Prediction Models for Acid Mine Drainage

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Possible Prediction Objectives

- identification of soluble and mobile metals
- maximum metal concentrations
- maximum metal loadings
- comparison of decommissioning options
- duration of dissolved metal production
- concentration and loading vs time

Outline

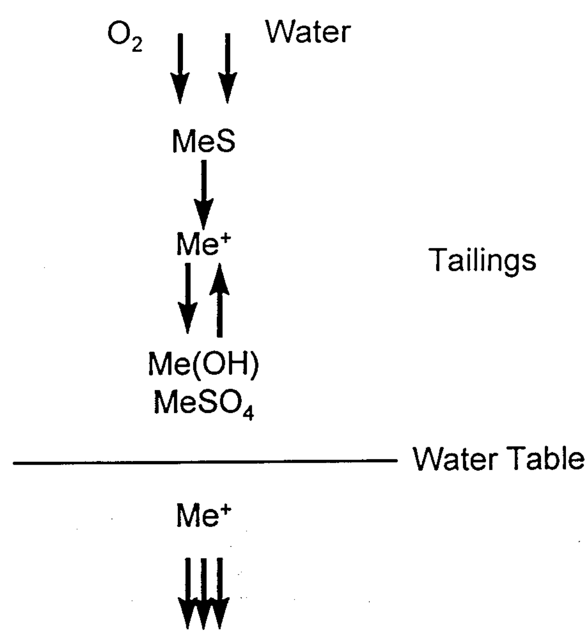
- Review of Physical and Chemical Systems
- Computer Models for AMD Prediction
  - Definitions
  - Classification
  - Applicability

Review of Physical and Chemical Systems

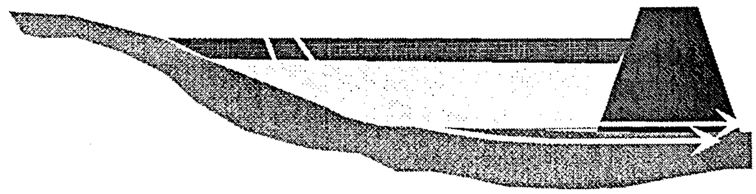
Acid-Base Balance

- Acid Potential (AP) %S
- Neutralization Potential (NP)

Acidity +	Carbonate Minerals	→	Metal Carbonates
Dissolved Minerals	Al-Si Minerals		Metal sulphates
			Metal hydroxides
			Dissolved ions

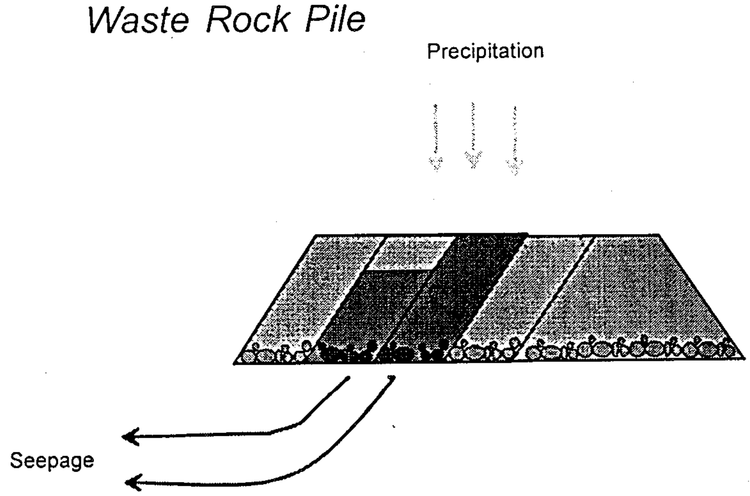


Flow System

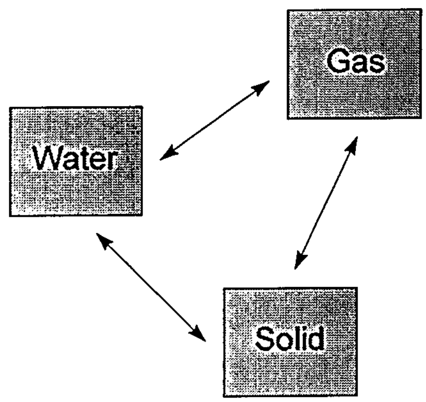


- define boundary conditions
- solve for hydraulic potentials
- calibrate to field data
- calculate velocities and discharges

Waste Rock Pile



Mass Transfer



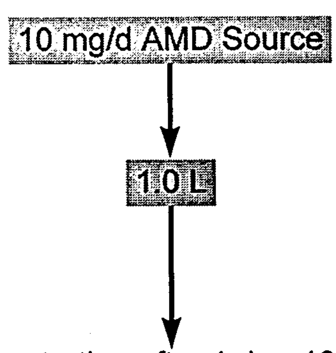
Geochemical Reactions in Mine Waste

PROCESS	*MASS TRANSFER EFFECT*
Oxidation of sulphides	H^+ and Me release
Precipitation of hydroxides	H^+ release and Me consumption
Dissolution and precipitation of sulphates	Me, H^+ release and consumption
Dissolution of hydroxides, carbonates, silicates	H^+ consumption
Co-precipitation	Me consumption

Geochemical Control
on contaminant release:

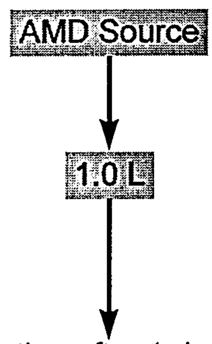
kinetic vs equilibrium

- kinetic control



Concentration after 1 d = 10 mg/L
after 2 d = 20 mg/L

- equilibrium control



Concentration after 1 d = 10 mg/L
after 2 d = 10 mg/L

Geochemical Reactions - Governing Principles

- Thermodynamics (Equilibrium)
  - determination of whether a reaction has sufficient energy to proceed
  - calculation of "effective" concentrations - activities
  - use of experimentally-determined thermodynamic constants

Geochemical Reactions - Governing Principles

- Kinetics
  - determination of reaction rates
  - use of experimentally-determined kinetic rate equations and constants

Geochemical Processes

Mass-transfer processes	Rate-controlling processes	Rate-modifying factors
DISSOLUTION / PRECIPITATION by: acid-base reactions hydrolysis redox reactions co-precipitation gas release/capture Wetting-drying ION EXCHANGE / SORPTION RADIOACTIVE DECAY	DIFFUSION - macroscopic - microscopic - atomic-scale NUCLEATION SURFACE REACTION ADSORPTION/ DESORPTION	CATALYSIS bacterial galvanic abiotic TEMPERATURE PRESSURE SURFACE AREA

Models for AMD Prediction

Definitions

- Model: a theoretical or physical construct that simulates a system

- Geochemical model: ...for geochemical systems

- Computer model: computer program incorporating theoretical or physical construct

Classification of Geochemical Models

- Equilibrium thermodynamic models
- Mass transfer models
- Coupled mass transfer-flow models
- Empirical and engineering models

Equilibrium thermodynamic models

- Solve the equilibrium distribution of mass among various solid or dissolved species and complexes
- Results reported as saturation indexes (SI) for minerals
- examples: MINTEQ, PHREEQE

Mass transfer models

- Simulate the kinetic evolution of solution chemistry as the system progresses towards equilibrium
- Results give aqueous concentrations and solid masses vs time
- examples: EQ6, PATHARC

Coupled mass transfer-flow models

- Simulate the evolution of solution chemistry in open fluid-rock systems
- Consider flow and solute transport
- examples: MINTRAN, PHREEQM

Empirical and Engineering models

- Simulate solution chemistry by using simplifying assumptions
- Focus on comparison of containment conditions
- examples: WATAIL, ACIDROCK

Data Requirements

MODEL	CLASS ---->	EQUIL.	M.T.	M.T./FLOW	EMP/ENG
Input	Parameters				
Field	Water Chem.	+++	++	++	+
Data	Mineralogy	+	+++	++	+
	Surface Area	0	+++	+++	+
	Temperature	+	+	+	+
	Oxygen	+	++	++	++
	Water Balance	0	+	++	++
	Pile Structure	0	0	0	++
Lab Data	Column Test	0	0	0	+
	Humidity Cell	0	0	0	+
Database	Thermodynamic	+++	+++	+++	++
	Kinetic	0	+++	+++	+

Model Applicability vs Prediction Objectives

Model	Class ---->	Equil.	M.T.	MT/Flow	Emp/Eng
Prediction Objective	I.D. Species	+++	++	+	0
	Max. Conc.	+	++	+	0
	Max. Loads	+	++	++	+
	Duration	0	++	+++	++
	Conc. - Time	0	+	++	+
	Decomm. Option	0	0	++	+++

Relative applicability of models
0 = none or not used
+ = the least
++ = intermediate
+++ = the most

Summary

- Physical, geochemical systems described
- Incorporation in computer models
- Computer model classification - levels
- Data requirements
- Applicability vs prediction objectives

Summary (cont'd)

1) Identify objectives
2) Characterize processes
3) Select model
4) Interpret results

Recommendations (1)

- Field dataset collection
- Better determination of reaction mechanisms
- Collect thermodynamic equilibrium constants
- Develop kinetic rate equations

Recommendations (2)

- Do not expect existing geochemical models to accurately predict water chemistry with time
- Encourage the application of mass transfer models to well-defined systems
- Use empirical models

Recommendations (3)

- Coordinate model development to follow developments in the understanding of geochemical and physical processes