

Model for predicting drainage quality from mine wastes

Muhammad Muniruzzaman

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Kuopio



Programme for Sustainable Growth and Jobs

Leverage from
the EU
2014–2020



Introduction

- Quantitative modelling is instrumental in effective predictions of water quality from mine wastes
- Prior understanding about the future series of events in waste settings may help performing more robust risk assessment and designing remediation measures
- Increasingly recognized not only in data interpretation but also in long-term predictions
- Received a great deal of research attention and led to the development of a variety of modelling approaches
- However, there is still a lack of attention towards utilizing predictive models at early (e.g., planning) phases of a mine

Governing Equations

- **Water Flow**

$$S_s S_w \frac{\partial h}{\partial t} + \theta \frac{\partial S_w}{\partial t} - \nabla \cdot (k_r \mathbf{K} \nabla h) = Q_i^w$$

- **Solute Transport**

$$\frac{\partial}{\partial t} (\theta S_w C_i) = -(\mathbf{q} C_i) + \nabla \cdot (\theta S_w \mathbf{D}_i \nabla C_i) - \sum_{r=1}^{N_r} \nu_{ir} R_r - \sum_{m=1}^{N_m} \nu_{im} R_m - \sum_{g=1}^{N_g} \nu_{ig} R_g$$

- **Gas Transport**

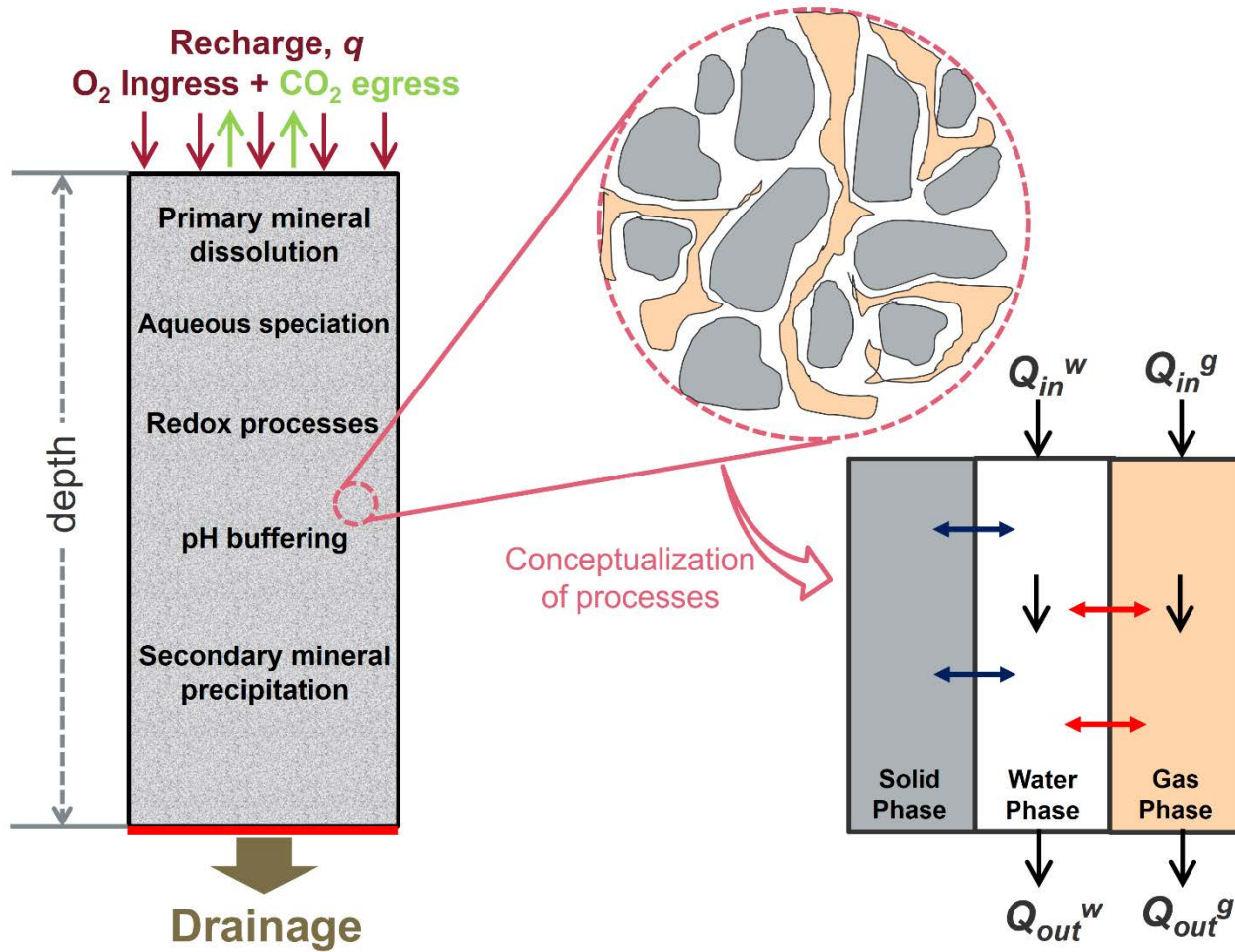
$$\frac{\partial}{\partial t} (\theta S_g C_i^g) = -(\mathbf{q}_g C_i^g) + \nabla \cdot (\theta S_g \mathbf{D}_{p,i}^g \nabla C_i^g) - Q_i^g$$

- **Mineral Reactions**

$$R_j = k_j \prod (\gamma_j C_j)^\nu \left[1 - \frac{IAP_j}{K_j} \right]$$



Modelling Approach

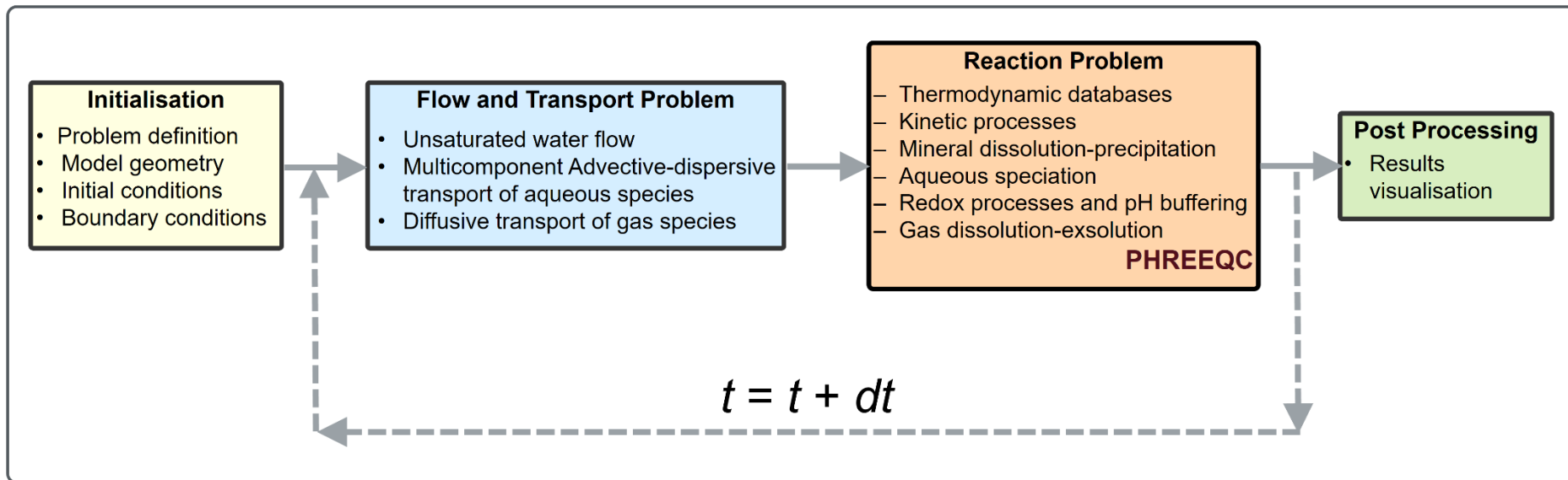


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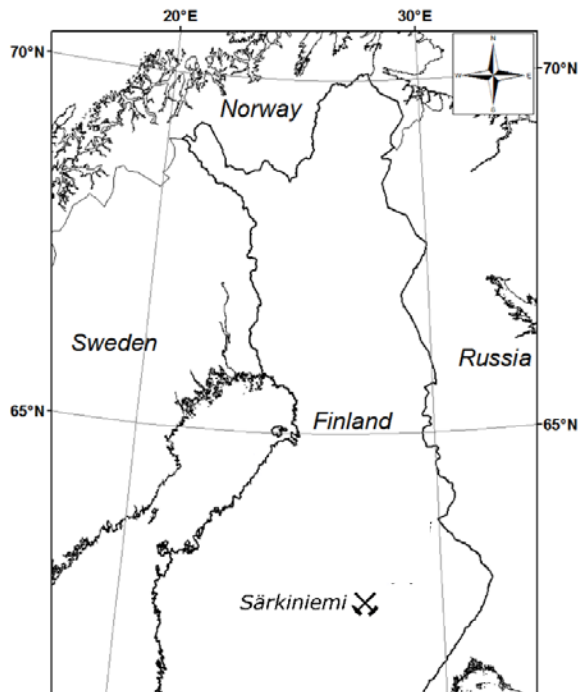
Modelling Approach (cont'd)

Structure of the Model



➔ *Numerical Method:* cell-centered Finite Volume Method

Example 1: Särkiniemi Waste Rock Pile



Mineral	Mineral Content		Surface Area, A	Rate coefficient, k	Reference
	[wt%]	[mol L _w ⁻¹] ^a	[m ² L _w ⁻¹]	[mol m ⁻² s ⁻¹]	
Biotite	33.56	2.12	0.65	10 ^{-10.97}	Nagy (1995)
Hornblende	6.07	0.58	0.05	10 ^{-8.10}	Palandri & Kharaka (2004)
Serpentine	3.52	0.33	0.05	10 ^{-9.08}	Declercq & Oelkers (2014)
Albite	1.45	0.15	0.60	10 ^{-10.16}	Palandri & Kharaka (2004)
Chlorite	1.35	0.06	0.50	10 ^{-11.11}	Palandri & Kharaka (2004)
Pyrrhotite	1.52	0.50	0.30	10^{-8.19}	Williamson & Rimdstidt (1994)
Anthophyllite	0.45	1.53×10 ⁻²	0.50	10 ^{-11.94}	Palandri & Kharaka (2004)
Pentlandite	0.03	1.03×10⁻³	0.70	10^{-8.19}	Williamson & Rimdstidt (1994)
Pyrite	0.02	4.42×10⁻³	0.30	10^{-8.19}	Williamson & Rimdstidt (1994)
SiO ₂ (a)	-	-	-	10 ^{-10.5}	Rimdstidt & Barnes (1980)

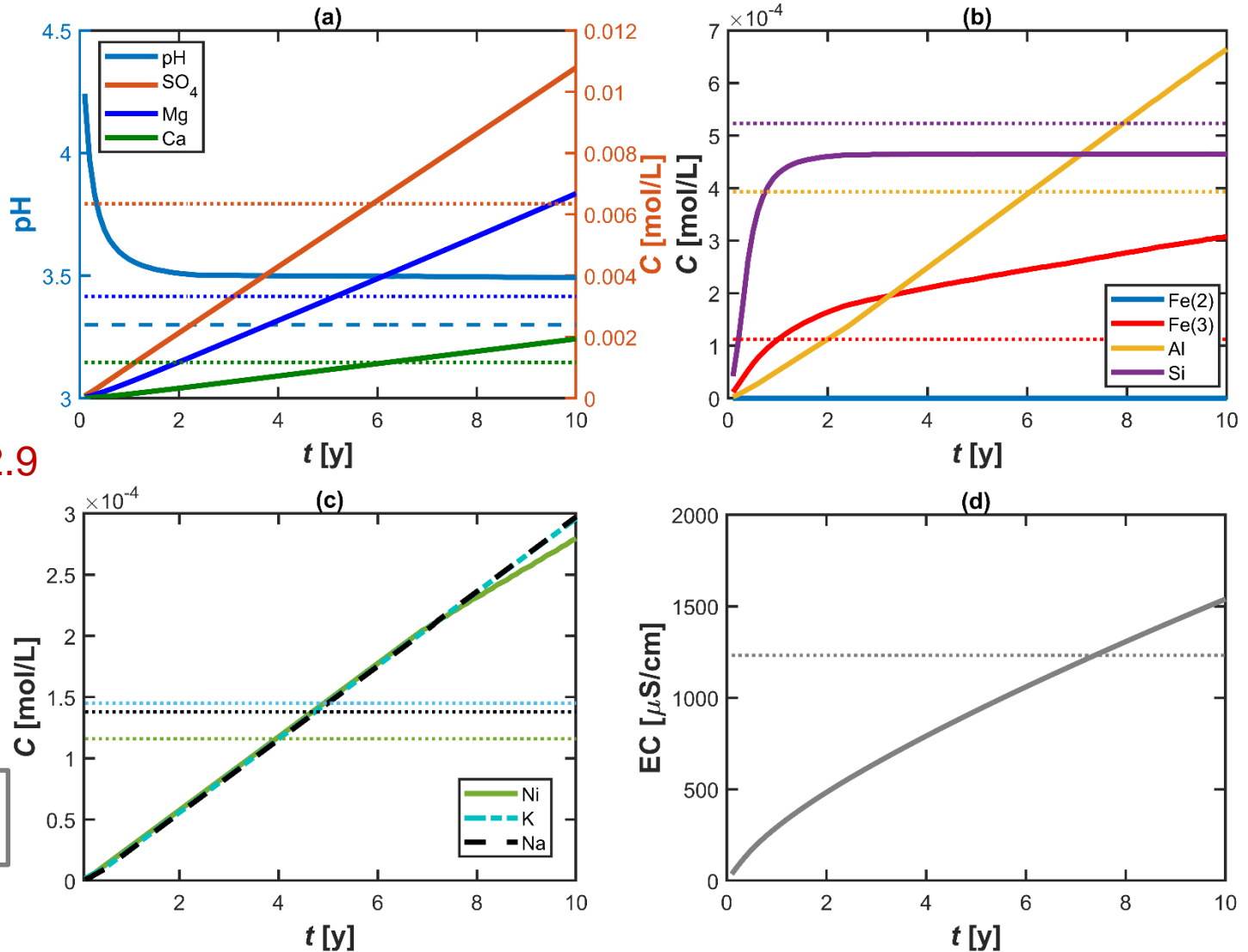
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Example 1: Särkiniemi Waste Rock Pile (cont'd)

Drainage Chemistry:

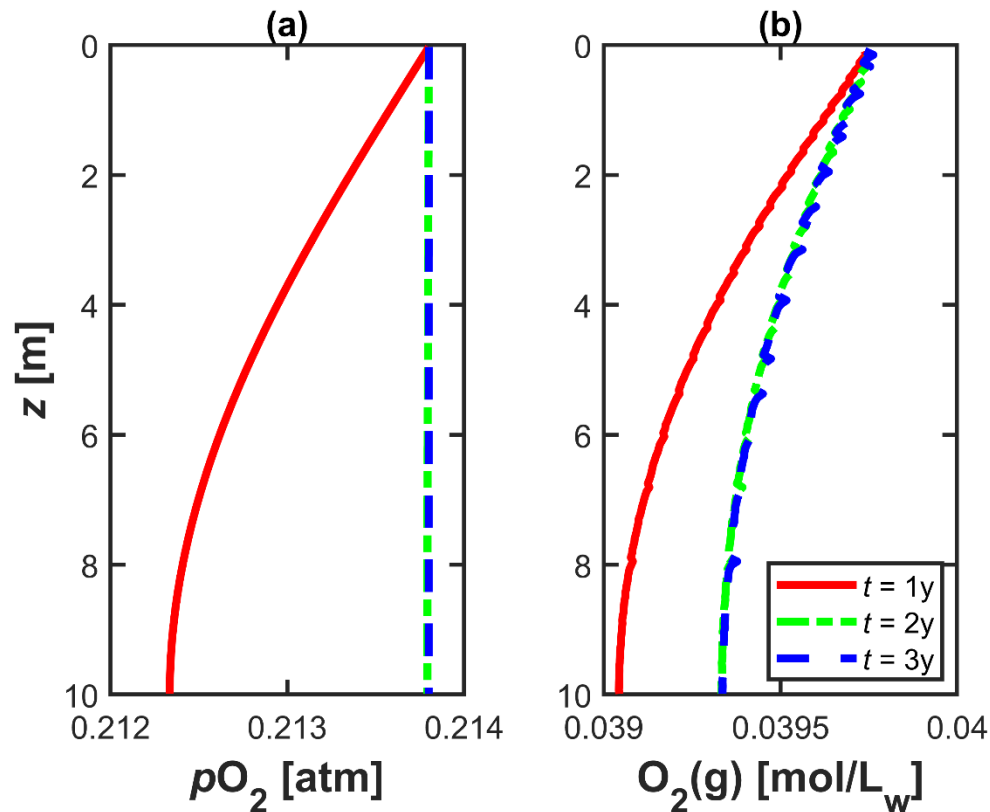


NPR = 0.2 – 0.4
 NAG pH = 2.7 – 2.9

Solid Lines – Model
 Dashed Lines - Data

Example 1: Särkiniemi Waste Rock Pile (cont'd)

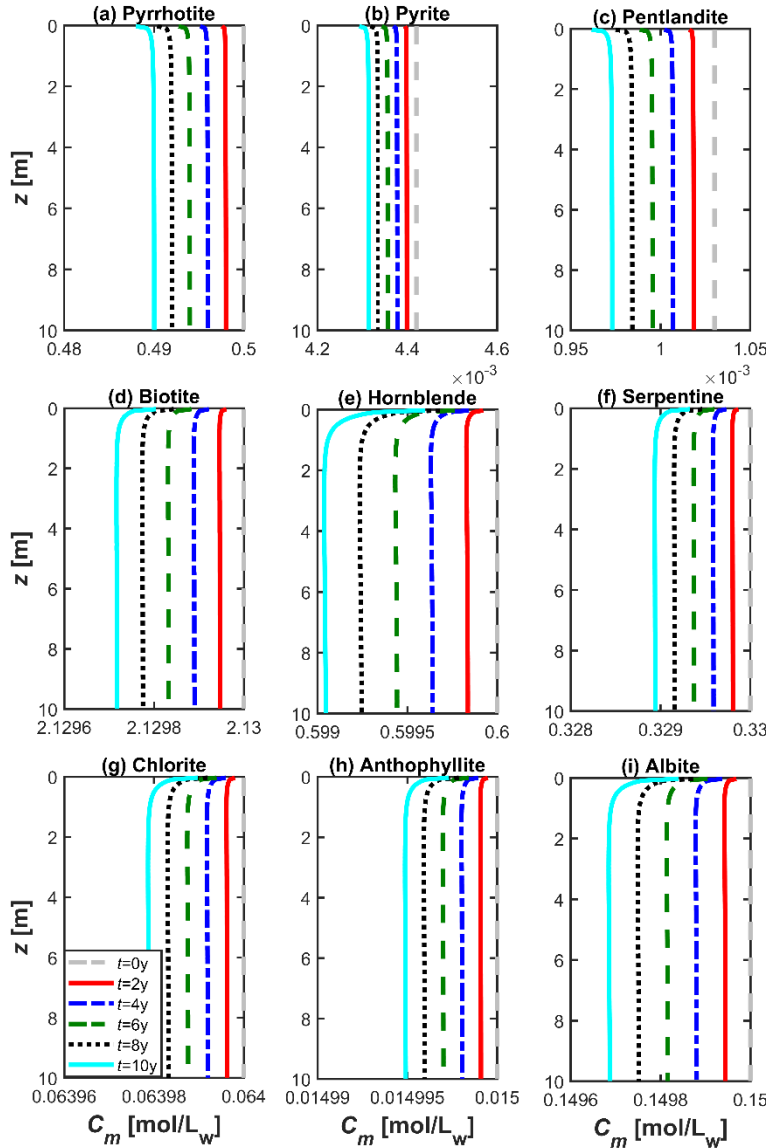
Transport of oxygen:



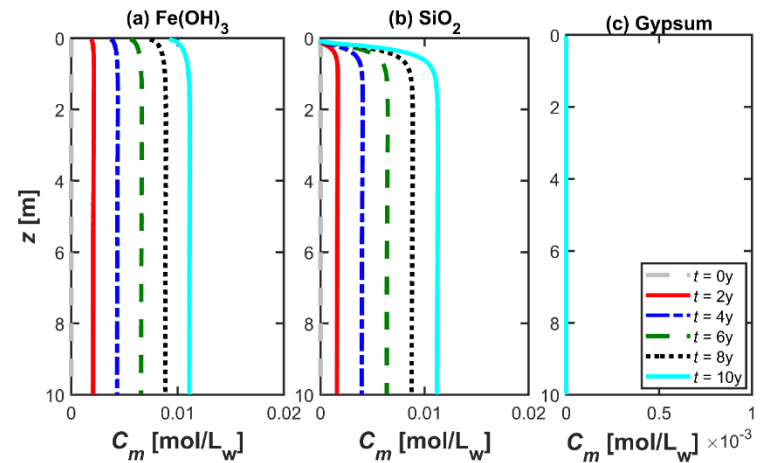
Example 1: Särkiniemi Waste Rock Pile (cont'd)

Evolution of minerals:

Primary minerals

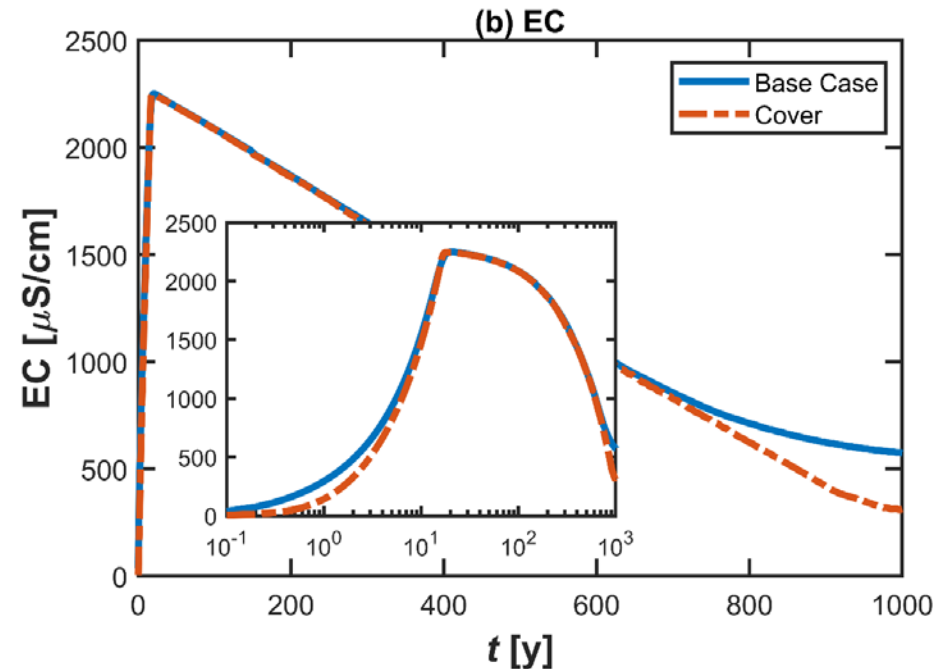
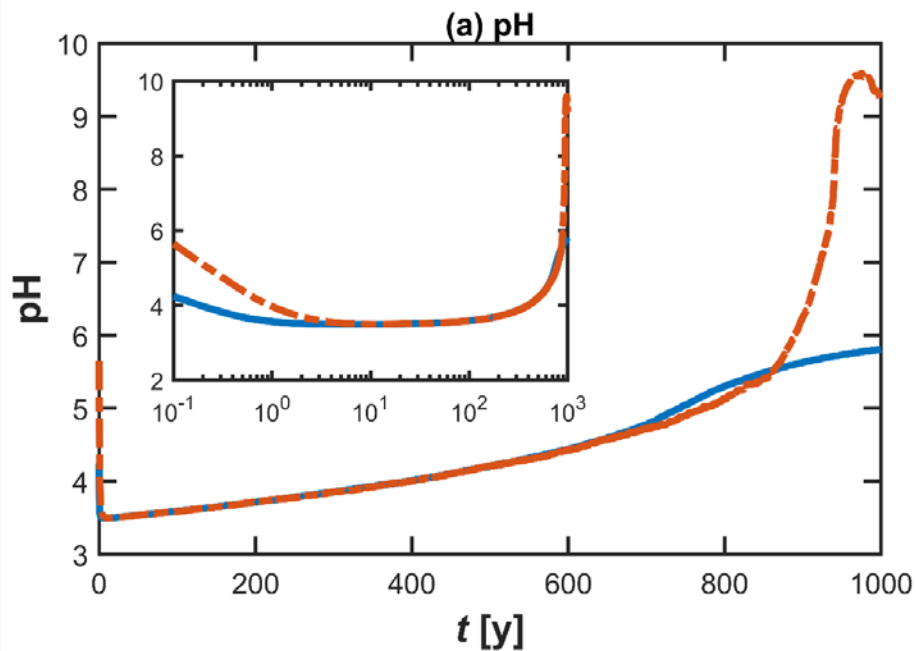


Secondary minerals

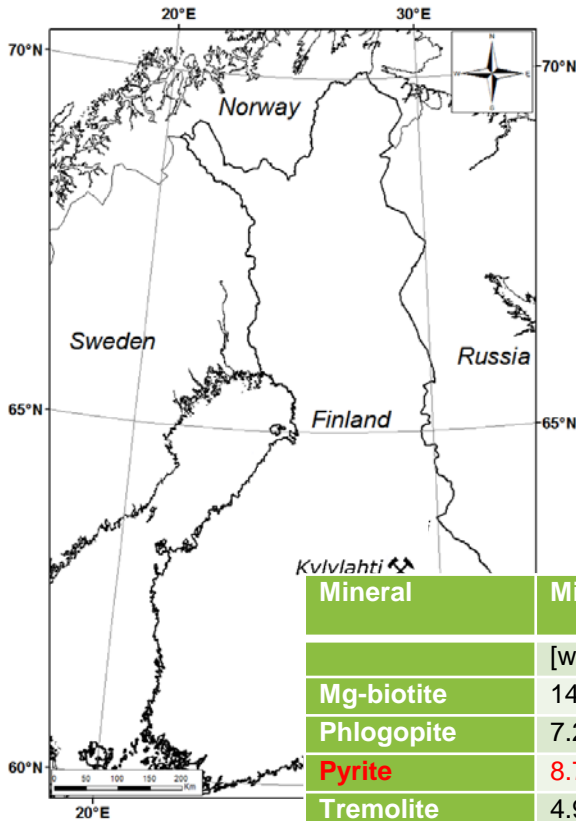


Example 1: Särkiniemi Waste Rock Pile (cont'd)

Long-term predictions and cover scenario:



Example 2: Kylylahti Waste Rock Pile

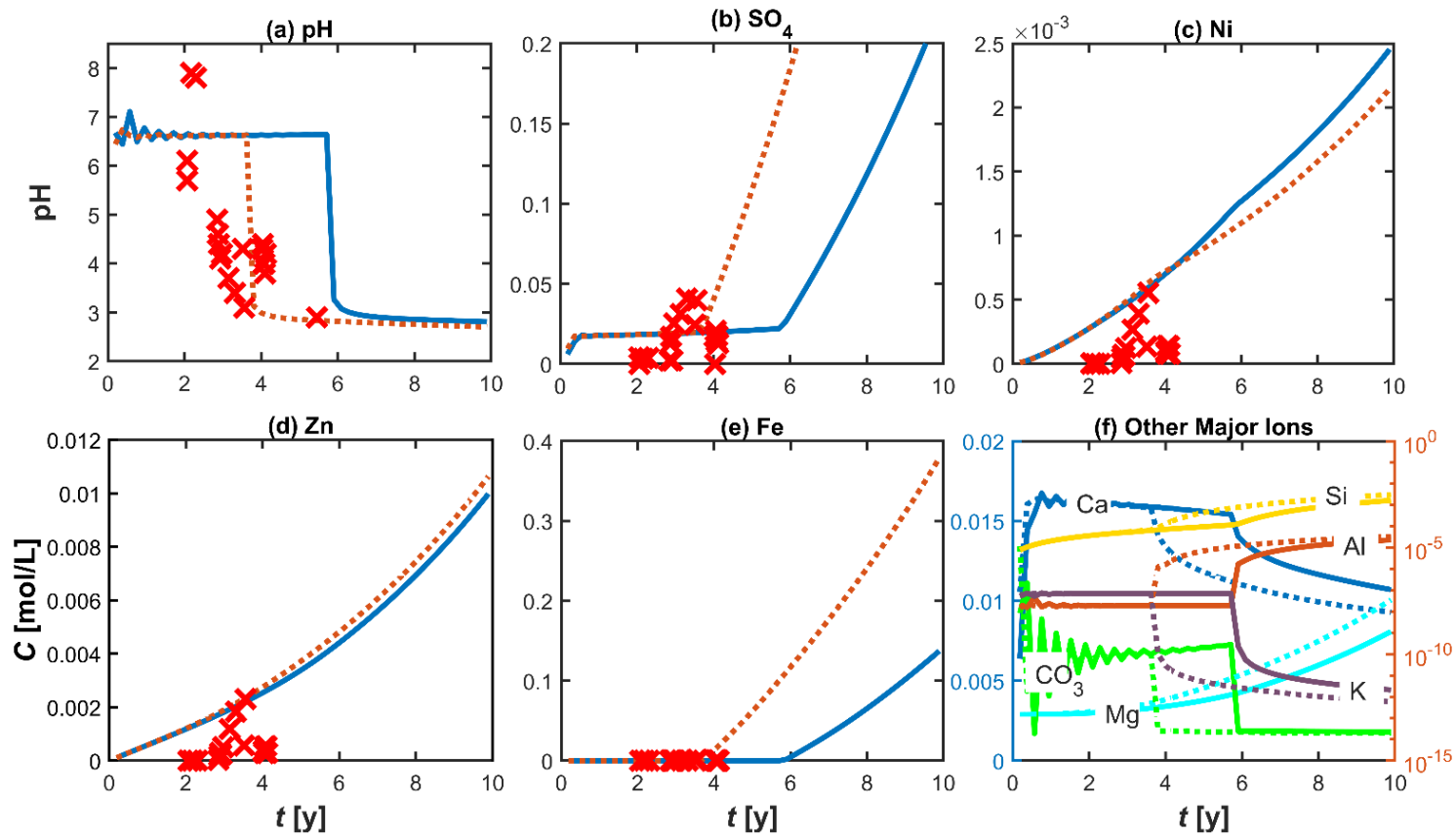


Mineral	Mineral Content		Surface Area, A [m ² L _w ⁻¹]	Rate Coefficient, k [mol m ⁻² s ⁻¹]	Reference
	[wt%]	[mol L _w ⁻¹] ^b			
Mg-biotite	14.49	0.92	0.05	10 ^{-10.97}	Nagy (1995)
Phlogopite	7.25	0.46	0.05	10 ^{-10.97}	Nagy (1995)
Pyrite	8.79	1.94	1.43^c	10^{-10.19}	Williamson & Rimdstidt
Tremolite	4.92	0.16	0.05	10 ^{-8.40} (k ₁) 10 ^{-11.98} (k ₂)	Palandri & Kharaka (2004)
Albite	3.83	0.39	0.06	10 ^{-10.16}	Palandri & Kharaka (2004)
Calcite	1.89	0.50	5 ^d	10 ^{-1.29} (k ₁) 10 ^{-4.46} (k ₂) 10 ^{-6.92} (k ₃)	Plummer et al. (1978)
Pyrrhotite	0.61	0.20	1.43^c	10^{-10.19}	Williamson & Rimdstidt (1994)
Sphalerite	0.08	2.17×10⁻²	1.43^c	10^{-9.22}	Domenech et al. (2002)
Pentlandite	0.05	1.72×10⁻³	1.43^c	10^{-10.19}	Williamson & Rimdstidt (1994)
Dolomite	0.02	2.87×10 ⁻³	5 ^d	10 ^{-3.19} (k ₁) 10 ^{-5.11} (k ₂) 10 ^{-7.53} (k ₃)	Plummer et al. (1978)

Example 2: Kylylahti Waste Rock Pile (cont'd)

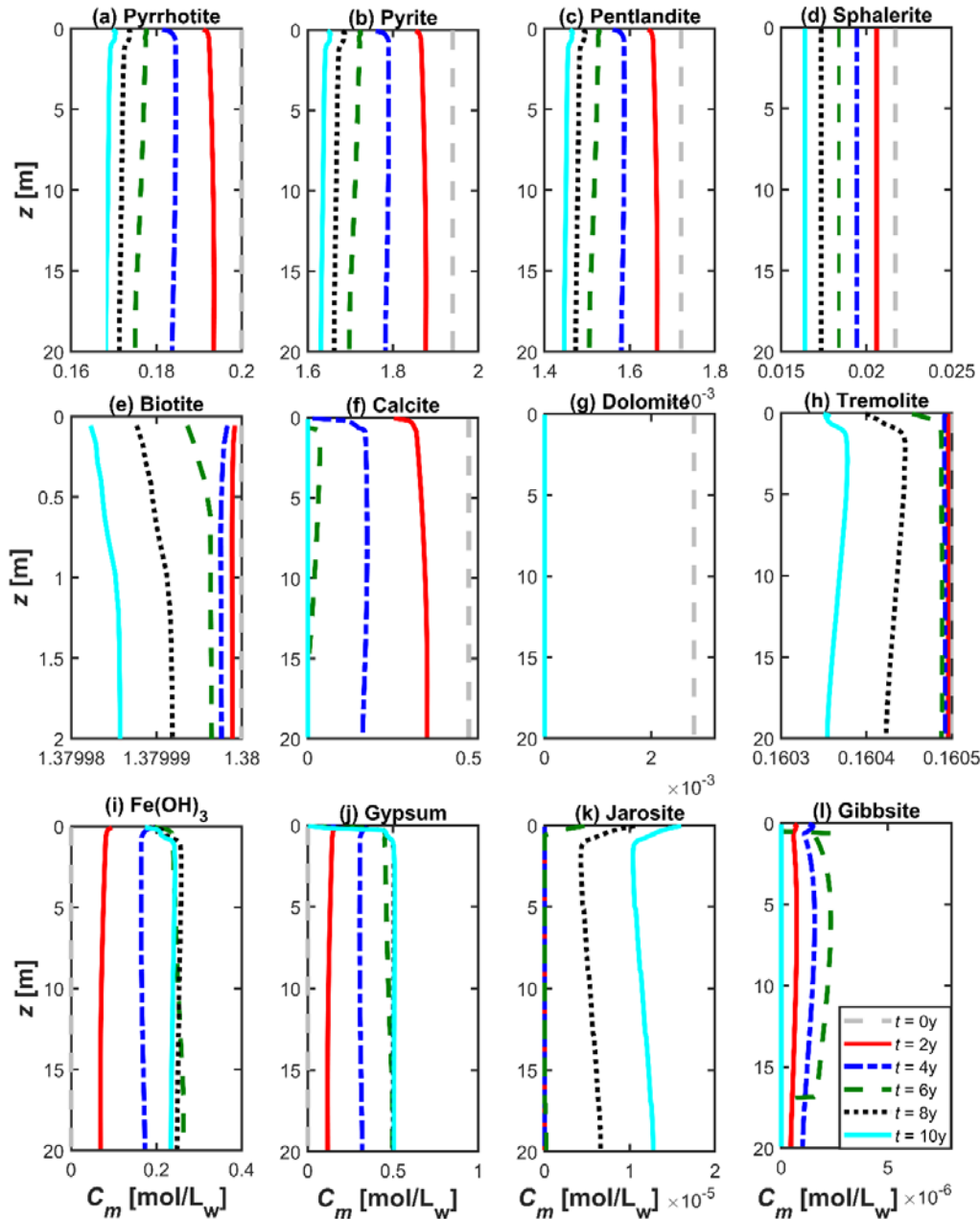
Evolution of Drainage Chemistry:

Blue Lines – lower oxidation rate
Orange Lines – higher oxidation rate

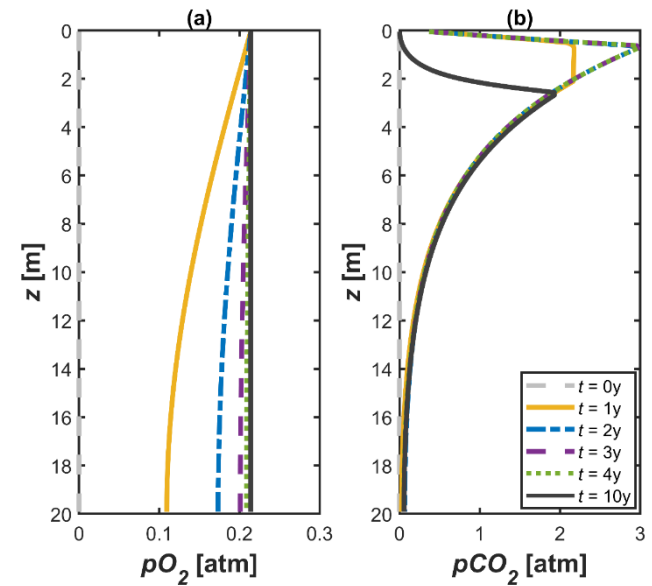


Example 2: Kylylahti Waste Rock Pile (cont'd)

Evolution of minerals



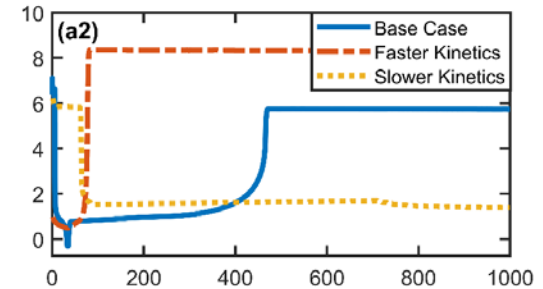
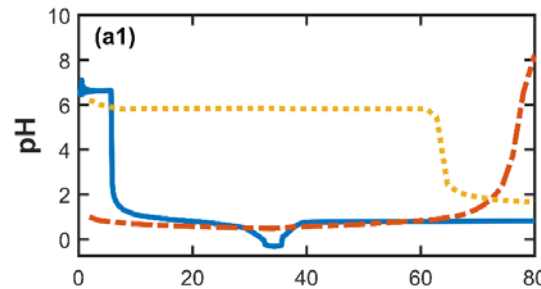
Gas transport



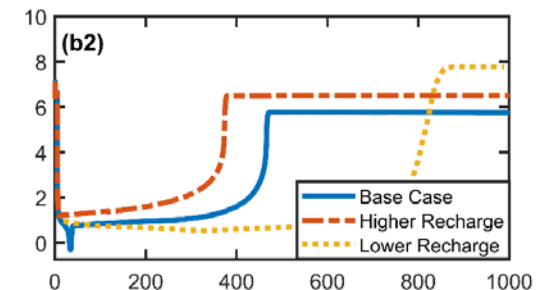
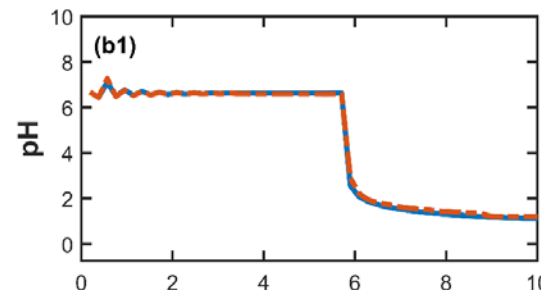
Example 2: Kylylahti Waste Rock Pile (cont'd)

Sensitivity Analysis:

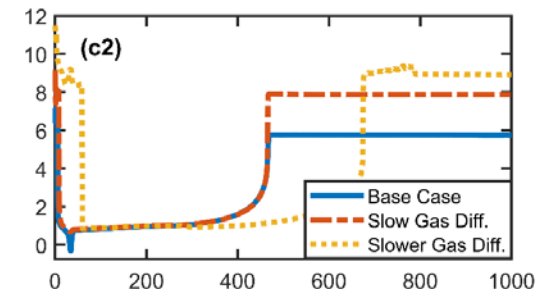
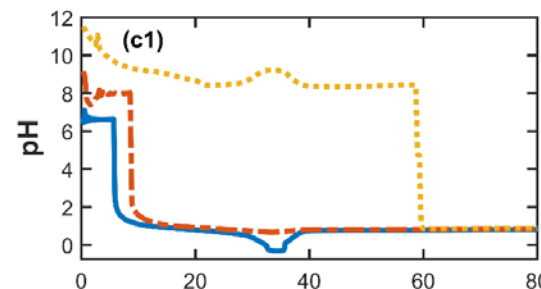
Reaction rate



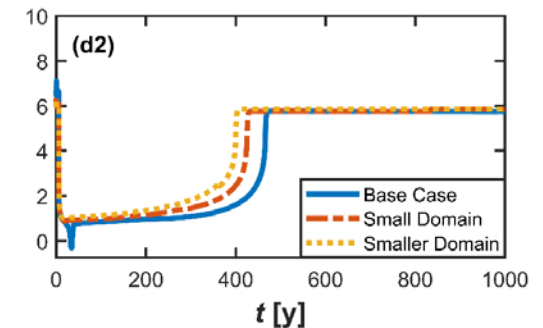
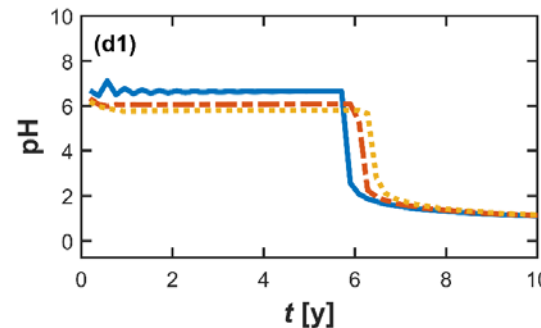
Recharge rate



Gas diffusion

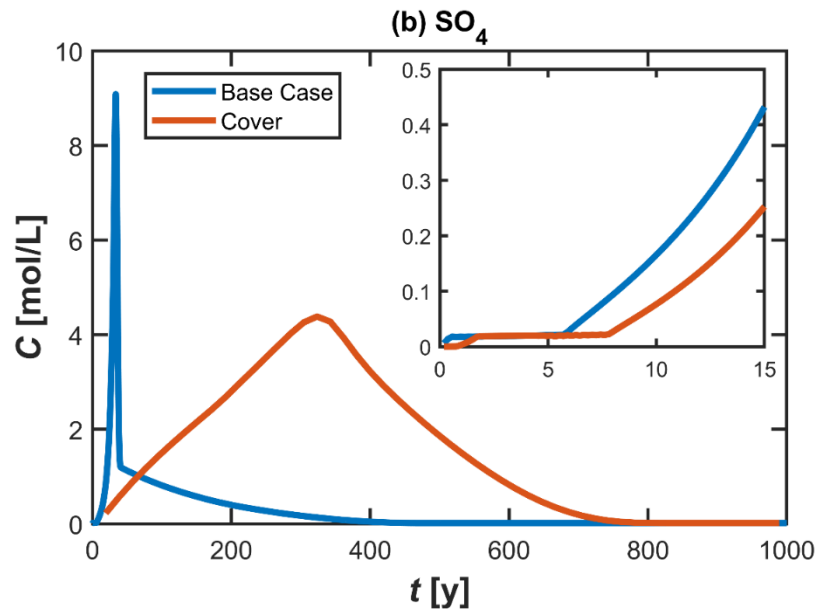
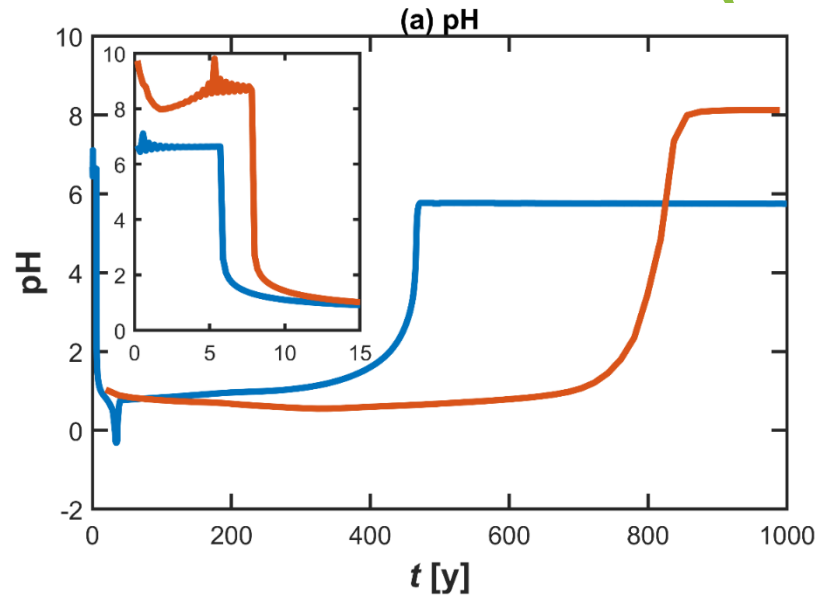


Domain size



Example 2: Kylylahti Waste Rock Pile (cont'd)

Long-term simulation
and cover scenario:

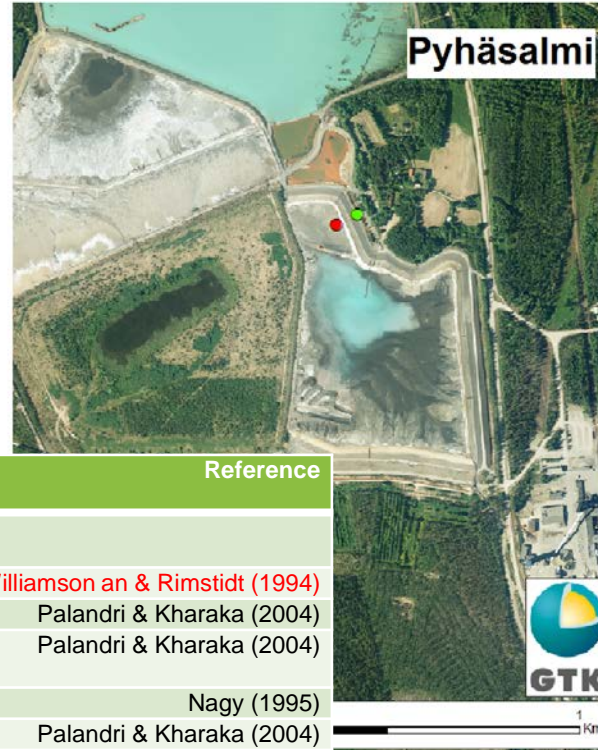
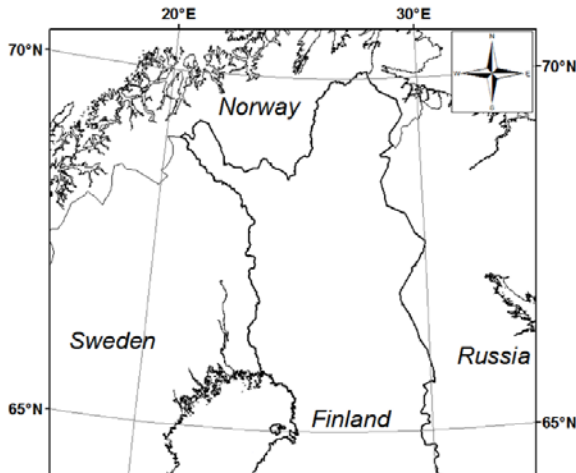


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Example 3: Pyhäsalmi Tailings Facility



Mineral	Mineral Content		Surface Area, A [m ² L _w ⁻¹]	Rate Coefficient, k [mol L _w ⁻¹ s ⁻¹]	Reference
	[wt%]	[mol L _w ⁻¹] ^b			
Pyrite	29.9	9.82	1.43 ^c	10 ^{-8.19}	Williamson an & Rimstidt (1994)
Hornblende	9.2	1.42	0.50	10 ^{-8.11}	Palandri & Kharaka (2004)
Tremolite	5.0	0.24	0.50	10 ^{-8.4} (k ₁) 10 ^{-11.98} (k ₂)	Palandri & Kharaka (2004)
Biotite	3.0	0.29	0.30	10 ^{-10.97}	Nagy (1995)
Albite	1.9	0.29	0.50	10 ^{-10.16}	Palandri & Kharaka (2004)
Serpentine	1.8	0.25	0.05	10 ^{-7.08}	Declercq & Oelkers (2014)
K-feldspar	1.7	0.25	0.50	10 ^{-10.06}	Palandri & Kharaka (2004)
Dolomite	1.7	0.36	5 ^d	10 ^{-3.19} (k ₁) 10 ^{-5.11} (k ₂) 10 ^{-7.53} (k ₃)	Plummer et al. (1978)
Chlorite	1.4	0.10	0.50	10 ^{-11.11}	Palandri & Kharaka (2004)
Calcite	1.1	0.42	5 ^c	10 ^{-1.29} (k ₁) 10 ^{-4.46} (k ₂) 10 ^{-6.92} (k ₃)	Plummer et al. (1978)
Anthophyllite	0.9	0.05	0.50	10 ^{-11.94}	Palandri & Kharaka (2004)
Phlogopite	0.8	0.07	0.30	10 ^{-10.97}	Nagy (1995)
Pyrrhotite	1.0	0.50	1.43 ^c	10 ^{-8.19}	Williamson an & Rimstidt (1994)
Chalcopyrite	0.2	0.04	1.43 ^c	10 ^{-8.19}	Williamson an & Rimstidt (1994)
Sphalerite	0.1	0.05	1.43 ^c	10 ^{-9.22}	Domenech et al. (2002)

● Drainage sample

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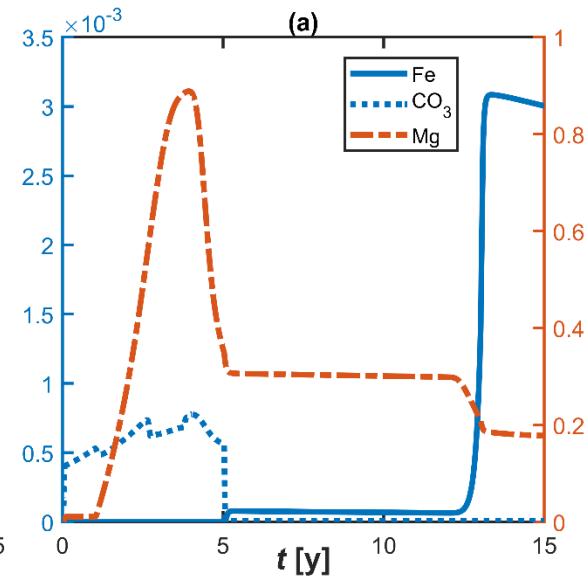
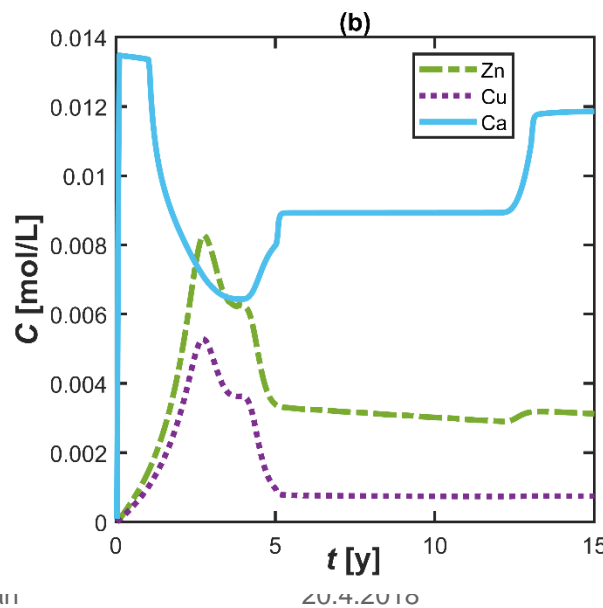
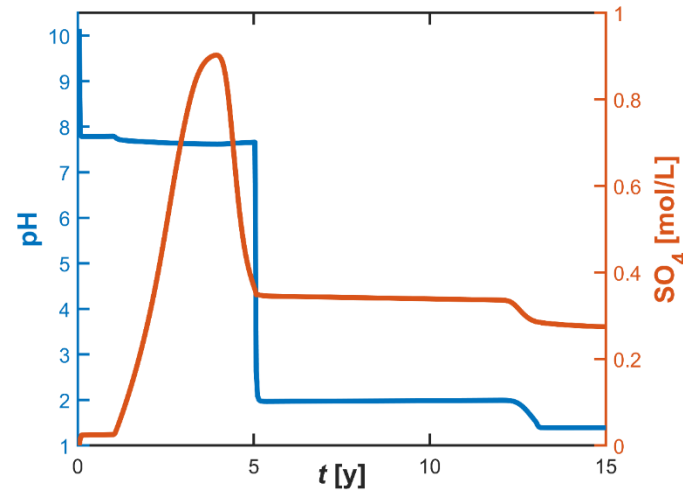
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Example 3: Pyhäsalmi Tailings Facility (cont'd)

Predicted Drainage Quality:

measured seepage water pH = 2.87
 NAG pH = 2.14



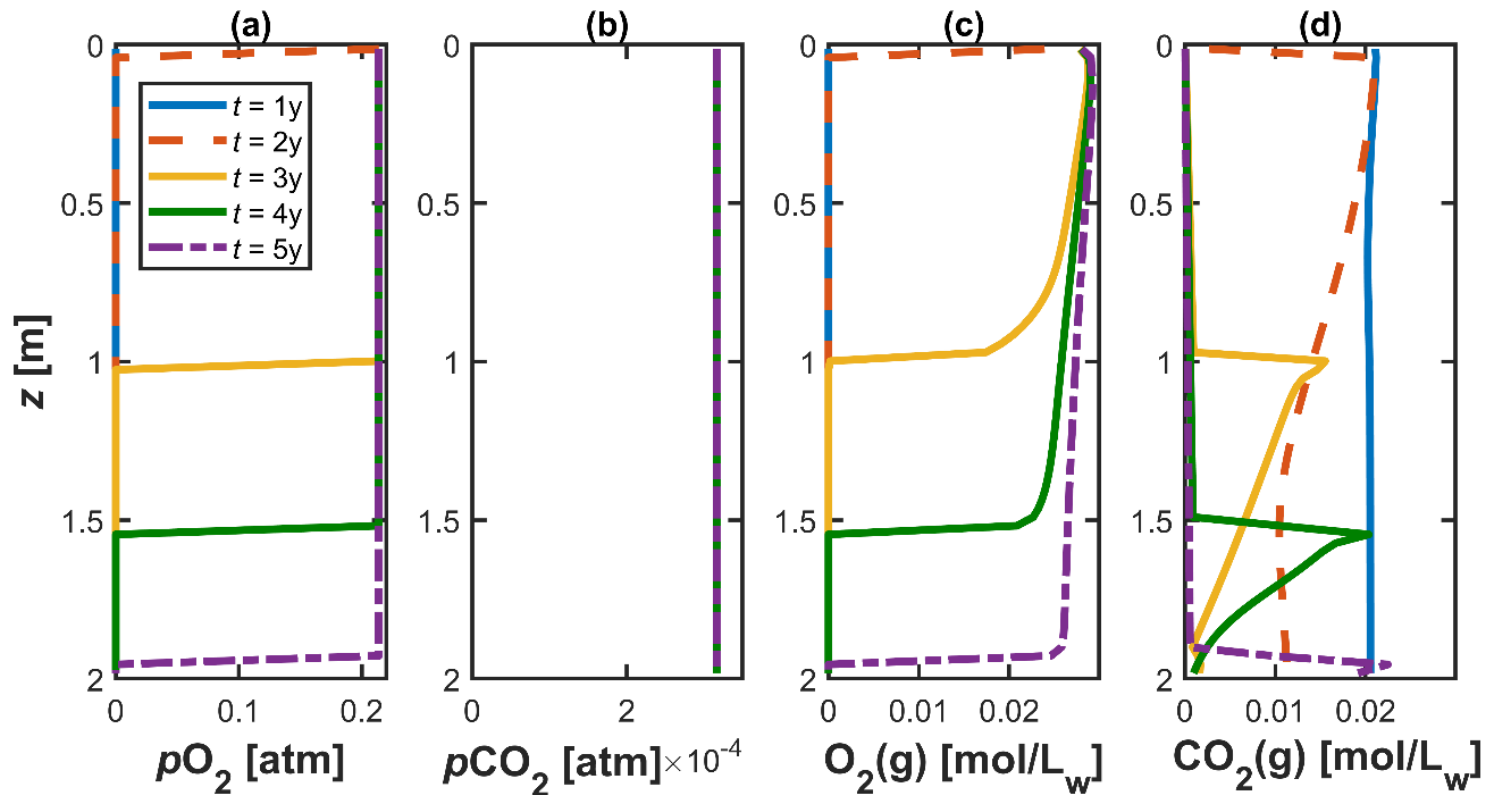
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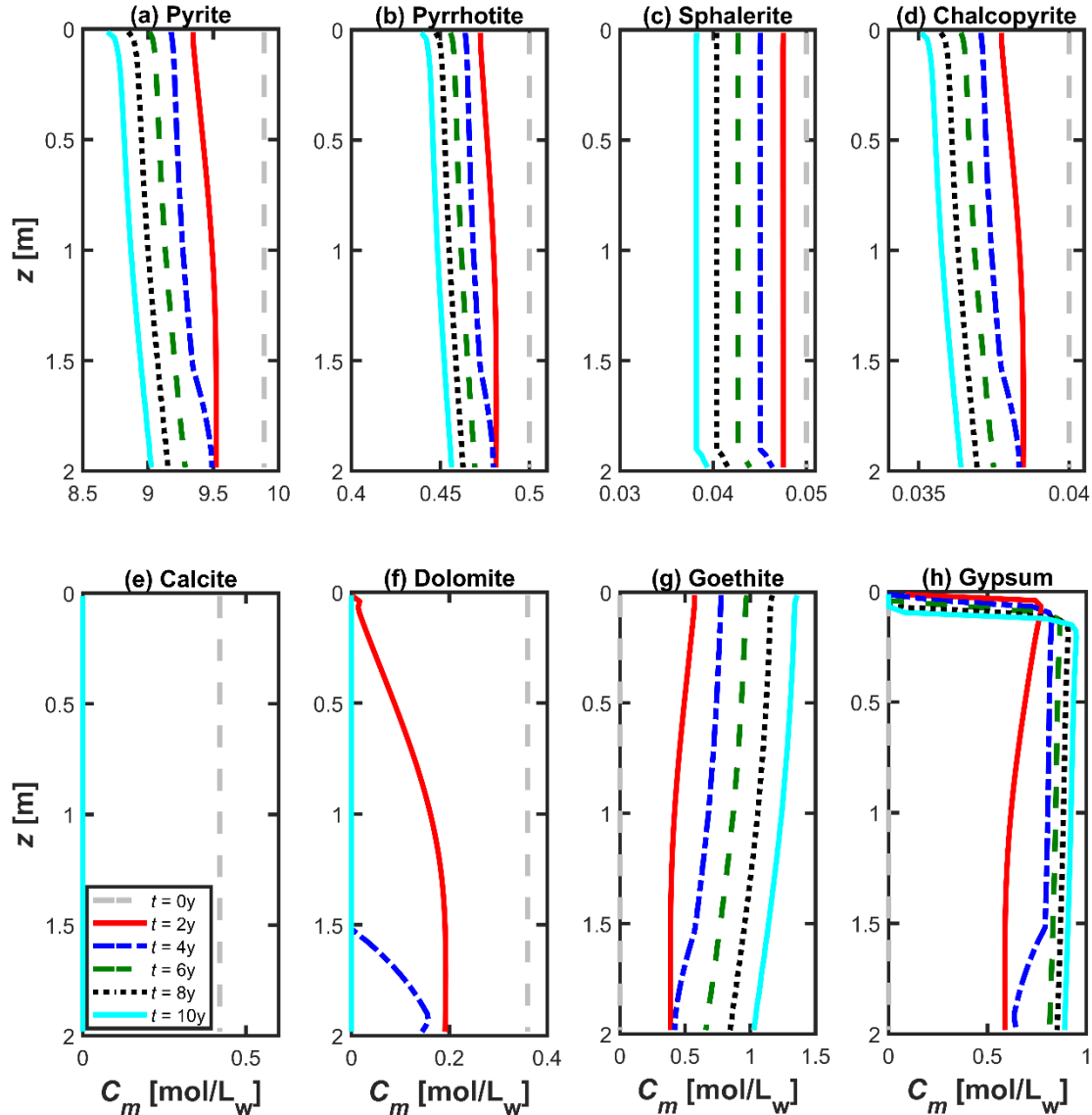
Example 3: Pyhäsalmi Tailings Facility (cont'd)

Transport of Gases:



Example 3: Pyhäsalmi Tailings Facility (cont'd)

Evolution of mineral phases:



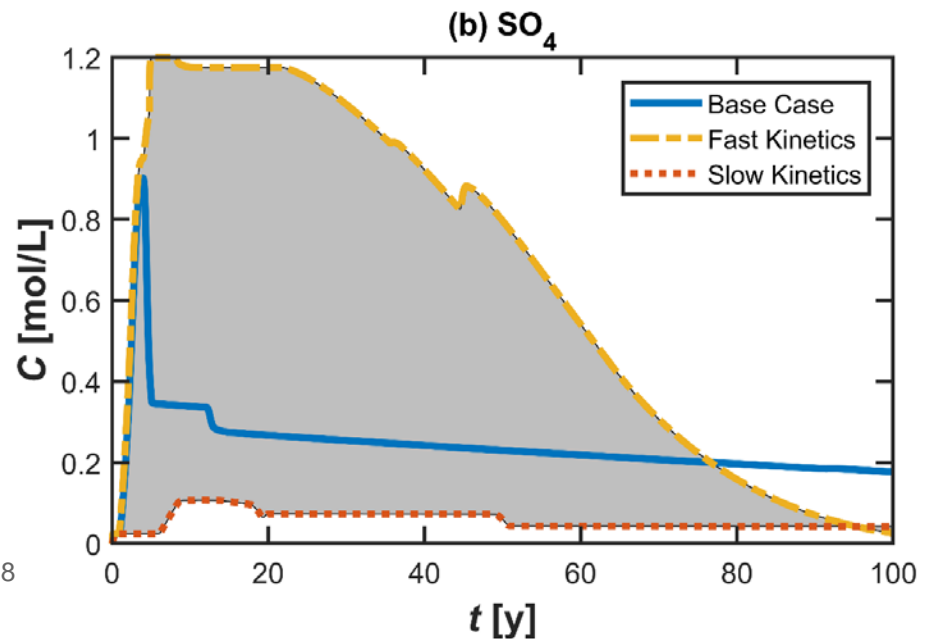
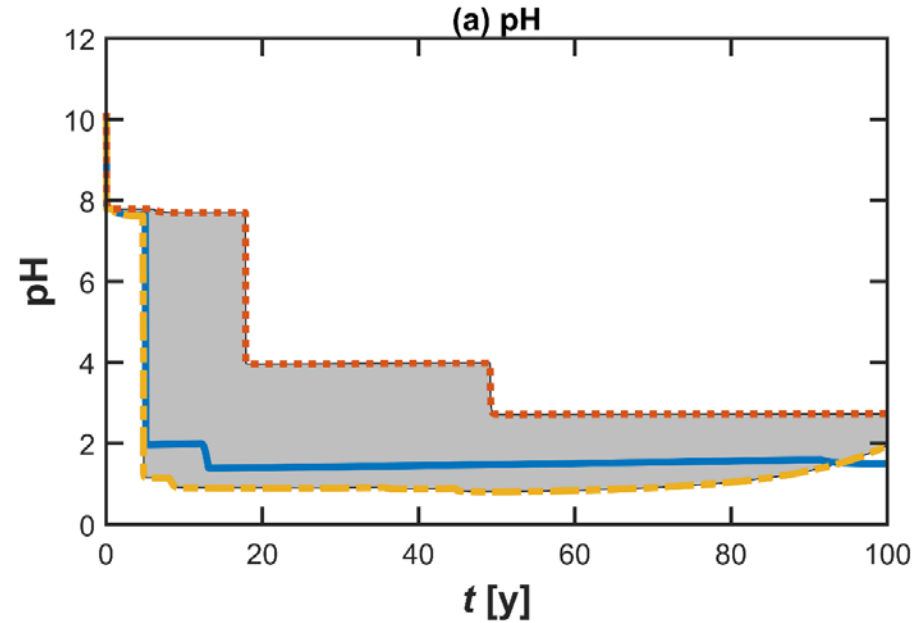
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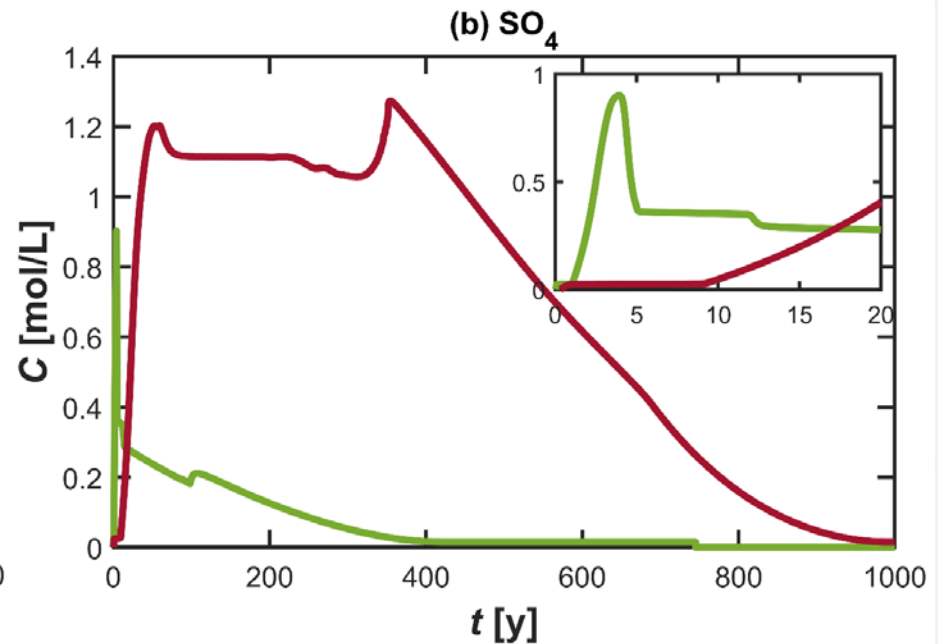
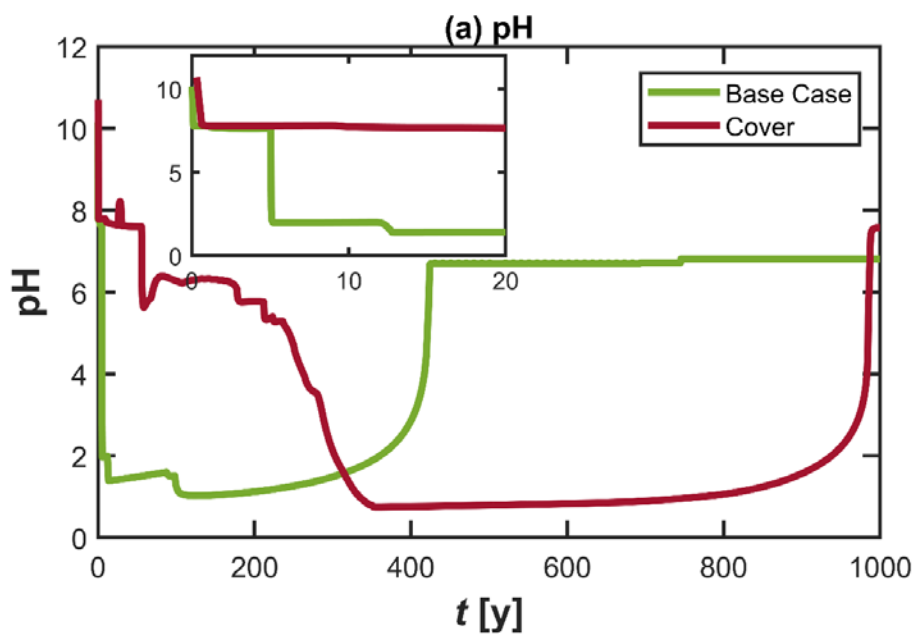
Example 3: Pyhäsalmi Tailings Facility (cont'd)

Long-term prediction of drainage water quality:



Example 3: Pyhäsalmi Tailings Facility (cont'd)

Cover scenario:



Major Sources of Uncertainties

- Heterogeneity: a problem cannot be solved with more computational resources!
 - Existing analogues can be used
 - Stochastic concepts can be applied to estimate the likelihood
- Reaction parameters and microbial mechanisms
 - Mineral reaction parameters should be obtained from the static and kinetic test results
- Seasonal fluctuations
- Water saturation and moisture profiles
- Retardation and sorption like processes
- Dimensionality → 1D, 2D or 3D dominated system!
- Coupling of gas and heat transport



Conclusions

- The proposed model seem to be capable of predicting the future key events
 - Simulation outcomes correspond to the static test results and the measured drainage quality
- Predictive modelling can be performed in an early stage of a mine with limited data
 - Prediction accuracy is only as good as the conceptual understanding about involved processes
 - Objective of such modelling would be achieve the right order of magnitude instead of obtaining the exact values
- Effects of uncertainty and the model limitations should be properly acknowledged
 - especially when such prediction results are used in decision making processes
- Predictive models should be continuously updated with the increasingly collected data during the operational phases



Thank you for your attention!

Contact:

Dr. Muhammad Muniruzzaman

Research Scientist

Geological Survey of Finland

Email: md.muniruzzaman@gtk.fi

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