Part 1: Reactive Transport Modeling in Mine Waste Management – Examination of its Role Based on Past and Present Applications

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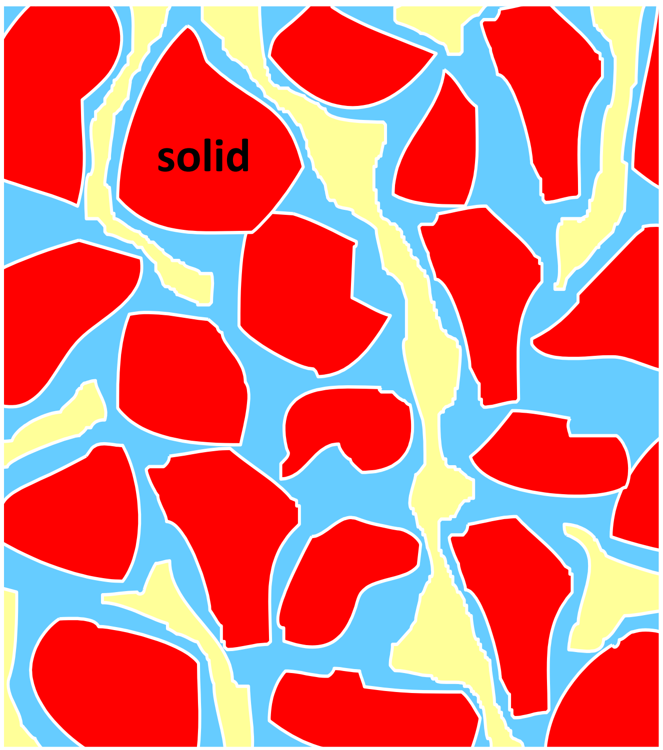
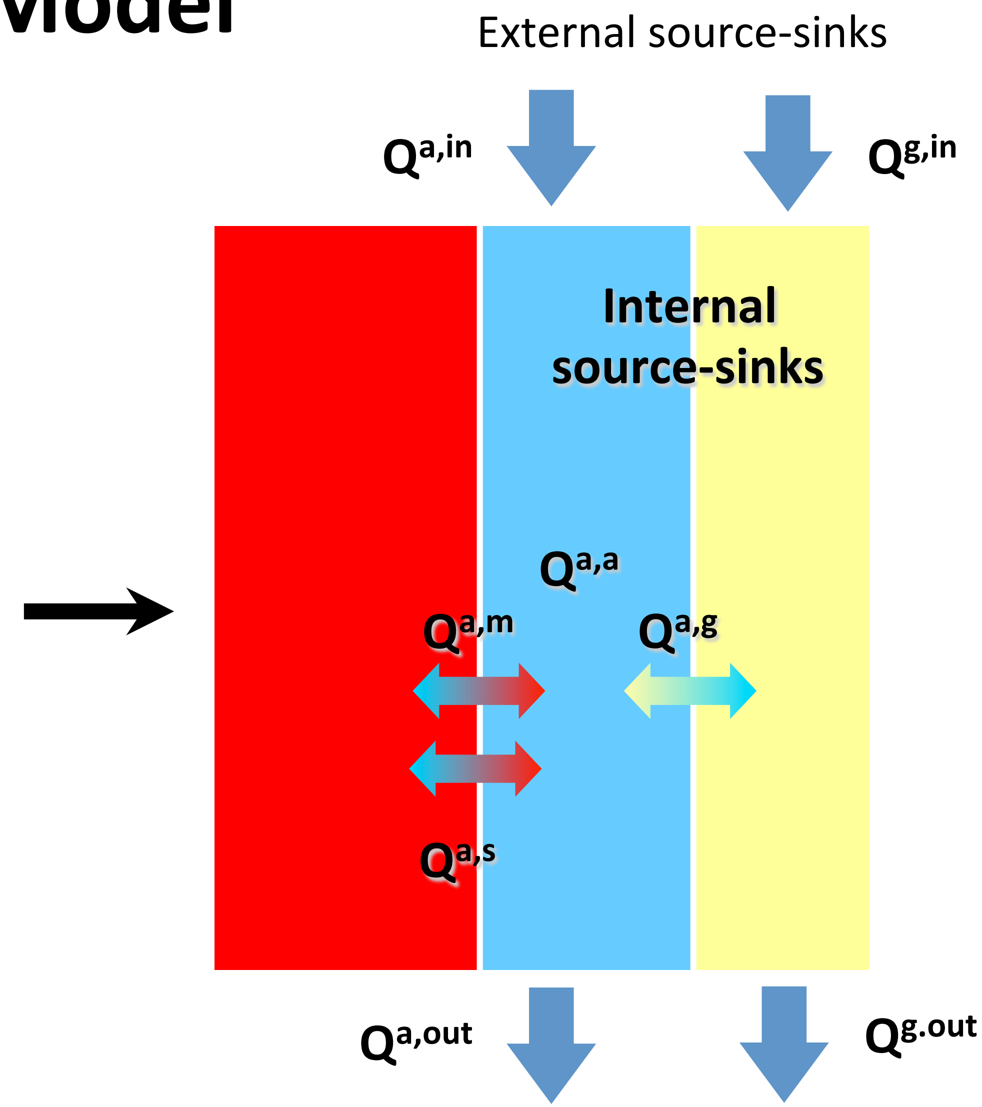
Presentation Outline

- What is "**Reactive Transport Modeling**"?
- **Can we trust these models**?
  - **Model verification** through an international **benchmarking** exercise - code intercomparison
- **Case studies - Applications of RTM in tailings**:
  - Long-term evolution of ARD release from mine tailings
  - Effect of reactivity and permeability distribution on ARD release from tailings
  - Carbon sequestration in ultra-mafic mine waste

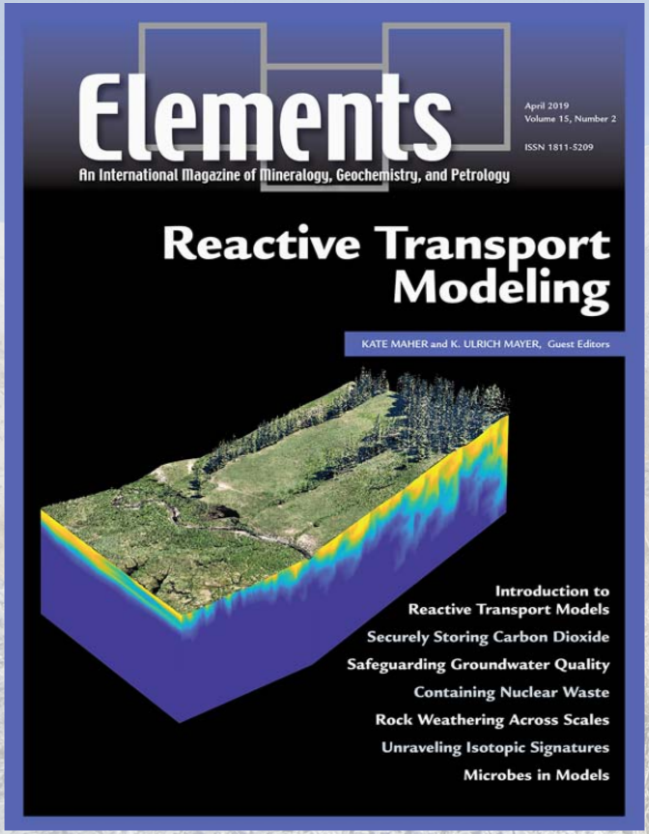
Basic Conceptual Model

Physico-Chemical System





What is Reactive Transport Modeling?



Book (in press):

Advances in Mine Waste Characterisation, Engineering and Management: A sustainable approach towards mine closure and rehabilitation

Editors: Anita Parbhakar-Fox, Matthew Lindsay and Michael Moncur

- **Will include a Chapter on RTM and application in mining**

What is Reactive Transport Modeling good for?

- Helps to **build conceptual models and evaluate conceptual models in a quantitative fashion**
- Explore "**what-if**" scenarios
- **Bracket** expected behavior
- Allows for ***comparison* of different environmental management options**
- **Data interpretation tool**
    - In order to develop predictive capabilities: Model needs to be **calibrated** and **constrained by lab/field data. Can be TRICKY!**

Available Reactive Transport Models

- PHREEQC in RT mode
- Geochemist's Workbench
- But also many others:
  - MIN3P
  - HYTEC
  - TOUGH-React
  - CrunchFlow
  - Flotran
  - HP1

Important Capability for Simulation of ARD generation:

Flow and transport in the unsatured zone

Can we trust these models?

- Trust comes from ***verification*** and ***validation***
- **Model verification**
  - Check that the governing equations are solved correctly
  - Completed using international benchmarking exercise through code intercomparison
- **Model validation**
  - Comparison between field/observational data and model output (**match** with ***real data***)
  - *Beware of* **non-uniqueness!**

Comput Geosci
DOI 10.1007/s10596-015-9476-9

ORIGINAL PAPER

Benchmark problems for reactive transport modeling of the generation and attenuation of acid rock drainage

K. Ulrich Mayer[1] · Peter Alt-Epping[2] · Diederik Jacques[3] · Bhavna Arora[4] · Carl I. Steefel[4]

Models compared in study: CrunchFlow, Flotran, HP1, MIN3P

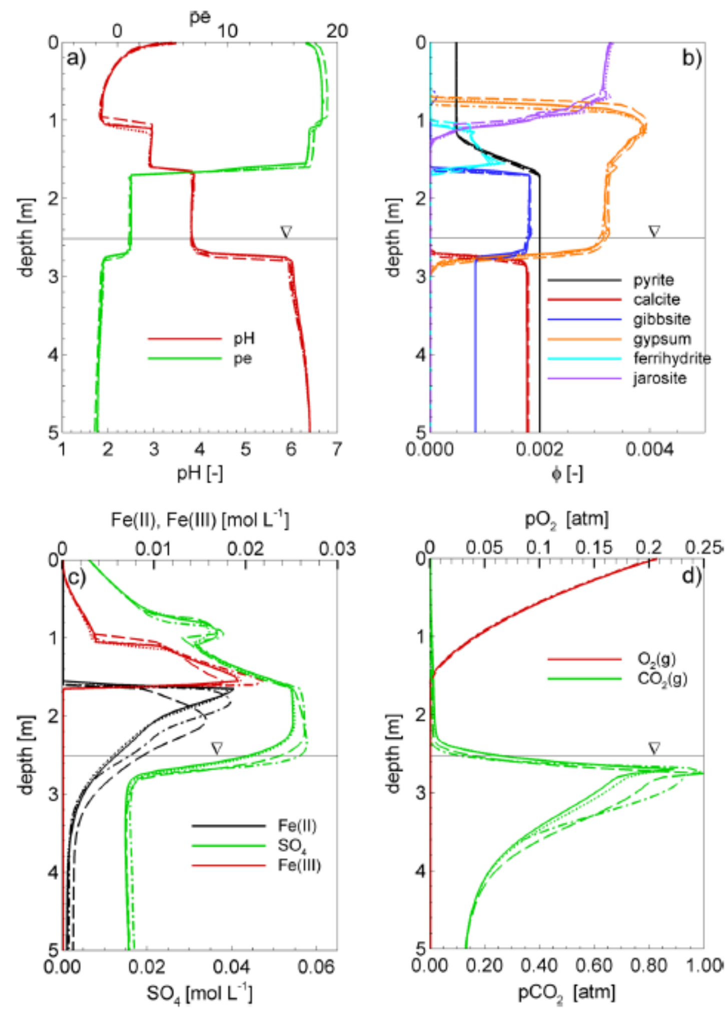


Fig. 5 Simulated profiles after 10 years for benchmark level II: **a** pH and pE; **b** mineral volume fractions; **c** total aqueous component concentrations of Fe(II), Fe(III), and SO_4; **d** pO_2 and pCO_2—*solid lines*: MIN3P, *dashed lines*: HP1, *dot-dashed lines*: Flotran, *dotted lines*: CrunchFlow

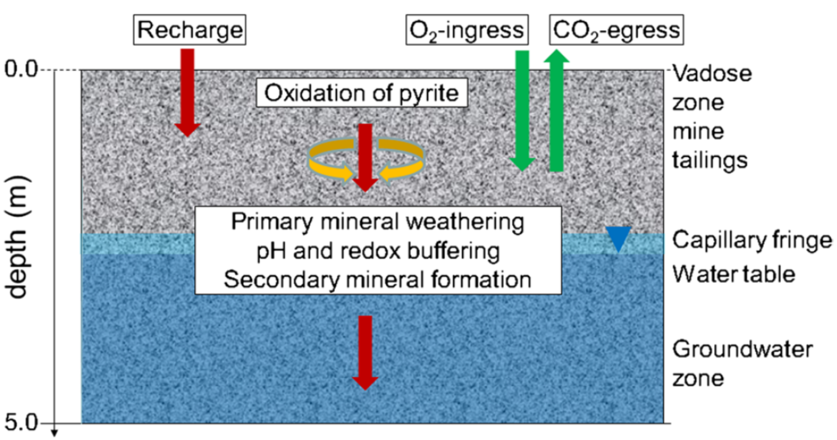


Fig. 1 Conceptual model of ARD generation and attenuation

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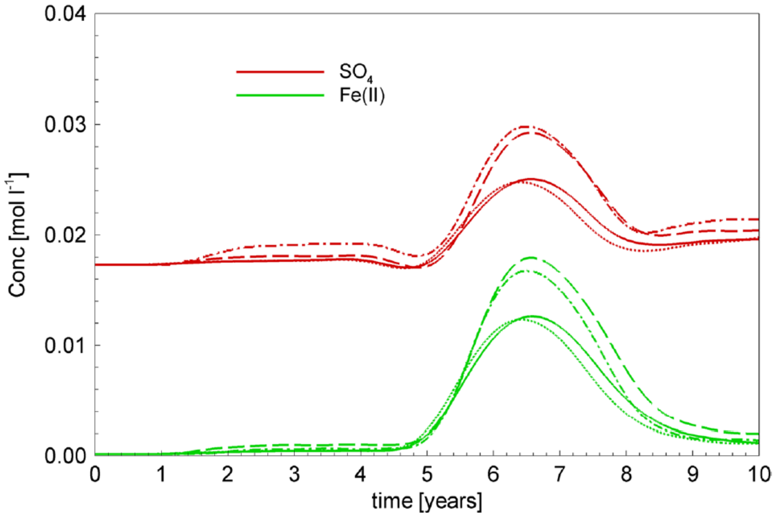


Fig. 8 Breakthrough curves for Fe(II) and SO_4 for benchmark ARD-B3 at z=2.5 m, *solid lines*: MIN3P, *dashed lines*: HP1, *dot-dashed lines*: Flotran, *dotted lines*: CrunchFlow

Table 6 Cumulative oxygen ingress, cumulative SO_4 and Fe(II) release after 10 years—benchmark ARD-B3

Mass ingress/release/egress [mol]	CrunchFlow	Flotran	HP1	MIN3P
O_2(g) ingress	344.3	345.8	350.0	343.5
SO_4 release	53.6	53.9	54.6	53.9
Fe(II) release	3.6	3.3	4.9	3.8
CO_2(g) egress (gas phase)	85.0	84.6	87.2	84.5

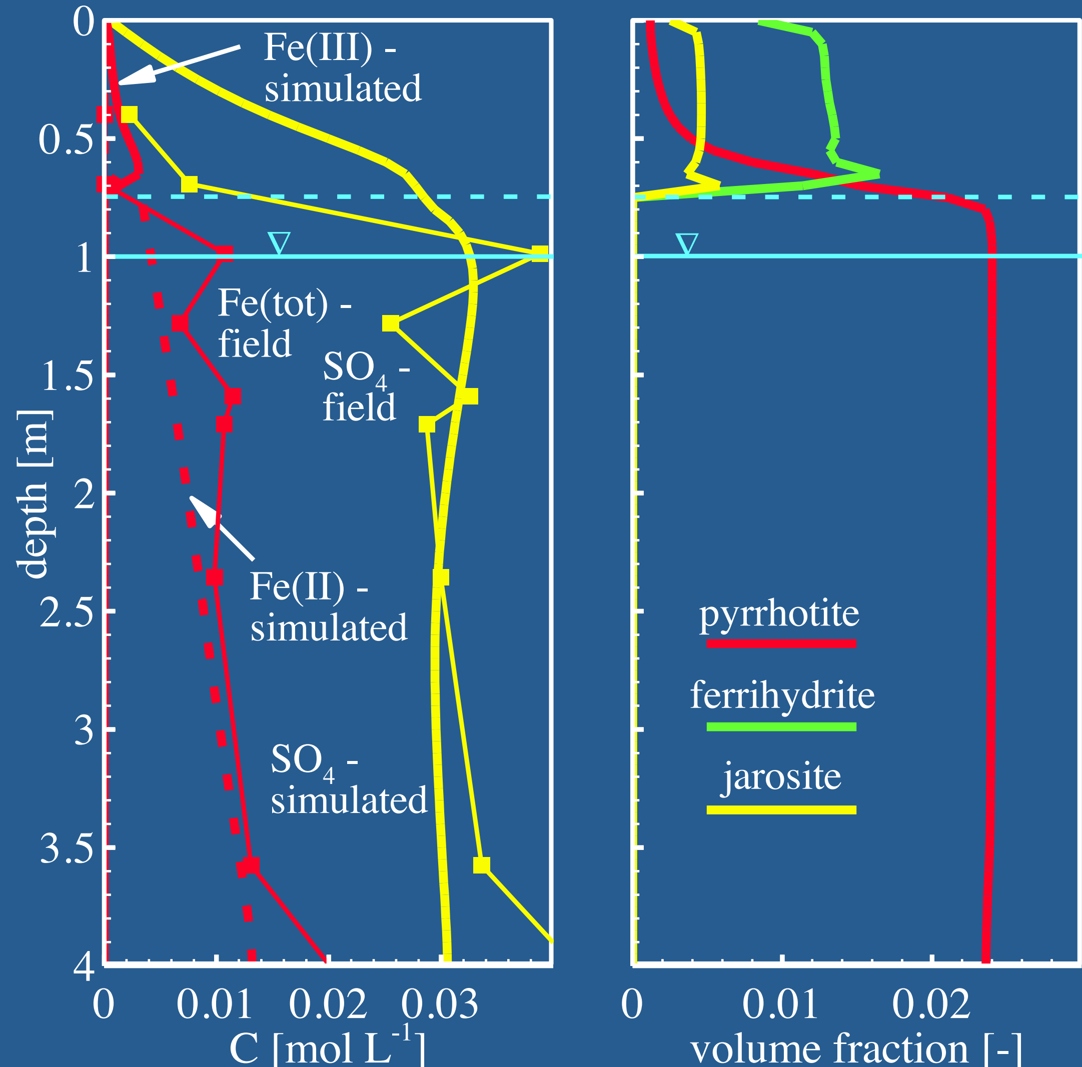
Photo: Canadian Mining Journal

Case Study 1: Nickel Rim, Sudbury

Acid Mine Drainage Generation and Attenuation

- Field site: **Nickel Rim Mine Tailings**, Sudbury, Ontario
- **Controlling Processes**:
  - **O_2 ingress** by gaseous diffusion
  - **Sulfide mineral oxidation** in **unsaturated zone**
  - **pH-buffering** due to the dissolution of **carbonate** and **aluminosilicate minerals**
  - **Secondary mineral precipitation** and **re-dissolution**

Nickel Rim - Fe and SO_4

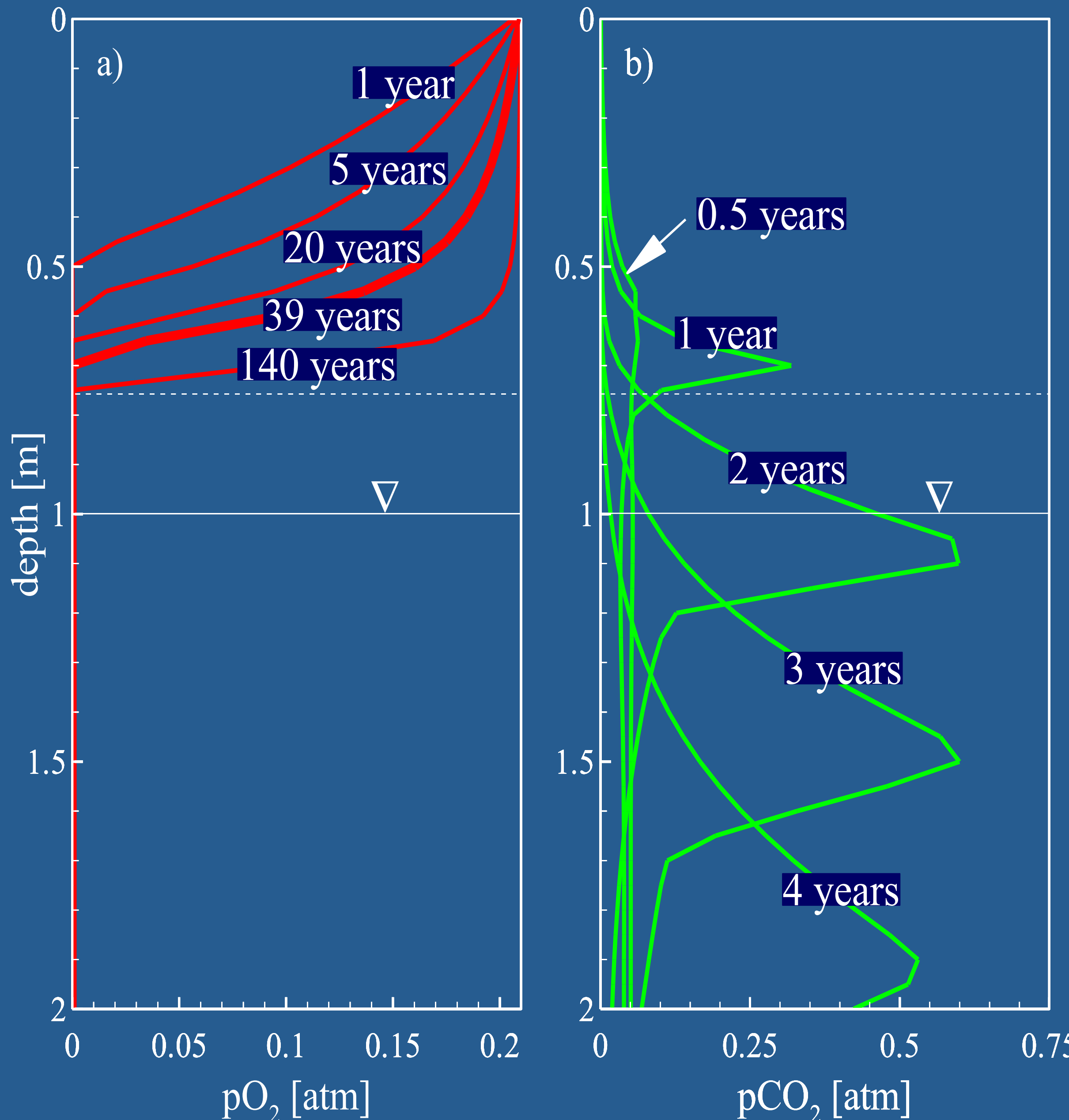


Data from

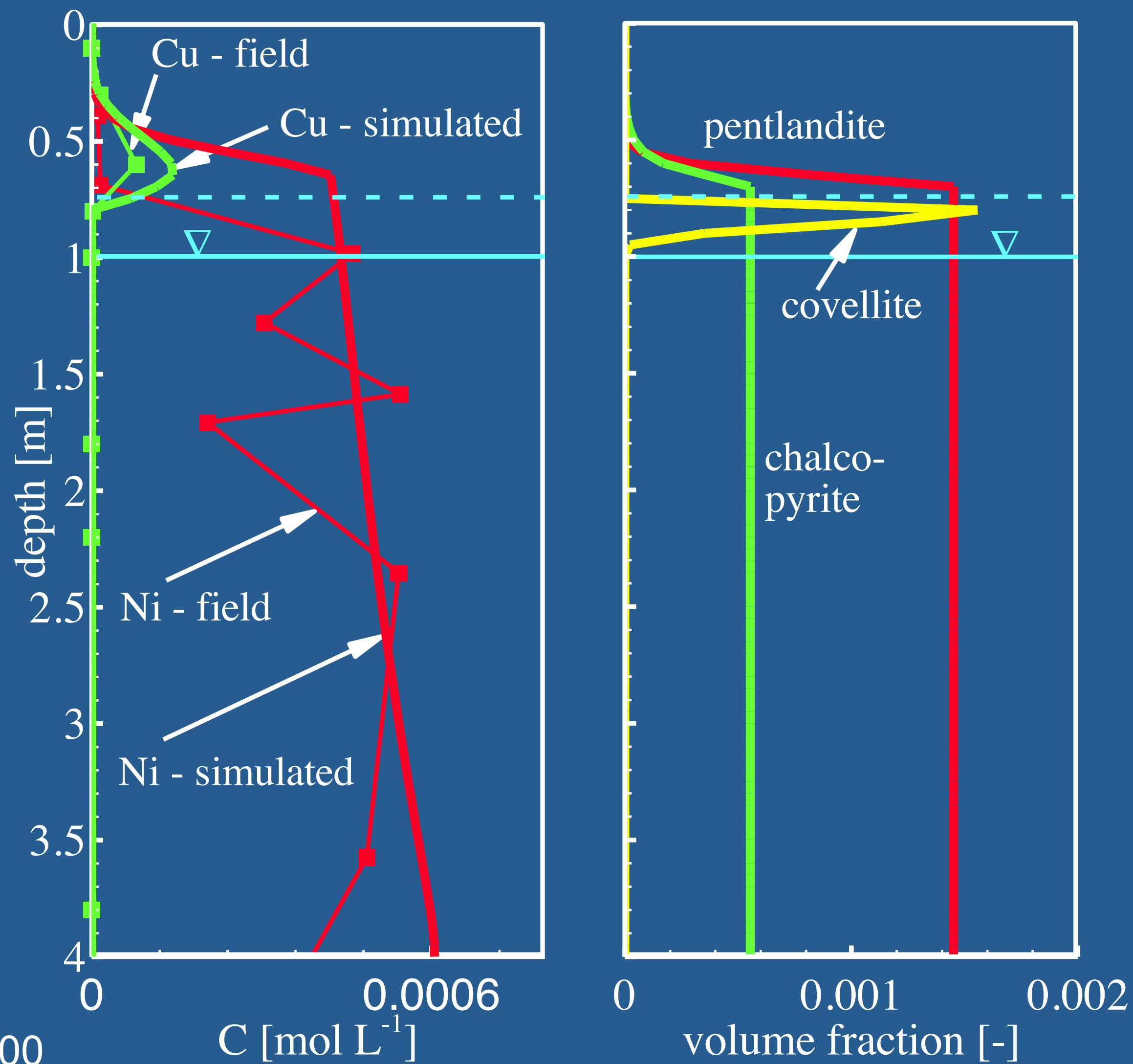
Benner et al., 2000

Nickel Rim

Partial gas pressures: O_2 and CO_2

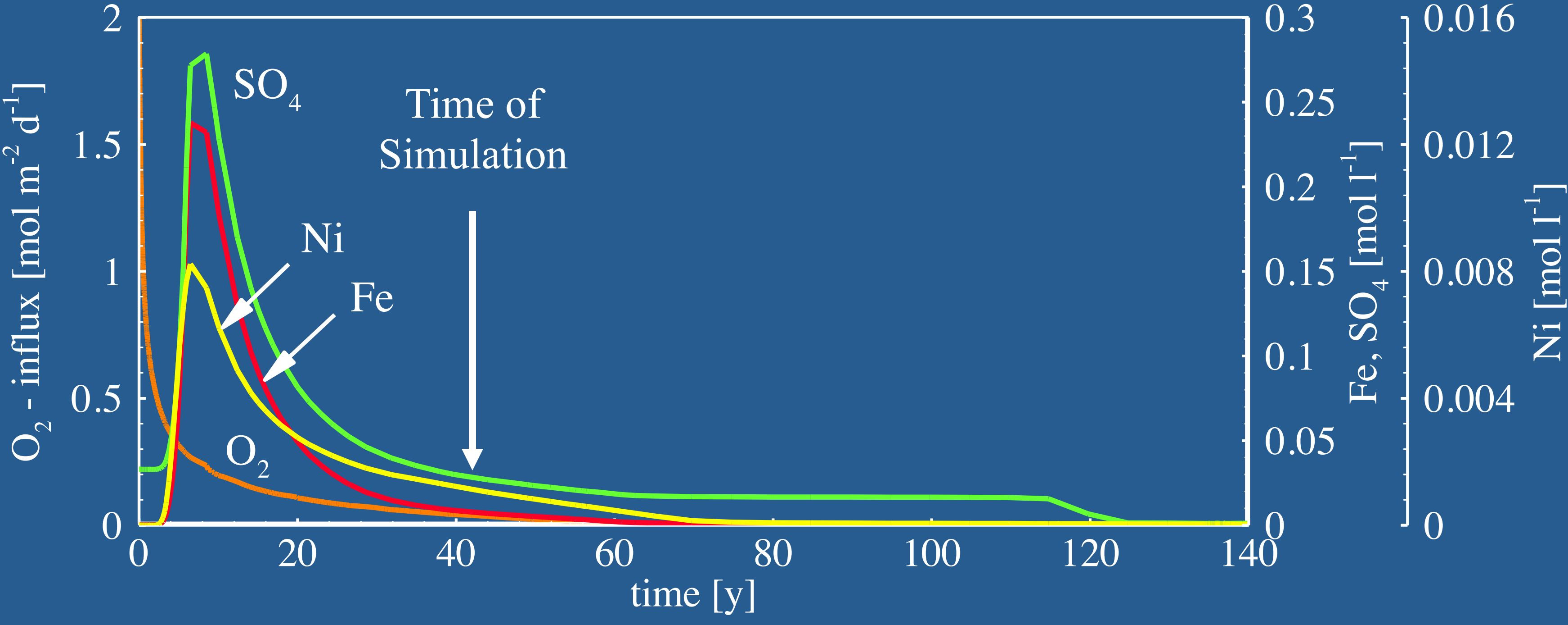


Nickel Rim - Cu and Ni



Data from
Benner et al., 2000

Potential for Long Term AMD-Generation

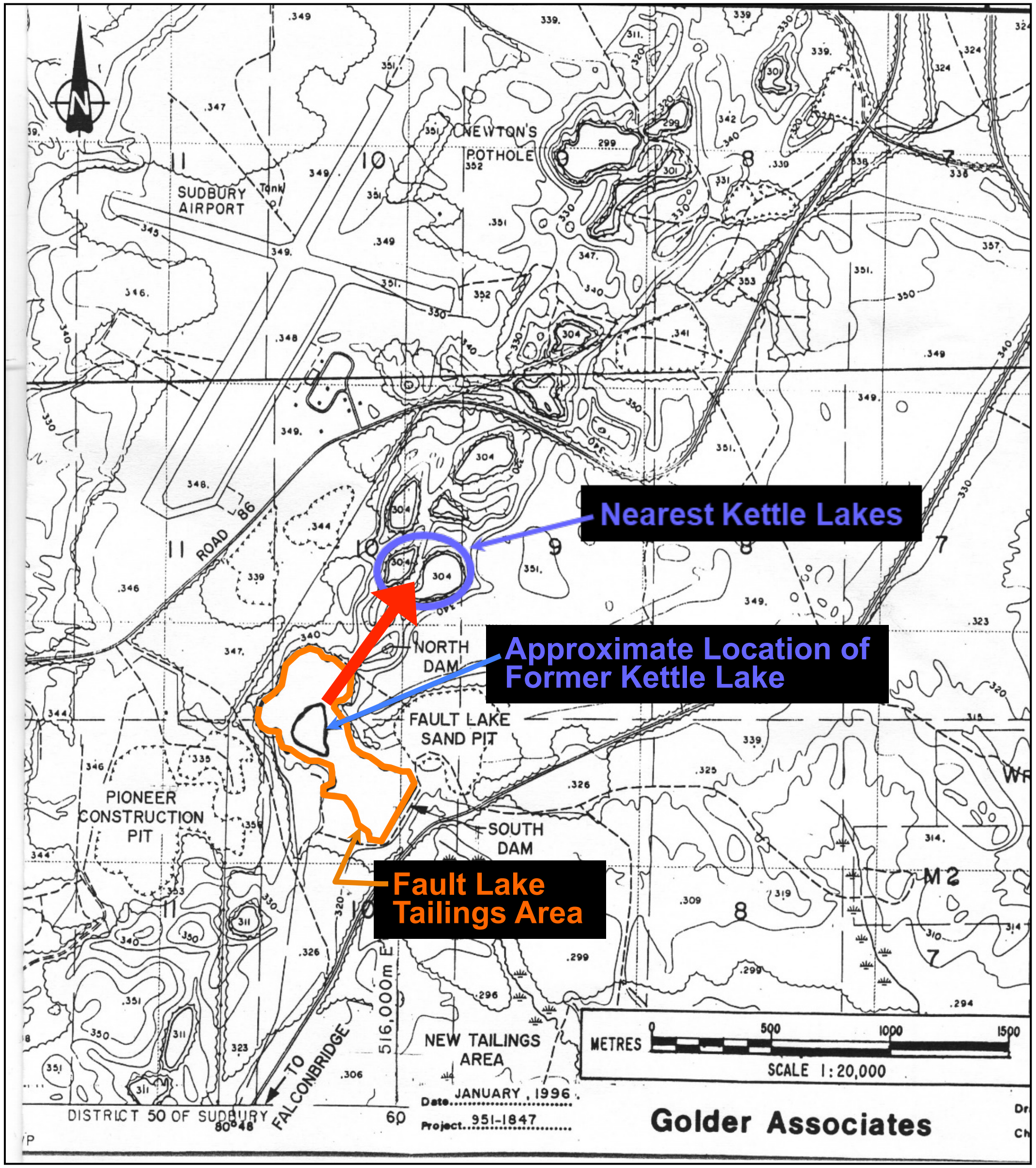


Lessons learned – Case Study 1

- RT models are well capable of "history matching" data, issue of non-uniqueness remains
- Concentration breakthough below the water table illustrates very clearly that unsaturated portion of the tailings are nearly "burnt out". A statement that could be made with confidence.
- Remedial measures to limit O_2 ingress would have been ineffective. "The train has left the station."

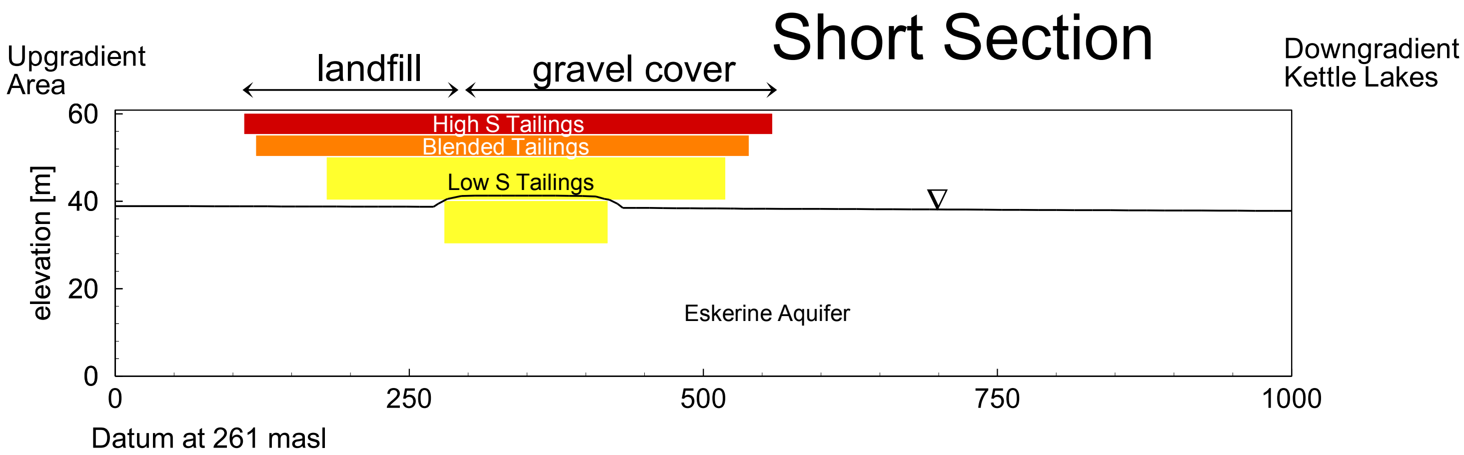
Case Study 2: Fault Lake Tailings, Falconbridge, ON

- 5.7 M tonnes tailings deposited 1964-1978
- Up to 50 wt % sulfide minerals
- Determine potential long-term impacts to groundwater and downstream receptors



Romano et al, ICARD (2006)

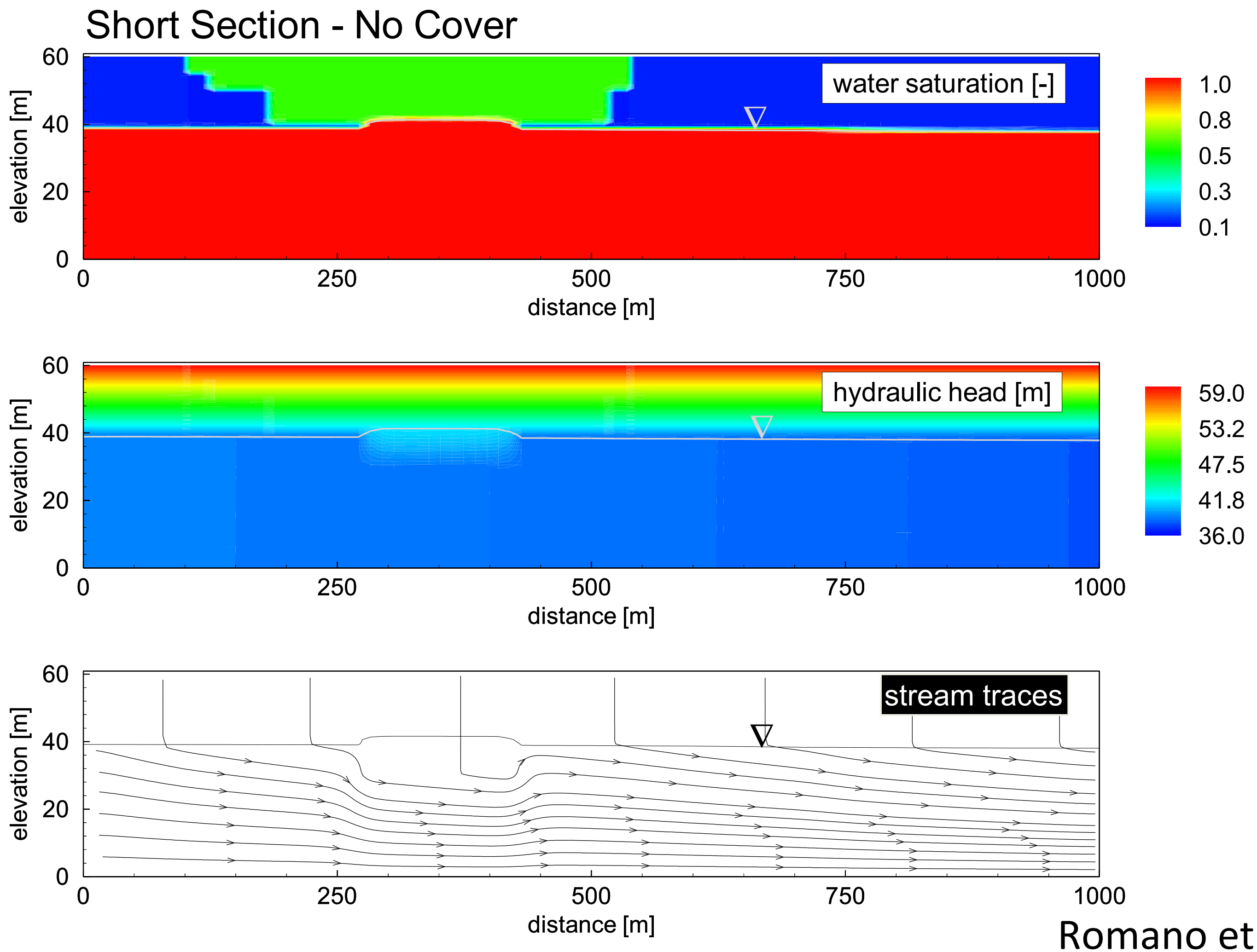
2D Simulation Domain



- High S tailings over low S tailings
- Thick unsaturated zone
- Tailings:
  - Mostly above water table, but not all
  - Higher carbonate content than aquifer
  - Lower hydraulic conductivity than aquifer

Romano et al, ICARD (2006)

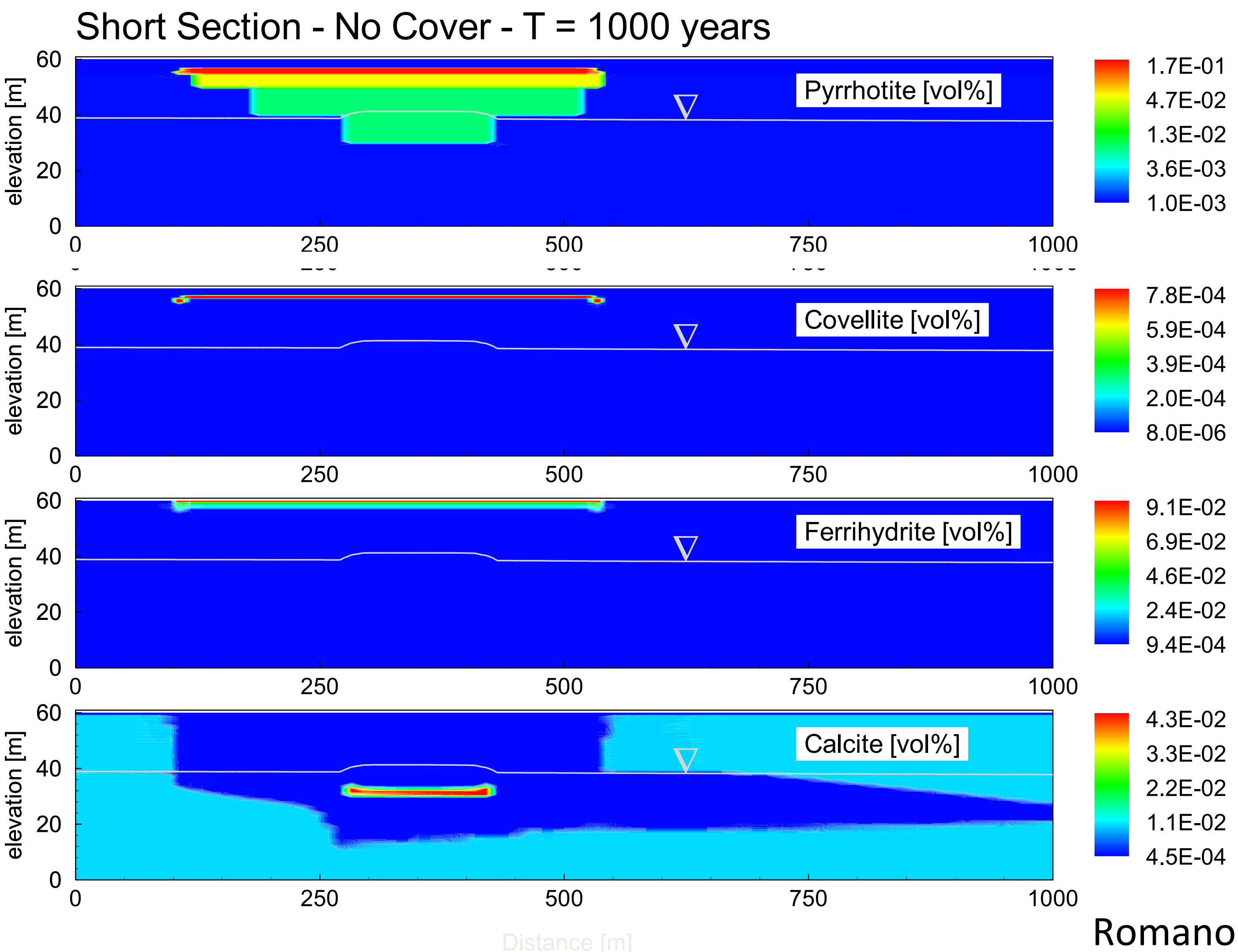
Steady State Flow Field Short Section



Downgradient Kettle Lakes

Romano et al, ICARD (2006)

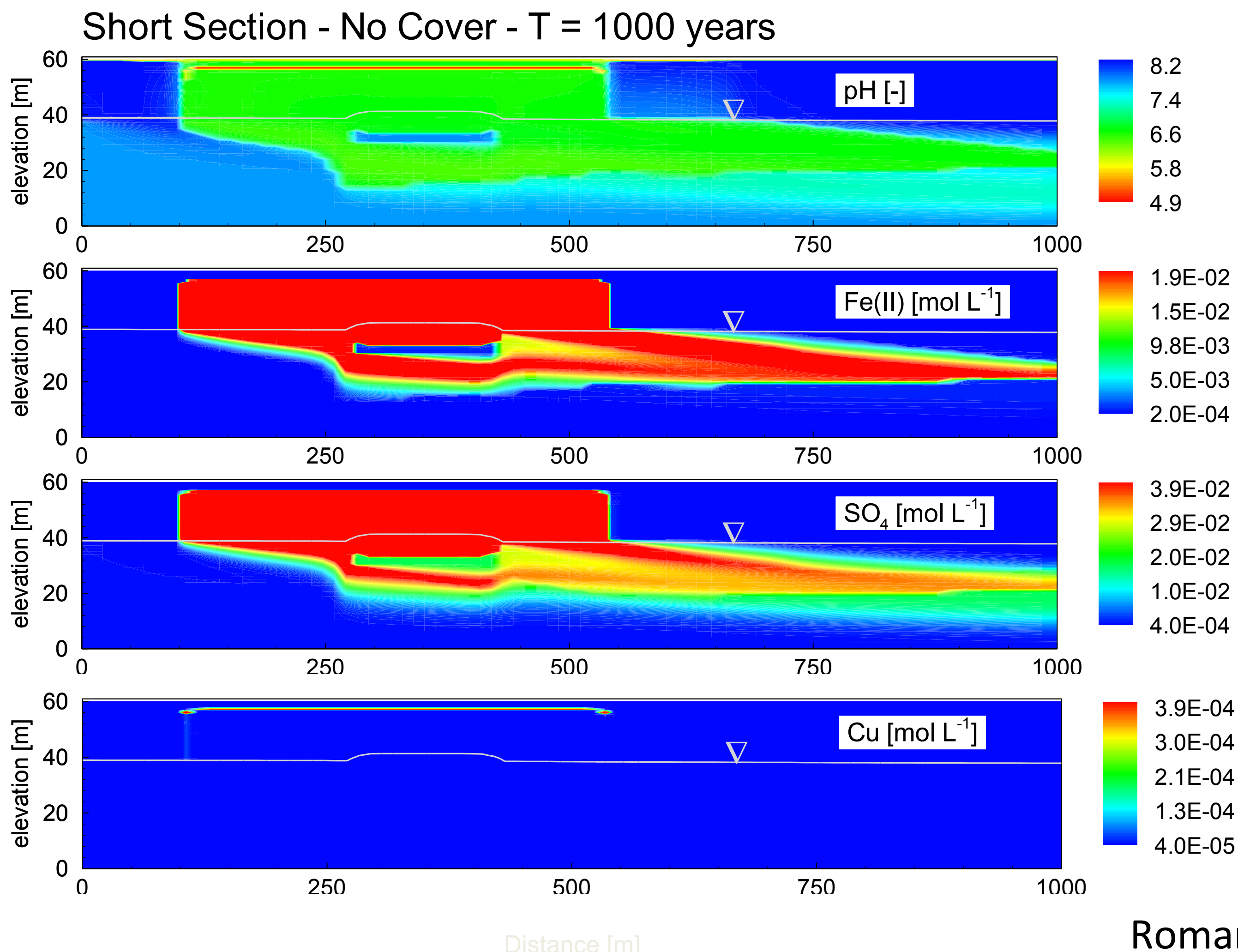
Mineral Volume Fractions
Short Section



Downgradient Kettle Lakes

Romano et al, ICARD (2006)

Aqueous Concentrations
Key Components – Short Section



Downgradient Kettle Lakes

Romano et al, ICARD (2006)

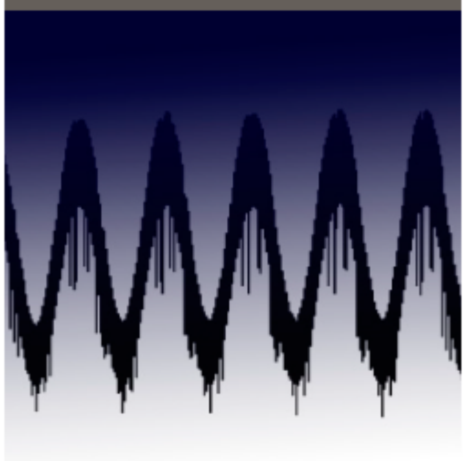
Lessons learned – Case Study 2

- Simulation results suggest formation of tailings plume characterized by sub-neutral pH, elevated Fe, SO_4
  - An example for predictive modeling
  - There are uncertainties regarding non-uniqueness, long term evolution, use in a supportive fashion
- Some not so obvious results, which provide additional information, food for thought:
  - ARD is preferentially generated in periphery of impoundment, where tailings are thin
  - Hydraulic exclusion of pH-buffer capacity in saturated portion of tailings
- An excellent example of interactions between flow, transport and geochemical reactions

Case Study 3: CO_2 Sequestration in Ultramafic Mine Tailings

Special Section:
Reactive Transport Modeling

S.A. Bea*
S.A. Wilson
K.U. Mayer
G.M. Dipple
I.M. Power
P. Gamazo



Vadose Zone J.
doi:10.2136/vzj2011.0053
Received 3 June 2011.

Reactive Transport Modeling of Natural Carbon Sequestration in Ultramafic Mine Tailings

Atmospheric CO_2 is naturally sequestered in ultramafic mine tailings as a result of the weathering of serpentine minerals [$Mg_3Si_2O_5(OH)_4$] and brucite [$Mg(OH)_2$], and subsequent mineralization of CO_2 in hydrated magnesium carbonate minerals, such as hydromagnesite [$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$]. Understanding the CO_2 trapping mechanisms is key to evaluating the capacity of such tailings for carbon sequestration. Natural CO_2 sequestration in subaerially exposed ultramafic tailings at a mine site near Mount Keith, Australia is assessed with a process-based reactive transport model. The model formulation includes unsaturated flow, equations accounting for energy balance and vapor diffusion, fully coupled with solute transport, gas diffusion, and geochemical reactions. Atmospheric boundary conditions accounting for the effect of climate variations are also included. Kinetic dissolution of serpentine, dissolution-precipitation of brucite and primary carbonates—calcite ($CaCO_3$), dolomite [$MgCa(CO_3)_2$], magnesite ($MgCO_3$), as well as the formation of hydromagnesite, halite (NaCl), gypsum ($CaSO_4 \cdot 2H_2O$), blödite [$Na_2Mg(SO_4)_2 \cdot 4H_2O$], and epsomite [$MgSO_4 \cdot 7H_2O$]—are considered. Simulation results are consistent with field observations and mineralogical data from tailings that weathered for 10 yr. Precipitation of hydromagnesite is both predicted and observed, and is mainly controlled by the dissolution of serpentine (the source of Mg) and equilibrium with CO_2 ingressing from the atmosphere. The predicted rate for CO_2 entrapment in these tailings ranges between 0.6 and 1 kg m^{-2} yr^{-1}. However, modeling results suggest that this rate is sensitive to CO_2 ingress through the mineral waste and may be enhanced by several mechanisms, including atmospheric pumping.

Abbreviations: BET, Brunauer–Emmett–Teller; SWCC, soil water characteristic curve; TIC, total inorganic carbon; TSF, tailings storage facility; XRPD, X-ray powder diffraction.

www.VadoseZoneJournal.org

Conceptual model

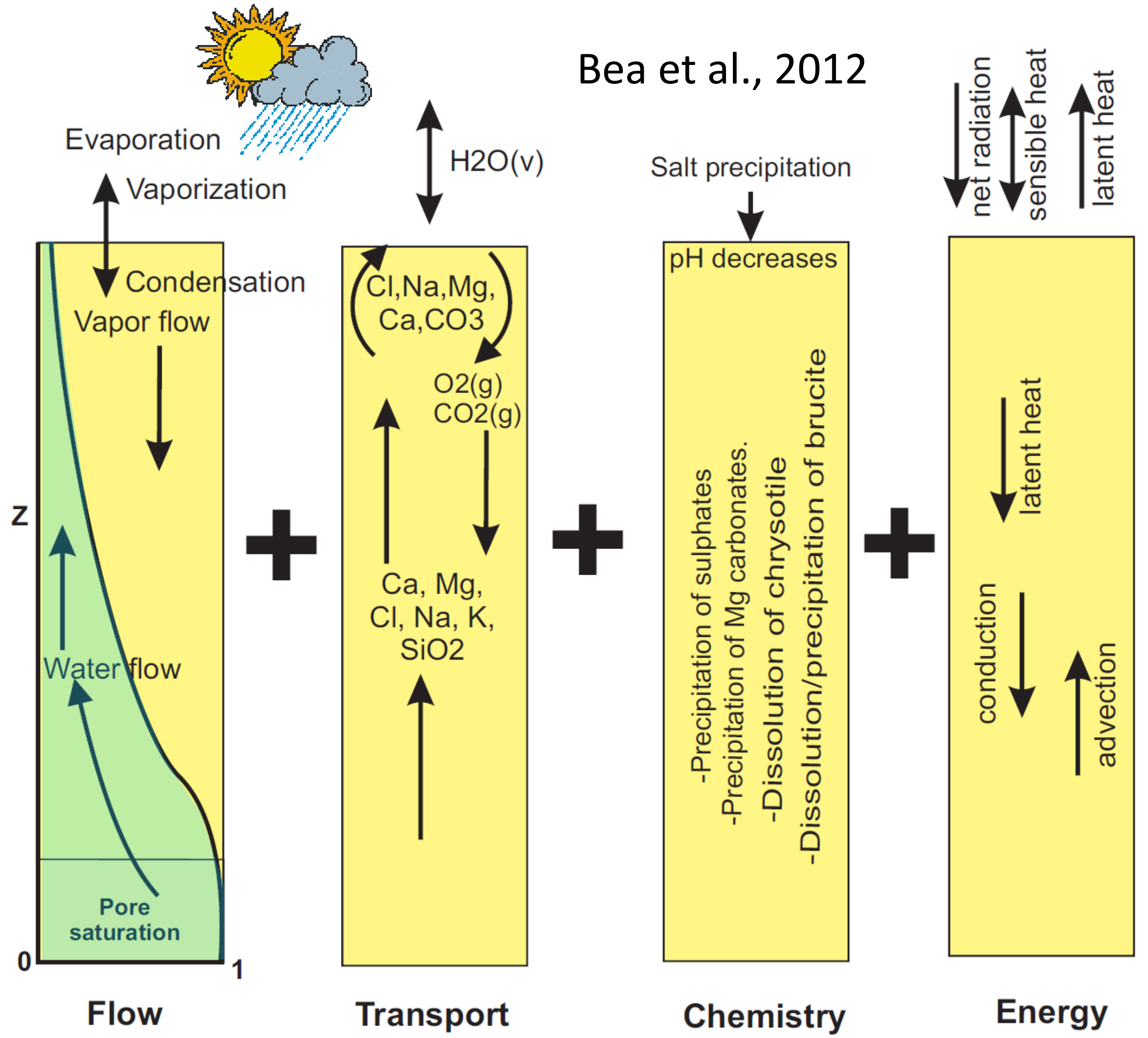


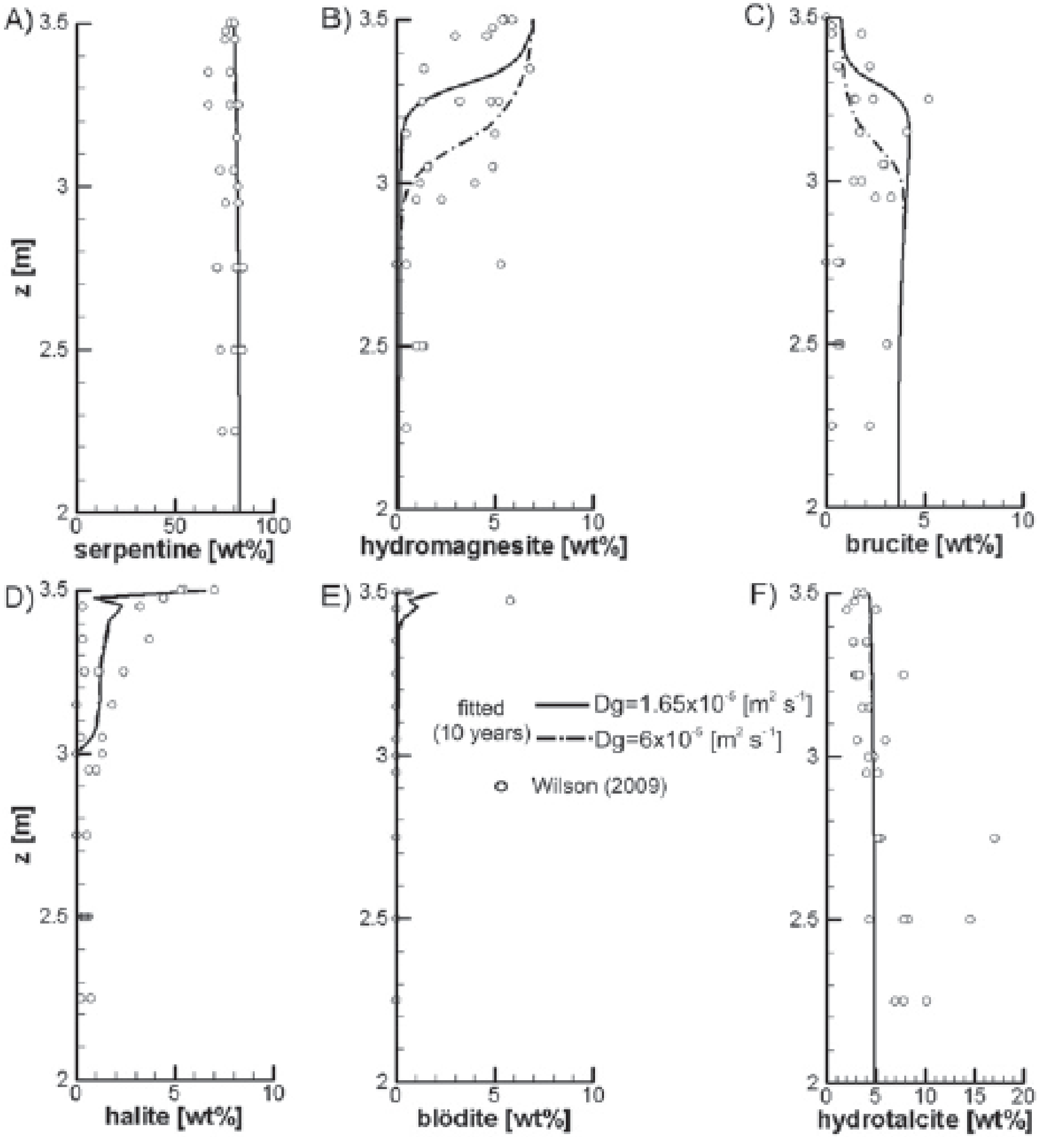
Figure 3.3 *Discontinuous* cover system trials at Mt Keith (June 2004)

Figure 3.104 Salt crust development at Mt Keith, TSF 1 (November 2002)

Stolberg, D. J.. Rehabilitation Studies on Tailings Storage Facilities in an Arid Hypersaline Region. Division of Civil Engineering, School of Engineering, The University of Queensland, Brisbane, Australia, 2005 .

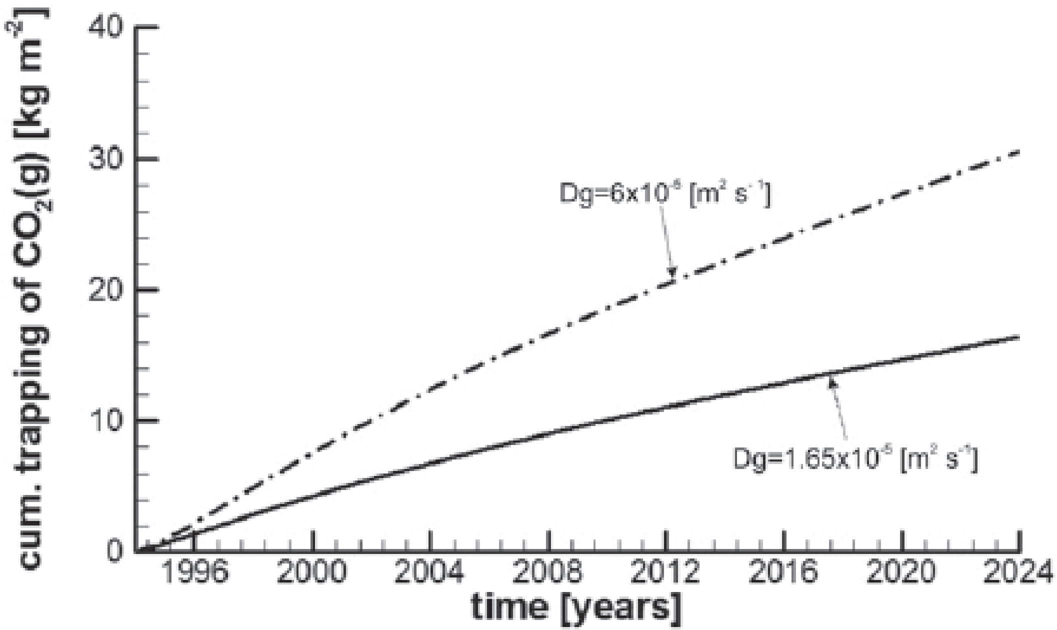
Modeling results of mineralogical evolution

- Model capable of capturing mineralogical evolution, BUT:
- Results suggest that gas diffusion alone is insufficient in supplying CO_2



Bea et al., 2012

Modeling results of cumulative CO_2 trapping in Mt. Keith tailings



Bea et al., 2012

- CO_2 trapped over 20 year time period:
  - D_g = 1.65 x 10^{-5} m^2 s^{-1}: 17 kg m^{-2}
  - D_g = 6.0 x 10^{-5} m^2 s^{-1}: 31 kg m^{-2} (more in-line with observations)

Lessons Leaned – Case Study 3

- Although the model is already complex, the simulations suggest that additional processes that were not considered in the simulations may lead to enhanced ingress of CO_2.
- These processes may include:
  - temperature dependence of diffusion coefficients
  - gas advection due to barometric pressure fluctuations
  - advective CO_2 displacement in the gas phase due to displacement by ingressing precipitation water
  - wind effects
- Sometimes we learn most, if the model does not fit the data

Now what?

- Reactive transport models for simulating processes in mine tailings are available
- These models have been verified
- We could use them to support investigations of ARD generation, attenuation within mine tailings and aquifers
- We could also use them to simulate neutral drainage, CO_2 sequestration, CO_2 release, etc …

References

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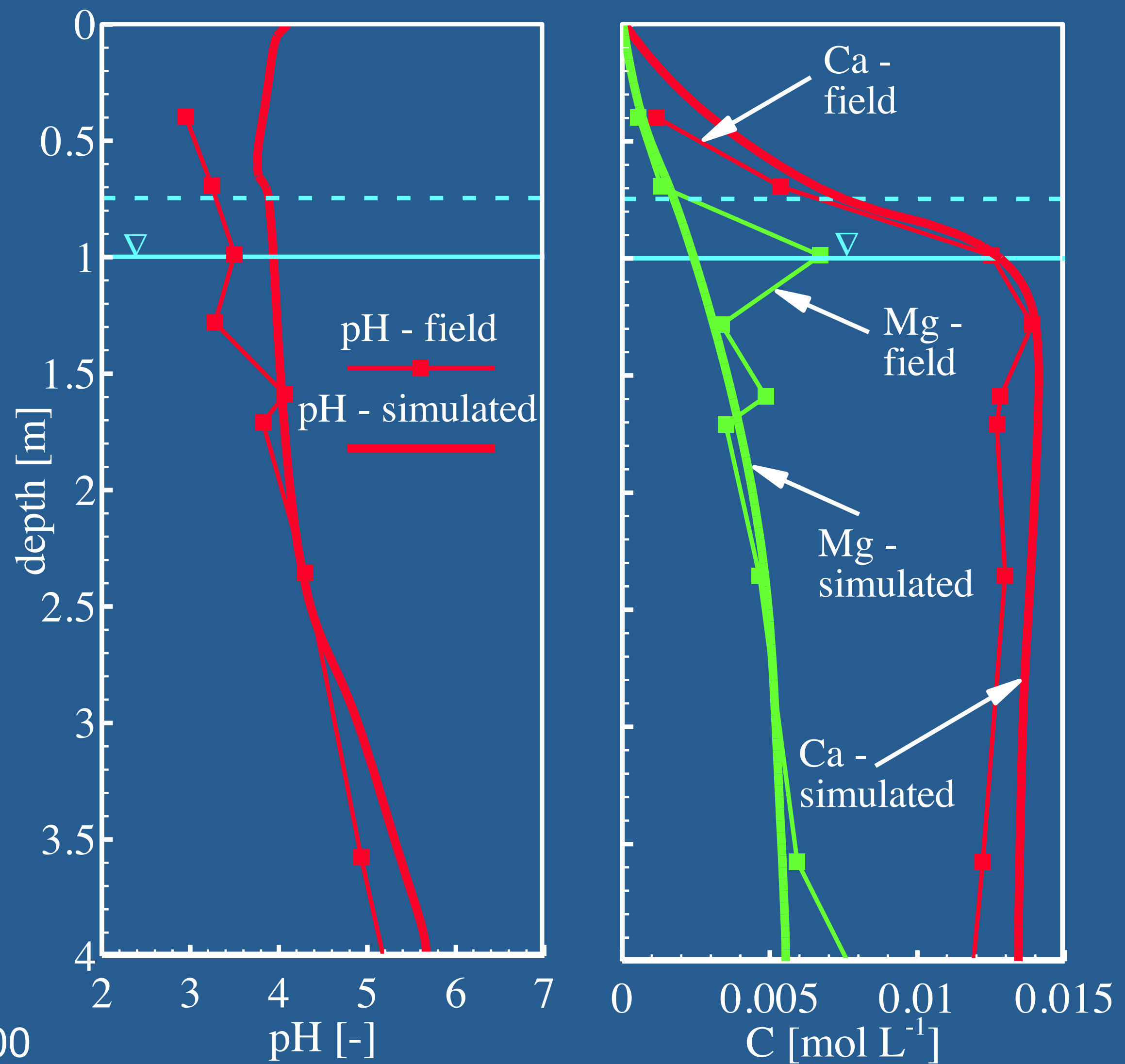
Nickel Rim - pH, Ca and Mg



Data from

Benner et al., 2000

Solid Phase Cu, Ni and S

Data from Johnson et al., 2000