



Predictive Modeling of Drainage Quality from Mine Wastes

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Endomines



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Transport and the Environment

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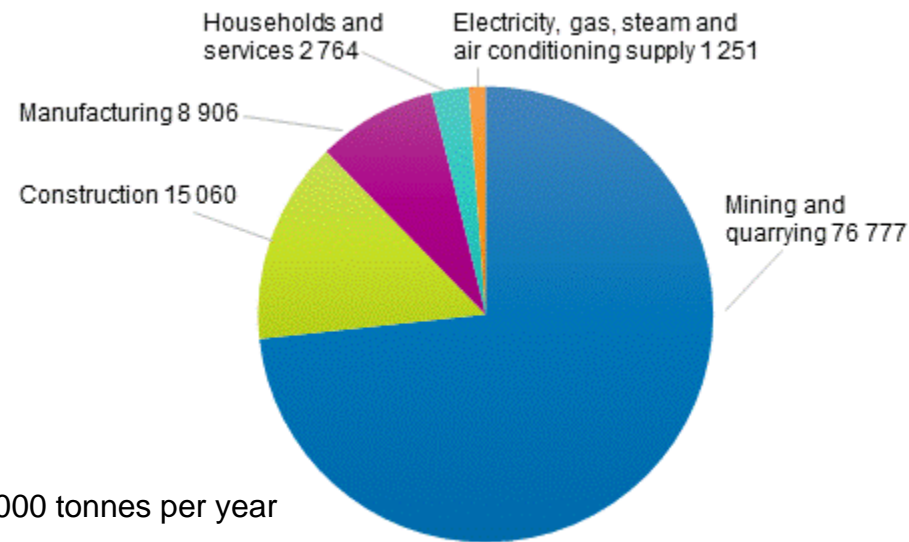
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Mine Wastes – Scale of the problem

- Mine wastes are the largest volume of materials handled in the world!
- In 1982, annual worldwide production of mine wastes was **>4.5 billion tonnes**
 - in Canada, mine waste production: **~980 Mt**
 - in Finland, mine waste production in 2015: **~77 Mt**



Waste generated by sector and type in 2015, 1,000 tonnes per year

(http://www.stat.fi/til/jate/2015/jate_2015_2017-06-15_tie_001_en.html)



Mine Wastes – Scale of the problem (cont'd)

- **>6400 km** of rivers and streams in the Eastern U.S. and **8000–16000 km** of streams in the Western U.S. are affected by mine drainage
- Estimated costs for remediating mine wastes internationally → ***tens of billions dollars***

(Blowes et al., 2014, Treatise on Geochem.)

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Mathematical Modeling

- Representation of a real world problem in mathematical forms derived from e.g., first principles such as the conservation of mass, energy and momentum
- Based on theory and experiments, and often apply approaches to integrate them
- Assumptions related to the simplification of reality are often made
- Mathematics is the language for quantitative process descriptions

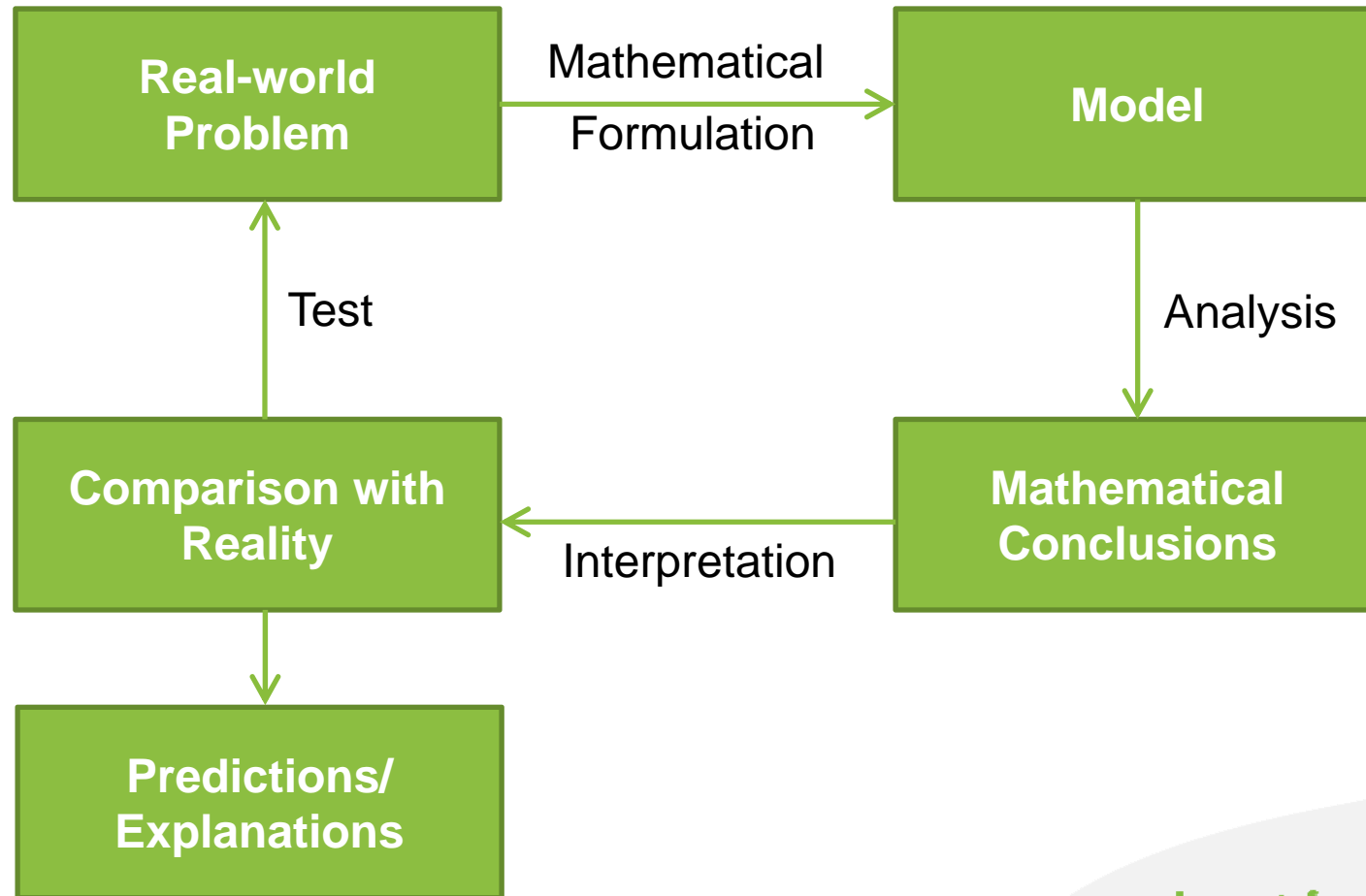
Why Models are Important?

- Processes (e.g., geochemical reactions) typically occur in open systems where fluxes drive physicochemical mechanisms
- “Slowness” and “nonlinearity” of processes requires predictive capabilities
- Difficult to evaluate quantitatively the importance of time-dependent processes without considering them as a part of a complex coupled system
- Models can provide testing of hypothesis as well as quantitative predictions
- For risk assessment and design of adequate measures for waste management

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Basic Philosophy of Predictive Modeling



Why Predictive Modeling?

Predictions

What will happen?
When it will happen?
Why it will happen?

Predictive analysis

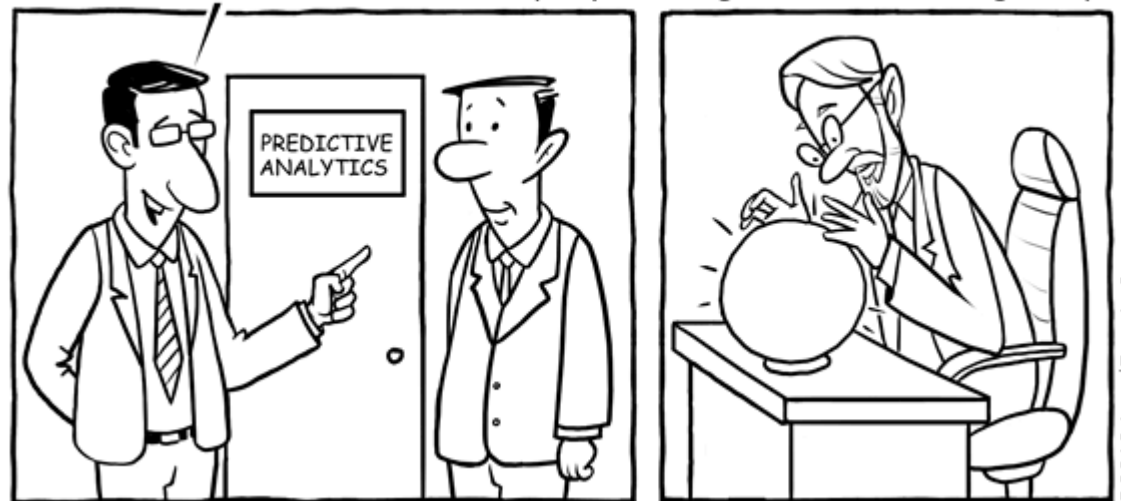
Decisions

How do we benefit from these

Effects

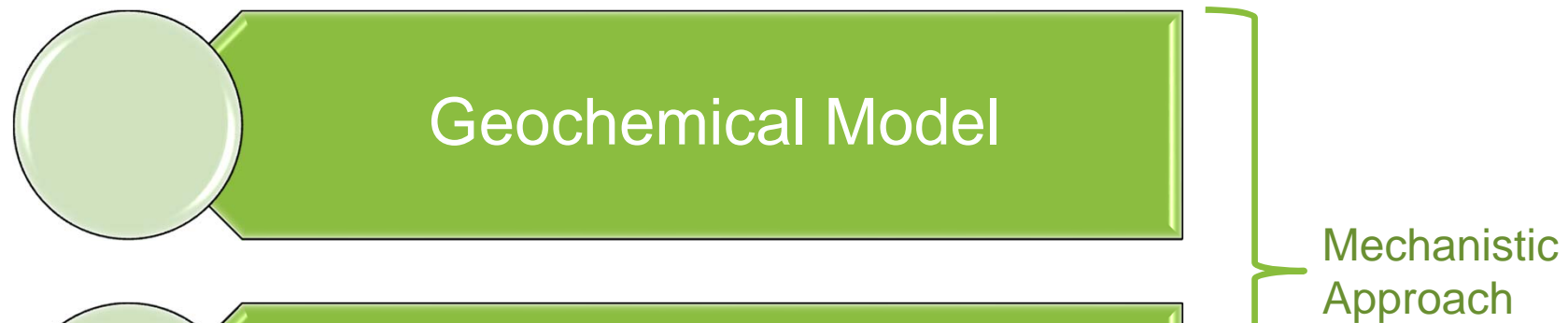
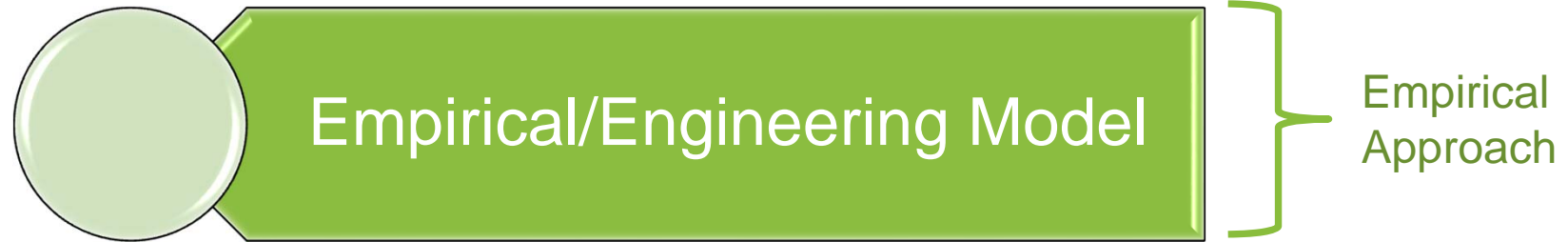
How will these decisions impact everything else?

Since he came on board, our accuracy in predicting visitor intent has gone up



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Typical Models in Mining Environments

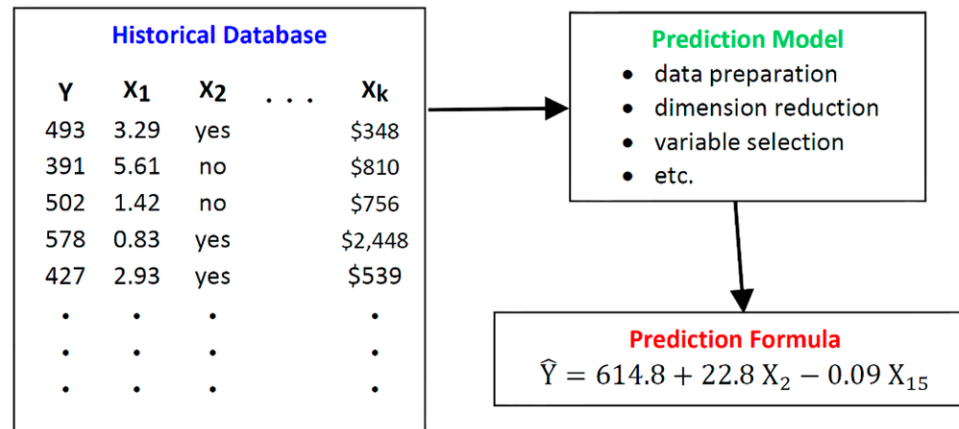


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Engineering/Empirical Model

- Based on statistical relationships (e.g., regression/correlation analysis)



Examples codes:
RATAP (MEND, 1990)
WATAIL (MEND, 1993)
MINEWALL (MEND, 1995)
etc.

- Relies on empirical data and ignores detailed physicochemical mechanisms
- Can be computationally inexpensive
- Lacks theoretical rigor and predictive capability is limited!

Geochemical Model

- Describes chemical reactions occurring in mine wastes
- Based on the theoretical equations describing geochemical reactions → *mechanistic formulation*
- Uses thermodynamic databases
- Can simulate a plethora of geochemical processes:
 - Aqueous complexation/speciation reactions
 - Acid-base reactions
 - Redox reactions
 - Cation exchange and surface complexation
 - Sorption/desorption
 - Dissolution-precipitation reactions (equilibrium and kinetics)
 - Solid/gas phases
 - Microbial reactions

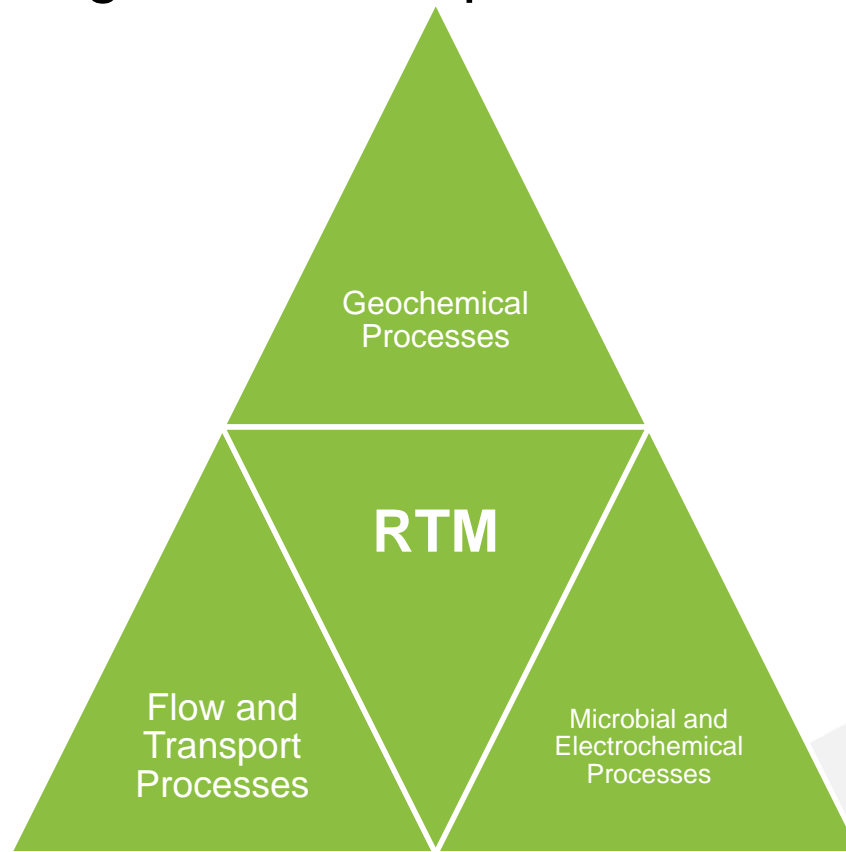
Geochemical Model (cont'd)

Popular computer codes:

- WATEQ4F (Ball and Nordstrom, 1991)
- MINTEQA2 (Allison et al., 1991)
- GEOCHEM (Parker et al., 1995)
- EQ3/6 (Wolery et al., 1992)
- CHESS (van der Lee et al., 2003)
- PHREEQC/PHREEQM (Parkhurst and Appelo, 1999)

Reactive Transport Model

- Most comprehensive model among these model types
- Solves simultaneous system of PDEs describing physical and geochemical processes



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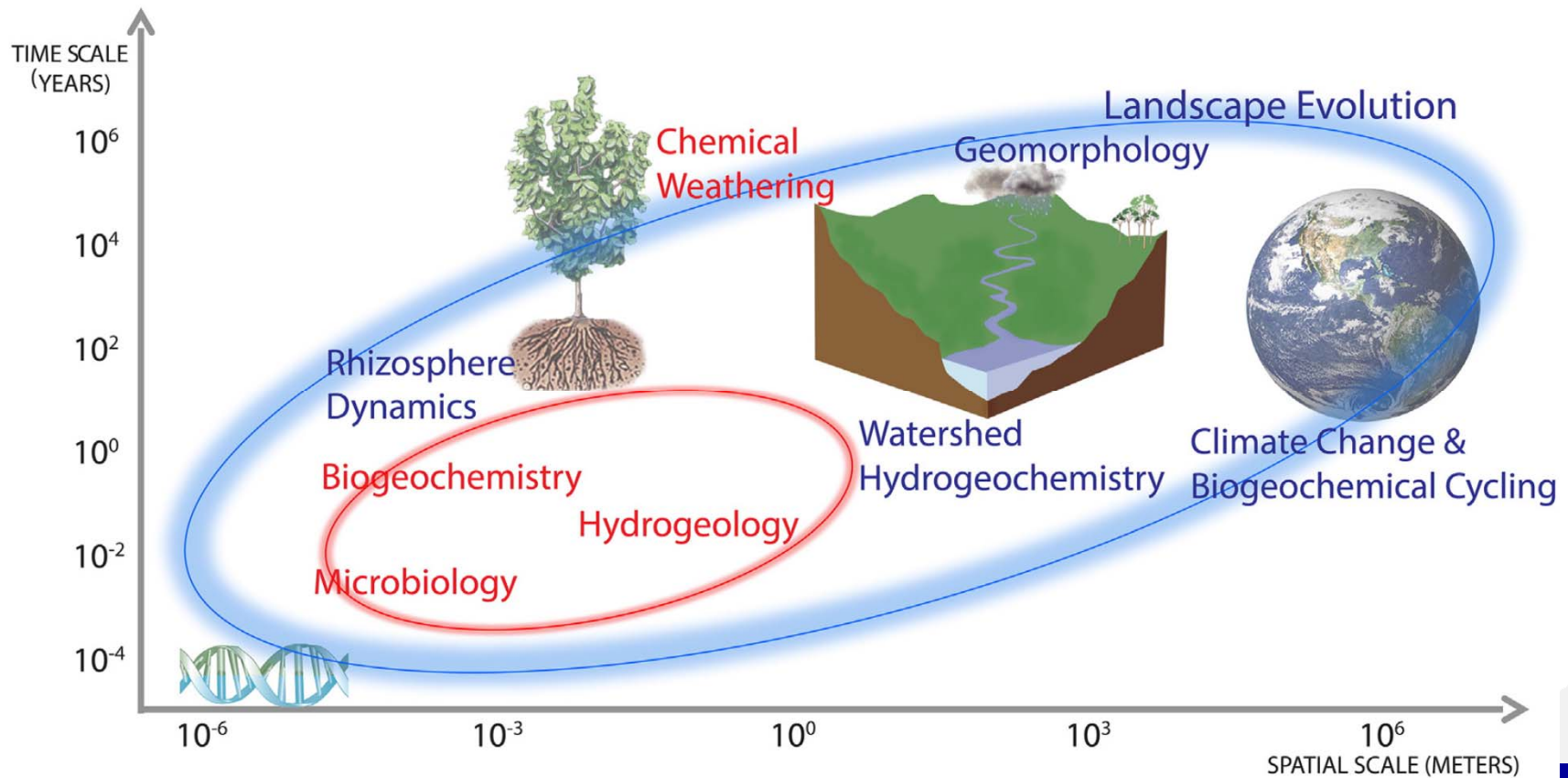
Reactive Transport Model (cont'd)

- Capable to simulate multidimensional fluid flow, multicomponent solute/gas transport, and biogeochemical reactions
 - a hybrid between hydrogeological and geochemical models
- Can predict non-intuitive system behavior when multiple processes are coupled and they collectively control system dynamics
- A high resolution model calculations can be computationally heavy!

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Reactive Transport Model (cont'd)



(Li et al., 2017, Earth-Science Reviews)

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Reactive Transport Model (cont'd)

Popular computer codes:

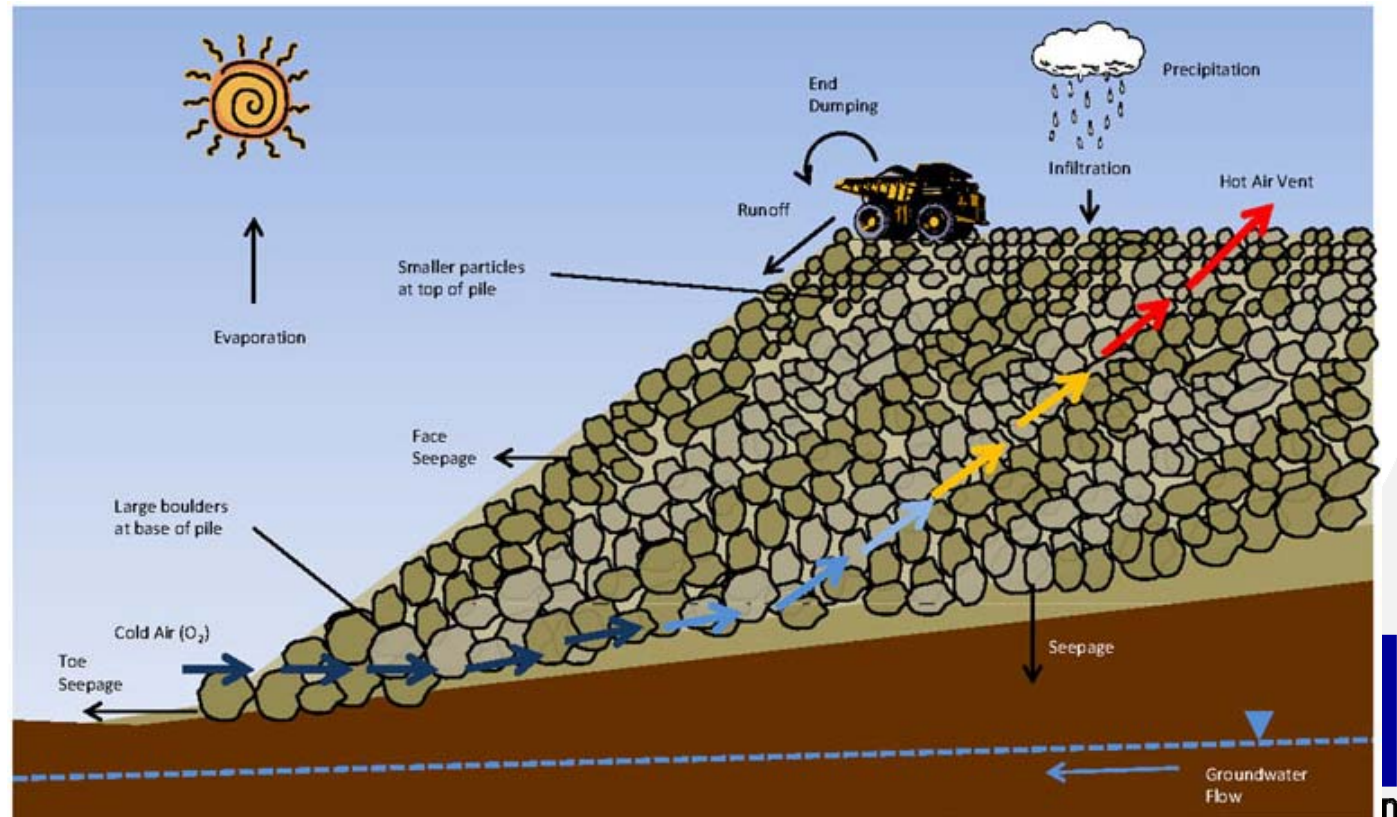
- PHREEQC (Parkhurst and Appelo, 2013)
- MIN3P (Mayer et al., 2002)
- CrunchFlow (Steefel and Lasaga, 1994)
- PHT3D (Prommer et al., 2003)
- PHAST (Parkhurst et al., 2005)
- Geochemist's Workbench (Bethke, 1997)
- TOUGHREACT (Xu and Pruess, 2001)
- HYDROGEOCHEM (Yeh and Tripathi, 1997)
- PFLOTRAN (Lichtner et al., 2013)
- OpenGeoSys (Kolditz et al., 2012)
- HP1/HPx (Šimunek et al. (2012))
- eSTOMP (White and Oostrom, 2006)

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Prerequisites for Quantitative Modeling

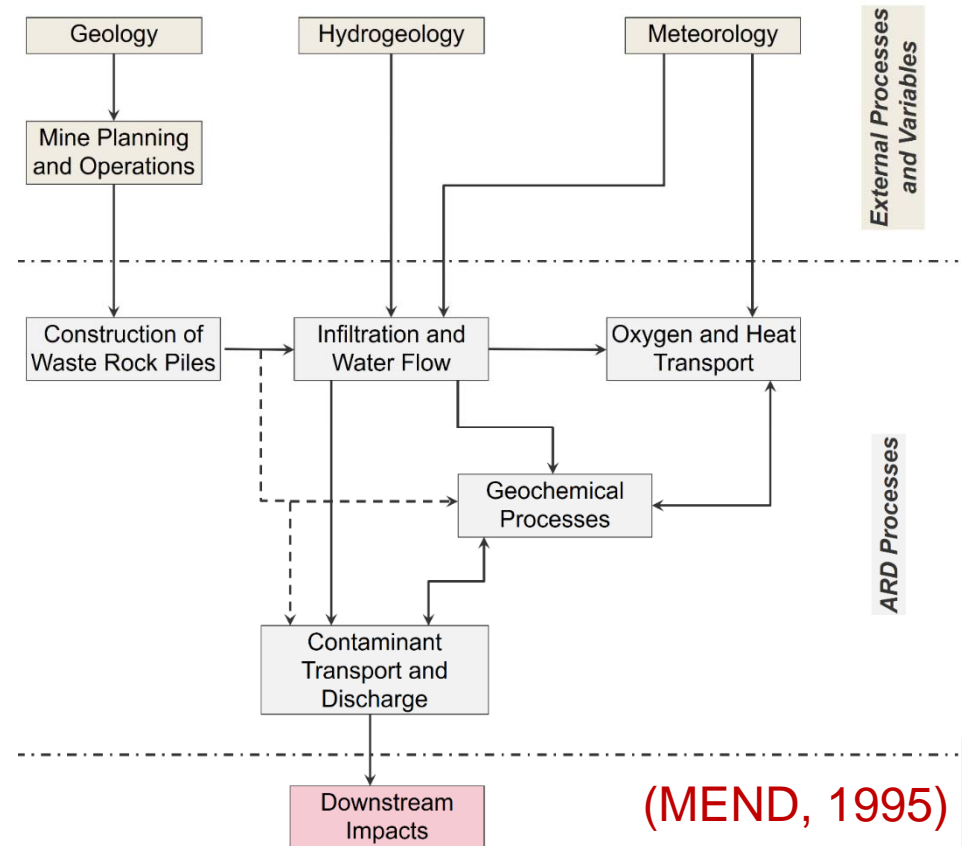
- Detailed site characterization
- A computer code



Data Requirements

- Data should be collected as much as possible
- Major processes must be identified
- Data must be representative of the domain of interest

If we are not able to formulate a system behavior by means of equations, we have not yet understood the system in a quantitative way!

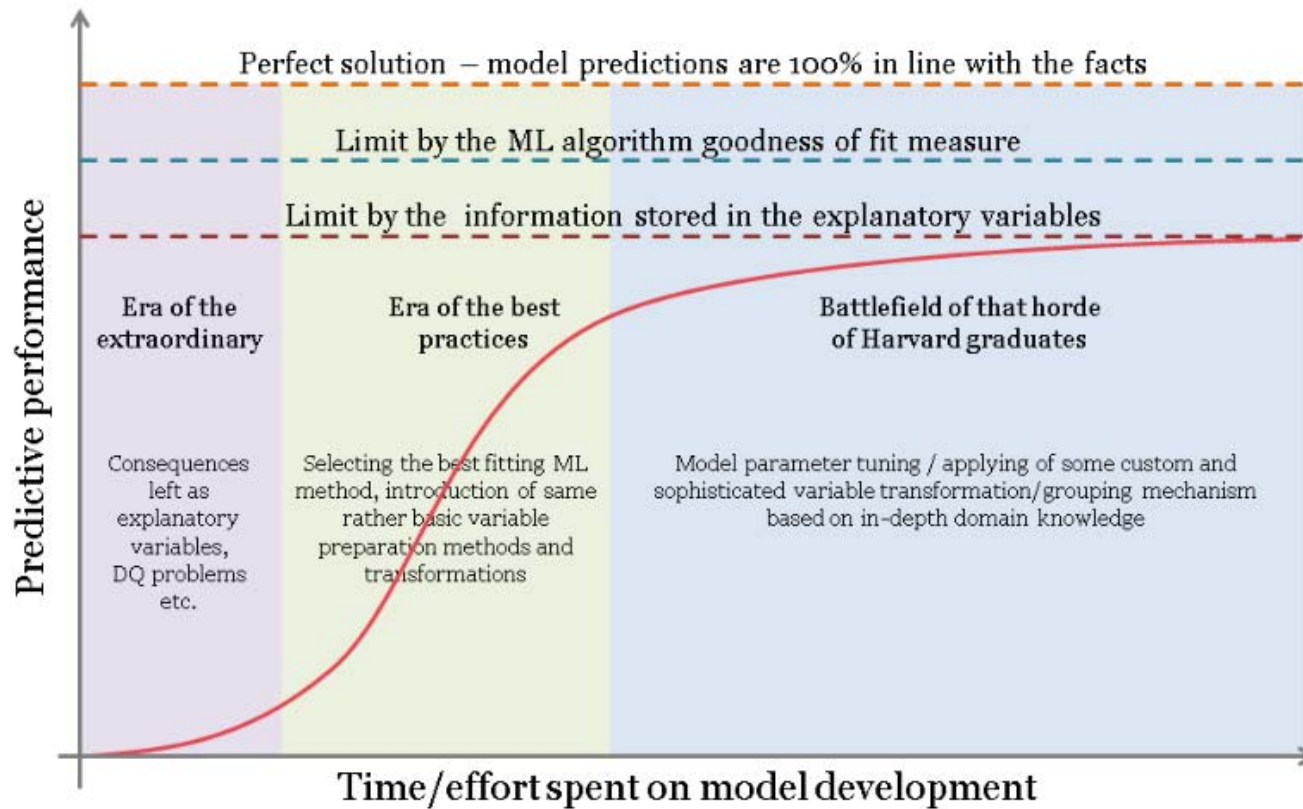


Challenges in Predictive Modeling

- Scarcity in collected data
 - inadequate data and heterogeneity
 - incomplete/partial system understanding
 - non-uniqueness and reproducibility of the collected dataset
 - unknown environmental conditions

- Numerical challenges
 - processes occurring at different scales
 - difficulties in defining boundary and initial conditions
 - numerical errors/uncertainties
 - computational limitations

Predictive Performance Curve



(<https://www.linkedin.com/pulse/well-trained-monkey-against-team-harvard-graduates-data-fodroczi>)

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Example Case Study: Acid Mine Drainage Generation and Attenuation

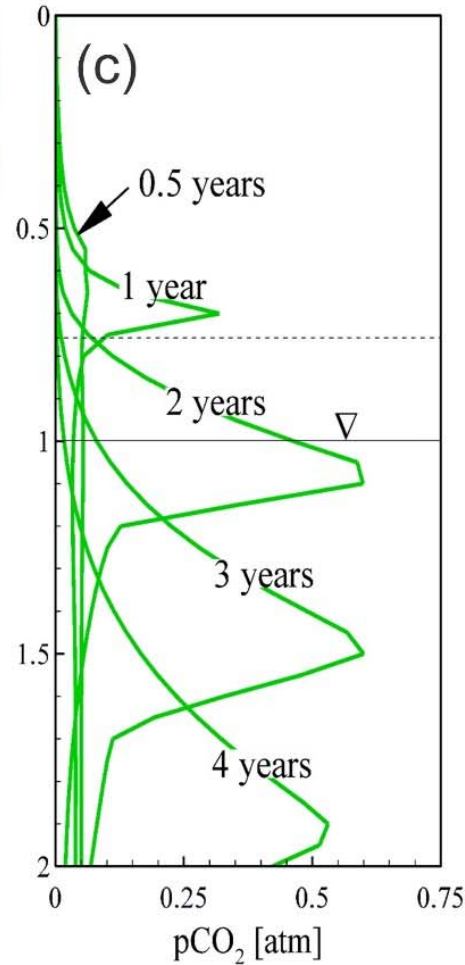
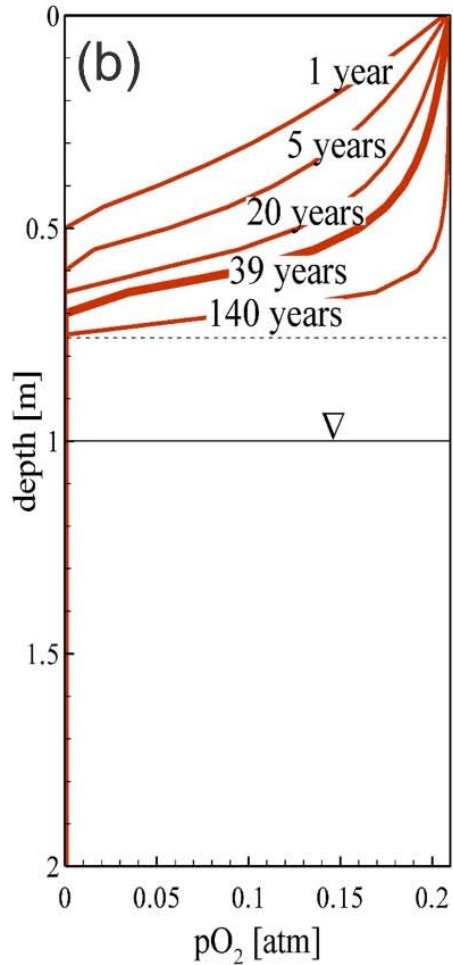
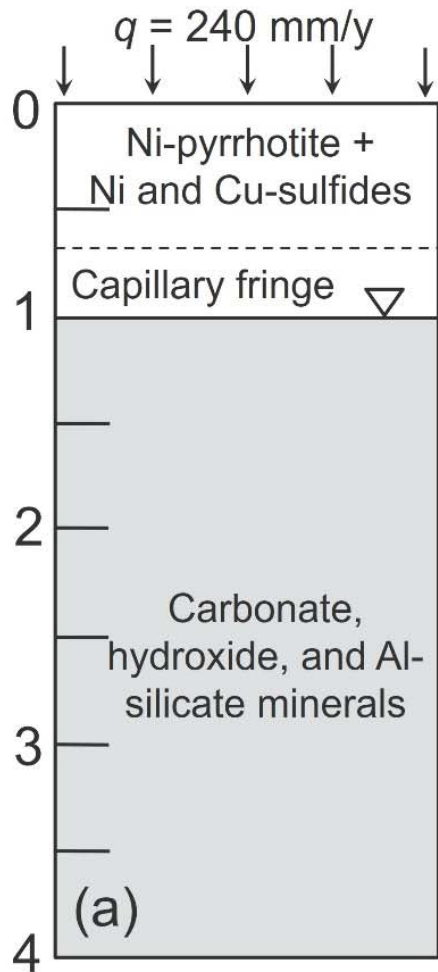
- Field Site: Nickel Rim Mine Tailings, Sudbury, Ontario, Canada (David Blows, Uni. Waterloo)
- Main processes:
 - O₂ ingress by gaseous transport
 - Sulfide mineral oxidation in unsaturated zone
 - pH buffering by Al-silicate minerals
 - Secondary mineral precipitation and re-dissolution

Mayer et al. (2002), WRR

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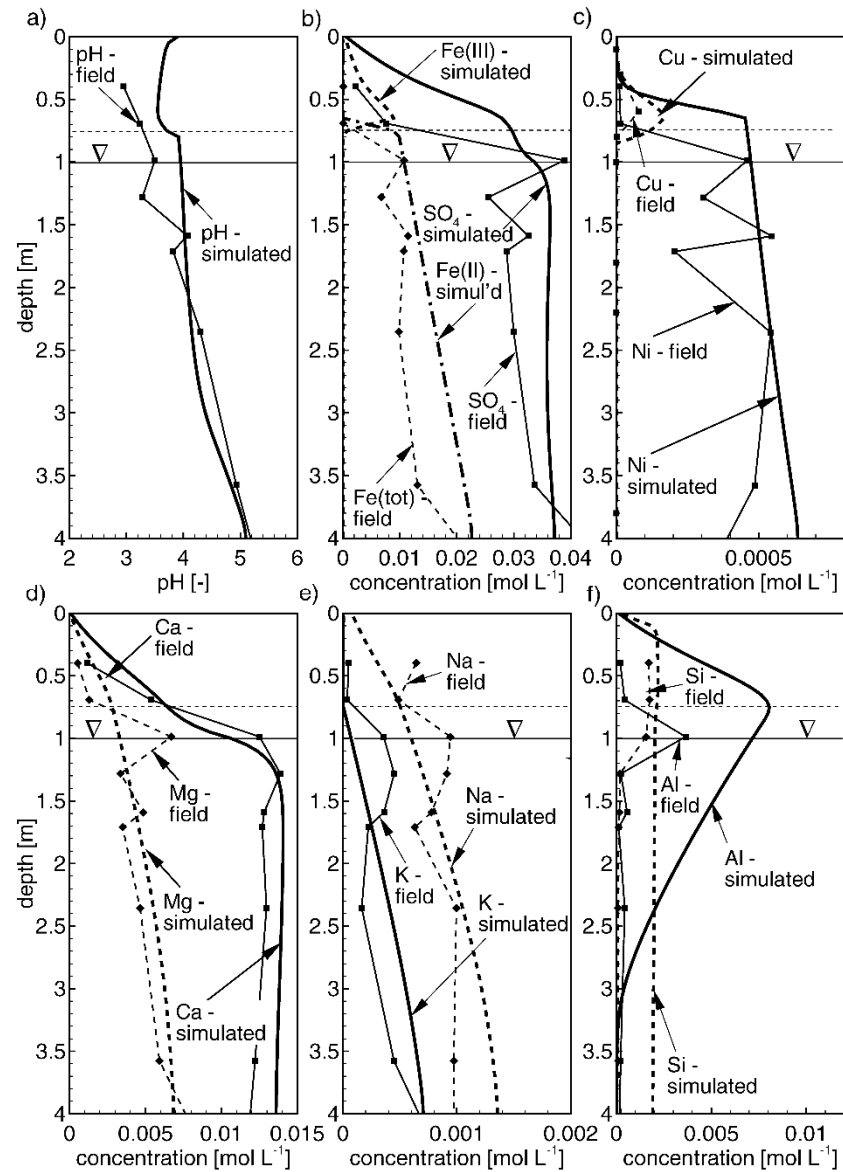


Conceptual Model

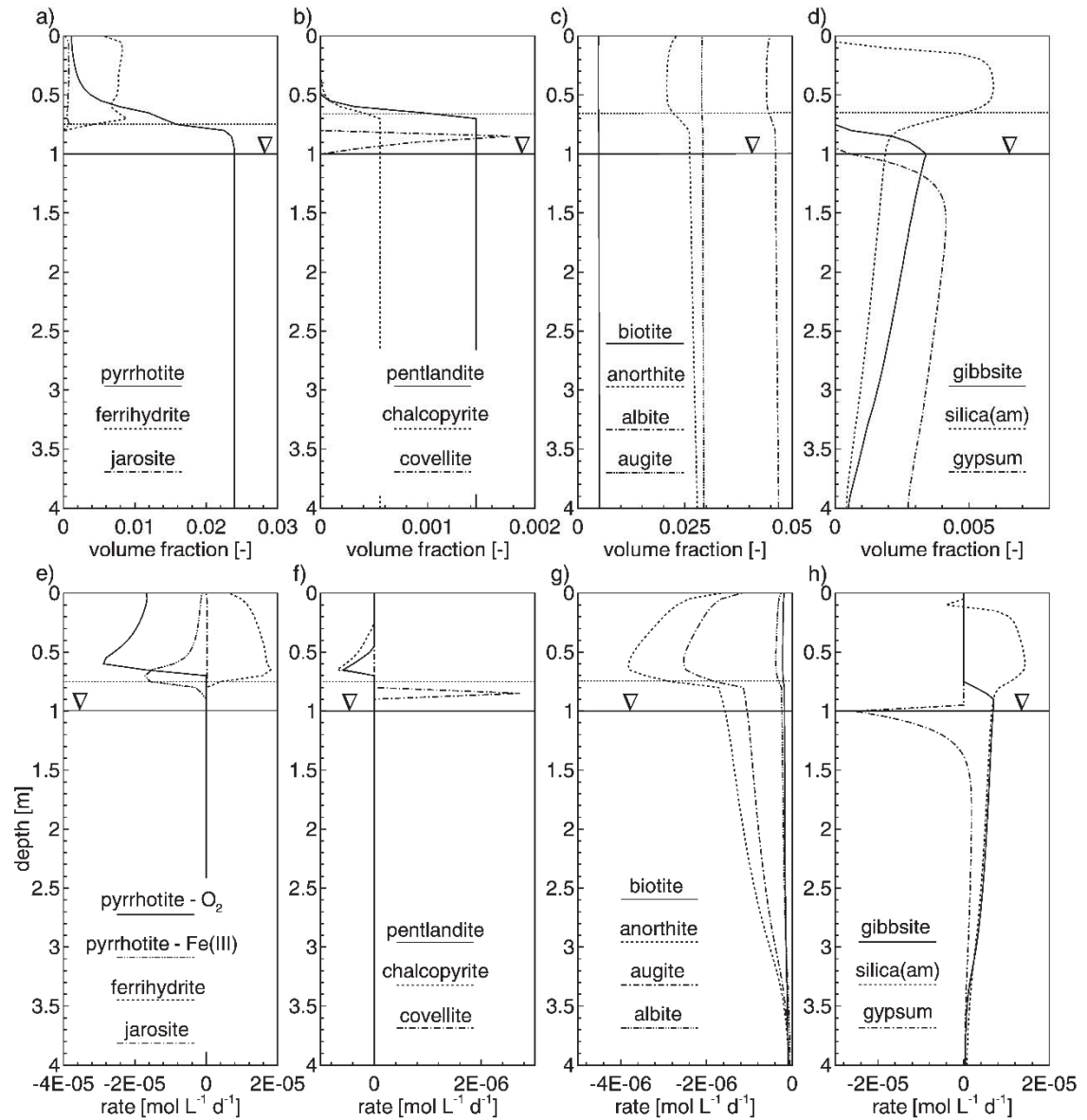


- | Mineral | |
|---------|--------------------------|
| (1a) | pyrrhotite ^a |
| (1b) | |
| (2) | chalcocrite |
| (3) | pentlandite ^e |
| (4) | calcite |
| (5) | anorthite |
| (6) | albite |
| (7) | biotite ^e |
| (8) | augite ^e |
| | |
| (9) | siderite |
| (10) | gibbsite |
| (11) | ferrihydrate |
| (12) | jarosite |
| (13) | gypsum |
| (14) | silica(am) |
| (15) | covellite |

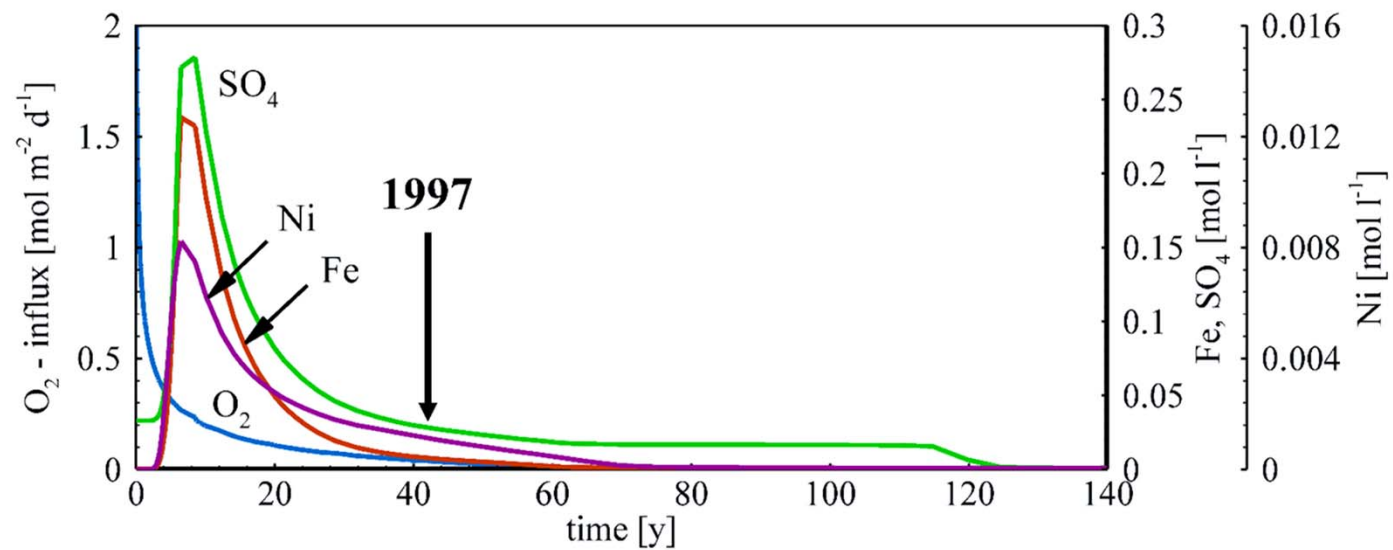
Aqueous concentration profiles



Mineral fractions



Potential for long term AMD generation?



Mayer et al., WRR, 2002

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Conclusions

- Detailed site characterization is **inescapable!**
 - A system simply cannot be predicted or modeled without understanding its internal processes!
- **Quality and quantity** of data will eventually determine the quality of predictions!
 - More budget and efforts should be dedicated to the quality data collection
- Predictive analyses should be performed already in the planning phase of a mine
- Theoretical rigor is mandatory in a prediction effort!

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Conclusions

time and costs. Many lawsuits and other legal proceedings involving hazardous waste can be simply avoided by collecting more and better field data. Some parties complain that collecting field data takes time and is expensive, but it is trivial compared to the costs and the length of legal proceedings.

(Nordstrom, 2012, App. Geochem.)

Thank you for your attention!

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