# A numerical study of oxygen flux through inclined covers with capillary barrier effects



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# ABSTRACT

Covers with capillary barrier effects (CCBEs) can be used to control the generation of acid mine drainage (AMD) caused by the oxidation of sulphide-rich mine wastes. In humid climates, CCBEs placed over reactive tailings are designed mainly to limit oxygen flux. Various studies have examined the influence of cover slope on the unsaturated hydrogeological behaviour of CCBEs. Results show that water distribution in inclined CCBEs depends on geometric factors (including slope inclination and length) as well as hydraulic properties of the cover materials and underlying wastes. Recently, numerical simulations performed with VADOSE/W (Geoslope Inc.) have been used to further assess the influence of slope geometry and sulphidic tailings properties on the ability of an inclined CCBE to limit oxygen diffusion. The simulated CCBEs are inclined at about 18 degrees and have a length of 10 m, 30 m and 50 m; the bulk oxygen reaction rate coefficient  $K_r$  of the tailings varied between 40 and 10,000/year (or 0.1 and 27.4/day). A highly interesting finding from the numerical calculations is the significant effect of tailings reactivity: for a given set of conditions, the oxygen flux through the cover tends to increase with the value of  $K_r$ . Furthermore, the results indicate that the oxygen concentration at the CCBE-tailings interface, which is typically assumed as being nil in most analytical calculations, can be much higher. This can lead to an underestimation of the CCBE efficiency.

# RÉSUMÉ

Les couvertures avec effets de barrières capillaires (CEBC) peuvent être utilisées pour limiter la production du drainage minier acide (DMA) provenant de l'oxydation de minéraux sulfureux que contiennent certains rejets miniers. En climats humides, ces CEBC jouent le rôle de barrières à la migration d'oxygène vers les résidus réactifs. Différentes études ont été réalisées afin d'évaluer l'influence de la pente de recouvrement sur le comportement hydrogéologique non saturé de CEBC. Les résultats ont montré que la distribution de l'eau dans la CEBC est influencée par les différents facteurs géométriques (incluant l'inclinaison et la longueur) et par les propriétés hydriques des matériaux de la CEBC et des rejets sous-jacents. Récemment, des simulations numériques ont été menées avec le code VADOSE/W (Geoslope Inc) pour évaluer l'influence de la géométrie de la pente et des propriétés des rejets sulfureux (générateurs de DMA) sur la capacité d'une CEBC inclinée à limiter la diffusion de l'oxygène. Les CEBC simulées avaient une inclinaison d'environ 18 degrés et une longueur de 10 m, 30 m et 50 m; le coefficient apparent du taux de réaction  $K_r$  des rejets variait entre 40 et 10000/an (ou 0.1 et 27.4/jour). Une des plus intéressantes conclusions de ces résultats numériques est l'effet significatif de la réactivité des résidus pour une série de conditions données: le flux d'oxygène à travers la couverture augmente avec la valeur de  $K_r$ . En outre, la concentration d'oxygène prédite à l'interface CEBC-résidus, que l'on considère souvent nulle pour des fins de simplification, peut être beaucoup plus importante que zéro. Cela peut conduire à la sous-estimation de la performance de CEBC.

# 1 INTRODUCTION

One of the main environmental challenges faced by mining companies is acid generation caused by oxidation of sulphide-rich mine wastes. To limit the environmental impact caused by acid mine drainage (AMD), several techniques have been developed in recent years. In humid climatic conditions, a cover with capillary barrier effect (CCBE) can be used to create an oxygen barrier to limit oxidation of the covered tailings (e.g., Collin 1987; Nicholson et al. 1989; Collin and Rasmuson 1990). In some instances, CCBEs are placed on inclined surfaces; such is the case, for example, when dykes have been constructed using AMD-generating mine wastes. Various studies have focused on the interpretation of laboratory and field measurements and numerical modelling to determine the behaviour of inclined CCBEs in relative humid climates (Aubertin et al., 1997, Bussière, 1999; Bussière et al. 2003; Maqsoud et al. 2005). To date, the performance of inclined CCBEs used as oxygen barriers has been mostly evaluated in terms of hydraulic response (volumetric water content ( $\theta$ ) and suction ( $\psi$ )). Results of these investigations have shown that a desaturation can sometimes occur uphill in the moisture retaining layer of the CCBE. Because oxygen migration is easier when the water content is reduced, the desaturation can affect the CCBE efficiency to control oxygen diffusion. Various means, including the use of suction breaks, have been proposed to attenuate the risk of desaturation near the top of the slope (Aubertin et al. 1996a,b, 1997; Bussière, 1999; Maqsoud et al. 2005).

Although hydraulic characteristics such as  $\theta$  can be linked to parameters controlling diffusive oxygen migration through CCBEs (e.g. Collin 1988; Aubertin et al. 2000; Mbonimpa et al. 2003; Aachib et al. 2004), it remains difficult to precisely quantify oxygen flux through an inclined CCBE. The volumetric water content is known to vary over time along slope and depth in a CCBE and in the underlying tailings. Averaging the materials characteristics to estimate oxygen flux involves several simplifying assumptions (Bussière et al. 2003), which can lead to less accurate results. It is much preferable to directly quantify the oxygen flux through the cover at various locations

The results presented here stem from a study recently performed to evaluate the effect of inclined cover configurations on oxygen migration using the numerical VADOSE/W (Geostudio 2004 - Geoslope code International 2004). Oxygen migration was quantified in terms of global cumulative oxygen flux reaching the tailings beneath the CCBE over time (Cissokho 2007). The numerical simulations were conducted to assess the effect of various parameters on CCBE behaviour, and to evaluate the efficiency in reducing oxygen flux. The parameters varied in the models include geometry (length and slope angle) of the inclined CCBE, hydraulic properties of the material used in the moisture-retention laver (water retention curve and saturated hydraulic conductivity) and reactivity of the underlying tailings. The effect of suction breaks added near the top of the slope was also studied.

The investigated CCBEs are inclined at about 18 degrees (i.e. about 1V:3H) and have lengths of 10 m, 30 m and 50 m. The apparent oxygen reaction rate coefficients of the tailings varied between 40 and 10,000/year (or 0.1 and 27.4/day). After a brief presentation of the model, the material properties and applied boundary conditions are described. Typical results expressed as vertical oxygen concentration profiles, oxygen concentration along the slope, global cumulative oxygen flux per m of width and global cumulative oxygen flux per m of width and m of length at the cover-tailings interface are then presented and discussed.

#### 2 MODELLING PROCEDURE

VADOSE/W was used to simulate water and vapour flows as well as gas (oxygen) diffusion. The governing equations for these processes are described in Krahn (2004). Only the oxygen transfer equations are recalled here. The two-dimensional models used to simulate the inclined CCBE, the applied boundary conditions and the material properties are also described in the following sections.

#### 2.1 Oxygen transfer equations in VADOSE/W

For two-dimensional molecular diffusion in an unsaturated porous medium which is consuming oxygen at a first order rate, the instantaneous oxygen flux F(x, y, t) [ML<sup>-2</sup>T<sup>-1</sup>] and concentration C(x, y, t) [ML<sup>-3</sup>] at position (x, y) and time t are determined from the Fick's first and second laws defined as follows (Krahn 2004; see also Collin and Rasmuson 1988; Yanful 1993; Mbonimpa et al. 2003):

[1] 
$$F(x, y, t) = -D_e \left( \frac{\partial C(x, y, t)}{\partial x} + \frac{\partial C(x, y, t)}{\partial y} \right)$$
  
[2]  $\frac{\partial}{\partial t} (\theta_{eq}C) = D_e \frac{\partial^2 C}{\partial x^2} + D_e \frac{\partial^2 C}{\partial y^2} - \theta_{eq} K_r C$ 

In these equations,  $D_e$  is the effective diffusion coefficient  $[L^2T^1]$ ,  $\theta_{eq}$  is the equivalent (diffusion) porosity  $[L^3L^3]$  (see Collin and Rasmuson 1988; Aubertin et al. 1995, 2000), and  $K_r$  is the bulk reaction rate coefficient  $[T^1]$ . Bulk and effective coefficients are related as follows:

[3] 
$$D_e = \theta_{eq} D^*$$
 and  $K_r = \theta_{eq} K_r^*$ 

Parameters  $D_e$  and  $K_r$  can be measured in the laboratory or *in situ* (Mbonimpa et al. 2003) or estimated from empirical models, such as the Collin and Rasmuson (1988) model which was modified by Aubertin et al. (2000) and Aachib et al. (2004) for  $D_e$ , and the Collin (1987, 1998) model which was modified by Gosselin et al. (2007) for  $K_r$ . VADOSE/W uses the Collin and Rasmuson (1988) model to estimate  $D_e$  from the volumetric water content  $\theta$  (Krahn 2004), while  $K_r$  needs to be specified (see below). In the code,  $K_r$  is defined from a half-life  $t_{1/2}^*$ , which can be expressed as in eq. [4]. The thermal properties required for the vapour flow solution are also derived by the software from the hydraulic parameters.

[4] 
$$t_{1/2} = \frac{\ln 2}{K_r} = \theta_{eq} \frac{\ln 2}{K_r}$$

VADOSE/W can calculate the flux as a global cumulative flux on a surface A ( $GCF_A$ ) (with  $A = L \times B$ , where L is the length and B is the width; usually a unit value of B is used – i.e. B = 1 m here) during a period of time  $t_d$ . This cumulative flux [M] can then be expressed as:

[5] 
$$\operatorname{GCF}_{A} = \int_{0}^{L} \int_{0}^{t_{d}} \operatorname{F}(x, y, t) dt dl$$

For a comparison of fluxes on surfaces having different lengths *L*, the global cumulative flux per unit length  $GCF_{UL}$  [ML<sup>-1</sup>] is defined as follows:

$$[6] \quad \text{GCF}_{UL} = \frac{\text{GCF}_{A}}{L}$$

Both parameters  $(GCF_{A,} GCF_{UL})$  will be used below to present the calculated fluxes through the simulated covers.

It should also been mentioned that the code SEEP/W was used in this investigation to validate some of the

water flow solutions given by VADOSE/W. Numerical solutions provided by VADOSE/W for the diffusion equation [2] were also validated for simple 1-D cases using POLLUTE (Rowe et al. 1994) and using analytical solutions developed by Mbonimpa et al. (2003) (details can be found in Cissokho 2007 and Gosselin 2007).

#### 2.2 Model description

Figure 1 shows a typical geometric model used for the numerical simulations. The CCBE configuration used in this study as a reference case has an inclination of 18° and a length of 30 m at the CCBE-tailings interface. Models with lengths of 15 and 50 m were also constructed. The CCBE contains three layers. The bottom layer (BL) placed directly over the reactive tailings consists of 0.5 m of sand and gravel. This layer acts as capillary break layer. A moisture retention layer (MRL) has a thickness of 0.8 m and is made of a non-plastic silty material. When kept at a high degree of saturation, this layer acts as an oxygen barrier (e.g. Collin, 1987; Nicholson et al. 1989). The top layer (TL), which acts as a drainage layer, is made of 0.3 m of sand and gravel. As shown in Figure 1, the model also includes an 8 msection of the flat surface of the dyke and cover. A toe drain (1m thick) made of highly pervious material (coarse gravel) is installed at the toe of the slope to evacuate the seeping water from the system. The tailings facility overlies a 2-m-thick low permeability silt, identified here as the foundation. The model grid was automatically generated with VADOSE/W. The simulations were conducted with quadrilateral element grids, with the average size of elements being about 10 cm x 45 cm in the CCBE layers. The grids typically contained 2172 nodes and 2078 elements.



Figure 1. A typical model used to simulate an inclined CCBE on a tailings dyke.

#### 2.3 Material properties

Table 1 presents the hydraulic properties of the different materials used in the various models. This includes the air entry value ( $\psi_a$ ), the residual volumetric water content ( $\theta_c$ ), the volumetric water content at saturation ( $\theta_s$ ), and the saturated hydraulic conductivity ( $k_{sat}$ ). These materials properties are based on actual measurements, and were

used by Bussière (1999) to demonstrate that capillary barrier effects were well developed in a cover constructed with such materials.

Table 1. Hvdraulic properties of the	different materials
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Materials	ψ <sub>a</sub> (kPa)	$\theta_r$	$\theta_s$	<i>k<sub>sat</sub></i> (m/s)
TL and BL	1	0.06	0.36	1.16×10 <sup>-3</sup>
MRL	12	0.05	0.44	5.0×10 <sup>-7</sup>
Tailings	15	0.05	0.31	7.0×10 <sup>-6</sup>
Foundation	23	0.01	0.38	2.5×10 <sup>-7</sup>

#### 2.4 Applied boundary conditions

The numerical calculations were performed under drainage conditions. Different boundary conditions were applied for steady-state and transient modeling.

In early spring, a CCBE built in a cold and wet climate (such as that of the Abitibi region, Quebec, Canada) is practically saturated with water due to cryogenic suction and to the subsequent melting of the snow cover. A complete saturation ( $S_r = 100\%$ , or  $\theta = \theta_s$ ) was therefore applied as the initial state of the MRL for the numerical modelling. Accordingly, zero water pressure was assumed for all CCBE surfaces. A zero water pressure condition, corresponding to the water table level, was also applied to the toe drain surface. A temperature of 15°C was used for the entire model, as the initial and boundary conditions. This value is low for the air temperature during the summer. However, Cissokho (2007) observed a negligible temperature effect when using 25°C and 45°C for the atmosphere in the calculations. There is no vegetation on the CCBE surface. Lastly, a zero initial oxygen concentration was considered throughout the model at the onset of water flow in the spring (at the end of the thawing period). It was thus assumed that oxygen cannot penetrate a CCBE that is frozen, and that the oxygen available below the cover at the beginning of winter is consumed by the reactive minerals. This is a conservative assumption regarding the diffusive oxygen flux.

The steady-state simulation results were used as a starting point for the transient simulations, after introducing new boundary conditions. The boundary conditions above the CCBE then become: a zero hydraulic flux, a temperature of 15°C and an oxygen concentration of 280 g/m<sup>3</sup> (atmospheric concentration). A zero pressure head was applied to the surface of the toe drain to simulate the water table level. The initial oxygen concentration is nil everywhere (at time t = 0) except above the cover. The transient calculations were performed for a drainage period of 46 days (this period was considered here as a worst case scenario, without any recharge of the cover). Strict convergence parameters were used, at a tolerance of 1x10-5 Convergence was also verified by comparing the predicted and initial unsaturated hydraulic conductivity functions.

As mentioned above, the main results of interest in this study are volumetric water content ( $\theta$ ), suction ( $\psi$ ), oxygen concentration (OC), and global cumulative oxygen flux beneath the CCBE.

# 2.5 Studied cases

Tailings reactivity with oxygen varies for different mines, depending on rock type and sulphide content, tailings grain-size, deposition method, degree of saturation, etc. Oxygen migration through CCBEs is also affected by the reactivity of the underlying tailings (Cissokho 2007). In this parametric study, apparent reaction rate coefficients  $K_r^*$  covering a large range of values were used: 40/year, 200/year, 1,000/year, 2,000/year, 4,000/year and 10,000/year. The case with  $K_r^* = 0$ /year, corresponding to inert tailings, was also studied as a reference state. It is used here for comparison purposes only (no CCBE would be required in this case). In this particular situation, the applied initial condition of zero oxygen concentration in the CCBE and tailings is unrealistic (this can also be the case for slightly reactive tailings). Nonetheless, the reference case will help assess the response of covers, for various possible scenarios, in a relative manner. It should be noted here that as the tailings have constant porosity n = 0.31, the effective reactivity rate coefficients  $K_r$  corresponding to the  $K_r^*$  values (see eq. [3]) depend only on the degree of saturation  $S_r$  in the tailings.

By combining the variations in  $K_r^*$  and CCBE length, 21 models were run. Representative results are presented below.

# 3 RESULTS

# 3.1 Vertical profiles of $\theta$ , $\psi$ , and OC

Typical vertical profiles of  $\theta$ ,  $\psi$  and OC for a CCBE with L=30 m and tailings with  $K_r^*$ =200/year, near the bottom and top of the slope, are presented for different drainage times in Figures 2 and 3, respectively. After 46 days of drainage, there is very little desaturation in the moistureretention layer (MRL) near the bottom of the slope, as  $\theta$ remains high (from 0.44 to 0.42) and the suction  $\psi$  is lower than the AEV =12 kPa in the middle of the MRL. However, profiles near the top of the slope indicate that  $\theta$ drops from 0.44 to 0.34 after 46 days of drainage in the middle of the MRL, whereas the suction varies from 0.5 to 30.5 kPa. Oxygen concentrations beneath the MRL are higher near the top (by about 30 mg/L - see Figure 3c) than at the bottom (about 15 mg/L- see figure 2c).

# 3.2 OC along the slope and cumulative flux at the interface

The oxygen concentrations in the middle of the MRL along the slope at different drainage times are presented in Figure 4 for a CCBE with *L*=30 m and tailings with  $K_r^*$ =200/year. At the onset of drainage, the oxygen concentration increases from the toe (where OC = 0, due to saturation) to the top of the slope. The OC remains nil for up to 2 days of drainage. For a each drainage time (t>2 days) shown, the oxygen concentration reaches a maximum before it tends to decrease; the distance from the toe at which this maximum is reached appears to decrease over time while the maximum value of OC increases (160 mg/L at about 20 m after 14 days, 180

mg/L at about 13 m after 25 days and 200 mg/L at about 7 m after 46 days). After a modest decrease, the OC remains almost constant (independent of the position) for a given time. These results can be explained, in part, by the desaturation of tailings beneath the CCBE, which increases their effective reaction rate (compared to saturated tailings) and reduces oxygen concentrations in the upper part of the slope.

VADOSE/W can also be used to determine the global cumulated oxygen flux (per m of width) at the CCBEtailings interface (as defined in eq. [5]). The evolution of this flux with drainage time is shown in Figure 5 for a CCBE with *L*=30 m and  $K_r^*$ =200/year. This figure shows that the global cumulative oxygen flux per m of width increases with time, reaching about 3 g, 158 g, 347 g and 682 g after 10, 25, 34 and 46 days of drainage, respectively.

3.3 Effect of  $K_r^*$  on vertical oxygen concentration profiles

Typical vertical oxygen concentration profiles near the top of the slope for various drainage times are shown in Figures 6 and 7 for a 30-m-long inclined CCBE. For the considered location, the elevation y of the CCBE surface is about 8 m (y is 0 at the tailings-foundation interface); this position is located on the slope at about 26 m from the toe (or about 4 m from the top). Results are presented in Figure 6 for  $K_r^*$  values of 0, 40, 200 and 1,000/year and in Figure 7 for  $K_r^*$  values of 2,000, 4,000 and 10,000/year. In all cases, the oxygen concentration decreases with depth for a given drainage time and increases with drainage time for a given depth in the CCBE and tailings. After 46 days of drainage, the oxygen concentrations near the bottom of the sloping CCBE are about 80 mg/L, 43 mg/L, 22 mg/L, 7 mg/L,  $\overline{4}$  mg/L and 0 mg/L for  $\kappa_r^*$ values of 0/year, 40/year, 200/year, 1,000/year, 2.000/year and 10.000/year, respectively. Results shown in Figures 6 and 7 also indicate that a nil concentration in the tailings occurs at different depths (at 46 days) depending on Kr\*. All oxygen concentration profiles are very similar when  $K_r^*$  is equal or higher than 2,000/year.

These results indicate that the oxygen concentration at the CCBE-tailings interface, which is assumed to be zero in most analytical calculations of oxygen flux through a CCBE, is often much higher. This would typically lead to an overestimation of the diffusive flux and to an underestimation of the CCBE performance. The tailings reactivity should therefore be taken into account when designing CCBEs to obtain a more precise evaluation.



Figure 2. Vertical profiles of (a) volumetric water content  $(\theta)$ , (b) suction  $\psi$  (kPa) and (c) oxygen concentration *OC* (mg/l) near the bottom of an inclined CCBE with *L*=30 m and  $K_{r}^{*}$ =200/year for different drainage times; for this location, the elevation *y* of the CCBE surface is about 2.1 m (*y* is 0 at the tailings-foundation interface) and the distance on the slope from the toe is about 7 m.



Figure 3. Vertical profiles of (a) volumetric water content ( $\theta$ ), (b) suction  $\psi$  (kPa) and (c) oxygen concentration *OC* (mg/l) near the top of an inclined CCBE with *L*=30 m and *K*<sub>r</sub>\*=200/year for different drainage times; for this location, the elevation *y* of the CCBE surface is about 8 m (*y* is 0 at the tailings-foundation interface) and the distance on the slope from the top is about 4 m.



Figure 4. Evolution of oxygen concentration (mg/L) along the slope in the middle of the MRL with drainage time for an inclined CCBE (L=30 m and  $K_r$ \*=200/year); distance 0 corresponds to the toe of the slope.



Figure 5. Evolution of global cumulative oxygen flux (g) (per m of width) with drainage time beneath an inclined CCBE with L=30 m and  $K_r^*$ =200/year.

#### 4 DISCUSSION

Global cumulative oxygen fluxes per unit length (GCF<sub>UL</sub>, g/m) calculated from equation [6], were used to compare cumulative oxygen fluxes of CCBEs with different lengths. The total length (*L*) of the inclined CCBE (at the tailings interface) includes the 8 m of horizontal section. For example, for a CCBE with *L*=30 m, the cumulative flux per unit length is calculated for a total length of 38 m. Figure 8 shows a typical evolution of global cumulative oxygen flux per unit length with drainage time for an inclined CCBE with *L*=30 m for different  $K_r^*$  values. For a given reactivity  $K_r^*$ , these fluxes increase with drainage time. For a given drainage time, the flux increases with  $K_r^*$ . One can also observe that the influence of  $K_r^*$  is small during the first 10 days.



Figure 6. Vertical oxygen concentration profiles near the top (y = 8m) of a 30-m-long inclined CCBE at various drainage times and for different apparent reaction rate coefficients:  $K_r^*$ : 0/year (a), 40/year (b) and 200/year (c).



Figure 7. Vertical oxygen concentration profiles near the top (y = 8 m) of a 30-m-long inclined CCBE at various drainage times and for different apparent reaction rate coefficients:  $K_r^*$ : 1,000/year (a), 2,000/year (b) and 10,000/year (c).



Figure 8. Evolution of global cumulative oxygen flux per unit length with drainage time for different values of  $K_r^*$  in an inclined CCBE with L=30 cm.

The evolution of global cumulative oxygen flux per unit length with reactivity  $K_r^*$  for the 3 slope lengths considered (*L*=15, 30 and 50 m) is presented in Figures 9 after drainage periods of and 46 days. For sloping cover lengths of 15 and 30 m, global cumulative oxygen fluxes per unit length are very similar, with values of approximately half the normalised flux of the *L* = 50 m CCBE. In all cases, the flux per unit length increases with reactivity, but it tends to stabilize when a  $K_r^*$  value of approximately 2,000/year is reached. This weak variation of the flux for  $K_r^*$  greater than 2,000/year can be explained by a lack of oxygen to support the imposed reaction kinetics in this range of reactivity (the oxygen concentration profiles are very similar, as explained in section 3.3).



Figure 9. Evolution of cumulative oxygen flux per unit length with reactivity  $K_r^*$  for 3 slope lengths (*L*=15, 30 and 50 m) after 46 days of drainage.

#### 5 CONCLUDING REMARKS

Numerical simulations with VADOSE/W have been used to assess the influence of sulphidic tailings reactivity on the ability of CCBEs inclined at about 18 degrees and having lengths of 10 m, 30 m and 50 m to limit oxygen diffusion under drainage conditions. The bulk oxygen reaction rate coefficients  $K_r$  of the tailings were varied between 40 and 10,000/year (or 0.1 and 27.4/day). A significant effect of tailings reactivity has been observed: global cumulative oxygen flux through the cover tends to increase with the value of  $K_r$ , particularly for values of  $K_r$  up to about 2,000/year (or 5.5/day). For  $K_r^*$  higher than 2,000/year, oxygen is almost completely consumed at the tailings surface, with the result that the gradients remain constant and oxygen fluxes tend to stabilize. The calculated results also indicate that the oxygen concentration at the CCBE-tailings interface can be much higher than zero. The typical assumption of a nil oxygen concentration in most analytical calculations can hence lead to an underestimation of the CCBE efficiency.

# ACKNOWLEDGEMENTS

This work was performed with the support of the NSERC Polytechnique-UQAT Industrial Research Chair in Environment and Mine Wastes Management (http://www.polymtl.ca/enviro-geremi/). The authors would like to acknowledge the support and participation of all their partners. The authors also thank Dr John Molson for helping improve the manuscript.

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