MODELING ACID MINE DRAINAGE IN WASTE ROCK DUMPS[1]

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Introduction

Acid mine drainage (AMD) results from the oxidation of sulfides present in mine wastes. The acidity generated by these reactions creates conditions under which metals can be leached and represent a threat for surface and ground waters. Even though leachate collection and neutralization are used to treat the problem, the industry is looking for methods to predict and prevent the generation of AMD at new sites and control methods for sites already producing AMD.

Waste rock dumps are generally very large accumulations of barren rocks extracted from open pits to access ore bodies. These rocks contain sulfides, most commonly pyrite, and often generate AMD at rates much higher than in mine tailings which are fine grained by-products of milling operations. Numerous coupled physical processes are involved in AMD production in waste rocks. Sulfide oxidation reactions are strongly exothermic and temperatures beyond 70 ºC have been mesured in some dumps. That heat is transfered by conduction and fluid advection. Dumps have thick partly saturated zones through which gases flow under thermal gradients and water infiltrates. Oxygen is required by the oxidation reactions and is supplied by diffusion and advection. The reaction products are carried in solution in very concentrated leachates.

Numerical modeling of AMD aims to 1) provide a better understanding of the physical processes involved in AMD, 2) allow the integration of available waste rock characterization data, 3) indicate new data or studies which are required to fill the gaps in our quantitative understanding of AMD processes, and 4) supply a tool for the prediction of AMD production, taking into account the impact of control methods. These objectives can only be met through sustained research efforts. This study is part of a wider research effort which as been on-going at La Mine Doyon since 1991 (Gélinas et al., 1994).

Reaction core model

In waste rock dumps, pyrite is contained in rock blocks and surrounded by other minerals and its oxidation proceeds from the surface of the blocks. As pyrite near the surface is oxidized, the oxidant must penetrate within the blocks to reach unreacted pyrite. A zonation appears within the blocks with an external zone in which pyrite is completely oxidized and an internal core where pyrite is unreacted. The whole of pyrite within a block is not oxidized simultaneously because the rate of oxygen consumption generally exceeds the rate of oxygen diffusion in the blocks. Our model uses features similar to those of Pantelis and Ritchie (1991), Cathles and Schlitt (1980), Jaynes (1983) and Levenspiel (1972). The volumetric oxidation rate Q_{Ox} (kg/m^3 s), observed in a unit volume of waste rocks, is related not only to surface oxidation but is also controlled by the oxygen diffusion rate in waste rock blocks:

$$Q_{Ox} = - K_{Ox} \cdot X_T \cdot X_{WO} \cdot \rho_{Ox}^{air} \cdot f(X) \ , \qquad (1)$$

where K_{Ox} is the global volumetric kinetic constant (s^{-1}), X_T and X_{WO} are kinetic factors related to temperature and oxygen partial density (0 to 1), ρ_{Ox}^{air} is the oxygen partial density in air (kg/m^3), and f(X) is the geometric factor which is a function of the proportion of pyrite remaining X.

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TOUGH AMD Capabilities

TOUGH AMD follows the same formulation as TOUGH2 (Pruess, 1991). However, the addition of a new component (oxygen) and a new primary thermodynamic variable (oxygen mass fraction in air) was required to represent AMD. Thus, in TOUGH AMD, there are three mass components (water, gases other than oxygen in air, oxygen) and one energy component (heat). Four equations, one for each component, have to be satisfied simultaneously to solve the system. Besides expanding components, other capabilities were added to represent AMD. Pyrite oxidation produces sinks for oxygen and sources of heat which are components of the system. Furthermore, that reaction consumes pyrite and produces sulfate, iron and acidity. The pyrite remaining has to be tracked since it affects the reaction rate and the production, accumulation and transport of sulfate is followed to represent AMD production outside the dump. The reaction core model is used to calculate the oxygen consumption rate Q_{Ox} (kg/m^3 s) to which the heat production rate is related. TOUGH AMD is thus adapted to the modeling of AMD and allows the representation of the main processes involved in waste rocks:

• Hydrology: Takes into account variable infiltration with time from the surface and represents unsaturated and saturated liquid flow within the dump.
• Gas transfer: Represents gas convection under pressure or temperature gradients as well as the diffusion of gas components, especially oxygen, under concentration gradients.
• Heat transfer: Includes the processes of conduction, fluid advection and gas diffusion. Takes into account the effect of phase changes on heat transfer and heat losses to confining beds.
• Geochemistry: Uses a reaction core model including the effects of surface reaction and diffusion on the volumetric oxidation rate. Computes the rates of consumption of pyrite and oxygen and the rates of heat and sulfate production.
• Mass transport: Uses sulfate to represent AMD production and tracks the production and advective transport of sulfate, its rate of mass accumulation and its release outside the dump.

Application of AMD numerical modeling

The first objective of numerical modeling is here to better understand the physical processes involved in AMD production in waste rocks. A general case is modeled to study the interaction of processes and identify the parameters having the greatest impact on the behavior of the system. The parameters and conditions used in the base case are representative of the South Dump at La Mine Doyon so that results may be compared to observations at this site (Gélinas et al., 1994). We are presenting here some of the findings of the modeling work for a base case. The application of the model to the evaluation of a control method, a border membrane, as well as a more detailled account of the modeling work is presented by Lefebvre (1994).

Model parameters and conditions

The base case is modeled for a period of 15 years and as such includes the period during which the dump has been in place (about 9 years) and provides a look at the potential future evolution of AMD production. It would be unrealistic to model the behavior of the dump for a longer period given the uncertainty in our knowledge of the site and in particular the absence of data on the evolution of physical properties with time which could affect significantly the behavior of the dump. This model actually supposes that physical properties remain constant even though we know from field observations that the material evolves and new minerals are formed and could alter the physical properties. Further studies are required to quantify the impact of this change in physical properties. The extensive characterization and monitoring program at La Mine Doyon allowed an evaluation of many physical properties of the waste rocks (Gélinas et al., 1994). Table I summarizes the physical parameters used in the model.

Table I - Physical properties of the base case.

Property	Symbol, value and units
Volumetric oxidation constant	$K_{ox} = 0.75x10^{-6}\ s^{-1}$
Diffusive / Chemical total times	$t_d/t_c = 2.5$
Pyrite mass fraction in solids	$w_{py} = 0.07$
Horizontal permeability	$k_h = 2.5x10^{-9}\ m^2$
Vertical permeability	$k_v = 1.0x10^{-9}\ m^2$
Porosity	$n = 0.33$
Solids density	$\rho_s = 2740\ kg/m^3$
Dry thermal conductivity	$\lambda_d = 0.9$ W/m ºC
Saturated thermal conductivity	$\lambda_w = 3.7$ W/m ºC
Heat capacity of solids	$c_{ps} = 837$ J/kg ºC
Thermal conductivity of the base	$\lambda = 1.55$ W/m ºC
Global density of the base	$\rho_b = 2008.6\ kg/m^3$
Heat capacity of the base	$c_p = 1504$ J/kg ºC
Standard diffusion coefficient	$D_o = 2.13x10^{-5}\ m^2/s$
Temperature diffusion coef.	$\theta = 1.80$
Tortuosity factor	$\tau = 0.7$
van Genuchten "m" factor	$m = 0.23$
van Genuchten "α" factor	$\alpha = 0.504\ Pa^{-1}$
Residual water saturation	$S_{wr} = 0.14$

The computation grid and limit conditions used in the base case are presented in figure 1. That grid represents a vertical half section within the dump and uses cartesian coordinates. The model has a 30 m thick unsaturated zone and a thin wedge-shaped saturated zone from zero to 1.5 m thick. Lateral dimensions are 87 m at the base and 57 m at the surface. The slope at the border is necessary to obtain representative air convection patterns (Pantelis and Ritchie, 1991). Since the internal boundary is a symmetry limit, the grid represents a system twice as wide. The limit conditions used are a water saturation of 0.42 generating an infiltration of about 35 cm per year, a temperature of 5 ºC and atmospheric oxygen mass fraction (0.2315). Atmospheric pressure is set at 100 kPa at the surface whereas a hydrostatic pressure profile is used at the sloping border. The system is supposed homogeneous. The same parameters are used as initial conditions.

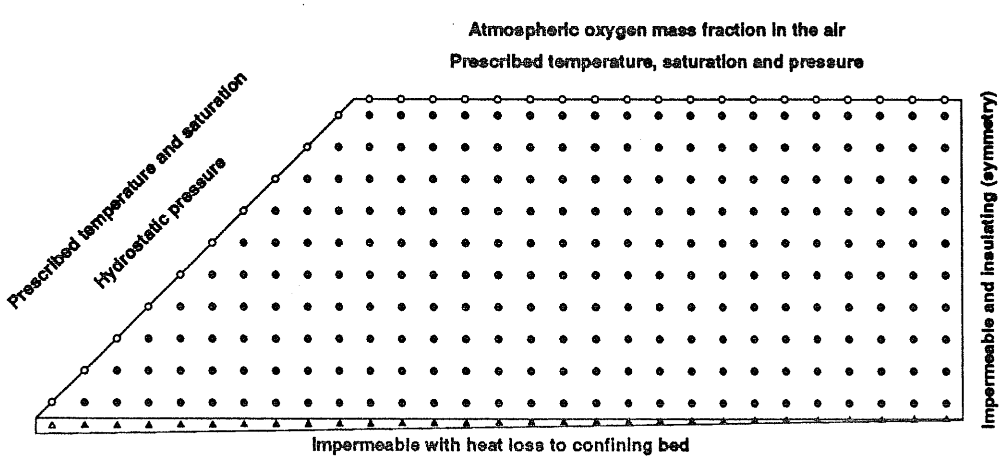

Figure 1 - Computation grid and limit conditions for the base case.

Physical conditions within the dump

Figure 2 shows the conditions prevailing in the dump after 9 years of AMD production: gas velocity and temperature, oxygen mass flux and relative concentration, and oxidation rate and remaining pyrite mass fraction. The key process in AMD production is oxygen supply to oxidation sites. Convection can provide oxygen in a much more efficient way than diffusion. Figure 2 (top) shows that air convection is controlled by temperature gradients. An increase in temperature reduces gas density and causes gas convection which is responsible for the supply of oxygen within the dump: figure 2 (middle) illustrates the oxygen mass flux and the relative oxygen concentration in the dump (with respect to atmospheric concentration). The oxygen flux is reduced along a given convection path within the dump because it is gradually consumed by the oxidation reaction. The oxygen concentration is thus maximum near air entry points and is gradually reduced within the dump. The central core of the dump is deprived of oxygen and does not produce much AMD. At this stage, the effect of diffusion is negligible compared with convection. Since pyrite oxidation is supposed to follow first order kinetics with respect to oxygen, its distribution has a direct impact on the oxidation rate. Figure 2 (bottom) shows the remaining pyrite mass fraction (contours) and the oxidation rate (circles). There is a sharp decrease in pyrite concentration at the border of the dump whereas the reduction is not as important near the surface. In the central part of the dump, very little pyrite is oxidized and a large potential for further AMD production remains.

Physical transfer processes

Transfer processes play an important role in AMD production. We will discuss the processes of heat transfer, water circulation and sulfate transport in waste rock dumps. Heat transfer in waste rock dumps occurs through the mechanisms of 1) conduction through the bulk of the material resulting from temperature gradients, 2) advection of fluids (liquid and gas) carrying heat and 3) diffusion of components in the gas phase. Figure 3 (top) shows the temperature distribution and the components of heat transfer. Three families of arrows represent respectively 1) the total heat flux, 2) the conductive heat flux (perpendicular to temperature contours) and 3) the diffusive heat flux. The difference between the total flux and the other components is the advective heat flux. At the outer limits of the dump, heat conduction is generally the dominant heat transfer mechanism. Conduction is also responsible for heating the center of the dump by carrying heat away from the zone of maximum temperature. Heat transfer by gas advection is dominant in the central hot zone where the gas phase contains more water vapor and carries a lot of heat. Water advection and its effect on heat transfer is very small in this case because of the low infiltration rate. However, this process can be significant in other cases. Heat transfer by diffusion in the gas phase is negligible because it is a binary process with diffusion and counterdiffusion of components with nearly equal heat capacity.

It is important to understand the modes of water circulation in a waste rock dump since the mass produced during AMD (sulfate, acidity, metals) is carried in solution. Figure 3 (middle) shows the distribution of water saturation and the mass fluxes of water in the liquid (downward pointing gray arrows) and vapor (black arrows) phases. Liquid water moves downward from the surface following infiltration in the unsaturated zone. Water is also transfered in the vapor phase by gas advection. Water transfer in the vapor phase is actually responsible for the redistribution of water within the dump. Relatively dry cold air entering the dump, mainly at the toe of the slope, acquires more and more water as it first moves horizontally and heats up. The gas phase carries the most water, as much as the liquid phase, as it moves upward through the hottest zone. Beyond that zone, in cooler areas near the surface, water vapor condenses and contributes to more infiltration. That process induces water saturation variations within the dump from 37.5% to 41.5%. The zone most influenced is near the toe of the slope at the base where water is withdrawn. Although important, the process of water vapor transfer by advection does not lead to important net water losses from the dump because most of the water withdrawn from the base recondenses near the top surface before the gas phase leaves the dump.

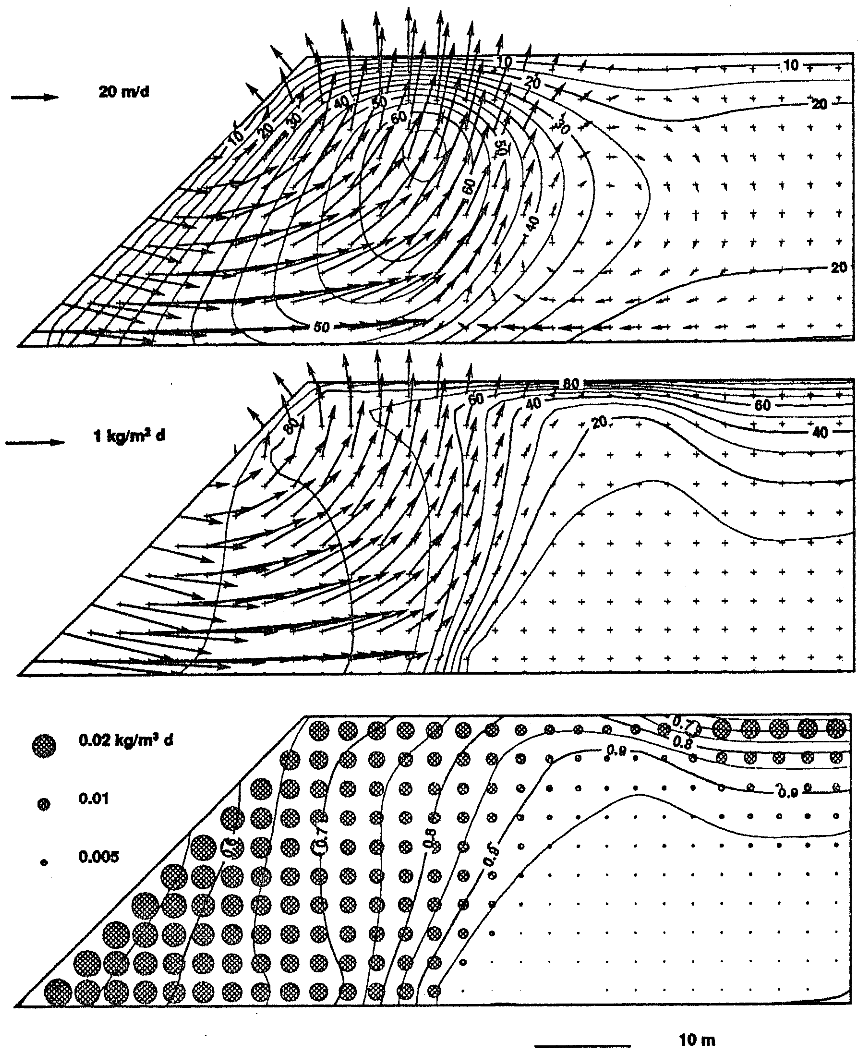

Figure 2 - Physical conditions (base case after 9 years).
Top: gas velocity (m/d) and temperature (ºC). Middle: oxygen mass flux (kg/m^2 d) and oxygen mass fraction in air with respect to atmospheric value (%). Bottom: unreacted pyrite mass fraction and oxidation rate (kg O_2/m^3 d).

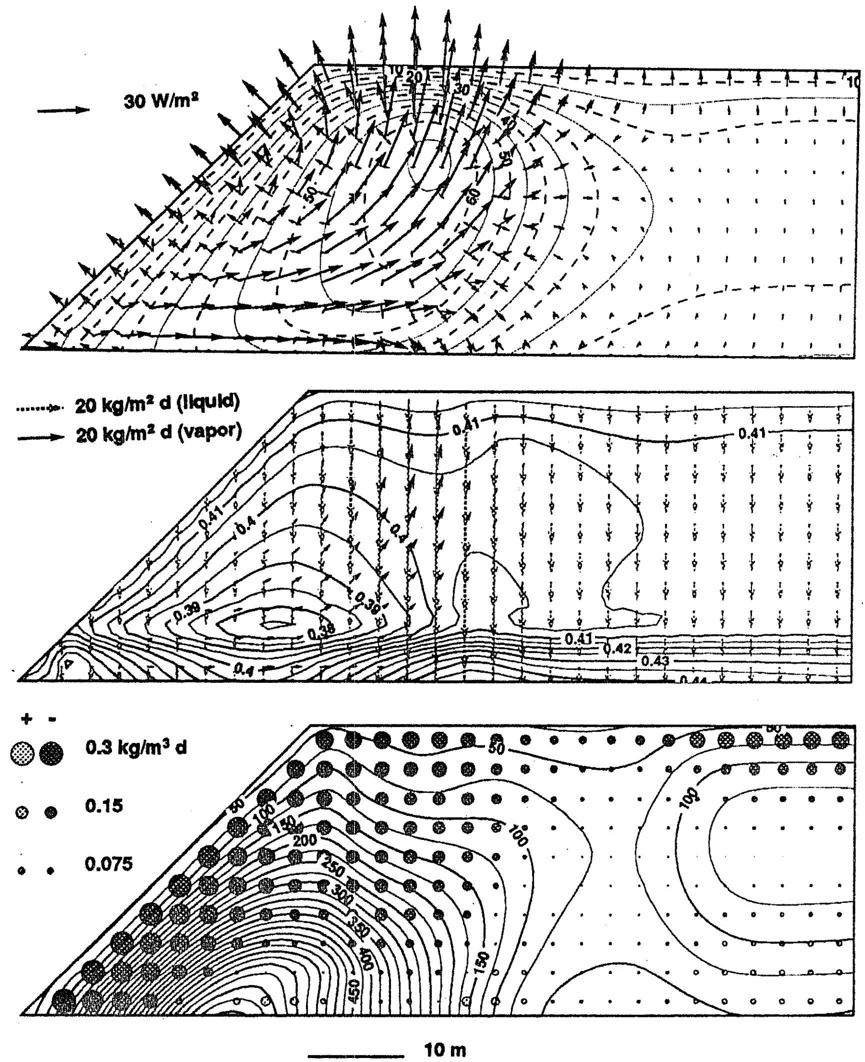

Figure 3 - Transfer processes (base case after 9 years).
Top: total, conductive and diffusive heat fluxes (W/m^2) and temperature (ºC). Middle: liquid (gray) and vapor (black) water mass fluxes (kg/m^2 d) and water saturation (-). Bottom: net sulfate flux (kg/d) and concentration (g/L).

AMD production is followed in the model by sulfate production, transport and release. Figure 3 (bottom) shows the distribution of sulfate concentration (contours) and the net sulfate flux in the grid elements. These net fluxes represent the difference in mass of sulfate entering and leaving an element. Net negative fluxes (dark circles) indicate that more mass exits the element than enters it whereas positive net fluxes (light circles) have an opposite meaning. Negative net fluxes occur in zones of high oxidation rate and consequently of high sulfate production. In these areas, more mass leaves the elements because internal production adds to the sulfate mass flux. Positive fluxes occur mainly at the core of the dump where sulfate mass production is low: in these areas, leachate of high concentration mixes with the leachate contained in the elements and comes out with less mass. This type of mass transport representation in the unsaturated zone supposes mixing of fluids instead of piston displacement and accounts for the limited leaching caused by small infiltration rates compared with the large volume of leachate stored in the unsaturated zone. This results in an increase in concentration and sulfate mass storage within the dump as more mass is produced than may be leached during the early years of AMD production. This representation of mass transport is simplistic and requires more work. Also, no account is taken in the model of mass loss due to new minerals precipitation (gypsum, jarosite). It is clear that the very high concentrations indicated by the model could not be reached in a real system because oversaturation and precipitation would occur to limit the concentration.

Conclusion

Further research is needed to develop the firm fundamental knowledge upon which applied numerical modeling must be based. Modeling is useful to better understand the coupled physical processes involved in AMD production in waste rocks. Also, modeling can be used to evaluate control methods mainly aimed at reducing air convection (Lefebvre, 1994). The processes of water infiltration in a coarse heterogeneous porous media, mass transport in the unsaturated zone, and the leachate geochemical behavior (interaction with rocks and mineral precipitation) need to be studied further both in the laboratory and in the field. The limited knowledge on these key processes limits further development of AMD modeling and our capability to predict the behavior of waste rock dumps. Further field studies are also required as we need more site characterization with integrated monitoring and modeling programs. For those sites, we have to develop methods to better characterize air permeability and its anisotropy as it affects both gas convection and water infiltration. We also have to be able to characterize, in the field and lab, the changes in physical properties of waste rocks through time and especially the effect of mineral precipitation.

References

Cathles, L.M., and Schlitt, W.J., 1980: A model of the dump leaching process that incorporates oxygen balance, heat balance, and two dimensional air convection. In Schlitt, W.J., ed., Leaching and recovering coper from as-mined materials. Proc. of the Las Vegas Symp., 26 Feb., 1980, Solution Mining Commitee, Soc. of Mining Eng. of AIME, pp. 9-27.

Gélinas, P., Lefebvre, R., Choquette, M., Isabel, D., Locat, J., and Guay, R., 1994: Monitoring and modeling of acid mine drainage from waste rocks dumps - La Mine Doyon case study. Report GREGI 1994-12 submitted to the MEND Prediction commitee, Sept. 1994.

Jaynes, D.B., 1983: Atmosphere and temperature within a reclaimed coal-stripmine and a numerical simulation of acid mine drainage from stripmined lands. Ph.D. Th., Penn. St., 198 p.

Lefebvre, R., 1994: Caractérisation et modélisation numérique du drainage minier acide dans les haldes de stériles. Ph.D. Thesis, Université Laval, 375 p.

Levenspiel, L., 1972: Chemical reaction engineering, 2nd ed. John Wiley & Sons, N.Y., 578 p.

Pantelis, G., and Ritchie, A.I.M., 1991: Macroscopic transport mechanisms as rate-limiting factor in dump leaching of pyritic ores. Appl. Math. Modeling, 15, March, pp. 136-143.

Pruess, K., 1991: TOUGH2 - A general-purpose numerical simulator for multiphase fluid and heat transfer. Lawrence Berkely Laboratory LBL-29400, 102 p.