Part 2: Reactive Transport Modeling in Mine Waste Management – Where to from Here?

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Mine Waste Environments

Mine Tailings



Decommissioned **Underground Mines**



Waste Rock Piles



Decommissioned **Heap Leach Pads**





RTM Examples Related to Waste Rock

• Case Study:

 Diavik Waste Rock Research Project - reactive transport model (RTM) to identify scaling relationships for ARD from laboratory experiments to full-scale piles



Case Study: Diavik Waste Rock Research Project David Wilson, David Blowes and coworkers (UWaterloo), Wilson et al (2018a,b)



Full Scale Pile Mechanistic scale-up **Test Piles** Active Zone Lysimeters 80 m (1.2 x 10¹¹ kg) Humidity Cells Wilson et al (2018a,b) 15 m (8.2 x 10⁷ kg) 2 m (9,300 kg) 0.1 m (1 kg)

Hypothesis: RTM can be *used to implement* an integrated conceptual model of sulfide waste rock weathering for laboratory experiments (i.e. humidity cells), then *scaled* to assess the geochemical evolution of a waste rock pile (i.e. full scale pile).

Humidity Cells

Test Piles

Temperature Constant: 22 °C and 5 °C

Hydrology Constant: 500 mL wk⁻¹

Geochemistry

Gas:

• Atmospheric P_{O_2} , P_{CO_2} Liquid:

• DI

Solid:

- Sulfides: pyrrhotite, chalcopyrite, sphalerite, pentlandite (total 0.18 wt.% S)
- Host: calcite, dolomite, biotite, muscovite, albite
- Secondary: jarosite, ferrihydrite, gibbsite, amorphous silica, gypsum, siderite

Temperature Spatially and temporally variable average daily temperature

Hydrology

Temporally variable FAO-PM calculated infiltration Constant K_s and soil parameters from characterization of site materials

Flow stopped under freezing conditions

Geochemistry

Gas:

- Atmospheric P_{O_2} , P_{CO_2} Liquid:
- Site precipitation

Solid:

- Sulfides: pyrrhotite, chalcopyrite, sphalerite, pentlandite
- Host: calcite, dolomite, biotite, muscovite, albite
- Secondary: jarosite, ferrihydrite, gibbsite, amorphous silica, gypsum, siderite

Wilson et al (2018a,b)



Geochemistry - Summary



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Annual Mass Flux – Test Pile



Wilson et al (2018a,b)



Lessons Learned – Diavik Case Study

- A reactive transport model calibrated to laboratory experiment results can be used to provide realistic multiyear assessment of waste rock geochemical evolution on the test pile scale
 - Geochemistry identical, BUT:
 - Scale-up requires consideration of additional processes (freezethaw, temperature fluctuations, hydraulic response)
- Commonly measured parameters can be used to constrain the modeling (does not need to be overly complex!):
 - Mineralogy (host rocks and sulfide minerals)
 - Infiltration
 - Temperature
 - Particle size distribution

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Scenario Analyses:

 Effect of internal structure, heterogeneity, and scale on ARD release: Do pile construction methods affect ARD release, and if so, how?



Effect of internal structure, heterogeneity, and scale on ARD release Katherine Raymond, MSc-student



Photo: Bas Vriens



Influence of Heterogeneity and Spatial Trends

Case		Max Mass Loading Rate	Decrease from Homogeneous		
		[mg ¹ kg ⁻¹ week ⁻¹]	Case		
Single Bench Models					
Homogeneous		61.8	-		
Heterogeneous	Push Dump	43.6	29%		
	End Dump	54.6	12%		
Structure	Push Dump				
	End Dump				



Total Basal Sulfate Mass Loading Release Rates



Influence of Structure (Traffic Surfaces and Trends)

Case		Max Mass Loading Rate [mg ¹ kg ⁻¹ week ⁻¹]	Decrease from Homogeneous Case	
Single Bench Models				
Homogeneous		61.8	-	
Heterogeneous	Push Dump	43.6	29%	
	End Dump	54.6	12%	
Structure	Push Dump	39.8	36%	
	End Dump	38.4	38%	





100

Influence of Structure Over Multiple Bench Models





100

Max Mass

Loading Rate

[mg¹ kg⁻¹ week⁻¹]

61.8

43.6

Single Bench Models

Case

Homogeneous

Push Dump

Decrease from

Homogeneous

Case

_

29%

Lessons learned – construction methods

- Inclusion of heterogeneity and construction methods in RTM can have a significant impact on predicted maximum mass loading rates (reduced from homogeneous model by 36 - 43%)
- Scale and presence of traffic surfaces are most important
 - Mass loading rates were comparable by the multi-lift pile for between construction methods (push vs. end dumping)

RTM Examples Related to Waste Rock

Case Study:

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Scenario Analyses:

- Effect of internal structure, heterogeneity, and scale on ARD release: Do pile construction methods affect ARD release, and if so, how?
- Effect of climate change on ARD generation and release under cold climate conditions: In search for the tipping point.



Permafrost and Mine Waste Storage Planning





ARD generation and release under cold climate conditions, Xueying Yi, MSc student

Current work:

- Consider heat from sulfide mineral oxidation
- Capture effects of freeze-thaw
- Insulation from snow cover
- Influence of TDS/solutes on water freezing-temperature
- Compare differences in potential mass loadings under different annual temperature changes due to climate change





Conceptual Model

- Sulfide mineral oxidation in active layer
 - Seasonally controlled
 - Exothermic: generation of heat with effects on active layer and permafrost

Seasonal climate forcing Precip, T **Active Layer** Waste Rock ARD release at base of waste rock?? Permafrost Natural sediments or rock Geothermal heat flux



Simulated temperature profiles as a function of average yearly temperatures

- Pyrite oxidation rate at 25 deg C: 1.7 x 10⁻¹⁰ mol dm⁻³ bulk s⁻¹
- Minor differences in active layer thickness
- No ARD release in any of the cases



Simulated temperature profiles as a function of average yearly temperatures

- Pyrite oxidation rate at 25 deg C: 1.7 x 10⁻⁸ mol dm⁻³ bulk s⁻¹
- Active layer reaches below based of WRP in all cases
- ARD release in all cases

Simulated temperature profiles as a function of average yearly temperatures

- Pyrite oxidation rate at 25 deg C: 1.7 x 10⁻⁹ mol dm⁻³ bulk s⁻¹
- Tipping Point!!
- ARD release due to increased MAAT

Basal sulfate loading of intermediate scenario over time with MAAT = -9 deg C and -6 deg C

Lessons learned – cold climate conditions and climate change

- Just starting to learn
- Preliminary simulation results suggest that climate change will have a limited effect in many cases
- On the other hand, effect can be substantial, if tipping point is reached
- Increase of active layer thickness to base of WRP may lead to short-lived high mass loadings. Food for thought.

Where do we go from here?

- Reactive transport models for simulating processes in mine tailings and waste rock are available
- MIN3P: 20+ year development and ongoing
- Complex geometry can now be included
- Computational efficiency allows to carry our larger scale 2D simulations, if needed
- Looking towards expanding model capabilities for non-isothermal, multiphase systems

Is there interest in the ARD community to use RTM models? If so, what are you looking for?

Reactive Transport Modeling Interest Survey <u>https://tinyurl.com/v5bw5dl</u> ...or grab a paper survey at reception table!

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Conceptual Model – Theory

Oxidation by O_{2(aq)}:

 $Fe_{0.852}Ni_{0.004}Co_{0.001}S + 1.9285O_{2(aq)} + 0.143H_2O \rightarrow$ $0.852Fe^{2+} + 0.004Ni^{2+} + 0.001Co^{2+} + SO_4^{2-} + 0.286H^+$

Oxidation by Fe³⁺:

$$\begin{split} Fe^{2+} &+ 0.25O_{2(aq)} + H^+ \rightarrow \mathrm{Fe}^{3+} + 0.5H_2O \\ &Fe_{0.852}Ni_{0.004}Co_{0.001}S + 1.714Fe^{3+} \rightarrow \\ &2.566Fe^{2+} + 0.004Ni^{2+} + 0.001Co^{2+} + S^0 \\ &S^0 + 1.5O_{2(aq)} + H_2O \rightarrow SO_4^{2-} + 2H^+ \end{split}$$

Sulfide oxidation simulated using shrinking core model

polysulfide mechanism of sulfide mineral oxidation

Schippers and Sand, 1999

Mayer et al., 2002