

Part II: Modeling Study of NMG's Backfill Concept of NAG and Waste Rock

- Mid-term Update Meeting with
Nouveau Monde Graphite Inc. (NMG)

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January 20th, 2020

DISCLAIMER

- The results presented in the following slides have been determined using experimental data provided by NMG
- Where experimental data was missing, literature data was used
- In future activities, these parameters will be determined experimentally, or refined, where applicable and possible
- As such, the results as presented may change
- For transparency, the major assumptions employed for this work will be clearly stated

Focus of Study

Task 2: Develop 1-D model containing layers of NAG over waste rock

- Study oxygen transport and consumption by sulphide-mineral oxidation through the boundary zone of the NAG layer
- Compare the concept of NAG over waste rock with dry-stacking of ordinary tailings over waste rock
- The concept of NAG over waste rock would be a configuration for the above-water-table portion of a pit backfill

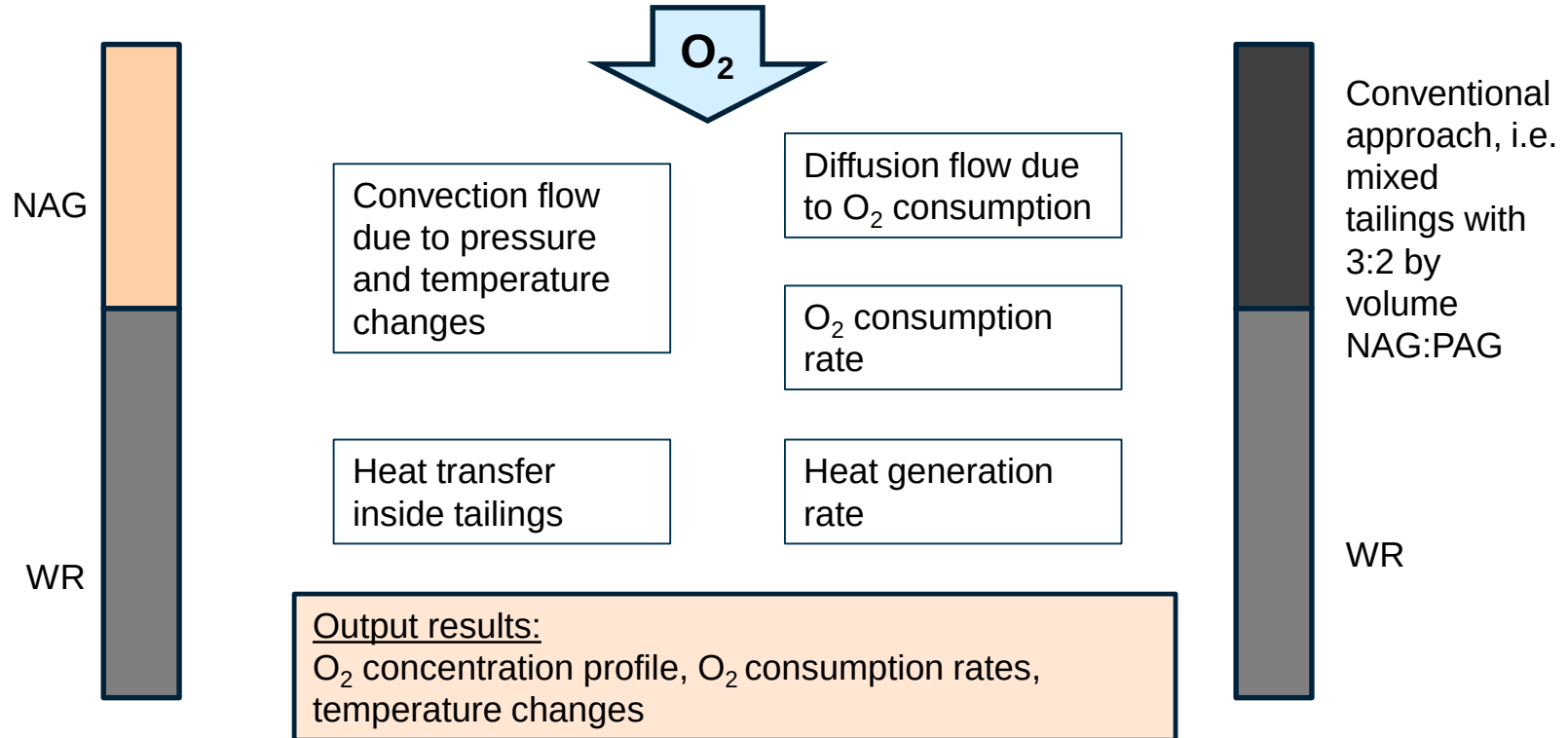
Summary of Preliminary Modeling Results

1. The NMG configuration of NAG over waste rock, for the above-water-table portion of a pit backfill, is able to hinder the transport of oxygen from the ambient into/through the waste rock layer, and as a result, the NAG layer functions as a layer that can reduce the total amount of oxygen consumed by pyrrhotite oxidation reaction inside the waste rock layer.
2. Our modeling results show that the amount of oxygen that is consumed by the tailings materials if dry stacked using a conventional concept is about 2.5 – 4.5 times the amount of oxygen consumed by the NMG configuration. That is to say, the NMG configuration indeed reduces sulfide oxidation reaction rates.
3. The transport of oxygen from the ambient into the NAG layer and the waste rock layer is a function of many parameters including the effective gas diffusivity and gas permeability, especially, inside the uppermost tailings layer. The smaller the porosity for gas transport and the thicker the top NAG layer, the more significant the advantage is.

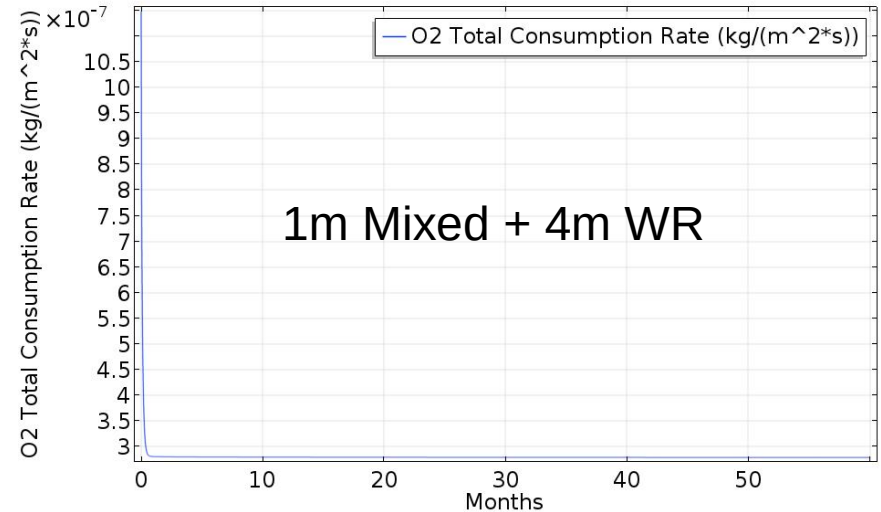
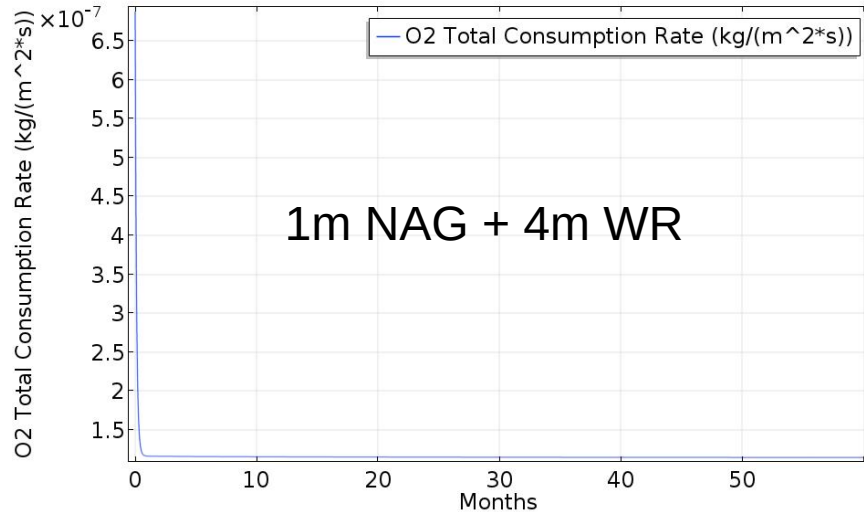
Summary of Preliminary Modeling Results

4. Although the sulfide oxidation reaction is an exothermic process, or, called self-heating process, the NMG configuration would not allow a high rate of heat production to the level of causing fire. The reason is: the transport of oxygen from the ambient through the NAG layer and the waste rock layer is significantly hindered by the top NAG layer and thus the sulfide oxidation reaction rates inside the waste rock layer is not high enough to make heat production rate high enough to cause fire.
5. The exothermic process of the sulfide oxidation reaction makes the temperature inside the NAG layer and the waste rock layer increase by a certain number of degrees C. Our modeling shows that the temperature would increase by about 15 degree C.
6. Although the sulfide oxidation reaction rates go up when temperature increases, the top NAG layer would reduce the effect of increased temperature on sulfide reaction rates due to the fact that the NAG layer hinders the transport of oxygen from the ambient into the waste rock layer. That is to say, the reduced level of oxygen transport reduces the effect of temperature increase on oxidation reaction rates.

Task 2: NAG+WR Simulated Phenomena

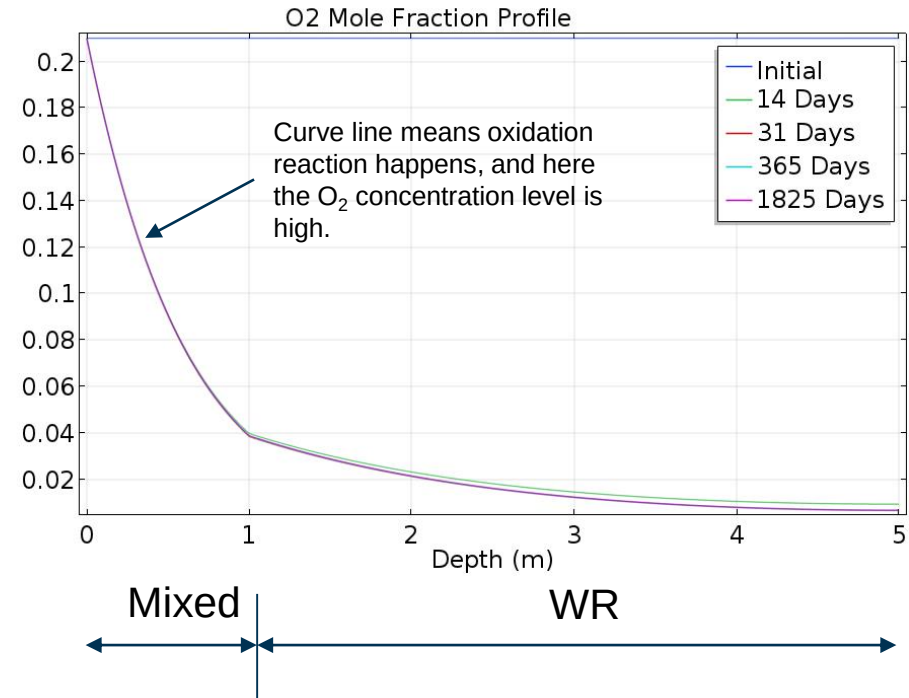
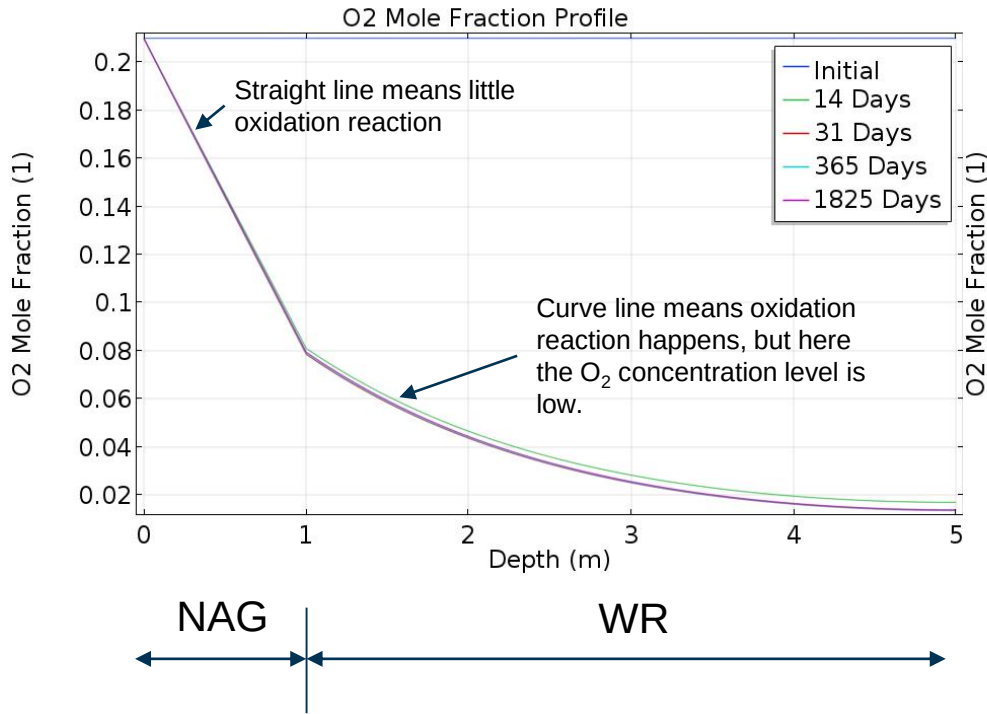


Comparison of O₂ Consumption Rates (kg/m²/s)



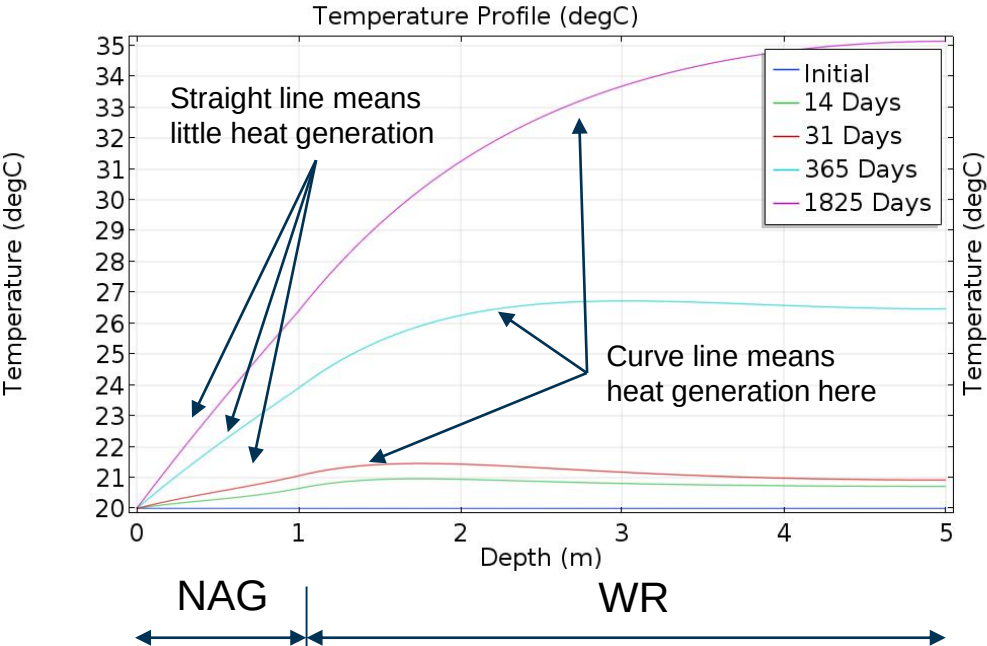
$$\frac{\text{O}_2 \text{ consumption rate in mixed tailings on top of waste rock}}{\text{O}_2 \text{ consumption rate in NAG on top of waste rock}} = \frac{2.79\text{e-}7}{1.14\text{e-}7} = 2.45$$

Comparison of O₂ Mole Fraction Profiles in 1m NAG on top of 4m WR

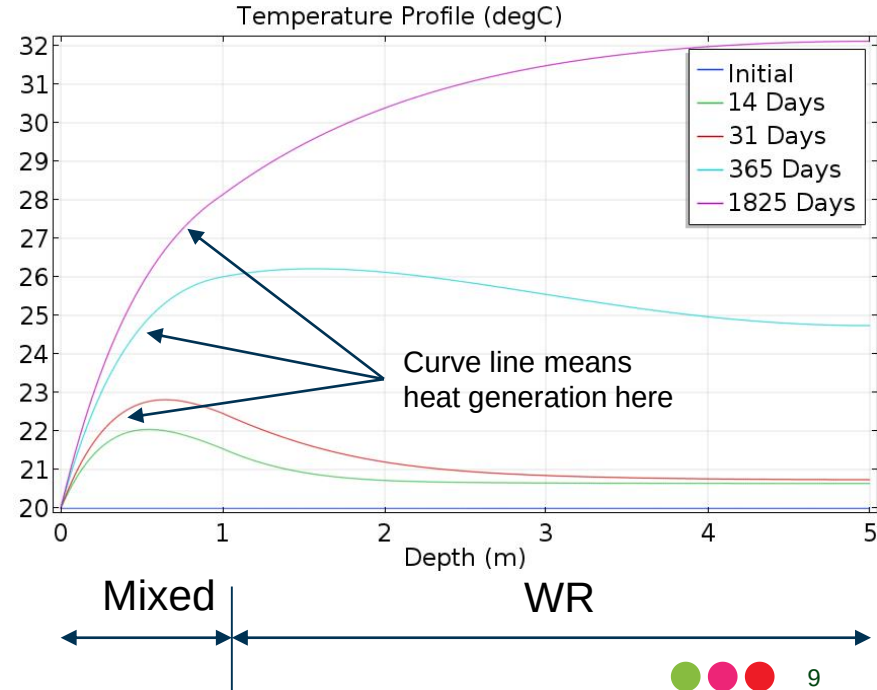


Comparison of Temperature Profiles in 1m NAG on top of 4m WR

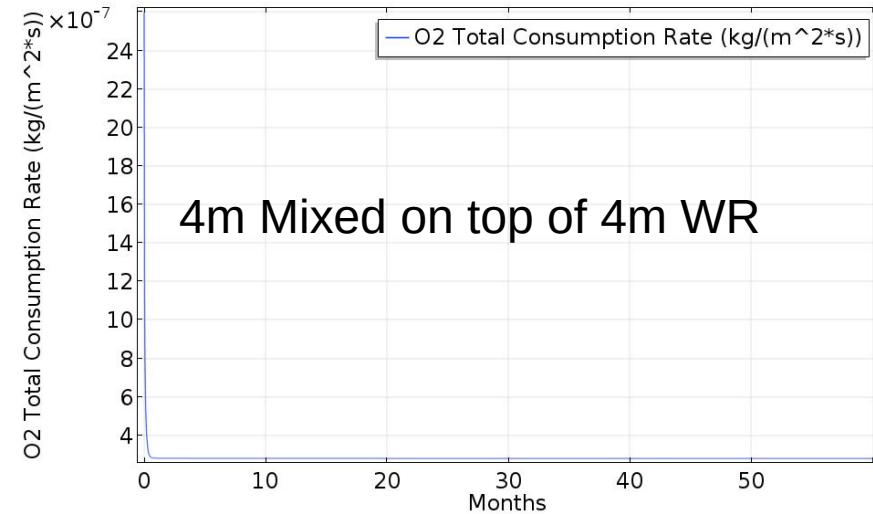
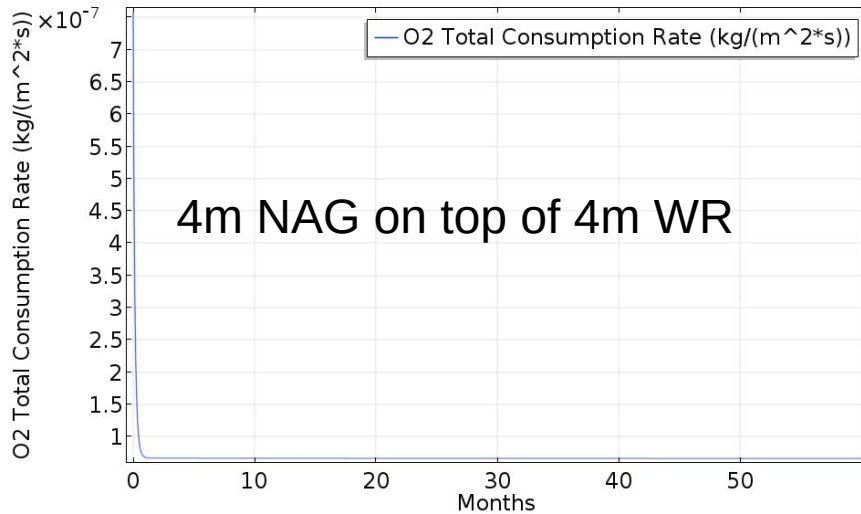
Heat is produced mainly in the WR layer, but with lower rate due to lower O_2 concentration level



Heat is produced mainly at the Mixed layer, with higher rate due to higher O_2 concentration level

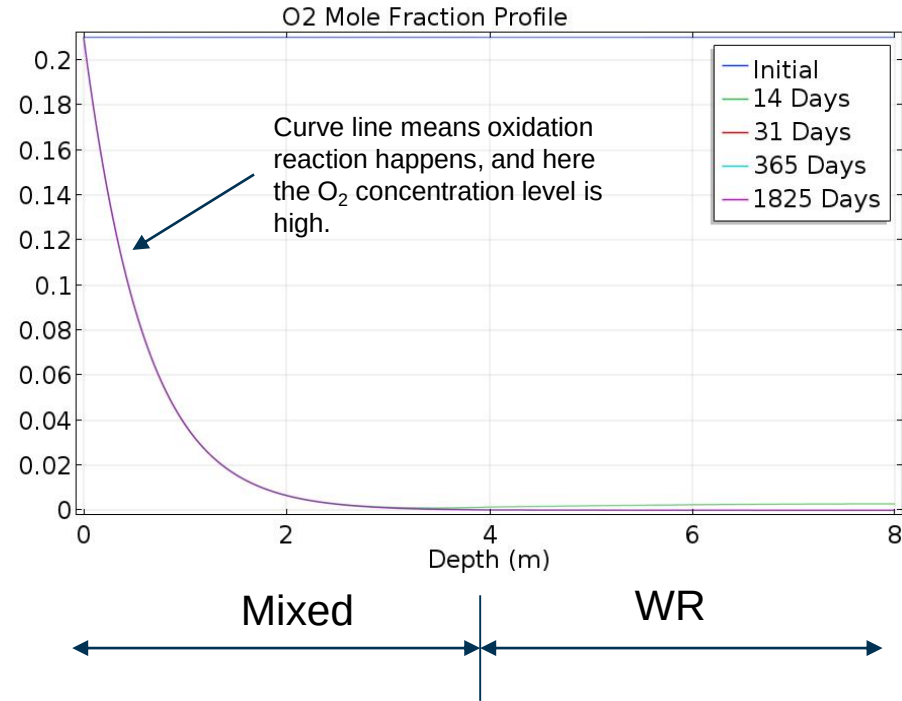
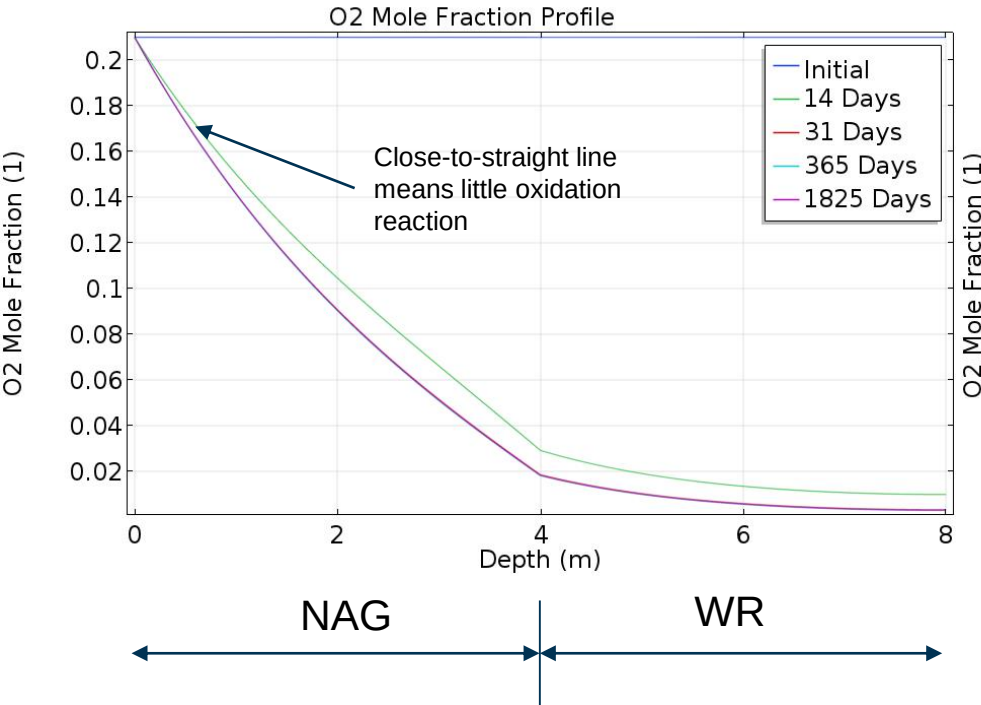


Comparison of O₂ Consumption Rate (kg/m²/s)



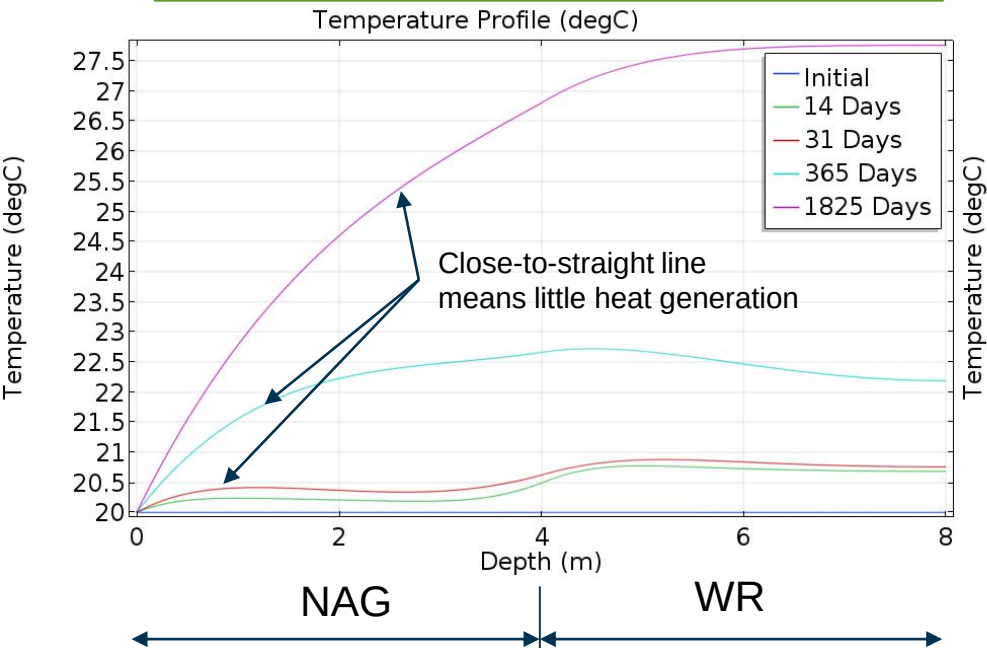
$$\frac{\text{O}_2 \text{ consumption rate in mixed tailings on top of waste rock}}{\text{O}_2 \text{ consumption rate in NAG on top of waste rock}} = \frac{27.95\text{e-}8}{6.6\text{e-}8} = 4.23$$

Comparison of O₂ Mole Fraction Profiles in 4m NAG on top of 4m WR

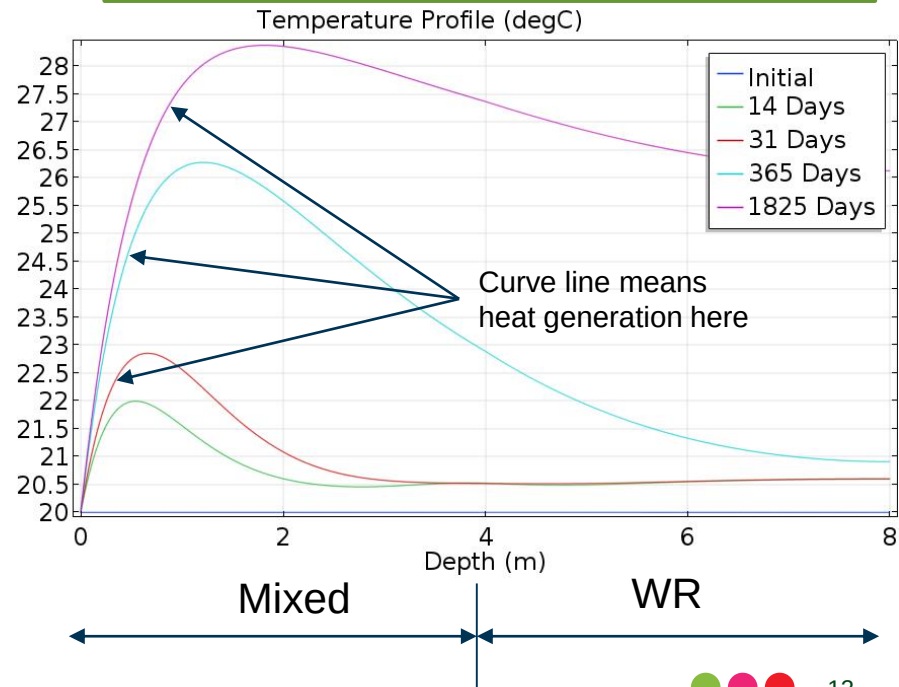


Comparison of Temperature Profiles in 4m NAG + 4m WR

Heat is produced mainly in the Waste Rock layer, but with lower rate due to lower O₂ concentration level



Heat is produced mainly in the Mixed layer, with higher rate due to higher O₂ concentration level



Parameters Used in the Simulations

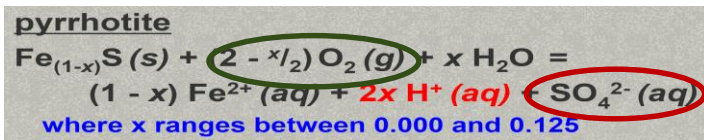
Name	Expression	Value	Description
L1	1.5[m]	1.5 m	NAG layer
L2	1[m]	1 m	PAG layer
L3	2.5[m]	2.5 m	WR layer
Por1	0.1	0.1	Effective Porosity in NAG
Por2	0.1	0.1	Effective Porosity in PAG
Por3	0.2	0.2	Effective Porosity in WR
Don1	$1.76e-5 \cdot \text{Por1}^{1.5} [\text{m}^2/\text{s}]$	$5.5656E-7 \text{ m}^2/\text{s}$	Effective Gas Diffusivity
Dcn1	$1.76e-5 \cdot \text{Por1}^{1.5} [\text{m}^2/\text{s}]$	$5.5656E-7 \text{ m}^2/\text{s}$	Effective Gas Diffusivity
Don2	$1.76e-5 \cdot \text{Por2}^{1.5} [\text{m}^2/\text{s}]$	$5.5656E-7 \text{ m}^2/\text{s}$	Effective Gas Diffusivity
Dcn2	$1.76e-5 \cdot \text{Por2}^{1.5} [\text{m}^2/\text{s}]$	$5.5656E-7 \text{ m}^2/\text{s}$	Effective Gas Diffusivity
Don3	$1.76e-5 \cdot \text{Por3}^{1.5} [\text{m}^2/\text{s}]$	$1.5742E-6 \text{ m}^2/\text{s}$	Effective Gas Diffusivity
Dcn3	$1.76e-5 \cdot \text{Por3}^{1.5} [\text{m}^2/\text{s}]$	$1.5742E-6 \text{ m}^2/\text{s}$	Effective Gas Diffusivity
Per1	$1.72e-13 [\text{m}^2]$	$1.72E-13 \text{ m}^2$	NAG Permeability
Per2	$1.52e-13 [\text{m}^2]$	$1.52E-13 \text{ m}^2$	PAG Permeability
Per3	$1.52e-10 [\text{m}^2]$	$1.52E-10 \text{ m}^2$	Waste Rock Sample Permeability...
Vis	$18.6e-6 [\text{Pa}\cdot\text{s}]$	$1.86E-5 \text{ Pa}\cdot\text{s}$	Air viscosity
Dens_s	$1810 [\text{kg}/\text{m}^3]$	$1810 \text{ kg}/\text{m}^3$	Tailings density
Hst	$1.2e6 [\text{J}/\text{K}/\text{m}^3]$	$1.2E6 \text{ J}/(\text{m}^3\cdot\text{K})$	Heat capacity of tailings
Hct	$0.2 [\text{J}/\text{K}/\text{s}/\text{m}]$	$0.2 \text{ W}/(\text{m}\cdot\text{K})$	Thermal conductivity of tailings
Hsg	$1012 [\text{J}/\text{kg}/\text{K}]$	$1012 \text{ J}/(\text{kg}\cdot\text{K})$	Specific heat of air
Hcg	$0.0251 [\text{W}/\text{m}/\text{K}]$	$0.0251 \text{ W}/(\text{m}\cdot\text{K})$	Thermal conductivity of air
Hp	$(744e3/2) [\text{J}/\text{mol}]$	$3.72E5 \text{ J}/\text{mol}$	Reaction Heat
Ko2	$4.2e-6 [1/\text{s}]$	$4.2E-6 1/\text{s}$	O2 Consp. Rate in PAG
Ko1	$8.33e-8 [1/\text{s}]$	$8.33E-8 1/\text{s}$	O2 Consp. Rate in NAG
Ko3	$5.95e-7 [1/\text{s}]$	$5.95E-7 1/\text{s}$	O2 Consp. Rate in WR
Y	$360 \cdot 24 \cdot 60 \cdot 60$	$3.1104E7$	
Rco	$8314.4598 [\text{J}/(\text{kmol}\cdot\text{K})]$	$8.3145 \text{ J}/(\text{mol}\cdot\text{K})$	Universal gas constant
Rs	$\text{Rco}/29 [\text{kg}/\text{kmol}]$	$286.71 \text{ J}/(\text{kg}\cdot\text{K})$	Specific gas constant
womin	$0.21 \cdot 32 / (0.21 \cdot 32 + 0.787 \cdot 28 + 0.003 \cdot 44)$	0.23262	O2 mass fraction in air
wnmin	$0.787 \cdot 28 / (0.21 \cdot 32 + 0.787 \cdot 28 + 0.003 \cdot 44)$	0.76281	N2 mass fraction in air
wcmin	$0.003 \cdot 44 / (0.21 \cdot 32 + 0.787 \cdot 28 + 0.003 \cdot 44)$	0.0045694	CO2 mass fraction in air

Parameters to be Characterized or Reassured for Future Engineering Designs

1. **O₂ concentration level inside the humidity cell testing needs to be confirmed to validate the reaction rate constants, on which these results are based**
2. **Effective diffusivities of gases inside the NAG need to be measured**
3. **Thermal properties, such as specific heat capacity and thermal conductivity of the NAG and the waste rock, also need to be measured**
4. **Water-retention curves of the NAG and the waste rock are needed for further calculation of effective gas permeability and liquid water flow**

Major Assumptions on Key Input Parameters

1. The porosity of NAG tailings is estimated as 10%, assuming that dewatered tailings has 85% solid content and 15% water content by weight throughout NAG tailings
2. Effective gas diffusion coefficients are estimated by $D_e = D_b * \epsilon^{1.5}$, where ϵ is porosity and D_b is gas bulk diffusivity
3. Thermal properties including specific heat capacity and thermal conductivity of the NAG and the waste rock, not available currently, are from literature
4. Sulfide oxidation reaction rates are assumed to be proportional to O2 concentration, and the oxygen consumption rate constant was extracted from the sulfate release rates obtained through humidity cell testing results by SNC-Lavalin
5. Sulfide oxidation reaction is pure pyrrhotite oxidation reaction



Acid-Base Accounting, David L. Fey, **USGS**. Billings Symposium / ASMR Annual Meeting. Assessing the Toxicity Potential of Mine-Waste Piles Workshop, June 1, 2003

THANK YOU

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Appendix: Equations

Boundary conditions:

comin
ccmin

NAG

WR



Por1=0.1
Per1=1.72e-13
Don1=1.76e-5*Por1^1.5[m^2/s]
Dcn1=Don1

Por3=0.2
Per3=1.52e-10
Don3=1.76e-5*Por3^1.5[m^2/s]
Dcn3=Don3

Concentrated species Transport (tcs)
Convection; mass transport in porous media

Equation

$$\rho \frac{\partial \omega_i}{\partial t} + \nabla \cdot j_i + \rho(u \cdot \nabla) \omega_i = R_i$$

$$N_i = j_i + \rho u \omega_i$$

$$j_i = - \left(\rho D_i^f \nabla \omega_i + \rho \omega_i D_i^f \frac{\nabla M_n}{M_n} - j_{c,i} + D_i^f \frac{\nabla T}{T} \right)$$

$$M_n = \left(\sum_i \frac{\omega_i}{M_i} \right)^{-1}, \quad j_{c,i} = \rho \omega_i \sum_k \frac{M_i}{M_n} D_k^f \nabla x_k$$

Rho (ideal gas)
 $R_{wo} = -Ko * wo * tcs.rho$
 $R_{wc} = Ko * wo * Roc * tcs.rho$
 M_n , constants
 D_k , constants (Por depend)
Variables: wo, wn, wc, (mass fractions)

T(ht)
tcs.rho

P_A (dl)
 u (dl)

tcs.rho

Darcy's law

Equation

$$\frac{\partial}{\partial t}(\epsilon_p \rho) + \nabla \cdot (\rho u) = Q_m$$

$$u = - \frac{\kappa}{\mu} \nabla p$$

Por

$K = Per ?$

$Q_m = Ko * wo * Roc * tcs.rho - Ko * wo * tcs.rho$

Variables: p

u (dl)

Heat Transfer in Porous Media

Equation

$$A_c(\rho C_p)_{eff} \frac{\partial T}{\partial t} + A_c \rho C_p u \cdot \nabla T + \nabla \cdot q = A_c Q + q_0 + A_c Q_{vd}$$

$$q = -A_c k_{eff} \nabla T$$

$$(\rho C_p)_{eff} = \theta_p \rho_p C_{p,p} + (1 - \theta_p) \rho C_p$$

$$k_{eff} = \theta_p k_p + (1 - \theta_p) k + k_{disp}$$

$C_{p,p}$, C_p , k_p , k , $\theta_p = 1 - Por$
 $Q_0 = Hp * Ko * wo / 0.032 [kg/mol] * tcs.rho$
Variables: T

Appendix: Reference of Standard Heats of Reactions

TABLE 1. - Standard heats of reaction
(ΔH_{298}°)

Mineral	Oxidation product	ΔH_{298}° kcal/mol
Chalcocite.....	CuO, CuSO ₄	-202.1
	Cu ₂ , SO ₄	-160.2
Chalcopyrite....	FeSO ₄ , CuSO ₄	-361.6
Galena.....	PbSO ₄	-197.0
Marcasite.....	Fe ₂ O ₃ , SO ₂	-200.4
	FeSO ₄ , SO ₂	-253.7
Pyrrhotite.....	Fe ₂ O ₃ , SO ₂	-132.1
	FeSO ₄ , SO ₂	-178.9
Pyrite.....	Fe ₂ O ₃ , SO ₂	-199.4
	FeSO ₄ , SO ₂	-252.7

Reimers, G.W and Hjelmstad, K.E., Analysis of the Oxidation of Chalcopyrite, Chalcocite, Galena, Pyrrhotite, Marcasite, and Arsenopyrite, United States Department of the Interior and Bureau of Mines, Report of Investigations 9118