Oxidation Modelling to Optimise Waste Rock Storage

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Abstract

Managing storage of potentially acid forming rock (PAF) requires a knowledge of the basic principles of acid mine drainage (AMD) generation; that a source, water and oxygen are required to generate AMD.

Waste rock characterisation through both static and kinetic methods combined with an understanding of the site geological model are commonly used in the early stages of mine planning and development to make inferences about waste storage design and/or potential treatment requirements. In wet environments of New Zealand, vadose modelling is also often undertaken to predict the saturation profile, seepage volumes and capping performance of PAF waste structures (e.g. embankments, constructed dumps). This conceptual modelling is often a crucial component in understanding the mine water balance and identifying zones of continued saturation as well as identifying zones of periodic desaturation. This modelling often defines the height and volume of PAF storage increasing or decreasing the reliance on non-acid forming (NAF) material (placed between the PAF and the surface) which is often in short supply.

However, this focus on saturation (which in very wet environments is a natural tendency) can at times forget the basic principles of AMD generation; that oxygen transport from the surface through to the stored PAF waste material is still a crucial factor for PAF material to generate AMD, and that it's reduction and/or absence (through limited transport mechanisms / pathways) can limit AMD production in unsaturated PAF material. This can result in the potential to optimise PAF storage in unsaturated zones and reduce the volumes of non-acid forming (NAF) material required.

This paper outlines vadose and oxygen modelling undertaken to help defend both saturated and unsaturated storage of PAF material on a waste dump in New Zealand and illustrates how a combined vadose/air model can be utilised to optimise the design of a PAF storage structure.

Keywords: Oxidation, PAF Storage, Unsaturated Zone, Vadose Zone

Introduction

Located in the Buller Coalfield on the West Coast of New Zealand, Bathurst Mining Limited (BT Mining) operate the Stockton Open Cast Coal Mine. The Cypress North Pit is located to the south of the Stockton area and the preferred closure option is to backfill the majority of the pit with Potentially Acid Forming (PAF) material to enable reestablishment of the wetland area present before mining and reduce the requirement for ex-pit storage. The climate on site is dominated by intense rainfall (>5,000 mm per annum), and an expected high groundwater table (post backfill and rehabilitation) within the pit has long been accepted as a viable solution to saturate the backfilled PAF material, prevent substantial sulfide oxidation and hence minimise long term risk (of AMD discharge) to the receiving environment.

Due to uncertainties in the final groundwater recharge level, the existing closure plan provides for a 2-meter buffer of Non-Acid Forming (NAF) material to be placed on top of the PAF backfill, but below the modelled phreatic recovery level to allow for anticipated groundwater response to drought periods that may occur on the West Coast. The previously accepted groundwater recovery level was at 697 m RL which when taking the 2-meter-NAF buffer into account, limited the extent of PAF backfill to a height of 695 m RL. Since this previous work was undertaken a large volume of hydrogeological data from around the site has been collected to reduce data gaps and uncertainty. This data has led to an increased understanding of the local groundwater conditions. GHD has utilised this data to develop a new three-dimensional groundwater model to reduce uncertainty around PAF backfill saturation and enable optimisation of backfill. The work undertaken has revised estimated phreatic recovery levels taking into account a conservative drought period, at a modelled 697 m RL or greater. This has provided confidence for additional PAF storage within the backfilled pit and has raised the possibility of additional PAF saturated storage which would offer relevant benefits in limiting ex-pit PAF storage.

In addition, the possibility of unsaturated PAF storage has been discussed as a potential option for additional in-pit storage above the phreatic zone in areas that are likely to have low oxidation rates and/or the risk of oxidation is deemed low. This is deemed preferable to ex-pit storage which is more likely to be exposed to higher rates of oxidation (depending on cover design) and ultimately will have a greater requirement for ongoing post closure treatment requirements. A large area of PAF backfilled North Pit is to be reinstated as a wetland. Due to the saturated nature of the wetland and the low permeability material between the wetland and the zone of saturation, it is considered unlikely that oxygen ingress through diffusive and/or advective processes (which are considered the dominant means of oxygen transfer) will be high enough to result in unacceptable acidification of the unsaturated PAF material. In addition, pit fill concepts include and increased storage option (ISO) which is likely to have greater oxygen ingress than the wetland cover option. The potential oxygen flux (and hence generation of AMD) needs to be quantified in order to define cover specifics and volume (and type) of PAF material placed in these areas.

To quantify this (theoretical flux of oxygen reaching the unsaturated underlying backfill material), GHD has undertaken oxidation transport modelling utilising the contaminant transport modelling software CTRAN/W. CTRAN/W is a finite element software product that can be used to model the movement of contaminants and gases through porous materials in response to the movement of water (in both saturated and unsaturated zones) and processes involving diffusion, dispersion, adsorption, decay and density dependency. The CTRAN/W model is integrated with its 'parent' vadose model in SEEP/W, which computes water flow velocity.

This paper outlines the modelling undertaken and the results from a series of conceptualised backfilled pit rehabilitation types. These rehabilitation types have been characterised as follows and are considered to broadly cover the ranges of surfaces likely to be present within the fully rehabilitated North Pit:

- Flat Wetland area; Flat topsoiled area; Topsoiled area with 20 degree slope; Transition area with 10 degree slope

Methods

Groundwater Modelling

A groundwater numerical model was developed to assist in the understanding of the groundwater flow dynamics at the Site and predict the groundwater recovery post-mining. The groundwater model was created using Groundwater Vistas 8.15 (Environmental Simulations, Inc, 1996–2021) as the graphic user interface (GUI) for MODFLOW NWT (Niswonger et al. 2011), developed by the United States Geological Survey (USGS).

A conservative model run was applied to the calibrated model depicting response to a derived 6-month minimum average rainfall (1,322 mm) with a return period of 100 years. It is worth noting that the West Coast region is expected to receive increases in rainfall over the next 30 years under predicted climate change scenarios (NIWA 2011) so it is implied that the applied drought scenario is considered a conservative assessment of likely minimum long term groundwater levels within the backfilled north pit. Sensitivity analysis suggested that the estimated minimum groundwater recovery (below which desaturation is considered unlikely) was between 697–698 m RL. A recovered groundwater level of 697–698 m RL was therefore utilised as a key boundary condition within the 2-dimensional oxygen model.

Oxygen Modelling

Diffusion and advection were considered the dominant oxygen transfer processes at Cypress and the modelling undertaken focussed on these processes without explicitly considering barometric pumping and/or convection. This approach is supported by the literature in which oxygen transport through molecular diffusion is considered the main transport mechanism in the majority of mine waste structures (e.g. Mbonimpa et al. 2002).

Modelling of oxygen transport within the backfilled North Pit (via diffusion and advection) was undertaken in the Geostudios modelling software SEEP/W and CTRAN/W (v.2021.3). The oxygen transport is modelled in CTRAN/W based on the steady state vadose modelling undertaken in SEEP/W. Both are finite element software products and together they can be utilised to model the movement of contaminants and gases through porous materials in response to the movement of water (in both saturated and unsaturated zones) and processes involving diffusion, dispersion, adsorption, decay and density dependency.

Four basic 2-dimensional meshes were constructed in SEEP/W for each of the range of surfaces expected. The cross sections utilised the soil properties as outlined in Table 1 which are thought to conservatively represent the varying main surface types and backfilled material. All materials were modelled as saturated/unsaturated within the SEEP/W model.

Boundary conditions applied to the vadose model are as outlined in Table 2. The groundwater level relates to the minimum conservative groundwater recharge within the drought scenario groundwater modelling within the flat backfilled level (700 m RL; GHD 2022). For the sloped scenarios, it is conservatively assumed that the groundwater mounding to the East (Highwall area) is minimal, and a conservative groundwater boundary condition is applied. Infiltration is assumed to reflect the drought scenario (GHD 2022) with a rainfall infiltration of 3 and 1% applied to the flat and sloped scenarios respectively.

The modelled cross-sectional 2-dimensional model mesh was based on a simplified cross-section of the backfill material, liner and cover type with results focussed on the middle of the model cross section to reduce

Table 1 *Soil Properties Utilised in SEEP/W Modelling*

Material	Thickness (m)	Saturated Hydraulic Conductivity (m/s)	Residual Water Content	Saturated Water Content	Anisotrophy (Ky/Kx Ratio)
Soil Cover	0.3	1×10^{-4}	0.05	0.3	1
Pit Liner	2	1×10^{-7}	0.05	0.41	0.1
Pit Backfill	45	5×10^{-5}	0.05	0.3	0.3
Wetland Material	0.3	1×10^{-8}	0.05	0.38	0.1

Table 2 *SEEP/W Boundary Conditions Applied*

Boundary	Boundary Type	Boundary Value
Groundwater Level (applied to extremes of model)	Water Total Head	697–698 m
Eastern Groundwater Level (ISO scenario)	Water Total Head	703 m
Infiltration / Rainfall – Flat Scenarios (A&B)	Water Flux	0.217 mm/day
Infiltration / Rainfall – Sloped Scenarios (C&D)	Water Flux	0. 0724 mm/day

boundary effects and provide results reflective of the various cover types being uniform over a large (ca. 100 m) area. All cross sections were constructed with a global element size of 1 m. The cover materials had a grid ratio of 0.1 (compared to the default grid) applied to ensure that results in the target area are provided in sufficient detail.

The effective diffusion coefficient (D_e) of oxygen into waste material is a combination of the diffusion coefficient in water (D_w) and the diffusion coefficient in air (Da). The transport of oxygen is substantially more rapid in air when compared to water and therefore the Da is many magnitudes of order greater than the Dw. Thus a layer remaining saturated (or close to saturated) impedes the passage of oxygen (in air) which results in reduced AMD generation (Mbonimpa et al. 2002).

The specific oxygen diffusion rates for both the gas phase and dissolved phase have been derived based on Fick's first and second law of diffusion which describe the relationship between the rate of diffusion and the three factors that affect diffusion-surface area, concentration difference and thickness of the substrate and Henry's constant which relates to the concentration of gas particles in the solution phase that is in equilibrium with the pressure of the gas in the vapor phase.

Based on the backfilled waste and cover/liner properties as outlined in Table 1, the oxygen diffusion rates based on the air and water content were then calculated and these relationships included in material properties in CTRAN/W. The equations utilised to calculate oxygen diffusion rates (equations 1–4) assume ambient temperatures and were modified from Aachib et al. (2004).

$$D_a = \frac{1}{n^2}\left(D_a^0 \theta_a^{Pa}\right) \quad (1)$$

$$Dw = \frac{1}{n^2}\left(HD_w^0 \theta_w^{Pw}\right) \quad (2)$$

$$Pa = 1.201\theta_a^3 - 1.515\theta_a^2 + 0.987\theta a + 3.118 \quad (3)$$

$$Pw = 1.201\theta_w^3 - 1.515\theta_w^2 + 0.987\theta w + 3.118 \quad (4)$$

Where n represents the porosity of the material; D_a^0 and D_w^0 represent the coefficient of free diffusion of oxygen in air and water respectively; H is Henry's constant (≈ 0.03 @ 20°C); Pa and Pw are calculated as a function of the volumetric air (θa) and water (θw) content.

Further considerations have been given to the oxygen reaction rate coefficient (Kr) within the modelling process as consumption of oxygen within the placed waste material will also drive advective processes within the backfilled material. The Kr has been estimated based on surface kinetics in which the rate considers the particle size distribution, reactivity of pyrite with oxygen, the pyrite content of the PAF material and the porosity of the material. Equation 5, 6 and 7 have been utilised as per Collin (1987).

$$Kr = K' \frac{6}{D_H}(1-n)Cp \quad (5)$$

$$D_H = [1 + 1.17\log(C_u)]D_{10} \quad (6)$$

$$C_u = D_{60}/D_{10} \quad (7)$$

Where K' is the reactivity of pyrite with oxygen; Cp is the pyrite content; n is the porosity; Cu is the coefficient of uniformity (D_{60}/D_{10})

The site-specific values adopted in the above equation and their sources are provided in Table 3.

The calculated Kr show small increases in Kr with corresponding increases in saturation. The increasing Kr (with increasing saturation) can be explained by low moisture content within the reactive materials becoming the limiting factor in the oxidation process (Gosselin et al. 2015), although it is likely the Kr value would decrease at very high saturation rates. The Kr values applied are therefore considered conservative.

The boundary conditions applied to the CTRAN/W model assume atmospheric oxygen at a concentration of 276.7 g/m³ with a base concentration of 0 g/m³.

Results

The flat Wetland scenario (Scenario A) showed a high degree of saturation at the surface with saturation not falling below >93 % throughout the backfill profile due to applied rainfall and the water retaining capacity of the material properties. The flat soil scenario (Scenario

Table 3 Oxygen Reaction Rate Coefficient Inputs

Input	Units	Source	Value
K^*	m^3 O_2/m^2 pyrite / s	Assumed from Literature	5×10^{-10}
C_p	%	Site Data	1.92
D_{10}	mm	Site Data	0.00002
D_{60}	mm	Site Data	0.0095

Table 4 Modelled Oxygen Flux

Scenario	Scenario Description	Oxygen Flux kg/d/m² (at top of PAF material)	Oxygen Flux kg/d/m² (at 2 m depth)
A	Flat Wetland area	5.6×10^{-10}	$<1.0 \times 10^{-10}$
B	Flat topsoiled area	1.1×10^{-5}	$<1.0 \times 10^{-10}$
C	Transition area with 10 degree slope	8.5×10^{-5}	$<1.0 \times 10^{-10}$
D	Topsoiled area with 20 degree slope	4.0×10^{-4}	$1.71 \times 10^{-6*}$

*Reduces to $<1.0 \times 10^{-10}$ kg/d/m² at 3m below surface.

B) showed a similar high degree of profile saturation with desaturation within the soil itself a function of the relatively higher water conductivity compared to the wetland (1×10^{-4} m/s compared to 1×10^{8} m/s for the soil/wetland covers respectively).

The sloped soil covers (Scenarios C and D) showed lower saturation levels in the sub-surface (to depths of approximately 5 and 10 below the landform) for the 10° and 20° slopes respectively which reflect the expected lower infiltration rates (and higher runoff rates) of rainfall on the sloped surfaces compared to the flat surface profiles and as per Scenario B, the relatively high assumed hydraulic conductivity value applied to the cover soil material.

Scenario A (Flat Wetland) has a low modelled flux of oxygen (5.6×10^{-10} kg/d/m²) infiltrating the cover material (Table 4). This is a reflection of the high saturation rates of the wetland and the high water groundwater table within the PAF material (the modelled minimum groundwater level is ca. 2 metres below the surface of the backfilled material). The modelled oxygen flux rate increases by several orders of magnitude in Scenario 2 (flat topsoiled scenario) which is largely a function of the assumed increased hydraulic conductivity within the soil (compared to the wetland cover). The sloped scenarios see increasing rates of oxygen flux reaching back-filled PAF, although this flux is limited to the upper 2–3 m of the stored material with very low oxygen flux rates still evident in all modelled scenarios ($<1.0 \times 10^{-10}$ kg/d/m²) below this point.

Discussion and Conclusion

The oxygen model suggests low rates of oxygen flux beneath the proposed wetland area within the backfilled North Pit. This is a result of the expected high groundwater table, flat profile of the surface materials and saturated state of the overlying materials. Organic material within the wetland will also likely consume oxygen resulting in a low risk of oxygen inundation into the stored PAF material. The modelling suggests that storage of PAF material in the unsaturated zone beneath the wetland presents a low overall risk of substantial oxygen ingress and hence acidification of that material upon mine closure.

Modelling suggests that backfilled areas covered in soil will likely result in greater rates of oxygen ingress and risk to acidification to underlying non-saturated PAF material compared to the wetland area. This effect is more pronounced in the sloped backfill scenarios where rainfall infiltration is reduced and the underlying groundwater table is potentially lower.

A number of oxygen probes are present within BTs Stockton Mine and the Northern Elevated Landform (NELF) adjacent the Cypress North Pit where monitored oxygen concentrations are reduced considerably (by several orders of magnitude) between the surface, the top 1m of backfill and the backfill below this depth. These observations align with predictions for the non-wetland cover scenarios presented here where a rapid decrease in concentration is observed within the top 1 m of backfill. This suggest that low ingress of oxygen through the cover surface at Stockton is common and that the modelled results here are reasonable and consistent with this.

The rate of oxygen ingress in the non-wetland scenarios may be reduced by material selection and/or soil conditioning. Terracing and/or slope reduction may also reduce the oxygen ingress and AMD generation in these areas. Likewise, the risk to acidification and generation of AMD may be reduced by placement of PAF material outside the zone of oxidation and/or the placement of low PAF material in the upper zones of the backfill. The risk to the receiving environment (in terms of AMD generation, flux and seepage) should be assessed based on these findings to optimise PAF placement within the North Pit.

The predicted oxygen flux rates for the non-wetland scenarios can be further refined once the conceptual cover design(s) are better understood. It is acknowledged that a 0.3 m soil cover is a very simplified cover and that in reality such a cover 'type' would consist of several layers of engineered material to enable vegetation growth, limit erosion and limit oxygen ingress with the sloped areas potentially containing terraces as well as sloped portions. The material would likely be limited to locally sourced/stockpiled material and soil properties could vary over different portions of the backfill. Once these variables are understood, the conceptual cover design can be developed further to better represent the conceptual design (rather than the presented simplified cross sections), allowing the placement of PAF to be optimised. Revised oxygen modelling will be able to provide oxygen flux over the entirety of the backfilled North Pit in order to better quantify likely ingress rates and ultimately AMD generation over the pit as a whole.

It is recommended that rehabilitated backfill covers be conceptualised in more detail with potential closure options (e.g. sloped, flat, terraced) replicated on site (to as close as feasibly possible). This should enable field calibration measures for the oxygen modelling and will enable further development of the oxygen model.

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