3.2. OPERATIONAL USE OF MATHEMATICAL MODELLING

Doug Chambers
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Operational Use of Mathematical Modelling

Prediction of Acid Mine Drainage

Douglas B. Chambers
Carol M. Pettit

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Outline

- Site Assessment and Data Review
- Data Collection, Sampling, Testwork
- Model Selection or Model Development
- Model Application
- Interpretation

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Site Assessment and Data Review

- Site Visit, Photographs
- Site Plans, maps, ...etc.
- Monitoring Data (exploration, development and operation)
- Laboratory Analyses, Testwork, Field Studies
- Mine Plan (development, operation, decomissioning)

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Data Collection, Sampling and Testwork

- Design Site-Specific Program
- Select Protocols for Sampling and Testwork
- Apply Reference Handbooks such as:
  - Waste rock sampling manual (MEND 4.5.1)
  - Environmental monitoring handbook (MEND)

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Why Model Tailings and Waste Rock Heaps ?

- To Examine Current State Of Acid Generation
- To Predict Future Contaminant Loads and Concentration Profiles
- To Assess Future Treatment Requirements
- To Compare Management and Decommissioning Options

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Mathematical Approach

- Empirical or Statistically-Based
  - Site water-quality database
  - Laboratory testwork
- Mechanistic or Based on Theoretical Equations
  - Kinetics of sulphide oxidation
  - Oxygen transport
  - Thermodynamic equilibrium
  - Mass transport

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Data Requirements for Geochemical Modelling (1)

- Climatic:
  - Monthly mean surface temperature
  - Monthly precipitation / evaporation/ evapotranspiration
- Physical:
  - Surface area, depth
  - Bulk density, porosity / void volume
  - Moisture content / saturation level (% void volume)
  - Particle size distribution

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Data Requirements for Geochemical Modelling (2)

- Hydrogeological:
  - Hydraulic conductivity (vertical & horizontal)
  - Infiltration flow
  - Seepage flow
- Water Quality:
  - Infiltration waters
  - Background water quality (surface, groundwater)
  - Porewater quality (with depth)
  - Seepage Quality

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Data Requirements for Geochemical Modelling (3)

- Mineralogical:
  - Mineralogical composition
  - Estimate of percent leachable pyrite (sulphide minerals)
  - Chemical and elemental analyses of solids
  - Chemical formulae of minerals
  - Proportion pre-oxidized (easily soluble) metals and radionuclides

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Data Requirements for Geochemical Modelling (4)

- Kinetic:
  - Biological and chemical oxidation rates for sulphide minerals
  - Weathering rates for silicates and carbonates
- Miscellaneous Data:
  - Description of historic as well as current activities
  - Visual observations reported during field visits

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Data Requirements for Geochemical Modelling (5)

- Transport Related Properties:
  - Diffusion coefficients
  - Convective air flow
  - Thermal conductivity
  - Temperature measurements with depth
  - Solid-liquid distribution coefficients (K_D) for metals and radionuclides

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Some Of The Major Uncertainties (1)

- Mineralogy:
  - Sulphide minerals (% fines)
  - Buffering minerals (carbonates and alumino silicates)
  - Secondary minerals (stored acidity, sorption)
- Proportion of Easily Leachable (pre-oxidized) Metals and Radionuclides

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Some Of The Major Uncertainties (2)

- Flows and Quality (infiltration, porewater, seepage)
- Porosity and Moisture Content
- Oxygen Transport (convection, diffusion)

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How to Deal with Uncertainty ?

- Perform Deterministic Sensitivity Analyses to Examine Influence of Particular Parameters or Assumptions
- Employ Distributed (probabilistic) Parameter Values
- Perform Preliminary Investigative Modelling (eg. empirical or physical modelling followed by geochemical)

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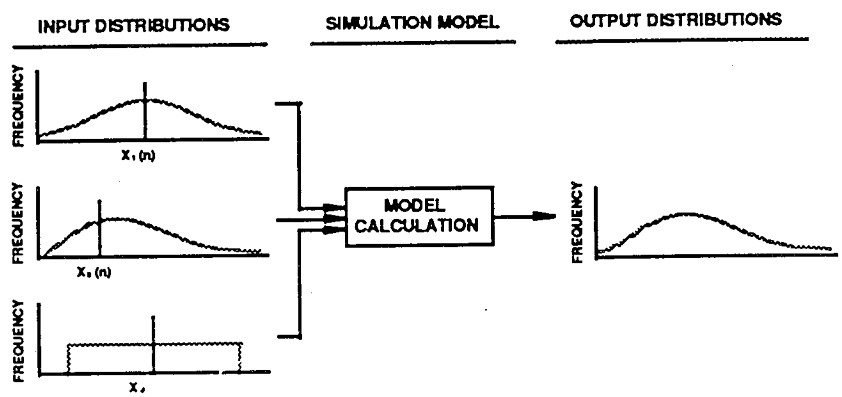
Concept of Probabilistic Analysis



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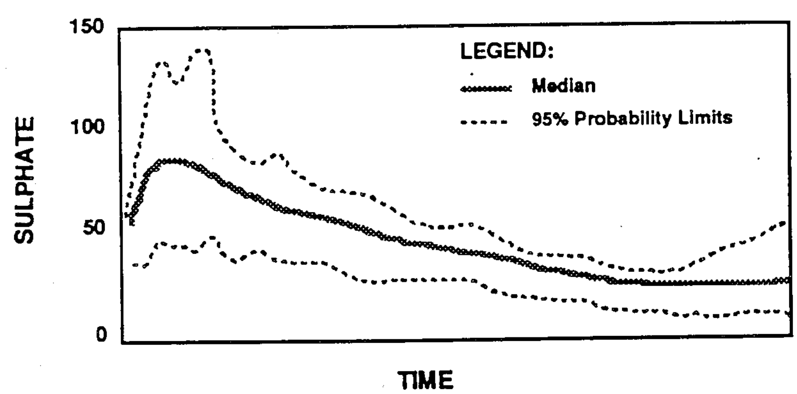
Defining Uncertainties



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Empirical Prediction (1)

- Examine Water Chemistry Database
  - Adequate data
  - Detection limits
  - Remove outliers
- Compile Summary Statistics (aqueous, solids)
- Uni or Bivariate Techniques
  - Time plots
  - Correlation analyses
  - Regression analyses

Empirical Prediction (2)

- Multivariate Techniques
  - Principle component analyses
  - Cluster, factor, discriminant, etc.
- Assess Cyclical or Repeating Trends
  - Time series modelling
- Develop a Model
  - Cross-validation
  - Assess confidence or reliability

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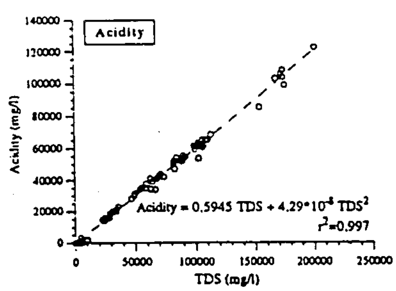
Parameters and Elements Correlation Matrix for Aqueous Species

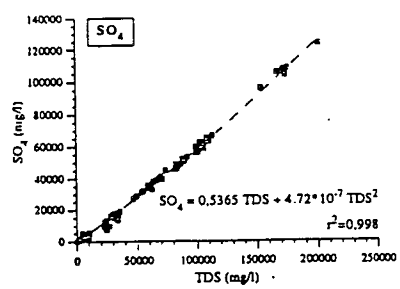
	Fe_{tot}	Acidity	TDS	SO_4	Conduc	pH	Ca	Al	SG*	Mg	Fe^{2+}	Fe^{3+}	E_H
Fe_{tot}	1												
Acidity	.971	1											
TDS	.978	.997	1										
SO_4	.973	.994	.998	1									
Conduct	.951	.958	.964	.959	1								
pH	-.409	-.402	-.377	-.354	-.380	1							
Ca	.734	.700	.723	.725	.804	-.257	1						
Al	.923	.979	.977	.977	.929	-.328	.665	1					
SG*	.971	.988	.998	.997	.949	-.855	.956	.977	1				
Mg	.931	.964	.970	.973	.937	-.233	.697	.965	.991	1			
Fe^{2+}	.800	.799	.819	.828	.819	-.029	.655	.822	.636	.876	1		
Fe^{3+}	.683	.636	.624	.604	.579	-.642	.419	.530	.936	.476	.108	1	
E_H	-.182	-.191	-.220	-.227	-.266	-.546	-.402	-.239	-.578	-.324	-.440	-.235	1
log(Fe2/Fe3)	.345	.353	.382	.392	.437	.429	.553	.404	.637	.477	.465	-.213	-.917

*Specific Gravity: only 15/93 samples.

MEND Report 1.14.2, Monitoring of Acid Mine Drainage: Chemical Data from Mine Doyon South Waste Rock Dump (GREGI 93-04, Université Laval)

Relationships Between TDS and Major Elements (TDS >25,000 mg/L)

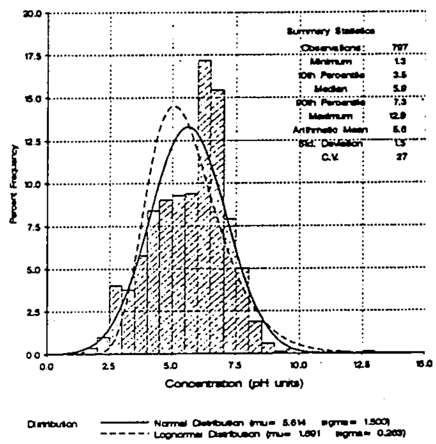




Note:
Used to reduce sampling frequency (costs)

MEND Report 1.14.2, Monitoring of Acid Mine Drainage: Chemical Data from Mine Doyon South Waste Rock Dump (GREGI 93-04, Université Laval)

Absetzerhalde
Paste pH



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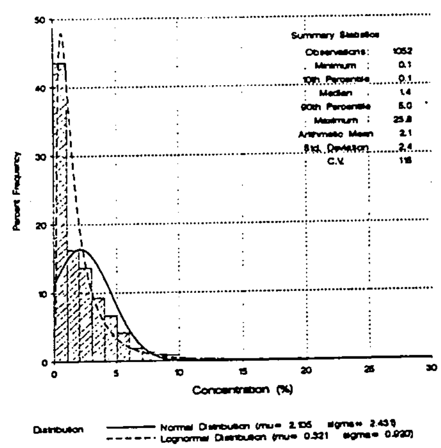
Absetzerhalde
Percent CO_2



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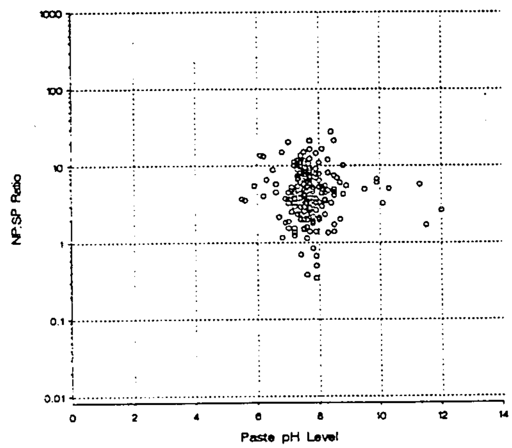
Drosen
NP / SP Ratio vs. Paste pH



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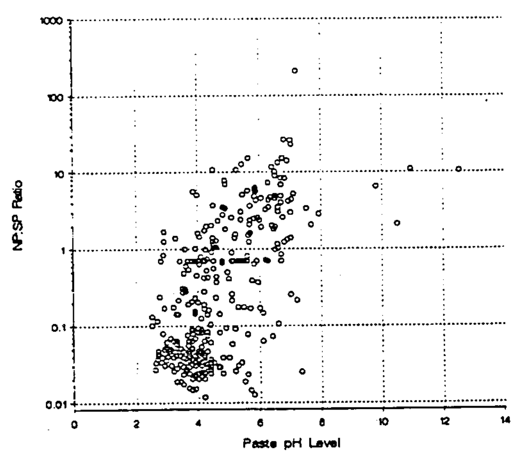
Nordhalde
NP / SP Ratio vs. Paste pH



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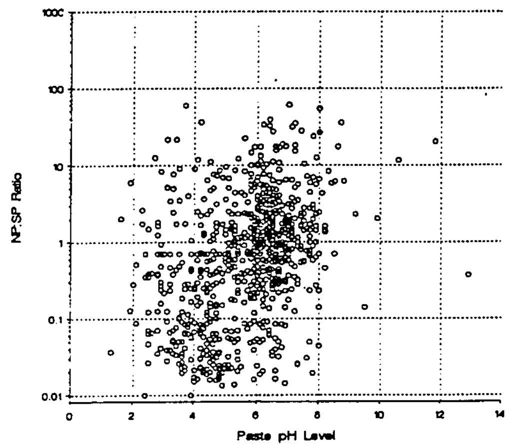
Absetzerhalde
NP / SP Ratio vs. Paste pH



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Cross Tabulation of NP:SP vs. NNP (Absetzerhalde)

Frequency Row Percent Column Percent	NNP Subset			
NP:SP Subset	NNP < -20 (Acid Generating)	-20 ≤ NNP < 20 (Uncertain)	NNP ≥ 20 (Non-acid Generating)	Total
NP:SP < 1 (Acid Generating)	434 68.24 100.00	202 31.76 88.99	0 0.00 0.00	636
1 ≤ NP:SP < 3 (Uncertain)	0 0.00 0.00	25 10.00 11.01	225 90.00 57.54	250
NP:SP ≥ 3 (Non-acid Generating)	0 0.00 0.00	0 0.00 0.00	166 100.00 42.46	166
Total	434	227	391	1052

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Empirical Prediction of Future Water Quality, SENES

- Analyse Results Obtained from Kinetic Testwork (e.g. humidity cell, columns)
- Develop an Empirical Expression Relating Constituent Concentration to Porewater Replacement Volume
- Apply this Expression Within a Mechanistic Framework (e.g. flow and mass transfer model)
- Perform an Environmental Pathways Assessment

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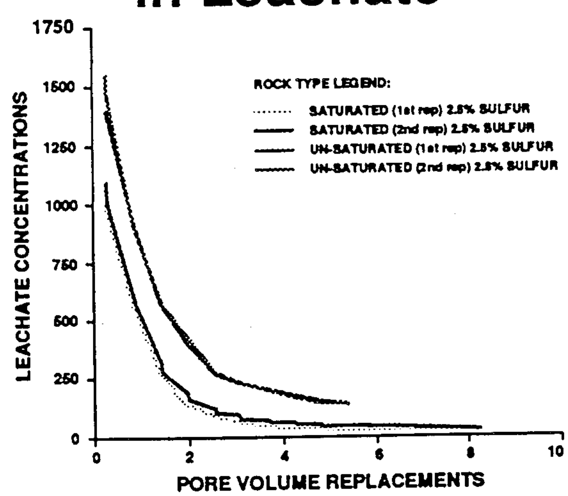
Sulfate Concentrations (mg/L) in Leachate



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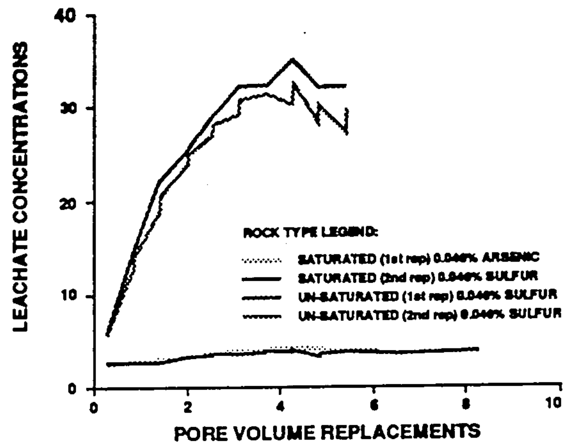
Arsenic Concentrations (mg/L) in Leachate



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Empirical Prediction

- Preliminary or "Order of Magnitude" Estimates of Annual Acid Generation Based on One Primary Factor:
  - Oxygen transport (diffusion)
  - Infiltration flow
  - Example → Equity Silver

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Estimates of Peak ARD Rates (t/a) for Main Dump and Bessemer Dump

	PEAK MEASURED (1990)	OXYGEN DIFFUSION	INFILTRATION	TECHNICAL COMMITTEE	MODEL RESULTS
No Cover	-	30,000	16,500	-	-
Loose Till Cover (1.4m)	8,900	12,500	11,000	17,100	7,800
Non-Compacted Clay (0.7m)	-	14,575	6,125	-	*
Semi-Compacted Clay (0.7m)	-	7,600	3,750	12,100	*
Compacted Clay (0.7m)	-	430	280	-	*

NOTE:
Peak Occurs Before Placement of Cover *

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Important Processes in Geochemical Modelling (1)

- Acid Generation Due to Biological and Chemical Oxidation of Sulphide Minerals
- Diffusion of Oxygen into Heaps and Tailings, and also into Tailings Rock Particles
- Convective Transport of Oxygen into Waste Rock Heaps

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Important Processes in Geochemical Modelling (2)

- Production and Transport of Heat (conduction and advection)
- Temperature With Depth and Effect of Temperature on Oxidation Rates
- Release (Leaching) of Metals and Radionuclides

Important Processes in Geochemical Modelling (3)

- Transport of Dissolved Chemical Species (eg. sulphate, aluminium, calcium, magnesium, iron, metals, radionuclides)
- Dissolution of Solid Buffering Minerals (eg. calcite, dolomite, sericite)
- Formation (precipitation) of Secondary Minerals (eg .ferric hydroxide, jarosite)

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Important Processes in Geochemical Modelling (4)

- Solubility of Solid Phases (eg. precipitates, minerals)
- Speciation of Dissolved Constituents
- Estimation of the pH

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Order of Selection for Buffering Minerals

pH	Minerals
> 6.2	Calcite
> 5.4	Siderite
> 4.8	Aluminium Hydroxide
	Magnesium Oxide
> 3.1	Ferric Hydroxide
< 3.1	None or Jarosite

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Important Processes in Geochemical Modelling (5)

- Solids Solution Equilibria for Metals and Radionuclides
- Adsorption of Metals and Radionuclides onto Aluminium and Ferric Hydroxides, Jarosite and Organic (Carbon) Surface
- Co-precipitation (e.g.. radium with gypsum, lead-210 with lead sulphate, lead carbonate ... etc.)

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General Approach to Mathematical Predictions (1)

- Identify Objectives
- Collect and Review Site Data
- Select, Adapt or Develop Model(s)
- Prepare Model Inputs and Parameter Estimates
- Calibrate Model to Field Data

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General Approach to Mathematical Predictions (2)

- Perform Simulations
- Interpret the Results
  - Identify controlling processes
  - Compare to concentrations at other sites
  - Compare to estimates obtained using alternate approach

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Overview of Models (1)

Types of Models	Typical Examples	SENES Models	Applications of SENES Models
Thermodynamic Equilibrium Models	MINTEQ PHREEQE	PHCALC GOLDTAIL	- water quality analyses / addition of alkaline amendments - treatment ponds
Mass Transfer Models	EQ6 PATHARC		- see below
Coupled Mass Transfer Models	MINTRAN PHREEQM	PITMOD UTAP	- mine wastes placed in flooded pits - source term module within environmental pathways models
		Site-specific empirical models	- kinetric experiments (eg columns, humidity cells)

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Overview of Models (2)

Types of Models	Typical Examples	SENES Models	Applications of SENES Models
Support or Physical Models (eg air/heat transport)	FIDHELM TOUGH AMD	CONVECT MINEVENT ROCKPIT	- waste rock heaps - underground mines - backfilled pit mines
Engineering Models	Q-ROCK MINEWALL WATAIL MINTOX RATAP	ACIDROCK ROCKSTAR URANTAIL	- Equity Silver heaps, Gessenhalde in-situ heap leach, coal spoil piles - Ronneburg heaps, Ronneburg mining region - gold, nickel, zinc and uranium tailings sites

CONVECT and ROCKPIT (1)

- **Steady State Physical (computer) Models**
- **Transport of Oxygen and Heat**
- **Waste Rock or Tailings**
- **CONVECT**
  - **Pyramidal Coordinates**
- **ROCKPIT**
  - **Cylindrical Coordinates**

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CONVECT and ROCKPIT (2)

- Depth Profiles for Oxygen, Temperature and Pyrite
- Diffusion or Convection ?
- Estimates of Convective Airflow Rates

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URANTAIL

- Dynamic Geochemical (computer) Model
- Acid Generating or Alkaline Tailings
- Gold, Base Metal, Uranium Tailings
- Wet or Dry Closure Alternatives
- Flooded (pond) With/Without Overflow or Recycle
- Simple to Complex Engineered Covers
- Predictions of Long-Term Water Quality

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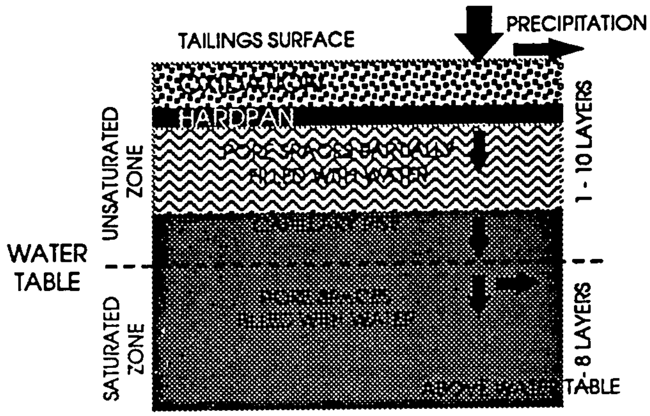
Concept for Modelling Tailings



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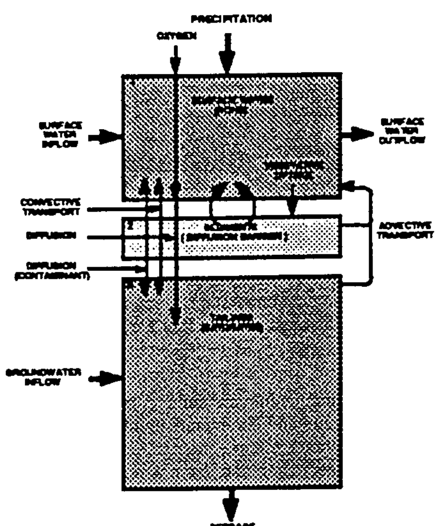
Concept for Modelling Submerged Tailings



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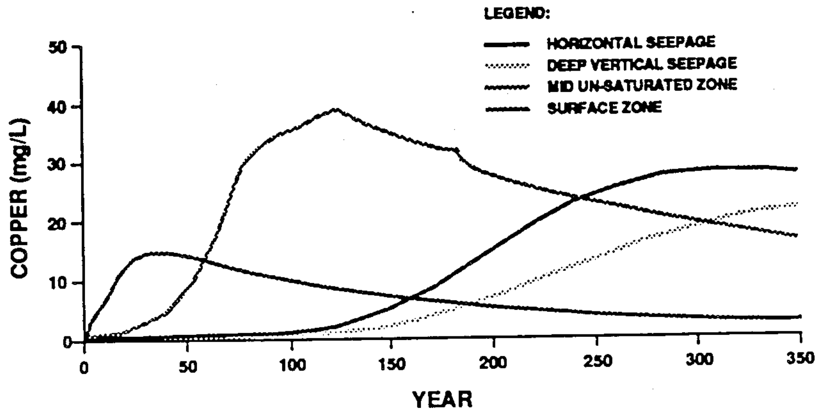
Simple Cover on Coarse (Gold) Tailings



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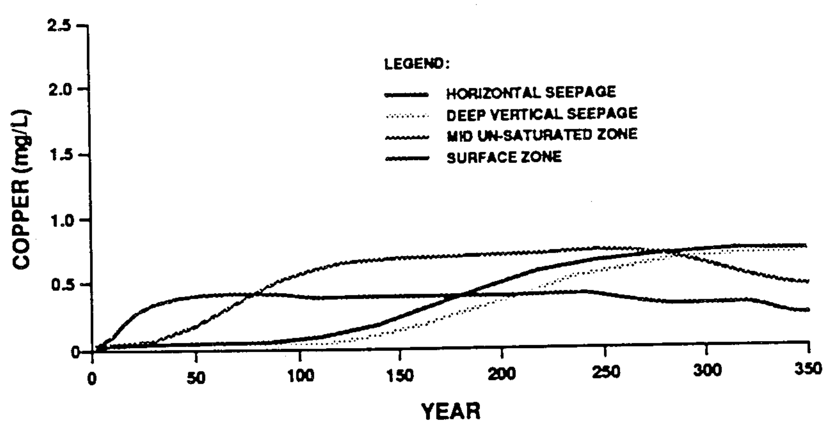
Engineered Cover on Coarse (Gold) Tailings



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ACIDROCK (1)

- Dynamic Geochemical (computer) Model
- Waste Rock Heap to Fines and Rock Particles
- Acid Generation and Neutralization Reactions

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ACIDROCK (2)

- Timed Events or Site - Specific Activities
  - Placement / removal of lifts
  - In-situ leaching
  - Recontouring, cover placement
- Equity Silver Waste Rock, In-Situ Uranium Leach Pile, Coal Refuse Piles

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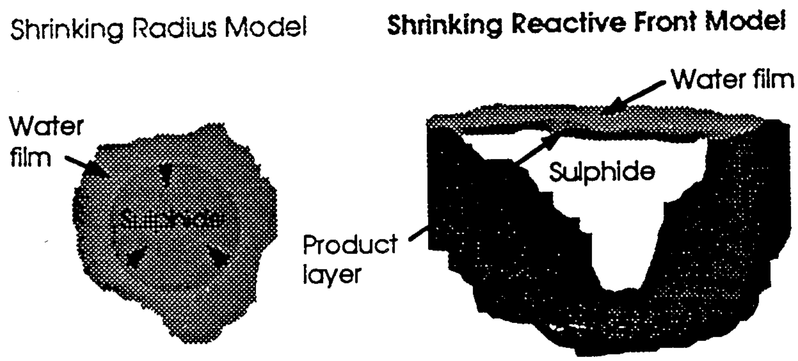
Mass Transport Processes



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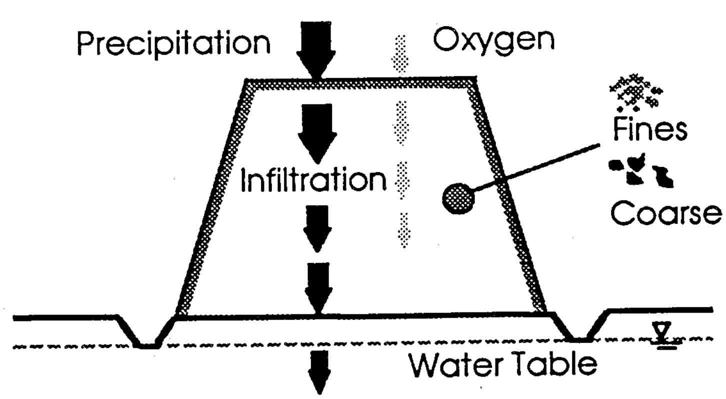
Concept for Modelling Waste Rock Heaps / Piles



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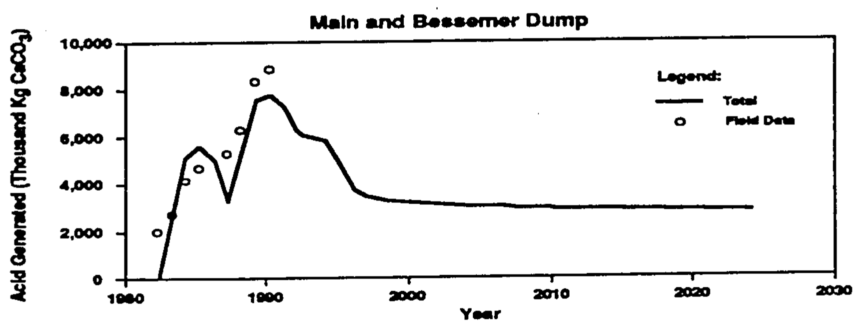
Equity Silver Waste Rock Heaps
Predicted Acid Generated



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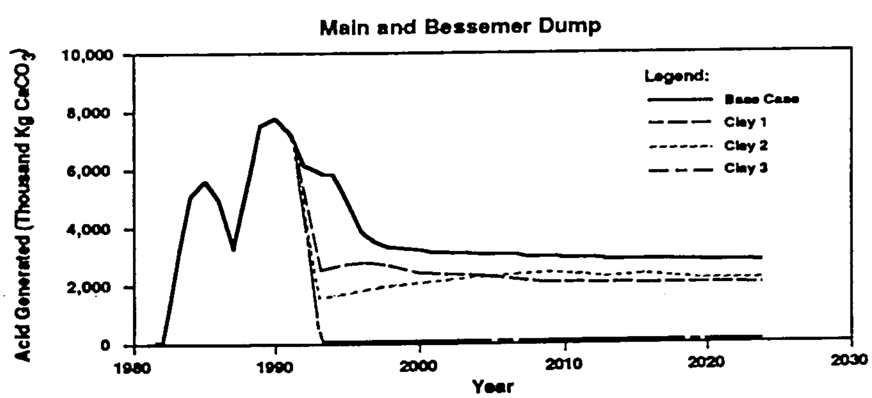
Equity Silver Waste Rock Heaps
Cover Effectiveness



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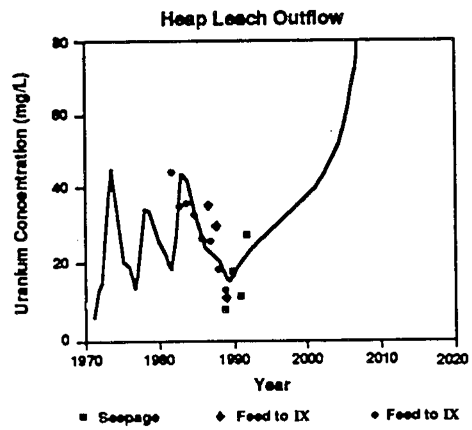
Gessenhalde Calibration: Predicted Uranium



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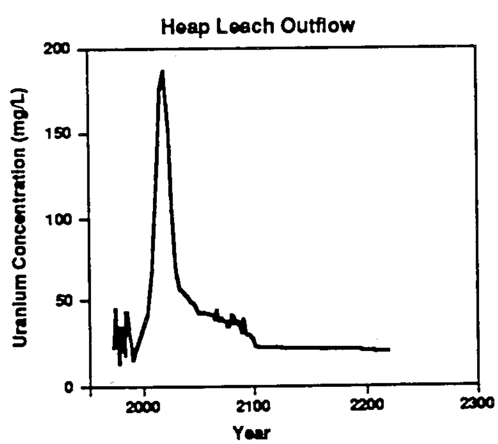
Gessenhalde Basecase Scenario: Predicted Uranium



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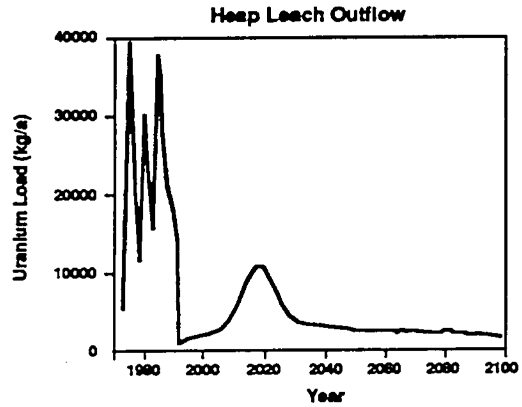
Gessenhalde Basecase Scenario: Predicted Uranium Load



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ROCKSTAR (1)

- Dynamic Geochemical (computer) Model
- Multi-Nodal Interconnected Compartments (20)
  - Waste rock piles, tailings, open pit, underground mines, surface water)
  - Each node has up to 20 layers
- Acid Generation / Neutralization and Release of Contaminants (aqueous species, metals, radionuclides)

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ROCKSTAR (2)

- Simultaneous simulation of 16 Waste Rock Heaps
- Detailed Simulation of Single Large Heap (10 nodes)
- Screening Simulation of Flooding of Mining Region (20 nodes)
- Detailed simulation of Flooding of Mining Region (60 nodes)

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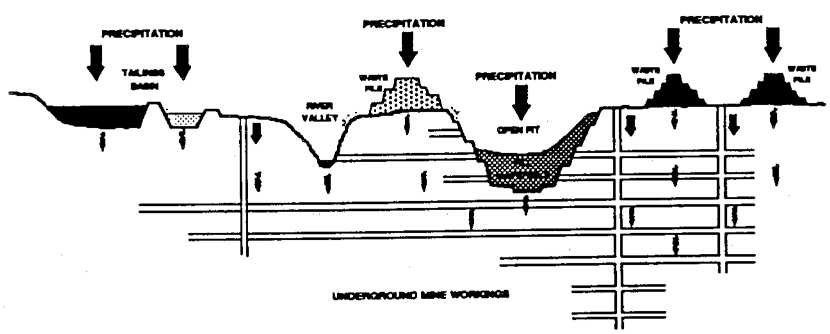
Schematic of Geochemical Modelling Compartments (Tailings Basins, Waste Piles, Mine, River ... etc.)



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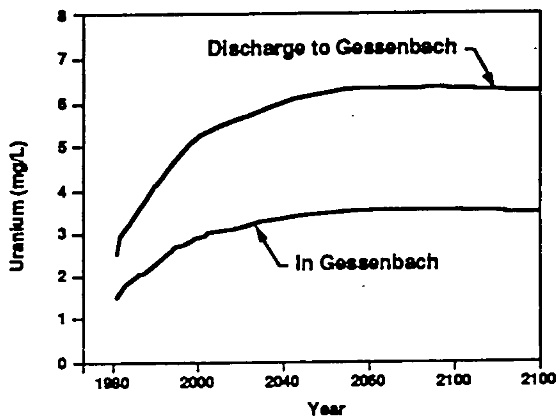
Gessenhalde Placed in Open Pit Predicted Uranium in River



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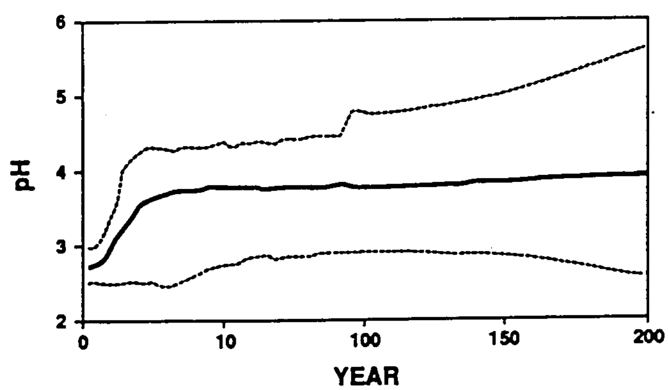
Probabilistic Results Large Waste Rock Pile (1)



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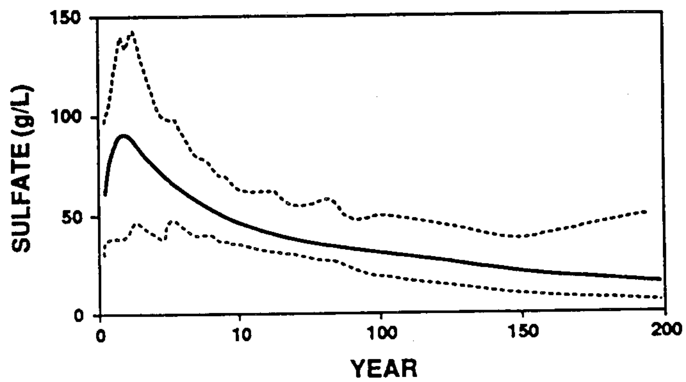
Probabilistic Results
Large Waste Rock Pile (2)



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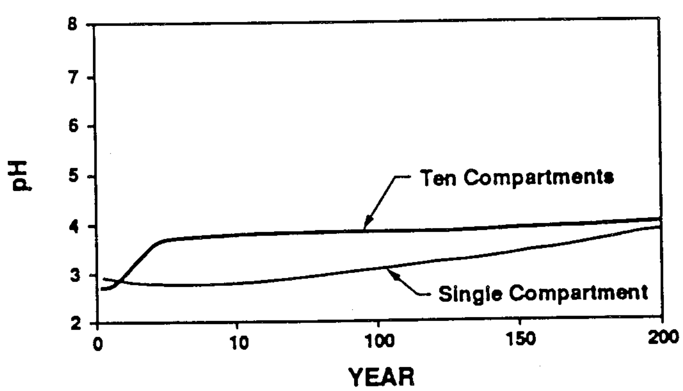
Simple Versus Detailed
Modelling of Heaps (1)



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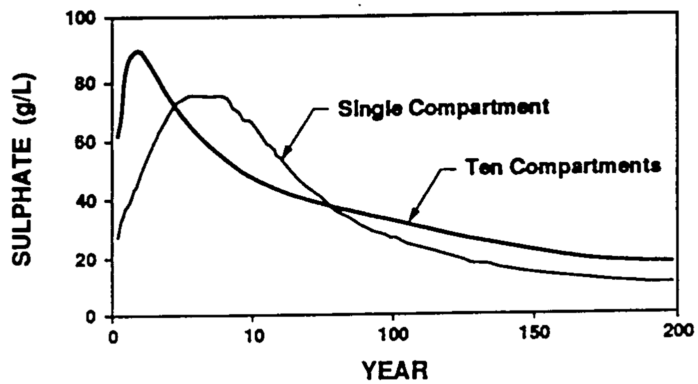
Simple Versus Detailed Modelling of Heaps (2)



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Conclusions (1)

- The Usefulness of Mathematical Prediction Models Has Been Demonstrated
  - Better understanding of mechanisms of AMD
  - Comparison of management options

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Conclusions (2)

- Areas for Improvement
  - Expansion of geochemical capabilities
  - Collection of mine site databases
  - Improved database of thermodynamic equilibrium constants, sorption coefficients, ...etc.
  - Consider kinetic rates for precipitation / dissolution, and surface-controlled reactions
  - Apply and develop empirical models

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Conclusions (3)

- Associated Assessments
  - Management options for mine water
  - Evaluation / comparison of treatment alternatives
  - Environmental pathways
  - Screening level and detailed risk assessments (human, ecological)
  - Monitoring program(s)
  - Decommissioning plan(s)

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3.3. REVIEW OF GEOCHEMICAL MODELS

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