

The main prediction I have to share today is that reactive transport models of mine waste facilities will become as common as groundwater models of mine sites. Why? Because they are powerful tools for assembling the numerous processes in waste rock and tailings and they offer a leap forward in development of source terms for water quality prediction. My story starts back in 2006, learning the basics of reactive transport modelling at UBC. Then, after three years studying how rain and snowmelt percolates through large waste rock piles, I realized it isn't as mysterious as people feared. Established hydrogeological methods and models could be used to predict the water flow. The geochemistry is complex: it took the U. of Waterloo team several more years to successfully model reactive transport in waste rock. But that moment in 2018 in this workshop signaled to the industry that there is a better way to predict metal leaching and acid rock drainage. For me as a consultant working with mining companies, I'm happy to share with you how we are using reactive transport modelling and modern mineralogy to improve how we predict water quality to support mine waste management and closure planning.



I'll introduce RTM, discuss ML/ARD prediction and how we apply modern mineralogy methods, and present a case study on modelling tailings for a base case of a no-cover scenario and evaluation of mitigation options



I'll start with a brief introduction to reactive transport modelling



Reactive transport models are numerical models that represent reactions, water flow, and transport in the subsurface. They integrate chemical and physical processes in a fully-coupled framework. Looking at the schematic here, we can simulate infiltration and unsaturated or saturated water flow. In each model cell we can simulate reactions between mineral, water, and gas phases: for example minerals like calcite dissolving or ferrihydrite precipitating according to thermodynamic equilibrium or pyrite transferring mass and acidity to the water according to oxygen levels and reaction kinetics. The water in each model cell can then equilibrate and we can specify particular redox reactions if we need to. Water flow is simulated according to hydraulic properties and heads, and mass is transported by advection, dispersion, and diffusion with the ability to simulate ion exchange and adsorption.



How do these models help us? We use them to check and refine conceptual models. We develop water quality predictions based on hydrogeological and geochemical processes, with those processes built right into the model, rather than using empirical scaling. And we can use these models to assess mitigation options.



Okay, now I'll discuss how we apply reactive transport models and results from modern mineralogy to the prediction of metal leaching and acid rock drainage



Thankfully, much work in the previous decades has resulted in clear and comprehensive guidance on how to predict ML/ARD from sulphidic materials. Probably most of you are familiar with Bill Price's prediction manual. After learning about a site and doing lots of characterization work, the last step is to predict the drainage chemistry. While chapter 20 discusses some options for geochemical modelling, the most common approach is to use empirical adjustments to static and kinetic test results to predict the drainage chemistry. But doing this accurately is a big challenge, to develop predictions for a full-scale mine waste facility based on 1 kg lab tests. Prediction is even challenging for mines that have operated for decades.



Here is a little more detail about prediction using the traditional approach. We start with static testing in the lab... Then we do kinetic tests in the lab... We then build a water quality model using a mass balance approach, using for example GoldSim or MineMod. We need some kind of a bridge to cross the orders of magnitude gap between mass loading rates in small lab tests and mass loading rates from huge mine waste facilities. So we use empirical scaling factors to try to account for the differences... If it is an existing mine, we have field measurements that we can use to calibrate the model. And then we run the model into the future to develop our forecast of water quality. But our greatest uncertainties in these forecasts are the source terms: the mass loading rates from the waste rock and tailings.



Now we're improving the approach by using automated SEM-EDS and sometimes laser ablation, which I'll discuss more. Sometimes we're using field tests, which can be a huge help. The key advance is that we're using reactive transport modelling to develop mechanistic models of mineral reactions in tailings and waste rock. This allows us to reduce uncertainty in closure planning.

Formula	Reaction	log Ki	Initial Volume Fraction m3 mineral m-3 bulk
	Primary Minerals		
Fe <sup>0.85</sup> Co <sup>0.00001</sup> Pb <sup>0.00002</sup> Ni <sup>0.00003</sup> S	$Fe^{0.85}Co^{0.00001}Pb^{0.000002}Ni^{0.00003}S + 1.925O^{2} + 0.15H^{2}O \rightarrow 0.85Fe^{2^{4}} + SO^{4^{2}} + 0.00001Co^{2^{4}} + 0.000002Pb^{2^{4}} + 0.00003Ni^{2^{4}} + 0.3H^{4}O^{2} + 0.00001Co^{2^{4}} + 0.000002Pb^{2^{4}} + 0.00003Ni^{2^{4}} + 0.0003Ni^{2^{4}} + 0.00003Ni^{2^{4}} + 0$	-	1E-02
FePb <sup>0.00001</sup> AsS	$FePb^{0.00001}AsS + 1.5H^{2}O + 3.25O^{2} \rightarrow Fe^{2^{4}} + SO^{4^{2^{4}}} + H^{3}AsO^{4} + 0.00001Pb^{2^{4}}$	-	3E-07
CuFeS <sup>2</sup>	$CuFeS^2 + 4O^2 \rightarrow Fe^{2*} + Cu^{2*} + 2SO^{4^{2*}}$	-	2E-06
ZnS	$ZnS + 2O^2 \rightarrow SO^{4^2} + Zn^{2+}$	-	1E-06
CaCO <sup>3</sup>	CaCO <sup>3</sup> + H <sup>+</sup> ↔ Ca <sup>2+</sup> + HCO <sup>3*</sup>	-8.48	2E-02
CaMg(CO <sup>3</sup> ) <sup>2</sup>	$CaMg(CO^3)^2 + 2H^+ \leftrightarrow Ca^{2+} + Mg^{2+} + 2HCO^3$	-17.1	7E-04
Ca(Mg,Fe, Mn)(CO <sup>3</sup> ) <sup>2</sup>	$Ca(Mg,Fe,Mn)(CO^3)^2 + 2H^+ \leftrightarrow Ca^{2+} + 0.1Mg^{2+} + 0.87Fe^{2+} + 0.03Mn^{2+} + 2HCO^{3+}$	-17.1	7E-04
KAI <sup>2</sup> (AISi <sup>3</sup> O <sup>10</sup> )(OH) <sup>2</sup>	KAI <sup>2</sup> (AISI <sup>3</sup> O <sup>10</sup> )(OH) <sup>2</sup> + 10H <sup>+</sup> ↔3H <sup>4</sup> SIO <sup>4</sup> + 3AI <sup>3+</sup> + K <sup>+</sup>	-	5E-02
KFe3(AISi3O10)(OH)2	K(Mg,Fe) <sup>3</sup> (AlSi <sup>3</sup> O <sup>10</sup> )(OH) <sup>2</sup> + 10H <sup>+</sup> ↔ 3H <sup>4</sup> SiO <sup>4</sup> + Al <sup>3+</sup> + 3Fe <sup>2+</sup> + K <sup>+</sup>	-	1E-02
	Secondary Minerals		
Fe(OH) <sup>3</sup> (am)	Fe(OH) <sup>3</sup> + 3H <sup>+</sup> ↔ Fe <sup>3+</sup> + 3H <sup>2</sup> O	4.89	1E-10
FeCO <sup>3</sup>	$FeCO^3 \leftrightarrow Fe^{2*} + CO^{3^2}$	-10.9	1E-10
AI(OH) <sup>3</sup>	AI(OH) <sup>3</sup> + 3H <sup>+</sup> ↔ AI <sup>3+</sup> + H <sup>2</sup> O	8.11	1E-10
CaSO <sup>4</sup> x 2H <sup>2</sup> O	$CaSO^4 \times 2H^{2O} \leftrightarrow Ca^{2*} + SO^{4^{2*}} + 2H^{2O}$	-4.58	1E-10
KFe <sup>3</sup> (SO <sup>4</sup> ) <sup>2</sup> (OH) <sup>6</sup>	KFe <sup>3</sup> (SO <sup>4</sup> ) <sup>2</sup> (OH) <sup>6</sup> + 6H <sup>+</sup> ↔ K <sup>+</sup> + 3Fe <sup>+3</sup> + 2SO <sup>42</sup> + 6H <sup>2</sup> O	-9.21	1E-10
	Formula           Fe <sup>0.456</sup> Co <sup>0.00001</sup> Pb <sup>0.00002</sup> Ni <sup>0.00003</sup> S           CuFeS <sup>2</sup> ZnS           CaCO <sup>3</sup> CaMg(FCO <sup>3)2</sup> Ca(Mg,Fe, Mn)(CO <sup>3)2</sup> XAP(AIS <sup>10</sup> O <sup>10</sup> )(OH) <sup>2</sup> XFe <sup>2</sup> (AIS <sup>100</sup> 10(OH) <sup>2</sup> )           Fe(OH) <sup>2</sup> (am)           FeCO <sup>3</sup> A(ICH) <sup>3</sup> CaSO <sup>4</sup> x 2H <sup>2</sup> O           Kre <sup>4</sup> (SO <sup>4</sup> ) <sup>2</sup> (OH) <sup>6</sup>	Formula         Reaction $F_{e0}^{0.85}C_{0}^{0.0001}Pb^{0.00002}N ^{0.00005} F = 1.9250^{2} + 0.15H^{2}O - 0.65Fe^{2*} + SO4^{2*} + 0.00001Co^{2*} + 0.000002Pb^{2*} + 0.00003N ^{2*} + 0.3H^{2*}$ $F_{e0}^{0.85}C_{0}^{0.0001}Pb^{0.00002}N ^{0.00005} F = 1.9250^{2*} + 0.5H^{2}O - 0.65Fe^{2*} + SO4^{2*} + 0.00001Pb^{2*}$ CuFeS2         CuFeS2 + 40^{2*} + Fe^{2*} + Cu^{2*} + 2504^{2*}           CaCO <sup>3</sup> CaCO <sup>3</sup> + M <sup>2*</sup> + Ca <sup>2*</sup> + HCO <sup>3*</sup> CaCO <sup>3</sup> CaCO <sup>3</sup> + H <sup>2*</sup> + Ca <sup>2*</sup> + HCO <sup>3*</sup> Ca(G)(CO <sup>3</sup> )2         Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2 + 2H <sup>4*</sup> + Ca <sup>2*</sup> + 0.1Mg <sup>2*</sup> + 0.1Tg <sup>2*</sup> + 0.03Mn <sup>2*</sup> + 2HCO <sup>3*</sup> Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2         Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2 + 2H <sup>4*</sup> + Ca <sup>2*</sup> + HO <sup>3*</sup> Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2         Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2 + 2H <sup>4*</sup> + Ca <sup>2*</sup> + 10.1Mg <sup>2*</sup> + 0.3FFe <sup>2*</sup> + 0.03Mn <sup>2*</sup> + 2HCO <sup>3*</sup> Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2         Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2 + 2H <sup>4*</sup> + Ca <sup>2*</sup> + 10.1Mg <sup>2*</sup> + 0.3FFe <sup>2*</sup> + 10.03Mn <sup>2*</sup> + 2HCO <sup>3*</sup> Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2         Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2 + 2H <sup>4*</sup> + Ca <sup>2*</sup> + 10.1Mg <sup>2*</sup> + 0.3FFe <sup>2*</sup> + 10.1Mg <sup>2*</sup> + 0.3FFe <sup>2*</sup> + 10.03Mn <sup>2*</sup> + 2HCO <sup>3*</sup> Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2         Ca(Mg,Fe, Mn)(CO <sup>3</sup> )2 + 2H <sup>4*</sup> + Ca <sup>2*</sup> + 10.1Mg <sup>2*</sup> + 0.3FFe <sup>2*</sup> + 10.1Mg <sup>2*</sup> + 0.3FFe <sup>2*</sup> + 10.1Mg <sup>2*</sup> + 0.2FFe <sup>2*</sup> + 10.1Mg <sup>2*</sup>	$ \begin{array}{c c c c c c c c c c c c c c c c c c c $

With reactive transport modelling, it is important that we understand the reactions and have good mineralogy testing. The mineralogy is the starting point. Here is an example of how we simulate the stoichiometry of mineral reactions. In this case, the main sulphide mineral is pyrrhotite, and if your eyesight is good, you can see we incorporate in MIN3P trace amounts of cobalt, lead, and nickel in the pyrrhotite. Other metals might be present in sulphide minerals such as arsenopyrite, chalcopyrite, and sphalerite, which in this case are present in trace amounts. To model the waste rock or tailings in this way, it is a huge advantage to have modern mineralogy methods. These methods are very helpful for quantifying bulk mineralogy, but are particularly useful for quantifying trace sulphides and carbonates and trace metals in minerals.



Traditional mineralogy methods are still helpful, but they have their limitations. X-ray diffraction has marginal resolution for the minerals of interest for metal leaching and acid rock drainage. Whole rock elemental analyses leave us wondering which minerals host the metals.



Automated scanning electron microscopy with energy dispersive spectroscopy provides us with the resolution we need for sulphides and carbonates. We can identify those trace metals-bearing minerals. And we can learn about mineral texture, size, liberation, and associations. Operators of metals mines have been doing this for over a decade to quantify orebodies, but commercial application to mine waste is new in the last several years.



Laser ablation ICP-MS or electron microprobe allows us to measure metals contents in specific mineral grains to part-per-million levels. Why do we need this? Since metals can be toxic at trace levels, we need to be able to model their trace levels in the solid phase.



We use several kinetic formulations for mineral reactions. One of these is the shrinking core model, which we often use within MIN3P to simulate sulphide mineral oxidation. Over time an alteration rim builds up on the sulphide mineral grains, as shown in the schematic and in the SEM image. The oxidant, oxygen or ferric iron, then has to diffuse through the reaction rim to reach the fresh sulphide mineral. Since the reaction rim grows over time, the reaction rate decreases.



In a reactive transport model, we may need to incorporate a mechanism for metals release and attenuation. The pH-dependent solubility inherently included in the thermodynamics might not explain observed attenuation and release. In the case studies I'll present next, we had to include pH-dependent adsorption and desorption reactions. In the humidity cell example shown here, lead released from pyrrhotite, adsorbed to iron oxyhydroxide surfaces at neutral pH, and then desorbed when carbonates were depleted and pH dropped.



This schematic shows the general work flow for a reactive transport model. First we choose the modelling tool. The model code has to go through verification and validation. If we use an established model code, this has been done already. We build the conceptual model that we'll apply in the numerical model, based on previous experience and site-specific data. We interpret field and lab data and build the numerical model using those results. We start simple and refine the model inputs by layering on complexity only as needed. We then may need to calibrate the model to lab or field data. (David Wilson showed us with the Diavik waste rock project how the processes can be defined well enough in a reactive transport model, that calibration might not even be needed.) After all of that, we then have enough confidence in a model to forecast future behaviour and assess mitigation options.

## MIN3P

- MIN3P selected features (Mayer 1999; Mayer et al. 2011, 2015; Steefel et al. 2015)
  - Transient, <u>variably-saturated</u> water flow in 1D, 2D, or 3D
  - Advective-dispersive transport with diffusion
  - Mineral water reactions: equilibrium or kinetic dissolution / precipitation
  - Adsorption, ion exchange, and aqueous complexation
  - <u>Gas diffusion</u>, partitioning, and reactions
  - Global Implicit Method: flow and geochem solved simultaneously
  - Adaptive time steps
- Other codes: PFLOTRAN, CrunchFlow, HP1, TOUGHReact
- Powerful tool for understanding weathering of mine waste



For the case studies I'll present next, we used the reactive transport code MIN3P, which was developed by Uli Mayer when he was at the University of Waterloo and has been further developed by he and his team at UBC for over 20 years. With MIN3P we can simulate all of the processes discussed in the previous slides. There are a few other codes that can represent a similar suite of processes. In particular, the ability to model variably-saturated flow, gas diffusion, and simultaneous solution of flow and geochemistry makes MIN3P a powerful tool for understanding the weathering of mine waste.

www.min3p.com

Physico-Che

External source-sinks

Q<sup>a,in</sup>

Interna

urce-sinks

17



Okay, now on to the case studies



The first case study is a tailings storage facility at a confidential gold mine site. The tailings are exposed to precipitation and evapotranspiration, so water percolates through them. Oxygen diffuses into the tailings, and in the unsaturated tailings, pyrrhotite oxidizes to release iron, sulphate, and acidity plus trace cobalt, lead, and nickel. Carbonate minerals buffer acidity, both in the unsaturated and saturated tailings, and metals are attenuated by adsorption to iron oxyhydroxide surfaces. The contact water seeps into the groundwater, so it is important for us to understand: will ARD develop? Will water treatment be needed? What type of cover is needed?



During operations, process water inundates most of the tailings. Tailings under the active beaches don't get much chance to oxidize, but tailings in an area that has been inactive for several years have oxidized. Seepage and porewater has neutral pH, except the porewater at the inactive beach. We modelled the facility during operations with a 1-D domain in MIN3P, with the upper 2 m unsaturated.



With the model we're able to represent more than a decade of measurements of neutral pH conditions that are due to the dominance of the process water, as well as the evident influence of reactions in the seepage at the toe of the dam. Sulphate and cobalt are among the constituents with elevated concentrations under the neutral conditions, and the model is able to represent this with appropriate kinetics assigned to the sulphide oxidation reactions. Not shown here, but we also simulated the acidic conditions in the unsaturated zone of the inactive beach, with much higher metals concentrations in the porewater. With the hydrogeological and geochemical mechanisms adequately modelled, we now have a tool we can use to forecast the post-closure conditions with some confidence.



Post-closure the tailings facility will be higher, and the water levels will drop resulting in a thick region of unsaturated potentially acid generating tailings. We simulated the facility with a series of 1-D model domains in MIN3P, with best-case, worst-case, and best estimate scenarios. One of the key questions was whether the carbonate minerals in the saturated tailings would be able to neutralize acidity generated in the overlying unsaturated PAG tailings.



The forecasts represent four hundred years, because that is a relevant timeframe for depletion of the pyrrhotite that is the main source of acidity and some of the metals. Porewater in the surficial tailings is shown with dashed lines, and seepage from the base of the tailings is shown with solid lines. The surficial tailings were simulated to go acidic in the initial decade post-closure, with elevated concentrations of most metals because the hydrogen ions dominate the sorption sites. But in the underlying saturated tailings, we forecasted that there will be enough carbonate minerals to maintain neutral pH seepage for most of the model runs, and some metals like nickel will be attenuated by adsorption. But even with the neutral pH, we forecasted seepage to have elevated sulphate, cobalt, and iron concentrations. We also couldn't rule out at this point the worst-case possibility that the seepage from the facility could go acidic with high metals concentrations, which you can see with the red lines. So we see that mitigation will be needed, especially for the runoff.



The third and final case study is using reactive transport modelling to evaluate cover options on a tailings facility. We modelled three options: a vegetative cover consisting of sand and gravel and topsoil, a multi-layer soil cover with a silty till layer between layers of sand and gravel, and a cover with an HDPE liner.



The improved covers, Cover Type 2 and 3, retained high water saturations, shown with the blue colour. This is not surprising for the cover with the HDPE liner, but certainly a good outcome for the multi-layer soil cover. Also, it was interesting to see that the moisture content in the tailings below the vegetative soil cover was a little lower than for the no-cover scenario due to transpiration through the vegetation.



The high moisture content in the multi-layer cover resulted in low oxygen concentrations in the tailings, shown in blue. Similarly the HDPE liner limited oxygen ingress to the tailings. These improved covers resulted in minimal sulphide mineral consumption modelled in the tailings.



Porewater quality in the tailings under the vegetative cover was similar as for the nocover scenario, as you can see with the low pH and high concentrations shown with the red and grey lines. But the porewater quality under the multi-layer cover and under the HDPE liner, shown with the green and blue lines, was much improved in the models. These results led our client to initiate a feasibility study for a multi-layer cover system, with the following step likely being test plots in the field.



Environmental success is critical for building trust in the mining industry.

## References

Amos RT, Blows DW, Smith L, Sego DC. 2009. Measurements of wind-induced pressure gradients in a waste-rock pile. Vadose Zone Journal, 8:953-962. https://doi.org/10.2136/vzj2009.0002 Appelo CAJ, Postma D. 2005. Geochemistry, groundwater and pollution, 2<sup>nd</sup> Ed. CRC Press, New York: 649p.

pp......

Ohlander B, Müller B, Axelsson M, Alakangus L. 2007. An attempt to use LA-ICP-MS to quantify enrichment of trace elements on pyrite surfaces in oxidizing mine tailings. Journal of Geochemical Exploration, 92:1-12. https://doi.org/10.1016/j.gexplo.2006.06.001

Kirchner T, Mattson B. 2015. Scaling geochemical loads in mine drainage chemistry modeling: An empirical derivation of bulk scaling factors. 10th International Conference on Acid Rock Drainage (ICARD) and IMWA Annual Conference, Santiago, Chile, April 21-24, 2015.

Kempton H. 2012. A review of scale factors for estimating waste rock weathering from laboratory tests. 9th International Conference on Acid Rock Drainage (ICARD), Ottawa, Canada, May 20-26, 2012.

Marcoline J. 2008. Investigations of water and tracer movement in covered and uncovered unsaturated waste rock. Ph.D. dissertation, U. of British Columbia, Vancouver, Canada. 317p.

Mayer KU. 1999. A numerical model for multicomponent reactive transport in variably saturated porous media. Ph.D. dissertation, Univ. of Waterloo, Waterloo, Canada.

Mayer KU, Frind EO, Blowes DW. 2002. Multicomponent reactive transport modeling in variably saturated porous media using a generalized formulation for kinetically controlled reactions, Water Resources Research, 38(9)1174, 13-1-3-21.

Mayer KU, Amos RT, Molins S, Gerard F. 2011. Reactive transport modeling in variably saturated media with MIN3P: Basic model formulation and model enhancements, inZhang F, Yeh G-T, Parker JC, Shi X, Groundwater Reactive Transport Models, 187-212.

Mayer KU, Alt-Epping P, Jacques D, Arora B, SteefelCI. 2015. Benchmark problems for reactive transport modeling of the generation and attenuation of acid rock drainage, Computational Geosciences, doi: 10.1007/s10596-015-9476-9.

Moncur MC, Ptacek CJ, Blowes DW, Jambor JL. 2005. Release, transport and attenuation of metals from an old tailings impoundment. Applied Geochemistry 20(3):639-659. https://doi.org/10.1016/j.apgeochem.2004.09.019 Neuner M, Smith LJ, Blowes DW, Sego DC, Smith LJD, Fretz N, Gupton M. 2013. The Diavik Waste Rock Project: Water flow though waste rock in a permafrost terrain. Appl. Geochem. 36, 222-233. http://dx.doi.org/10.1016/j.apgeochem.2012.03.011

Pham N, Sego DC, ArensonLU, BlowesDW, Amos RT, Smith L. 2013. The Diavik Waste Rock Project: Measurement of thermal regime in a waste rock pile under permafrost environment. Appl. Geochem. 36, 234–245.

Steefel CJ, Appelo CAJ, Arora B, Jacques D, Kalbacher T, Kolditz O, Lagneau V, Licthner PC, Mayer KU, Meeussen JCL, Molins S, Moulton D, Shao H, Šimūnek J, Spycher N, Yabusaki SB, Yeh GT. 2015. Reactive transport codes for subsurface environmental simulation. Computational Geosciences, 19:445-478, doi: 10/1007/s10596-014-9443-x.

Wilson D. 2018. A mechanistic approach to assessment of the geochemical evolution of low-sulfide mine-waste rock. PhD thesis, U. of Waterloo, Canada. 217p. https://uwspace.uwaterloo.ca/handie/10012/14311

## Ecometrix Environmental

