated pit surfaces for successive periods (2010–LOM) (Figure 3b). Then a new block model relating to truck-dumping locations and UGA classification was created for the waste dump. The results of the waste dump block model development show that it can represent the variability of periods and UGAs within the deposit. An overview of the block model with the location of UGAs is shown in Figure 4.

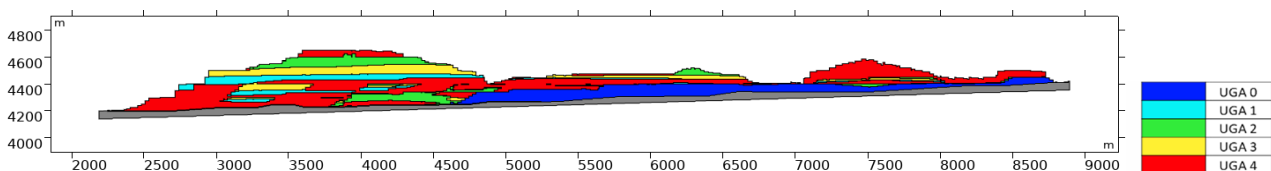


Figure 4 Projected surface of the dump in the year 2065, in terms of the geoenvironmental units

4 Predictive geochemical model

To predict the future water quality of the waste rock dump effluent, a predictive numerical model was carried out with iCP software.

4.1 Modelling code

The Comsol-PhreeqC interface (referred to as iCP) is a reactive transport simulator that allows the coupling of processes for different multiphysical phenomena such as unsaturated flow or heat transfer (Nardi et al. 2014). At this interface, unsaturated flux, heat transmission and solute transport are calculated with Comsol multiphysics software (Comsol 2020) while chemical reaction calculations are carried out in PhreeqC (Parkhurst & Appelo 2013).

4.2 Kinetic behaviour calibration using humidity cell tests

To understand the kinetic processes that occur between waste rock dump materials upon contact with oxidising agents (e.g. water and oxygen), numerical modelling of leachate qualities has been conducted, and calibrated using experimental data from the HCT.

4.2.1 Input data

The sample mineralogical composition and the surface areas of the mineral phases have been used as an input for the model to reproduce the results obtained in the HCTs through numerical modelling.

The HCTs are based on the ASTM D5744-18 methodology (ASTM International 2024), which allows the weathering reactions of a solid sample in a controlled laboratory condition to be reproduced. These tests have been used to characterise the UGAs. In the specific case of UGA-04 they were conducted to define and confirm the geochemical long-term behaviour.

In iCP a 1D geometry was considered, designing cells 10.2 cm wide by 20.3 cm long with an element size of 1 cm, where the first 8 cm of the cell are occupied by the sample. Additionally, the empty part of the cell (12.3 cm) has been included because, upon saturating the sample with 1 L of water, a portion of water accumulates over the sample.

The flow of water and air enters through the top of the cell in one-week cycles. The water flow within the cell under unsaturated conditions is calculated using the Richards equation, considering a sample porosity of 43% and a hydraulic conductivity of 4.5 m/d.

At the beginning of each cycle, 1 L of water is injected at the upper boundary of the model. After one hour of contact, the experimentally measured amount is extracted through the lower boundary (this amount varies from cycle to cycle and ranges between 0.79–0.99 L). Meanwhile, the remaining water in the sample evaporates with dry air circulation through the cell.

The sample selected for modelling corresponds to UGA-04 with a median grain size (0.06 to 0.14 cm). The mineralogical composition of this sample was determined through X-ray diffraction (XRD) and is summarised in Table 2.

Table 2 UGA-04 mineralogical composition

Mineral phase	Formula	UGA-04 wt%
Albite	$\text{NaAlSi}_3\text{O}_8$	0.57
Chlorite	$(\text{Mg,Fe})_3(\text{Si,Al})_4\text{O}_{10}$	9.15
Muscovite	$\text{KAl}_2(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$	34.72
Oligoclase	$(\text{Na,Ca})(\text{Si,Al})_4\text{O}_8$	3.54
Pyrite	FeS_2	5.58
Quartz	SiO_2	45.72
Rutile	TiO_2	0.72
	Total	100

Regarding the modelled minerals, quartz has not been explicitly included as it is considered chemically stable. Similarly, rutile was not considered due to insufficient thermodynamic data. In addition to these mineral phases, 0.25% of carbonates (calcite) has been included, recalculated from the NP result of the ABA test conducted during the 2022 campaign.

4.2.2 Results

In an initial estimation, the reactive surface area of the minerals was calculated considering a particle diameter of 2.37 mm. However, in the calibration process, adjustments were made to the surface areas to fit the results to the HCT. The initial, final and increment surfaces used are detailed in Table 3.

Table 3 Surface areas (Sa) used for the kinetic reaction calculation of each mineral, initially and after model calibration, as well as the resulting increment factor

Mineral phase	Sa initial (m ² /L)	Sa calibrated (m ² /L)	Increase factor
Pyrite	0.10	2	20
Calcite	0.0086	3,000	3.5 × 10 ⁵
Albite	0.02	0.4	20
Clinocllore (chlorite)	0.32	64	200
Muscovite	1.15	20.3	20
Oligoclase (plagioclase)	0.12	2.46	20

Furthermore, calcite was modelled as a kinetic phase. Indeed, when calcite is modelled as an equilibrium phase it depletes after just a couple of cycles, ceasing to mitigate pH and leading to very acidic pH values, which does not represent what happens in field conditions, where such low pH values are not seen. However, experimental results indicate a gradual dissolution. Therefore, the kinetic expression for calcite dissolution includes an exponent that considers the evolution of the surface area as dissolution progresses:

$$S_a = S_{a,0} \cdot m_0 \cdot \left(\frac{m}{m_0}\right)^n \quad (1)$$

where:

S_a and $S_{a,0}$ are the surface area of calcite at each moment and at the beginning, respectively

m and m_0 correspond to the amount of moles of calcite at each moment and at the beginning

n is the exponent.

The model calibration results in $n = 3$. As indicated in Table 3, the surface area of calcite has had to be substantially increased (five orders of magnitude). This is equivalent to considering conditions close to equilibrium. Figure 5 shows the evolution of the pH, sulphate and carbonate/bicarbonate concentration of the experimental results compared with the calibrated model results.

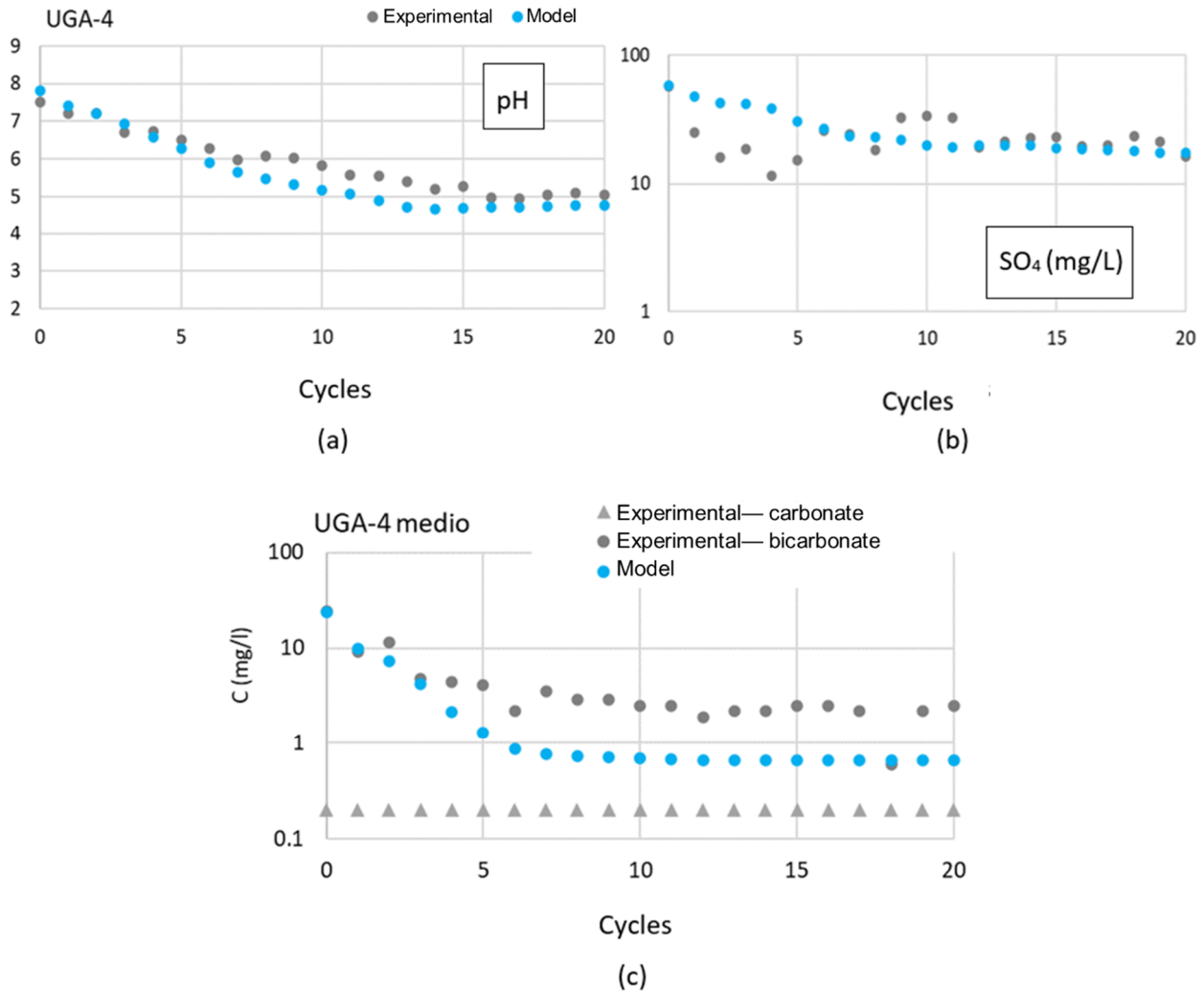


Figure 5 Evolution of the humidity cell tests (grey): pH (a); Sulphate (b); Carbonate/bicarbonate concentration (c) where carbonate concentration represented by grey triangles and bicarbonate concentration by grey circles, as compared with the calibrated model results (blue)

Regarding concentrations obtained for the drainage water from the cell after each modelled cycle, it was observed that the evolution of pH shows a decreasing trend from an initial value of 7.5 to stabilise around pH 5. This gradual decrease in pH in the effluent waters is attributed to a reduction in calcite dissolution, which mitigates acidification. The values obtained in the modelling are compared with the experimental data (Figure 5a).

As evidenced in Figure 5b, sulphate (SO₄) dissolution remains consistent across the various cycles and, overall, these results are well reproduced by the modelling.

On the other hand, the evolution of HCT carbonate concentration (CO₃ and HCO₃; Figure 5c) compared to the carbonate concentration obtained with the calibrated model (blue), is also reproduced by the model, although the calculated final concentration is slightly lower. This phenomenon can be attributed to the equilibrium with atmospheric CO₂, which generates greater transfer between dissolved inorganic carbon species and CO₂ in the gas phase. Figure 6 shows the evolution of calcium and iron concentrations for the experimental results compared with the calibrated model results.

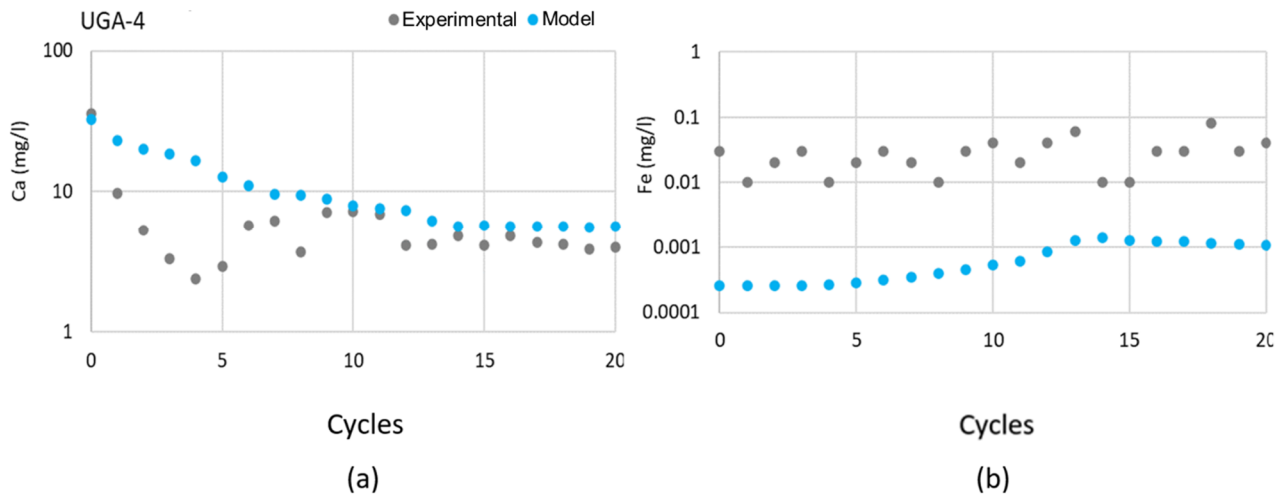


Figure 6 Evolution of humidity cell tests: (a) Calcium; (b) Iron concentration, in mg/L, compared with the calibrated model results (blue)

The calcium concentration is mostly derived from calcite dissolution and shows good agreement with the experimental results (Figure 6a). Meanwhile, the iron concentration obtained with the model is restricted by the solubility of ferrihydrite (Figure 6b). The experimental concentrations, which are slightly higher than the modelled ones, may be due to the presence of colloids.

4.3 Dump modelling

With the reaction surfaces calibrated, the numerical model of the waste rock dump was developed considering a variable saturation model.

4.3.1 Input data

The behaviour of the waste rock dump has been simulated using a multiphase approach that involves solid (UGAs), liquid (pore and infiltration water) and gas (air circulation inside the dump) interaction. Given the multiple variables of the problem, it has been solved using three 2D models of multiphase flow and non-isothermal reactive transport.

The three sections carried out were built following the traces of the main streams on which the dump will be located at the close of the operation (year 2065). The geometry of each section includes the different UGAs deposited in the dump, the presence of a drain in one of the streams and a generic hydrogeological unit under the dump. The UGAs distribution in the dump has been carried out based on a block model that integrates the mining plan with the past and future annual growth of the dump.

Figure 7 presents a simplified diagram of the unit arrangement within the dump. This diagram enables us to analyse the potential impacts that could arise from the placement of reactive materials in the landfill. It serves as a simplified example of a conservative scenario.

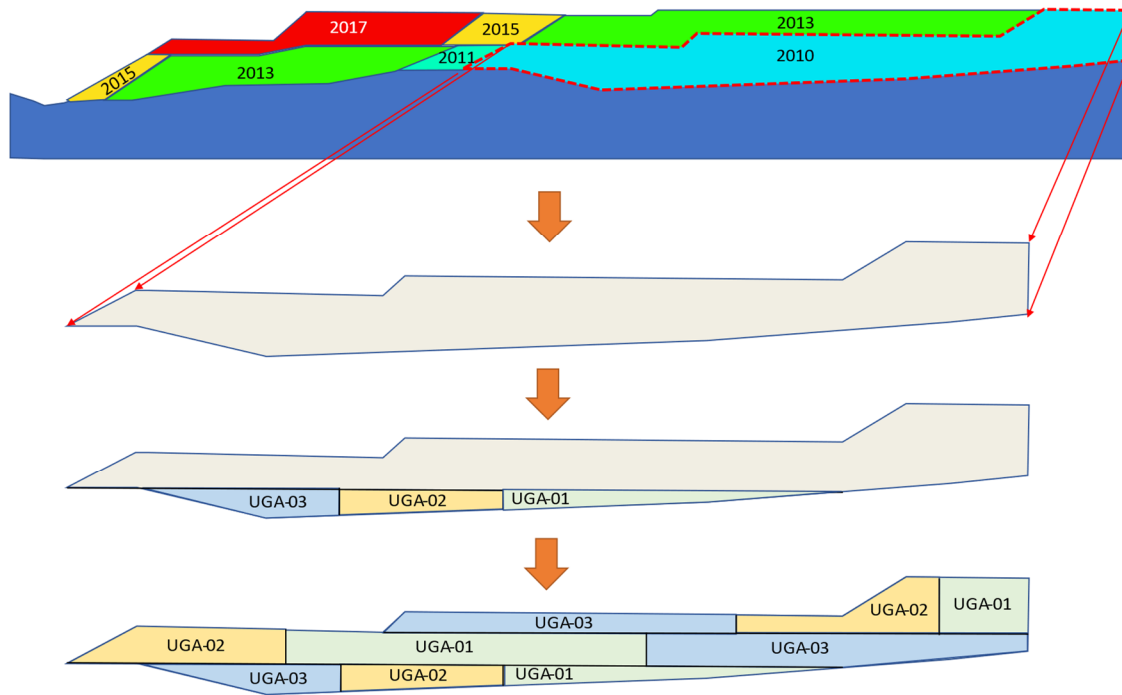


Figure 7 Conceptual model of geoenvironmental unit (UGA) disposal in the dump

Pyrite oxidation constitutes the main source of heat, and its transfer will occur through thermal conductivity (solid-liquid-gas) and advection (liquid-gas) processes. The thermal properties of the UGAs have been estimated as similar to those of homogeneous soils, considering thermal conductivity values of $150 \text{ kJ} \cdot \text{day}^{-1} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$, specific heat of $0.8 \text{ kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ and a pyrite reaction enthalpy of $1.546 \text{ kJ} \cdot \text{mole}^{-1}$. The importance of this process lies in the impact it has on the liquid and gas circulation inside the waste rock dump.

For gas solute transport, the processes identified as dominant have been advection, dispersion and diffusion. The advection and dispersion estimation has been based on velocity calculations from the multiphase flow model, while diffusion has been calculated using the Millington and Quirk model (Millington & Quirk 1961). Oxygen transport has been estimated with a simplified model since it is not a limiting factor in the oxidation processes, so the atmospheric concentration inside the dump was used at all times.

The mineralogy was defined by the average compositions of each UGA obtained by XRD (Table 4). These mineral phases will dissolve following a kinetic law or, in the case of relatively fast kinetics, following the laws of chemical equilibrium. Furthermore, the variation of water pore chemical composition can lead to secondary phases precipitation of minerals such as gypsum, jurbanite, basalite, jarosite, amorphous silica, calcite, alunite, azurite, malachite, and hydroxides of Al, Fe and Cu, which will precipitate and dissolve following the laws of chemical equilibrium.

The flow of water entering the dump comes from local rainfall, with seasonal variability.

Table 4 Mineralogical composition of geoenvironmental units

	Mineral phase wt%				
	UGA-01	UGA-02	UGA-03	UGA-04	UGA-0
Ferrihydrite	0	0	0	2.211	1.105
Pyrite	0	0	0.455	3.770	1.885
Chalcopyrite	0.088	0	0	1.818	0.953
Albite	7.200	7.185	3.251	0.574	3.887
Muscovite	8.275	9.510	4.887	27.433	17.854
Feldspar	5.700	5.707	15.784	5.719	5.710
Kaolinite	8.705	0.000	2.440	5.959	7.332
Chlorite	17.064	19.911	14.841	7.304	12.184
Biotite	0	0.850	1.075	0	0
Calcite	0	0	0	0.100	0.050

Regarding the reactive surface of the minerals, this has been calculated from the P20 average of values of different granulometric measurements carried out in the dump. The P20 selection is intended to give greater weight to the thinner material, which has a larger reactive surface.

4.3.2 Results

The minerals present progressively oxidise or dissolve due to contact with air and/or rainwater. Each UGA presents a different mineralogical evolution, with Figure 8 showing the dissolution percentages of each mineral as a function of time and in each UGA. The greatest reactivity occurs for calcite, chalcopyrite and pyrite.

The oxidation of sulphides generate acidity within the waste rock dump. This acidification is variable in the different UGAs due to the variable initial content of sulphides and carbonates. Figure 8 shows the temporal evolution of pH for different measurement points. In summary:

- UGAs 1 and 2 do not contain pyrite so their pH values remain neutral or alkaline.
- UGA-3 has pyrite but no carbonates so the pH of this domain drops to a value of three in less than one year and is maintained until the end of the simulation.
- UGAs 4 and 0 contain pyrite and the presence of carbonates (calcite), and show two stages
 - first stage (20–25 years) — the oxidation of pyrite is counteracted by the neutralisation of calcite and the pH drops to 5.5
 - second stage (> 25 years) — the carbonates have been completely dissolved and the pore waters have become more acidic, reaching a pH of 2.

In addition to a pH decrease (Figure 9), the sulphide oxidation leads to a dissolved sulphate concentration increase within the waste rock dump. Finally, Figure 10 shows the increase of sulphate concentrations: in the northern section the initial concentration is 1.44 mg/L and 43 years later it has increased to 100 g/L in UGA-4, 20 g/L in UGA-0 and 1 g/L in UGA-3.

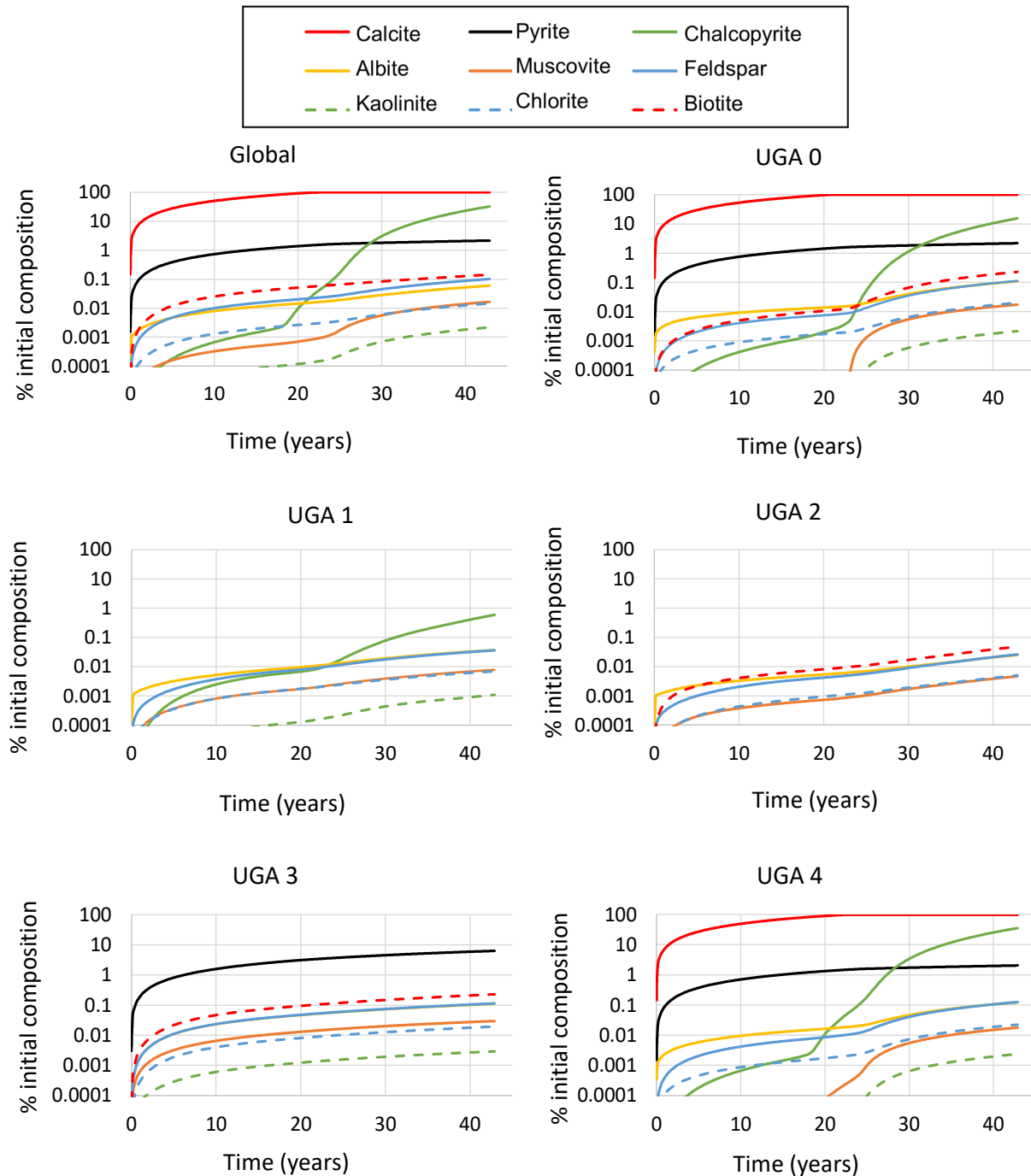


Figure 8 Mineral content/time evolution in the global model and for each geoenvironmental unit (UGA). The percentages refer to the total initial amount of each mineral in each UGA for the entire dump

Regarding the global behaviour of the waste rock dump:

- During the first stage (20–25 years), carbonates neutralise most of the acidity produced by pyrite oxidation. The waste rock dump produces slightly acidic water (pH 5.5–6) and the sulphate and copper concentrations exceed the chilean standard for water irrigation (Chilean National Normalization Institute [INN] 1987).
- During the second stage (> 25 years), carbonates are depleted and the UGAs lose their neutralisation capacity. Therefore, the acidity generation of the dump increases, producing outlet

waters with a pH of 2 and exceeding the chilean standard for water irrigation (INN 1987) for iron and aluminium concentrations.

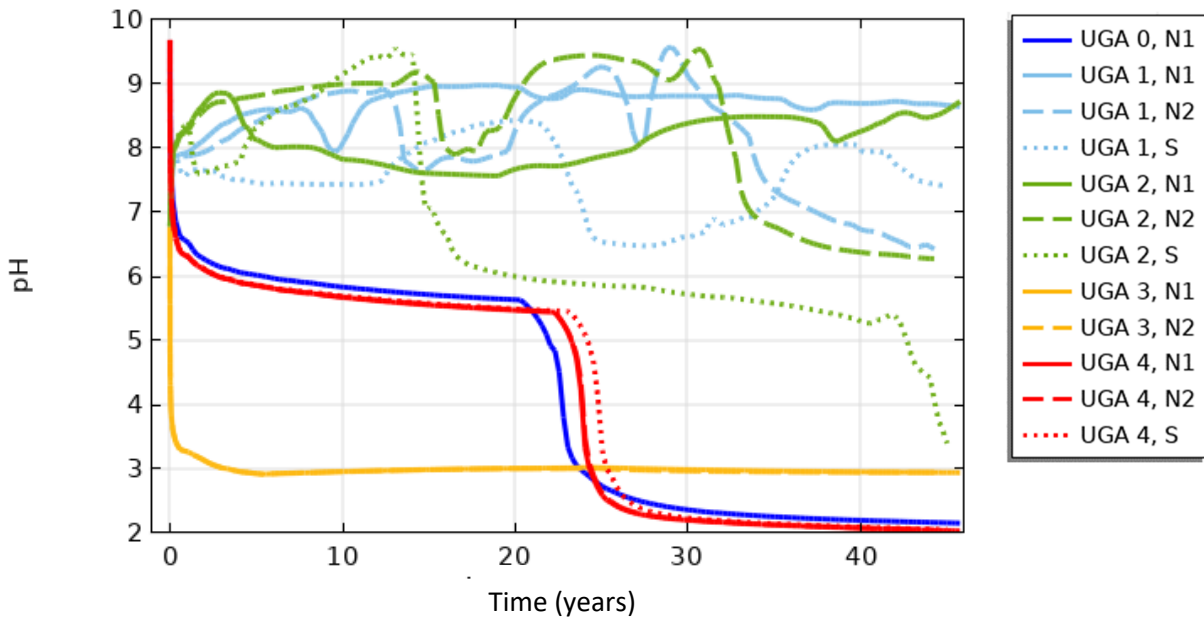


Figure 9 pH time evolution for each geoenvironmental unit (UGA)

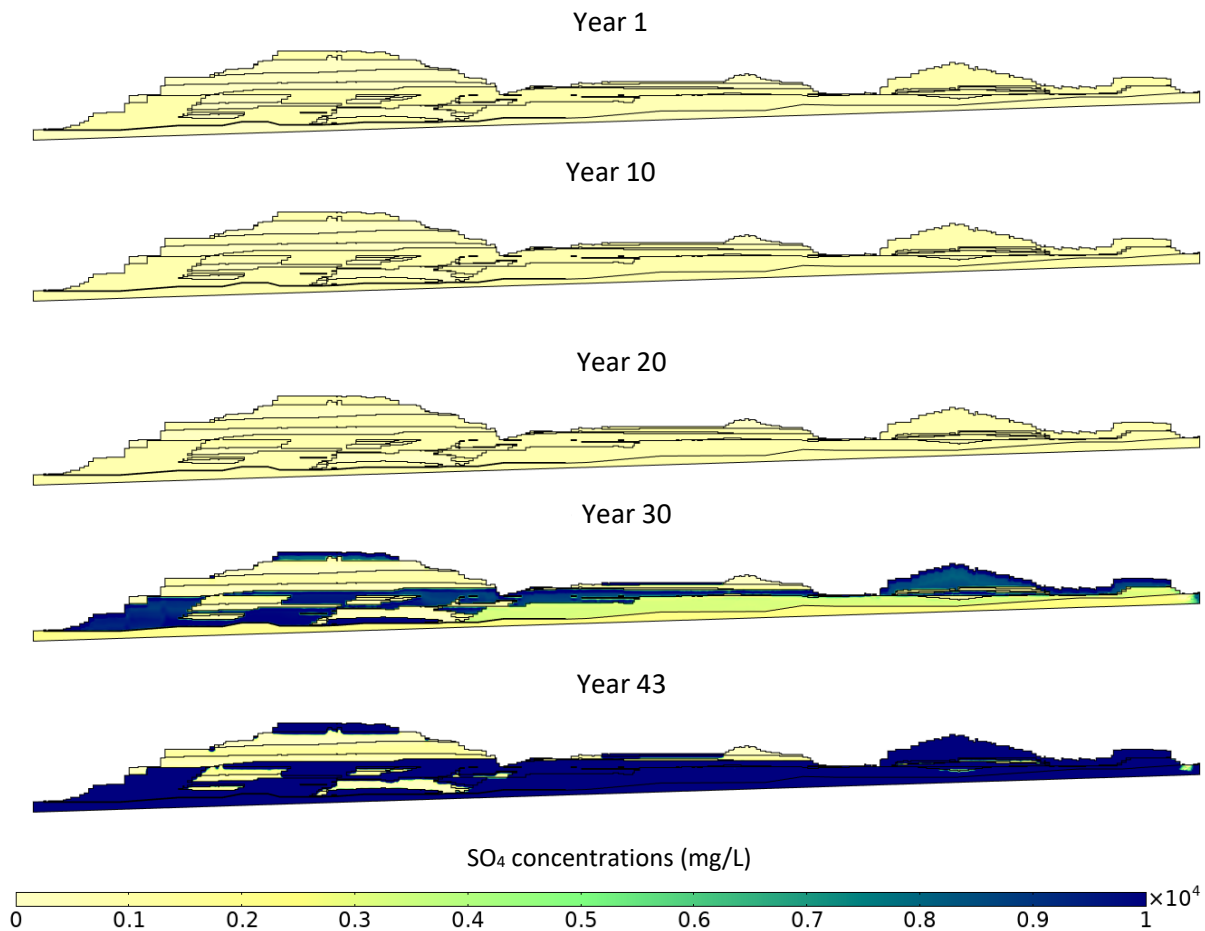


Figure 10 The evolution of sulphate concentration in the dump (2D)

5 Conclusion

Based on the results of the different geochemical static and kinetic tests conducted on many mineral waste samples, UGAs were defined according to their acid mine drainage potential.

The block model review shows that the estimation of the mineral zone and pyrite content is in accordance with the ranges determined by static and mineralogical tests, allowing the use of the UGA definition to create a block model for the waste rock dump. For the LOM, the material destined for the waste rock dump indicates that around 30% has no acid-generating potential, 41% has a low acid-generating potential and 29% presents a high acid-generating potential, as well as a high potential for metal leaching.

To predict the future water quality of the waste rock dump effluent, a predictive numerical model was generated with Comsol-PhreeQC interface (iCP) software: a reactive transport simulator for unsaturated flow. The results from HCT have been used to simulate the kinetic behaviour of the materials through numerical modelling to calibrate the waste rock dump predictive water quality model.

The calibration results indicated that the surface area and the reactivity of the minerals have been underestimated in the initial data and calculations.

Therefore, the following factors were addressed to correct the model:

- Consider equilibrium with CO₂(g).
- Calculate calcite dissolution using a kinetic behaviour.
- Adapt the reactive surfaces of the minerals according to the results of the study.

With these changes, the geochemical model has been able to reproduce experimental results.

Regarding the geochemical evolution of the dump, the most significant processes in the 45 years of simulation are the complete dissolution of calcite and the partial oxidation of pyrite and chalcopyrite.

The results allow for an estimation the waste rock dump effluent water quality evolution into the future. Acidification of the waste rock dump waters was observed due to sulphides' oxidation, together with the release of sulphates and metals. The release of sulphate and metals observed in the modelling allows for a prediction of exceedance of the relevant environmental standards, thus highlighting the need to implement mitigation measures for:

- sulphate and copper concentrations from the beginning
- iron and aluminium concentrations from year 25.

The mitigation measures implemented should lead to updated modelling that confirms their efficiency, with revised water quality projections.

In conclusion, predictive geochemical modelling allows the mining industry to prepare for closure by helping to achieve the chemical stability of applicable facilities that in turn allows for adequate effluent management.

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