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Part I: Modeling Study of NMG's Co-disposal of NAG+PAG and Waste Rock

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

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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 1: Develop 1-D model containing layers of NAG + PAG over waste rock

- **Study oxygen transport and consumption by sulphide-mineral oxidation through the central zone of the co-disposition cell**

- **Compare the concept of on-land co-disposal of NAG + PAG over waste rock with dry-stacking of ordinary tailings over waste rock**
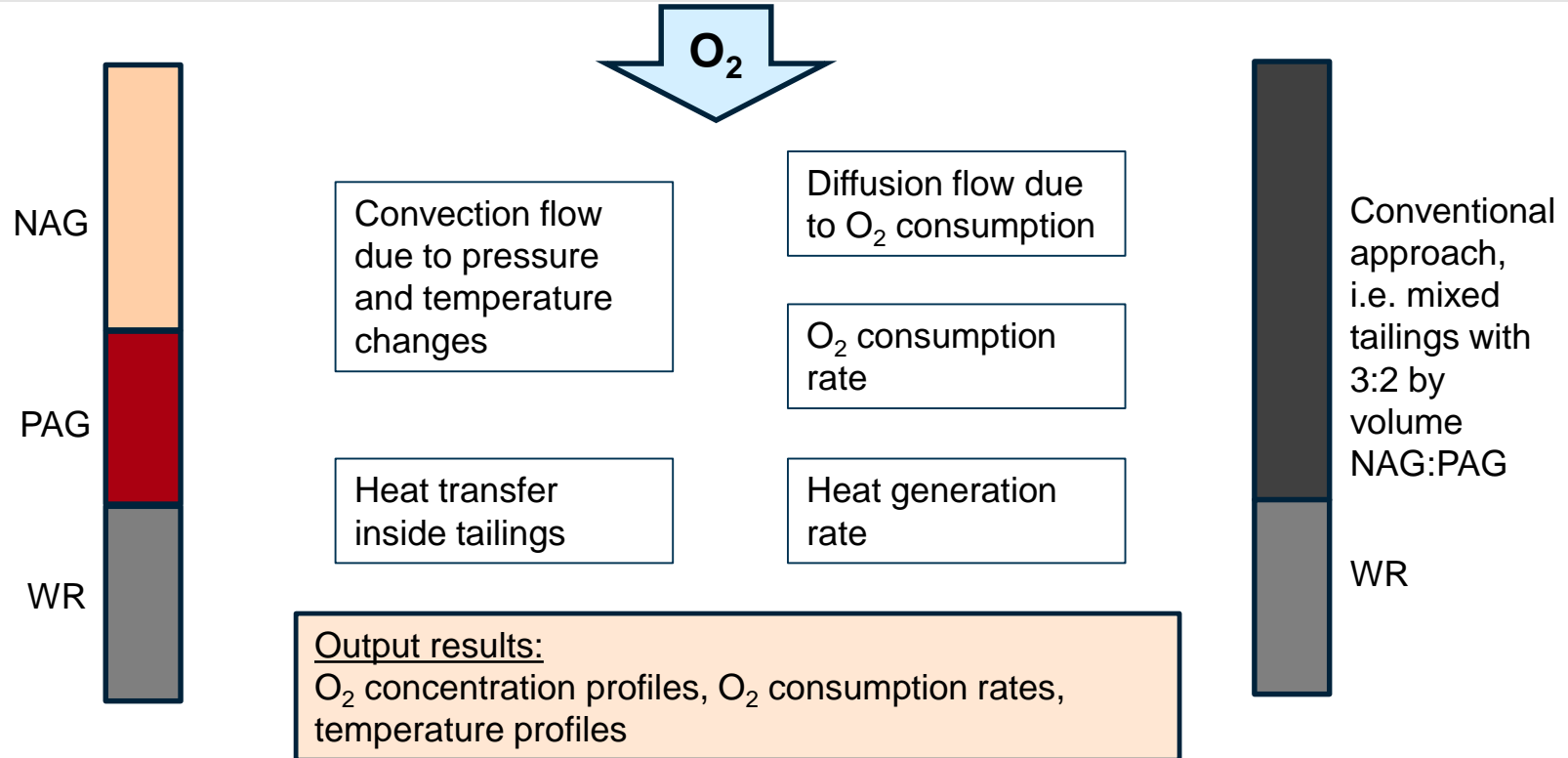
Summary of Preliminary Modeling Results

1. The NMG configuration of the tailings piles, i.e., a NAG layer that is put on the top of a PAG layer, which is on the top of a waste rock layer, is able to hinder the transport of oxygen from the ambient into/through the PAG layer and 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 PAG layer and 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 1.5 - 4 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 PAG 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.
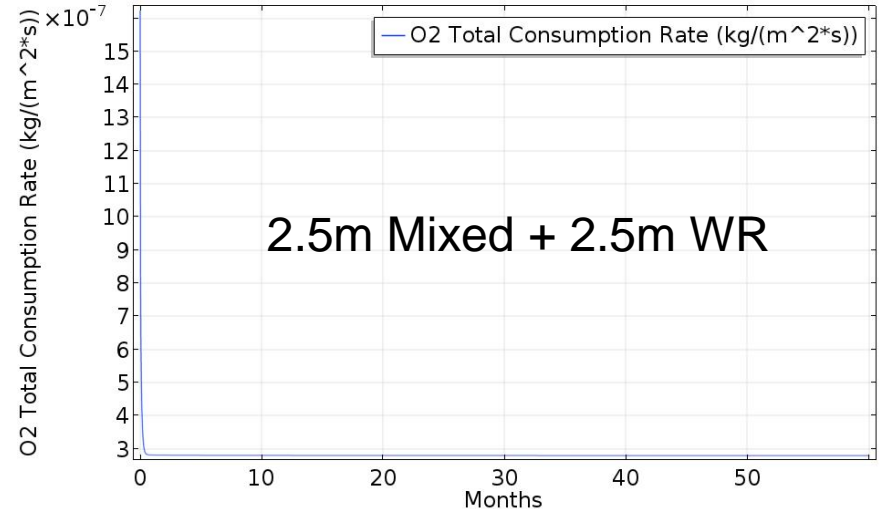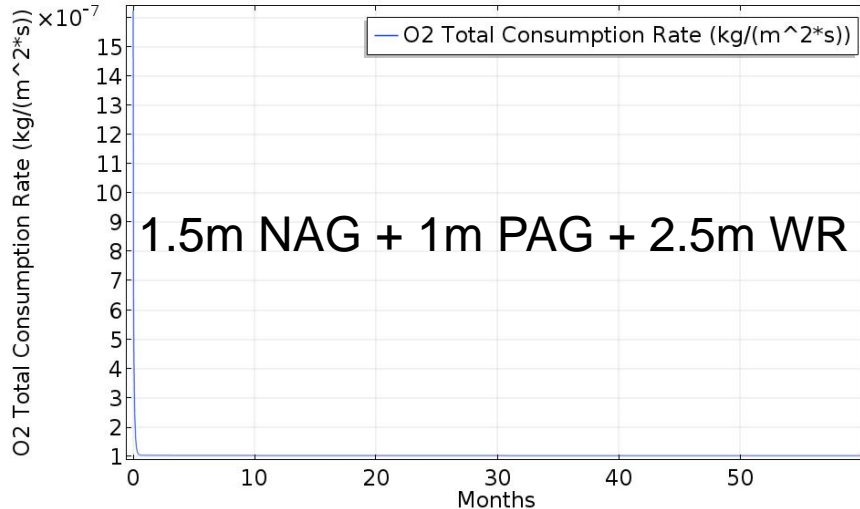
Summary of Preliminary Modeling Results

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 into the PAG layer and the waste rock layer is significantly hindered by the top NAG layer and thus the sulfide oxidation reaction rates inside the PAG layer and 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 PAG layer and the waste rock layer increase by a certain number of degrees C. Our modeling shows that the temperature would increase by about 10 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 PAG layer and the waste rock layer. That is to say, the reduced level of oxygen transport reduces the effect of temperature increase on oxidation reaction rates.
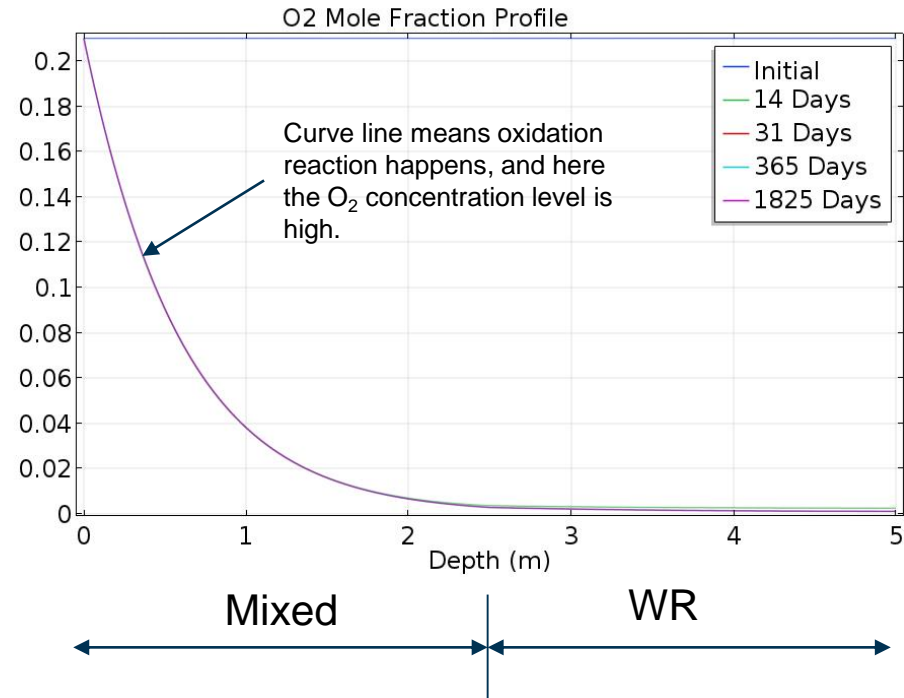
Task 1: NAG+PAG+WR Simulated Phenomena

O_2

NAG

PAG

WR

Convection flow due to pressure and temperature changes

Diffusion flow due to O_2 consumption

O_2 consumption rate

Heat transfer inside tailings

Heat generation rate

Conventional approach, i.e. mixed tailings with 3:2 by volume NAG:PAG

WR

Output results:
O_2 concentration profiles, O_2 consumption rates, temperature profiles

Comparison of O$_2$ Consumption Rates (kg/m²/s)

1.5m NAG + 1m PAG + 2.5m WR

2.5m Mixed + 2.5m WR
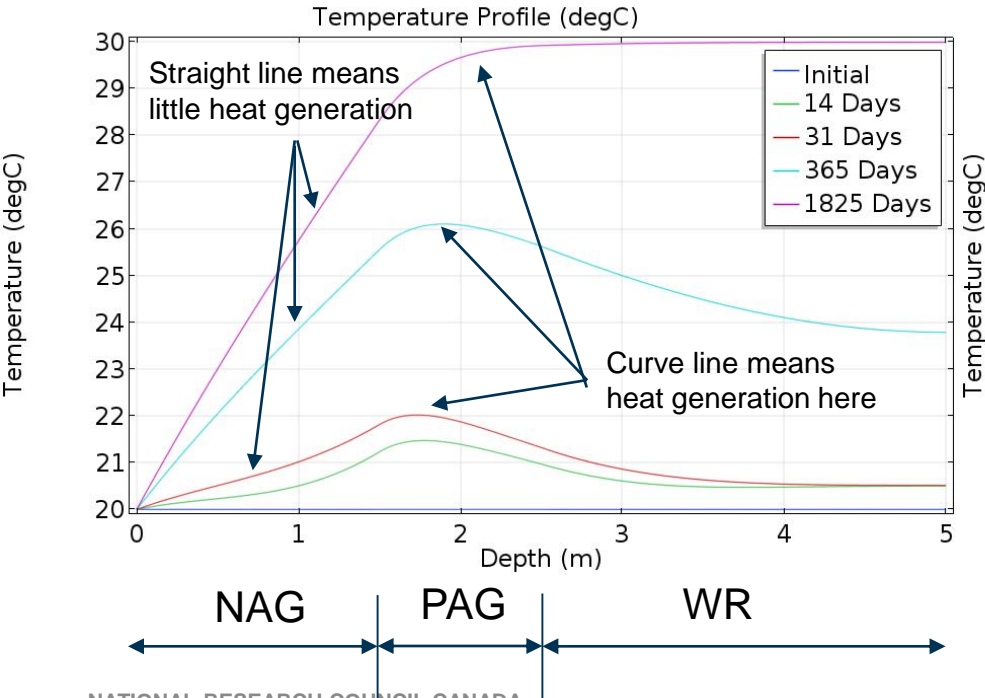
$$\frac{\text{O}_2 \text{ consumption rate in mixed tailings on top of waste rock}}{\text{O}_2 \text{ consumption rate in NAG + PAG on top of waste rock}} = \frac{2.79e\text{-}7}{1.03e\text{-}7} = 2.7$$

Comparison of O$_2$ Mole Fraction Profiles

O2 Mole Fraction Profile

Straight line means little oxidation reaction

Curve line means oxidation reaction happens, but here the O$_2$ concentration level is low.

Legend: Initial, 14 Days, 31 Days, 365 Days, 1825 Days

NAG   PAG   WR

O2 Mole Fraction Profile

Curve line means oxidation reaction happens, and here the O$_2$ concentration level is high.

Legend: Initial, 14 Days, 31 Days, 365 Days, 1825 Days
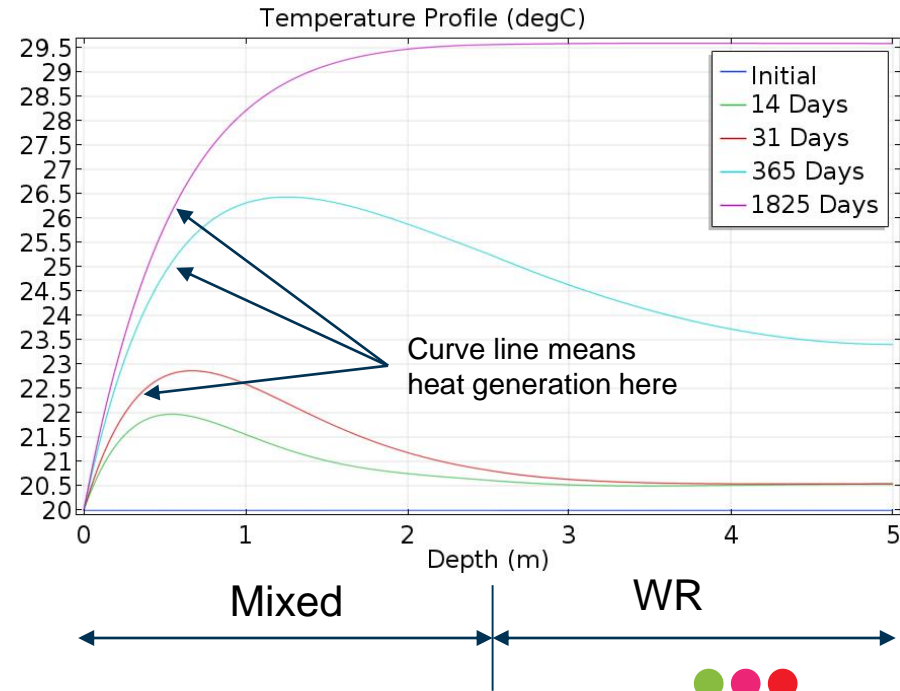
Mixed   WR

Comparison of Temperature Profiles

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

Heat is produced mainly in the Mixed layer, with higher rate due to higher O_2 concentration level
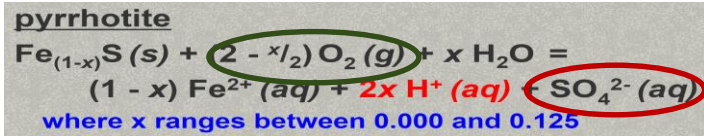
Straight line means little heat generation

Curve line means heat generation here

Curve line means heat generation here

NAG   PAG   WR

Mixed   WR

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*Por1^1.5[m^2/s]	5.5656E-7 m²/s	Effective Gas Diffusivity
Dcn1	1.76e-5*Por1^1.5[m^2/s]	5.5656E-7 m²/s	Effective Gas Diffusivity
Don2	1.76e-5*Por2^1.5[m^2/s]	5.5656E-7 m²/s	Effective Gas Diffusivity
Dcn2	1.76e-5*Por2^1.5[m^2/s]	5.5656E-7 m²/s	Effective Gas Diffusivity
Don3	1.76e-5*Por3^1.5[m^2/s]	1.5742E-6 m²/s	Effective Gas Diffusivity
Dcn3	1.76e-5*Por3^1.5[m^2/s]	1.5742E-6 m²/s	Effective Gas Diffusivity
Per1	1.72e-13[m^2]	1.72E-13 m²	NAG Permeability
Per2	1.52e-13[m^2]	1.52E-13 m²	PAG Permeability
Per3	1.52e-10[m^2]	1.52E-10 m²	Waste Rock Sample Permeabili...
Vis	18.6e-6[Pa*s]	1.86E-5 Pa·s	Air viscosity
Dens_s	1810[kg/m^3]	1810 kg/m³	Tailings density
Hst	1.2e6[J/K/m^3]	1.2E6 J/(m³·K)	Heat capacity of tailings
Hct	0.2[J/K/s/m]	0.2 W/(m·K)	Thermal conductivity of tailings
Hsg	1012[J/kg/K]	1012 J/(kg·K)	Specific heat of air
Hcg	0.0251[W/m/K]	0.0251 W/(m·K)	Thermal conductivity of air
Hp	(744e3/2)[J/mol]	3.72E5 J/mol	Reaction Heat
Ko2	4.2e-6[1/s]	4.2E-6 1/s	O2 Consp. Rate in PAG
Ko1	8.33e-8[1/s]	8.33E-8 1/s	O2 Consp. Rate in NAG
Ko3	5.95e-7[1/s]	5.95E-7 1/s	O2 Consp. Rate in WR
Y	360*24*60*60	3.1104E7	
Rco	8314.4598[J/(kmol*K)]	8.3145 J/(mol·K)	Universal gas constant
Rs	Rco/29[kg/kmol]	286.71 J/(kg·K)	Specific gas constant
womin	0.21*32/(0.21*32+0.787*28+0.003*44)	0.23262	O2 mass fraction in air
wnmin	0.787*28/(0.21*32+0.787*28+0.003*44)	0.76281	N2 mass fraction in air
wcmin	0.003*44/(0.21*32+0.787*28+0.003*44)	0.0045694	CO2 mass fraction in air

Parameters to be Characterized or Reassured for Future Engineering Designs

1. O_2 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 and the PAG need to be measured

3. Thermal properties, such as specific heat capacity and thermal conductivity of the NAG, the PAG and the waste rock, also need to be measured

4. Water-retention curves of the NAG, the PAG 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 and PAG tailings is estimated as 10%, assuming that dewatered tailings has 85% solid content and 15% water content by weight throughout NAG and PAG tailings

2. Effective gas diffusion coefficients are estimated by $D_e = D_b * \varepsilon^{1.5}$, where ε is porosity and D_b is gas bulk diffusivity

3. Thermal properties including specific heat capacity and thermal conductivity of the NAG, the PAG 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

pyrrhotite
$Fe_{(1-x)}S (s) + (2 - {}^x/_2) O_2 (g) + x H_2O =$
$(1 - x) Fe^{2+} (aq) + 2x H^+ (aq) + SO_4{}^{2-} (aq)$
where x ranges between 0.000 and 0.125

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

Appendix: Equations

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

Boundary conditions:

comin
ccmin

NAG

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

PAG

Por2=0.1
Per2=1.52e-13
Don2=1.76e-5*Por2^1.5[m^2/s]
Dcn2=Don2

WR

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

Equation

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

$$\mathbf{N}_i = \mathbf{j}_i + \rho \mathbf{u}\omega_i$$

$$\mathbf{j}_i = -\left(\rho D_i^f \nabla \omega_i + \rho \omega_i D_i^f \frac{\nabla M_n}{M_n} - \mathbf{j}_{c,i} + D_i^T \frac{\nabla T}{T}\right)$$

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

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)
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tcs.rho

Heat Transfer in Porous Media

Equation

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

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

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

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

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

Darcy's law

Equation

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

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

u (dl)

Por
K = Per ?
Q_m=Ko*wo*Roc*tcs.rho-Ko*wo*tcs.rho
Variables: p

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_2O_3, SO_2......	-200.4
	$FeSO_4, SO_2$......	-253.7
Pyrrhotite......	Fe_2O_3, SO_2......	-132.1
	$FeSO_4, SO_2$......	-178.9
Pyrite..........	Fe_2O_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 Stated Department of the Interior and Bureau of Mines, Report of Investigations 9118