Characterizing, Predicting and Modeling Water from Mine Sites

May 18-21, 2009
Sacramento, California

STRATUS CONSULTING

USGS science for a changing world

Kuipers & Associates, LLC

Water Boards Training Academy

Course Outline

- Day 1: Advanced acid generation, Mine site overview, Mine site characterization
- <u>Day 2: Modeling</u>
- Day 3: Site Tour of Jamestown Mine
- Day 4: Use of prediction information in mine permitting and case studies

Day 2: Muddling (Hobbit word for modeling)

May 19, 2009

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Day 2: Modeling Water at Mine Sites

- An overview of modeling to predict water quality and quantity at hardrock mine sites
- Conceptual models, codes, evaluation, and examples

Modeling Water Quantity and Quality at Mine Sites?

Why Model?

- Complex systems:
  - Surface runoff and infiltration, groundwater-surface water interactions, etc.
  - Geochemical precipitation and dissolution reactions, adsorption/desorption, redox reactions, etc.

- Models can:
  - Can be programmed to interface with large databases
  - Can provide new insights into complex problems
  - Can integrate and couple many different processes
  - Aid in site characterization
  - Aid in the evaluation of remedial alternatives
  - Aid in the prediction of remedial consequences

Models: Overview and Definitions

- **What is a model?**
  - a simplification of reality
  - "…a well-constrained logical proposition, not necessarily mathematical, that has necessary and testable consequences." (Greenwood, 1989)
  - "…a testable idea, hypothesis, theory, or combination of theories that provides new insight or interpretation of an existing problem (Nordstrom, 2004)".
  - "Every area of science uses models as intellectual devices for making natural processes easier to understand. The model that reliably predicts the outcome of real events, or that continues to fit new data, is essentially a kind of theory, a broad statement of how nature works." *Jay Lehr (1990) editorial in Ground Water*

Models: Overview and Definitions

- **What is NOT a model?**
  - a code; there is no such thing as the PHREEQC model, only the PHREEQC code
  - a representation of reality
  - "Models do not represent reality, they represent our thinking about reality" (Nordstrom, unpublished lectures, 1992)
  - "Mathematics and thermodynamics deal with models of reality, not reality itself" (Anderson and Crerar, 1993)

Models: Overview and Definitions

- **What is a hydrologic model?**
  - A theoretical construct, using physically based equations of motion, that permits the calculation of observable hydrologic properties
- **What is a chemical model?**
  - a theoretical construct, using principles of chemistry, that permits the calculation of chemical properties and processes
- **What is a geochemical model?**
  - A chemical model applied to a geologic system

"I find it the most difficult thing in the world to be a theorist and an honest man."
- A.S. Neill

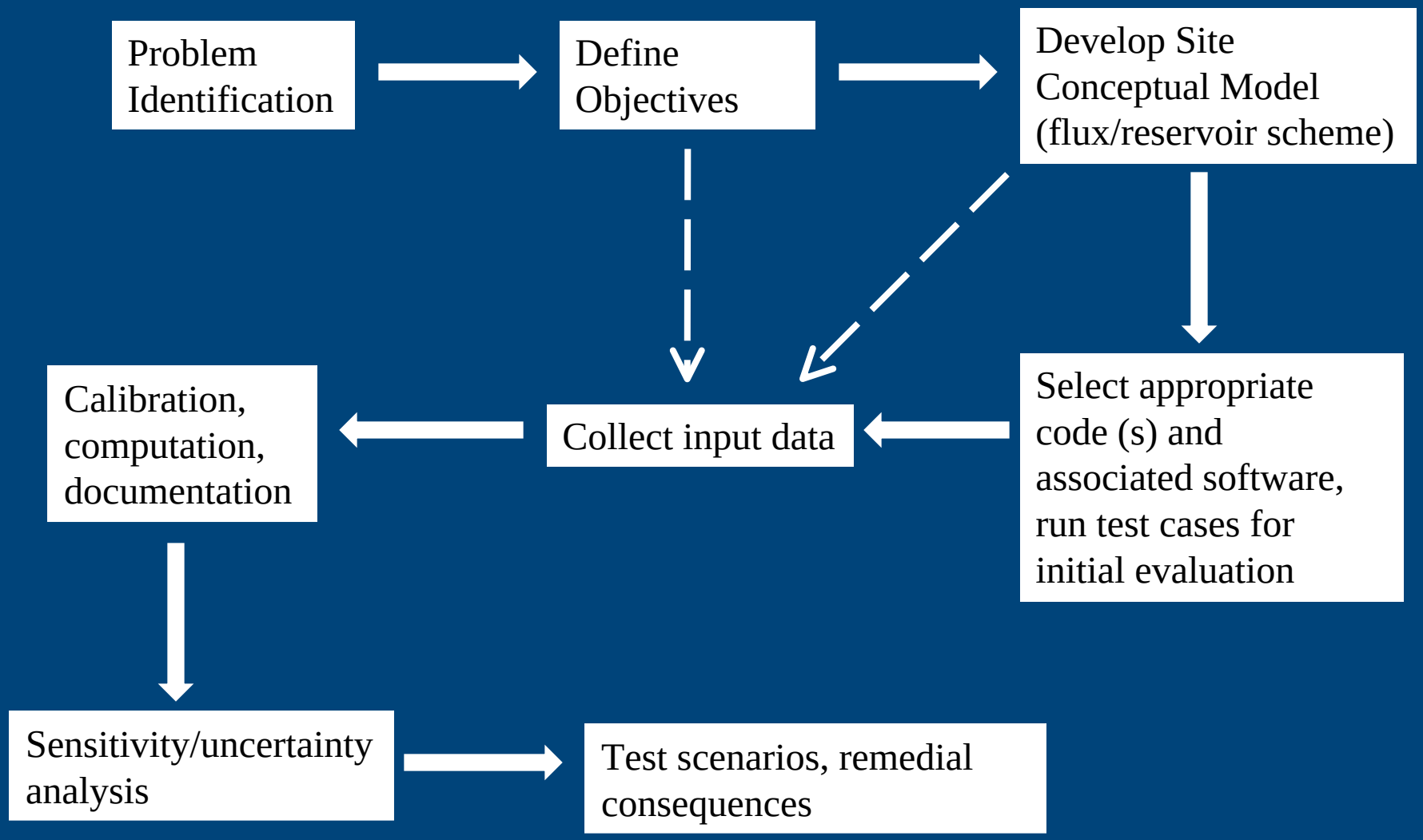
Models: Overview and Definitions

- **Mathematical models**
- **Numerical models**
- **Scale models or experimental models**
- **Analog models**

Overview of Models

- Garbage in = garbage out
  - Model is only as good as the inputs and assumptions
- Documentation is critical
  - A model without documentation is nearly useless
  - A proprietary code is also nearly useless for regulatory purposes

General Modeling Steps



Conceptual Models

What is a Conceptual Model?

- "The conceptual model is the basic idea, or construct, of how the system or process operates; it forms the basic idea for the model (or theory)." (Bredehoeft, 2005)
- …a qualitative description of the hydrology and geochemistry of the site
- Based on subjective judgment of the analyst
- Logic, analogs, scale models, numerical models, are all tools by which to test the adequacy of the prevailing concept
- Expect the conceptual model to be continuously updated as new information is acquired.

Correcting misconceptions about conceptual models

- "1. Modelers tend to regard their conceptual models as immutable.
- 2. Errors in prediction revolve around a poor choice of the conceptual model.
- 3. Data will fit more than one conceptual model equally well.
- 4. Good calibration of a model does not ensure a correct conceptual model.
- 5. Probabilisitic sampling of the parameter sets does not compensate for uncertainties in what are the appropriate conceptual models, or for wrong or incomplete models." (Bredehoeft, 2005)

Why is a Conceptual Model Necessary?

- It represents our understanding of the system under study
- It effectively communicates how we view the system
- Through its development, key factors relevant to the system are identified
- It facilitates appropriate selection of modeling codes and application of the codes

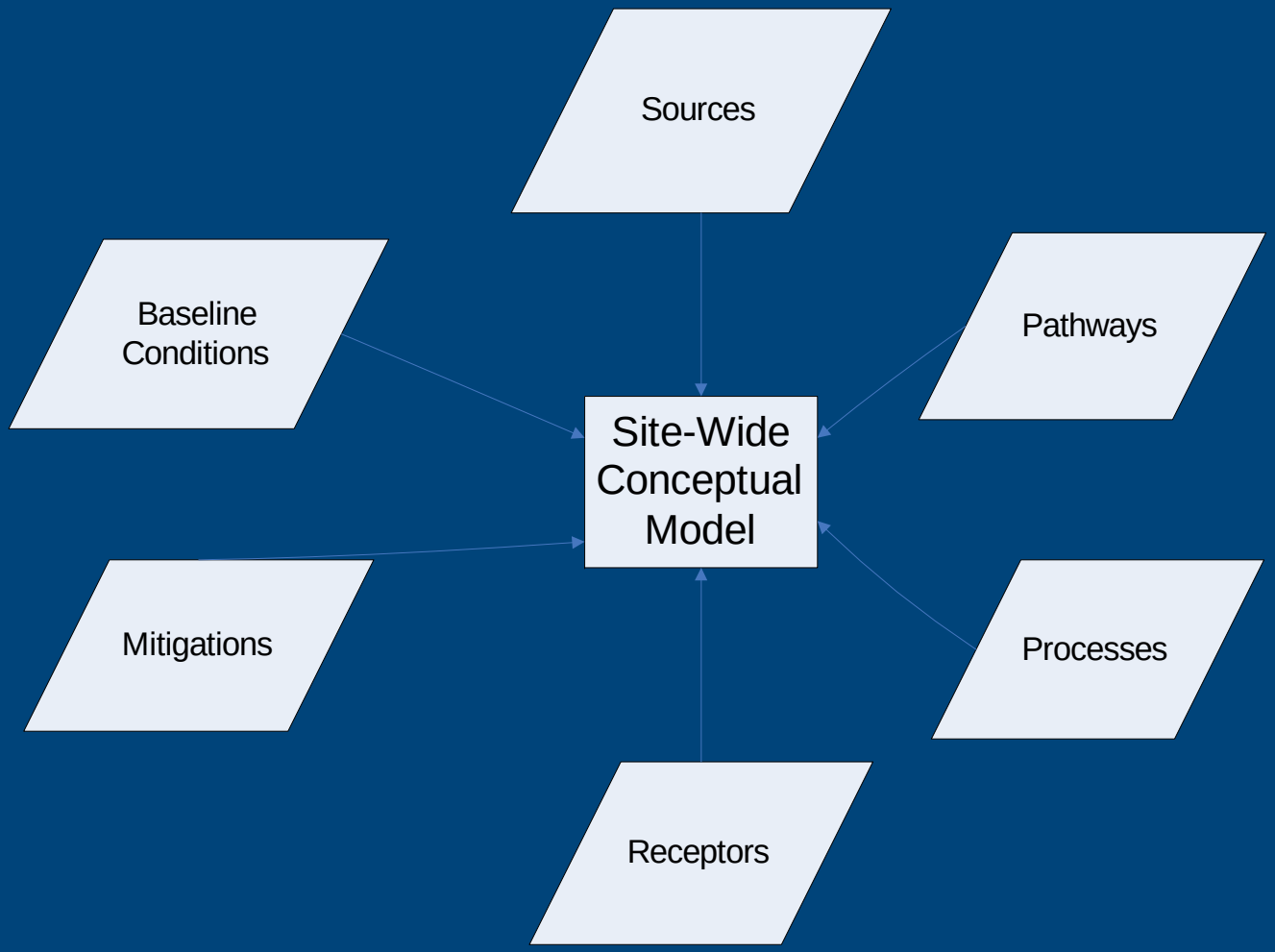
Development of a Conceptual Model

- Identify the problem/question
  - Will the waste dump be a source of acid and metals to the nearby creek?
  - What will be the rate of groundwater level rise after mining?
  - Will there be changes over time in flows or concentrations, and what will they be?
- Develop clear statement of objectives
- Characterize factors relevant to the system: sources, pathways, processes, etc.
- Define how these factors are inter-related, based on available data and assumptions

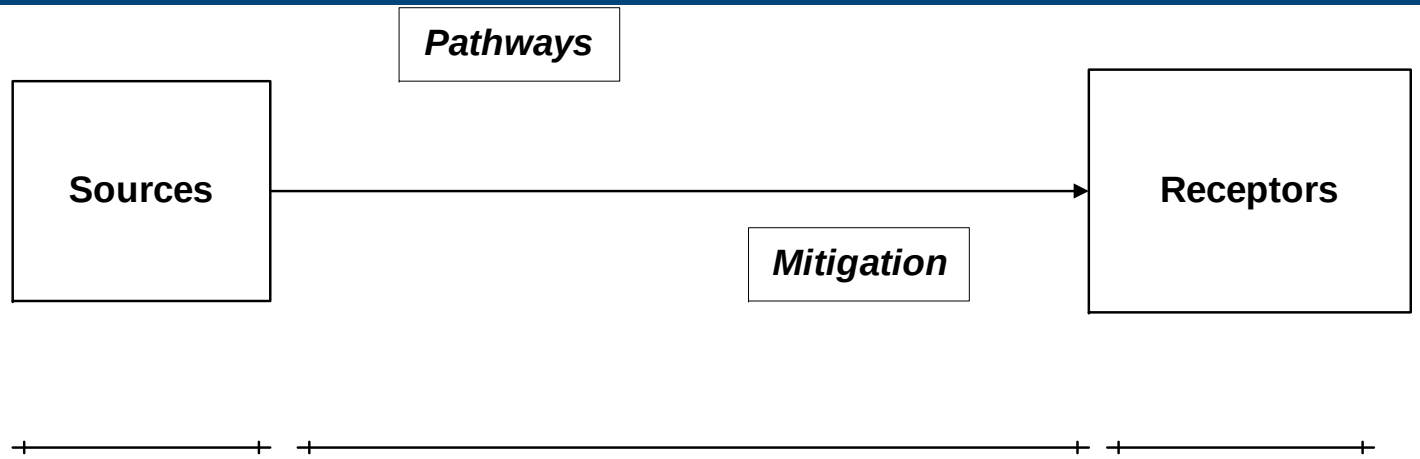
Conceptual Model Development

- Questions to ask:
  - What is the modeling objective?
  - What processes are we trying to represent in the model?
  - What variables should be quantified within the model?
  - Which of these variables are under the control of the modeler?
  - What relevant data are available?
  - How should the concept of time be treated?

General Elements of a Conceptual Model



Elements Specific to Hardrock Mining



Sources:
Tailings
Waste rock
Low-grade ore stockpiles
Heap and dump leach materials
Wall of pits or underground workings

Pathways:
Leaching from sources
Runoff
Infiltration through soil /vadose zone
Transport in groundwater
Discharge to surface water
Transport in surface water
Uptake by biota
Movement of mining process waters

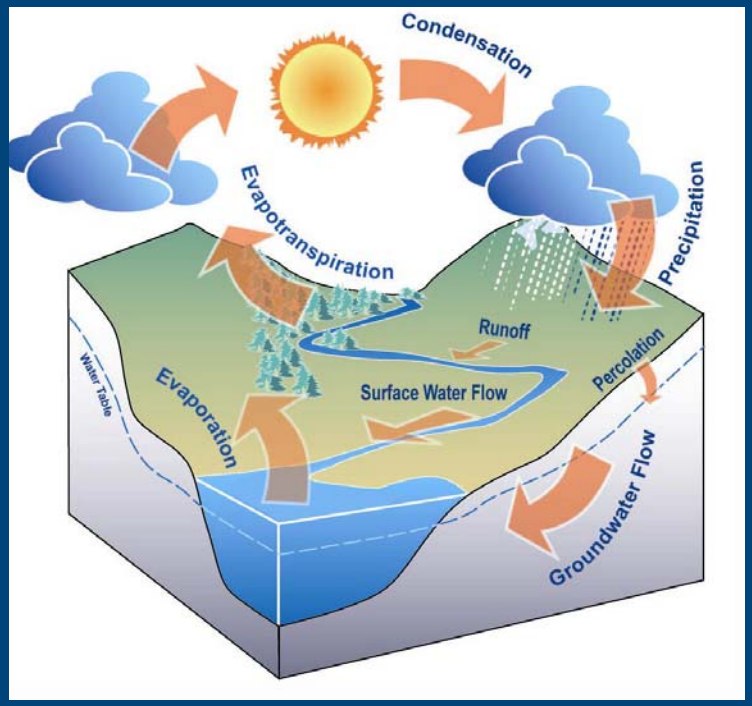
Receptors:
Groundwater
Surface water
Seeps
Pit lakes
Aquatic and terrestrial wildlife
Air
Vegetation
Humans

Mitigation Measures:
Mixing with lime or more benign materials
Runon/runoff controls
Liners
Water Treatment…

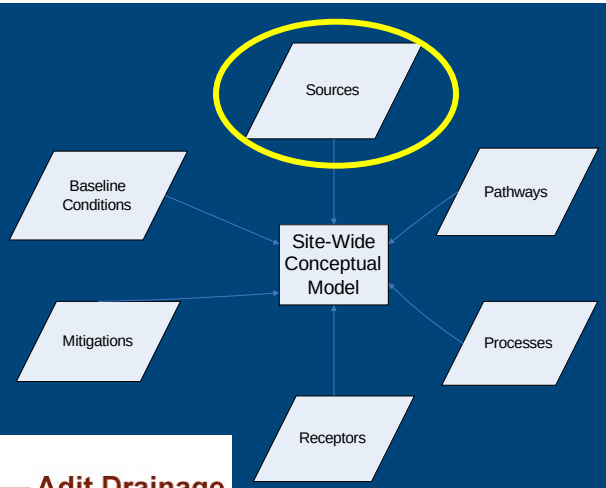
Maest et al. 2005

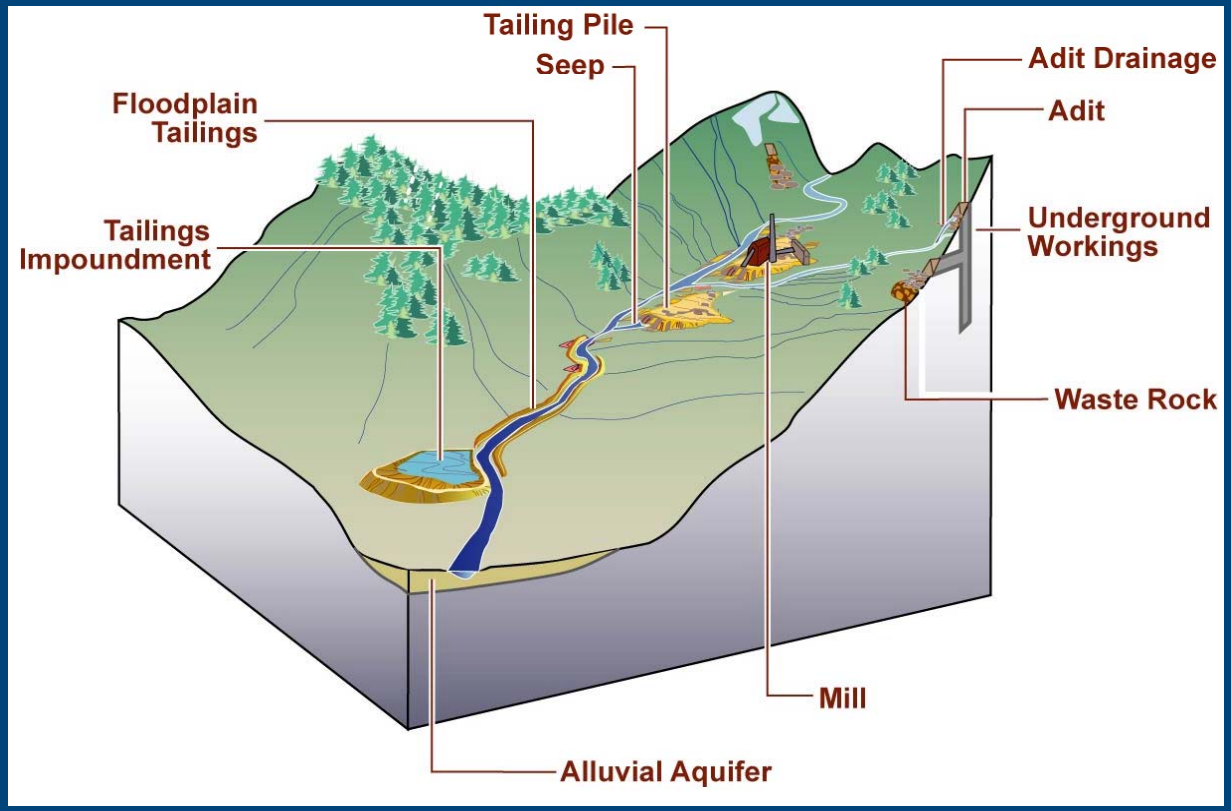
Impacts on the Environment: *Fate and Transport*

- Physical movement of chemical constituents from sources to receptors (water, aquatic life, people)
- Chemical changes and interactions along that pathway



Sources

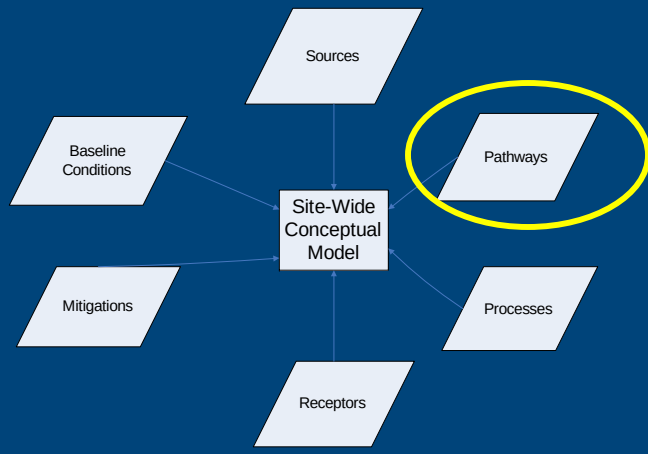

Sources
Baseline Conditions
Pathways
Site-Wide Conceptual Model
Mitigations
Processes
Receptors


Tailing Pile
Seep
Adit Drainage
Adit
Floodplain Tailings
Tailings Impoundment
Underground Workings
Waste Rock
Mill
Alluvial Aquifer

Contaminants of Concern

- Metals
- Acid
- Radionuclides
- Sulfate, nitrate
- Extraction/beneficiation reagents

Pathways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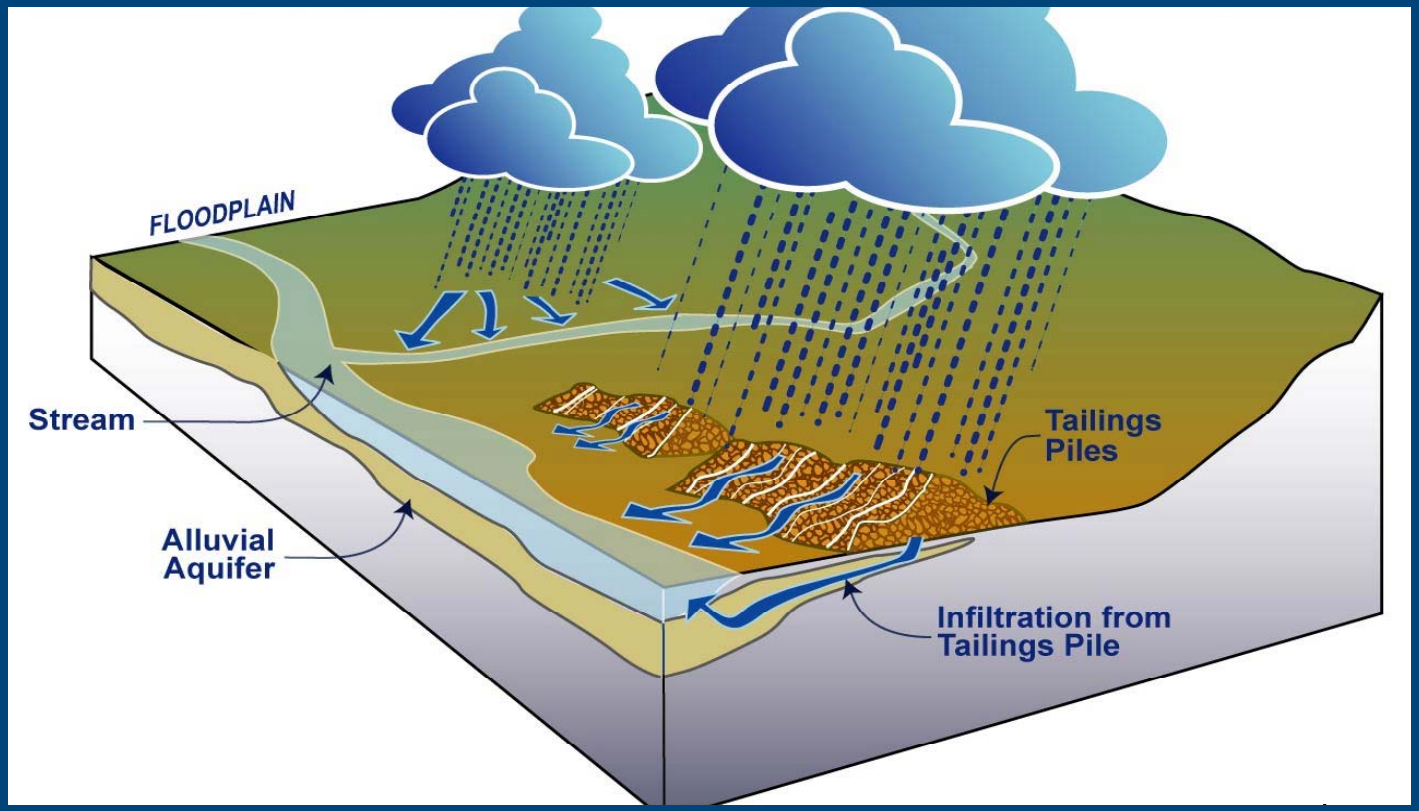
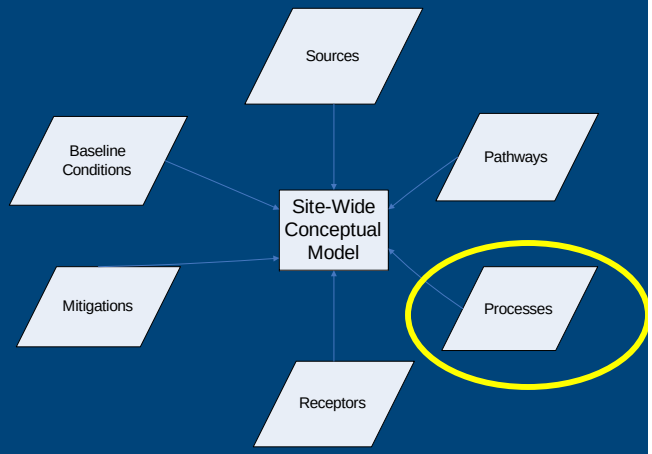

FLOODPLAIN
Stream
Alluvial Aquifer
Tailings Piles
Infiltration from Tailings Pile

Processes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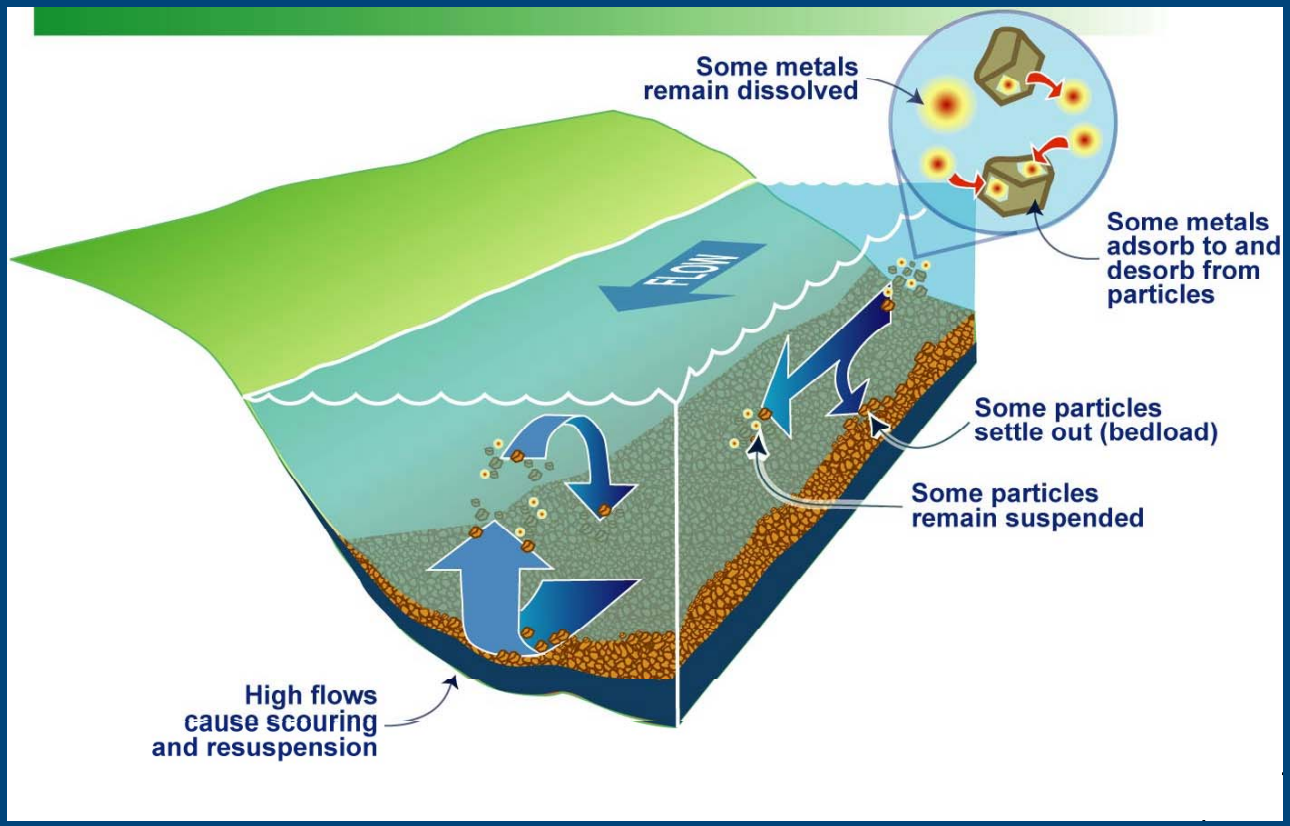
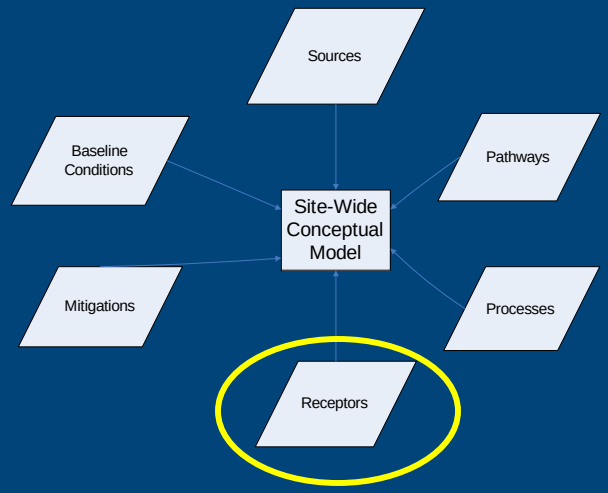

Some metals remain dissolved
Some metals adsorb to and desorb from particles
FLOW
Some particles settle out (bedload)
Some particles remain suspended
High flows cause scouring and resuspension

Receptors

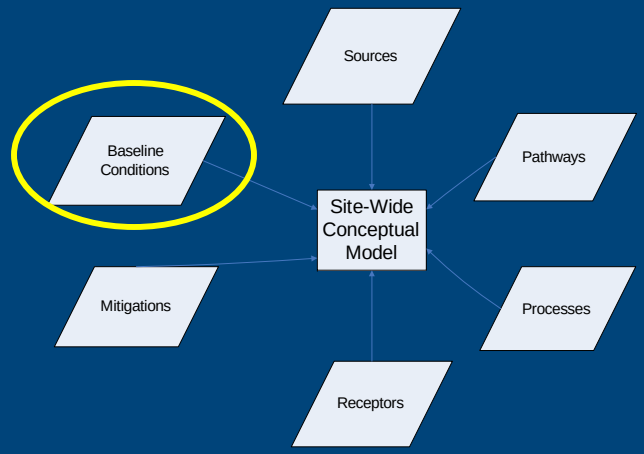


- Groundwater
- Surface water
- Seeps
- Pit lake
- Aquatic and terrestrial wildlife
- Air
- Vegetation
- Humans

Mitigations

- Mixing/blending of PAG/non-PAG wastes
- Runon/runoff controls
- Liners
- Covers
- Treatment
- Slurry cut-off walls

Baseline Conditions

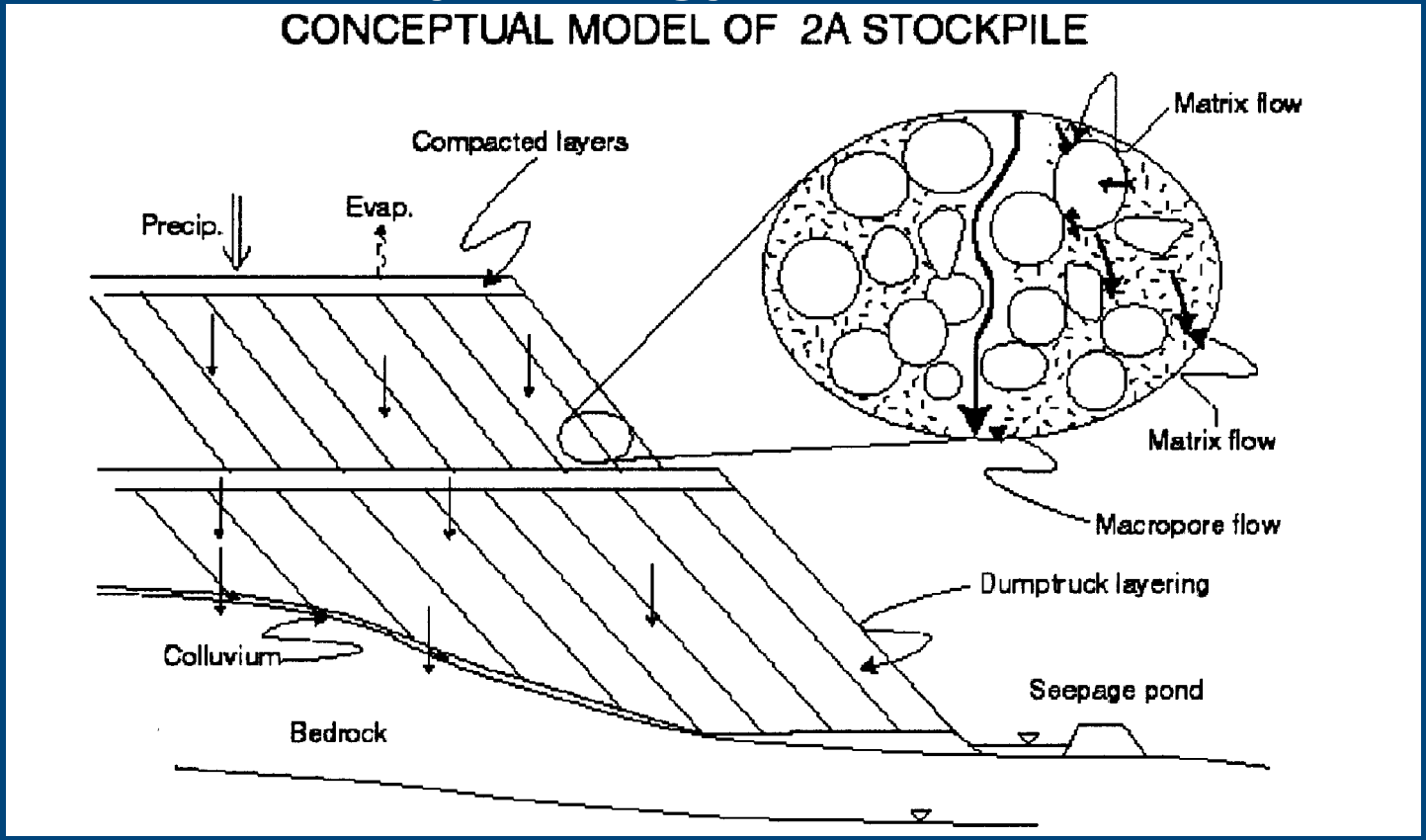


- Geologic units
  - Lithology/mineralogy, depth, thickness, locations
- Existing wastes/contaminant sources
  - Physical, hydraulic, geochemical characteristics, volumes, locations
- Groundwater, surface water, springs
  - Location, quality, quantity, seasonal/ temporal variability in water quality/quantity

Baseline Conditions (cont.)

- Hydrology and hydrogeology
  - Depth to groundwater, recharge /infiltration rates, groundwater flow directions and fluxes, gaining/losing reaches of stream, hydrologic parameters, seasonal/temporal variability
- Climatic conditions
  - Precipitation, evaporation, climate type, seasonal/long-term climatic variability, typical storm events, temperature

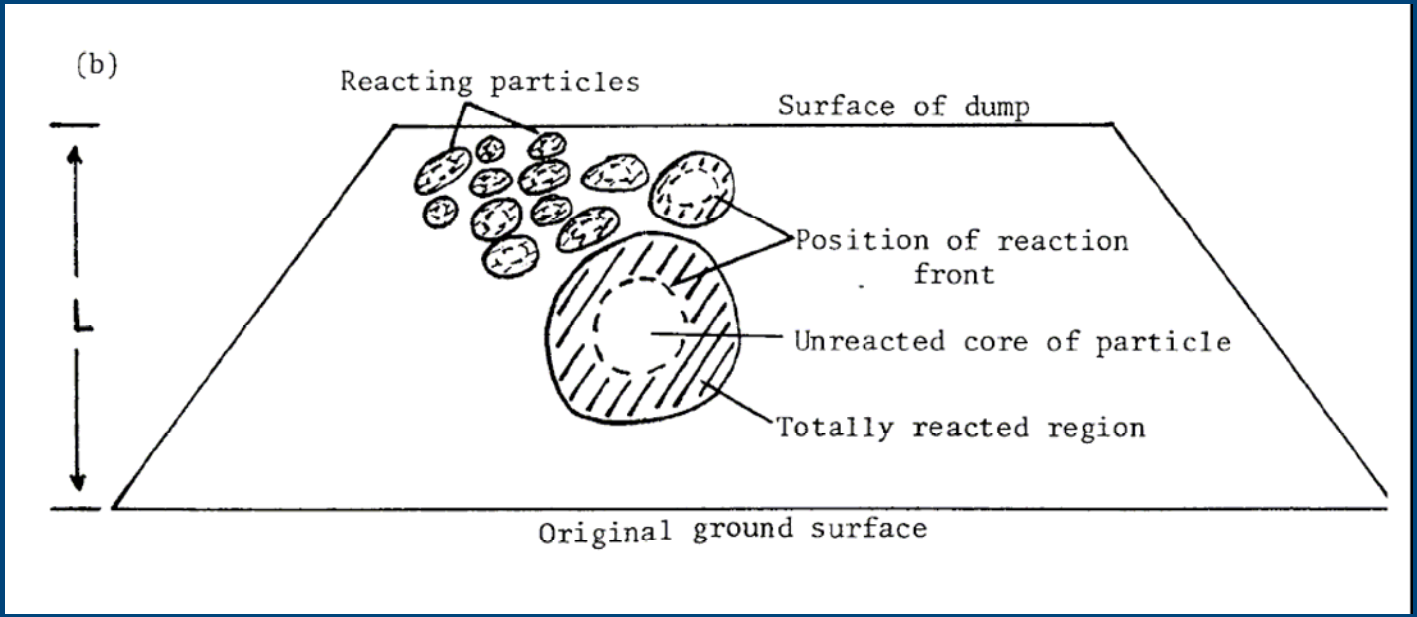
Conceptual Model Example: Tyrone Mine, New Mexico - Hydrology



Source: SARB Consulting, 1999.

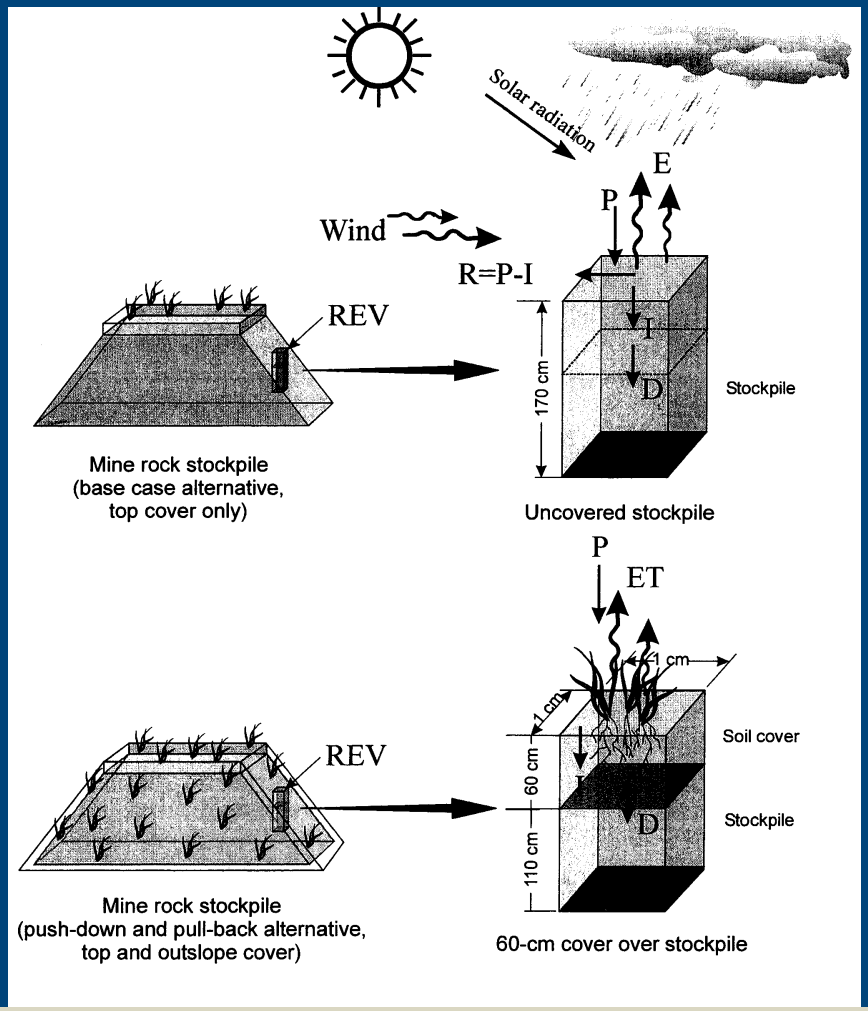
Pyrite Oxidation Conceptual Model Example

- Oxygen diffusion into unsaturated waste rock
- Reaction of oxygen with sulfides in dump
- Proceeds from surface down



Davis and Ritchie; 1986

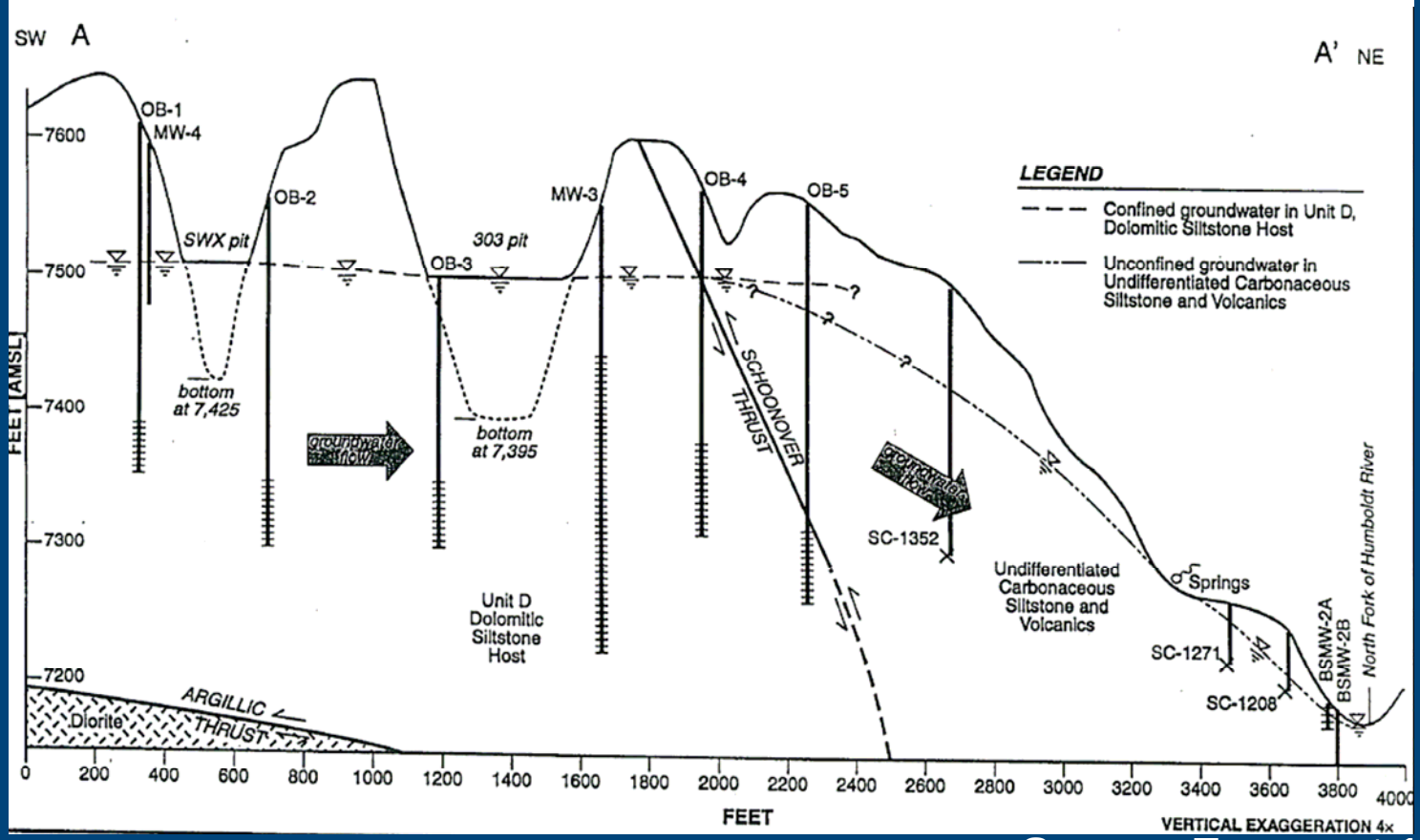
Conceptual Model Example: Chino Mine Stockpile Cover Alternatives



Source: DBS&A, 2001.

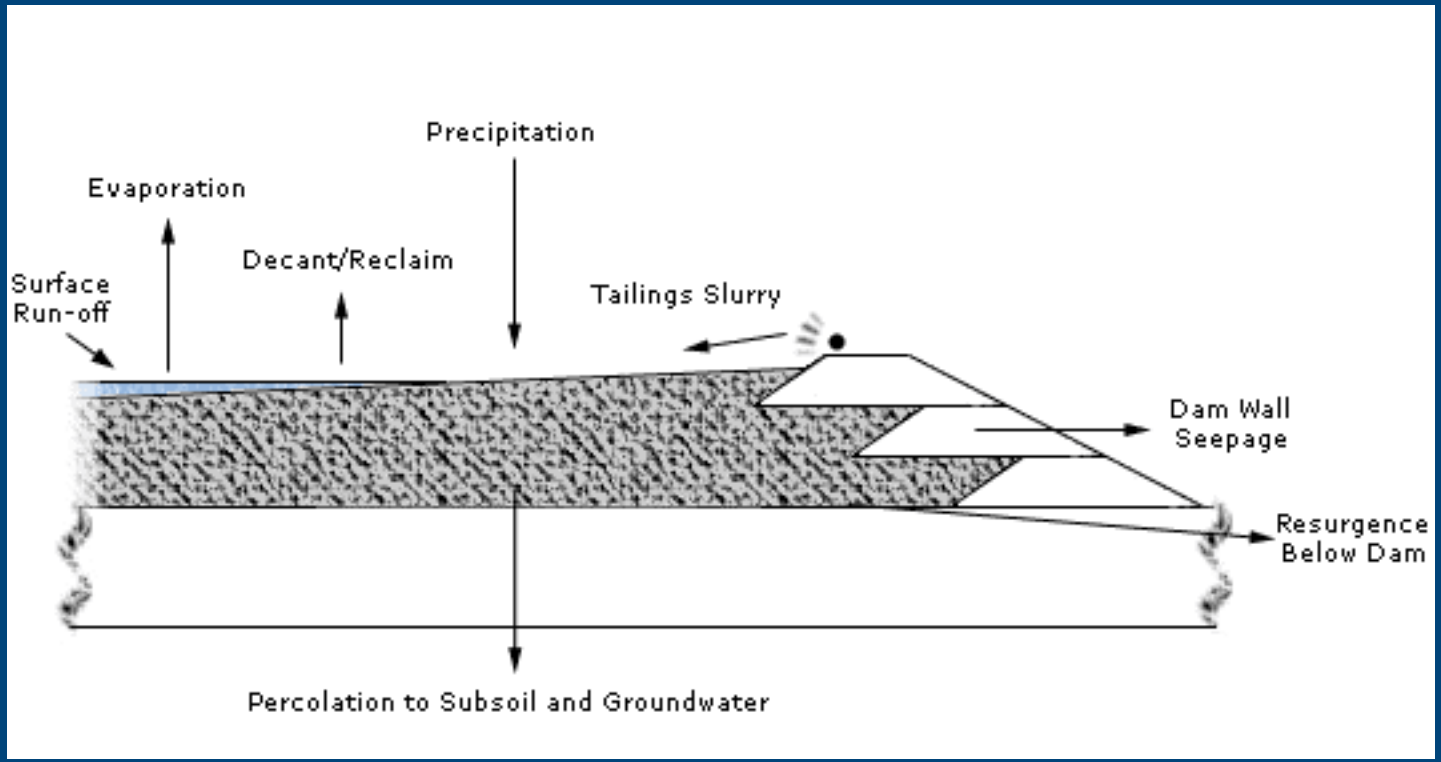
Conceptual Model Example: Groundwater

Big Springs Mine Hydrogeologic Section



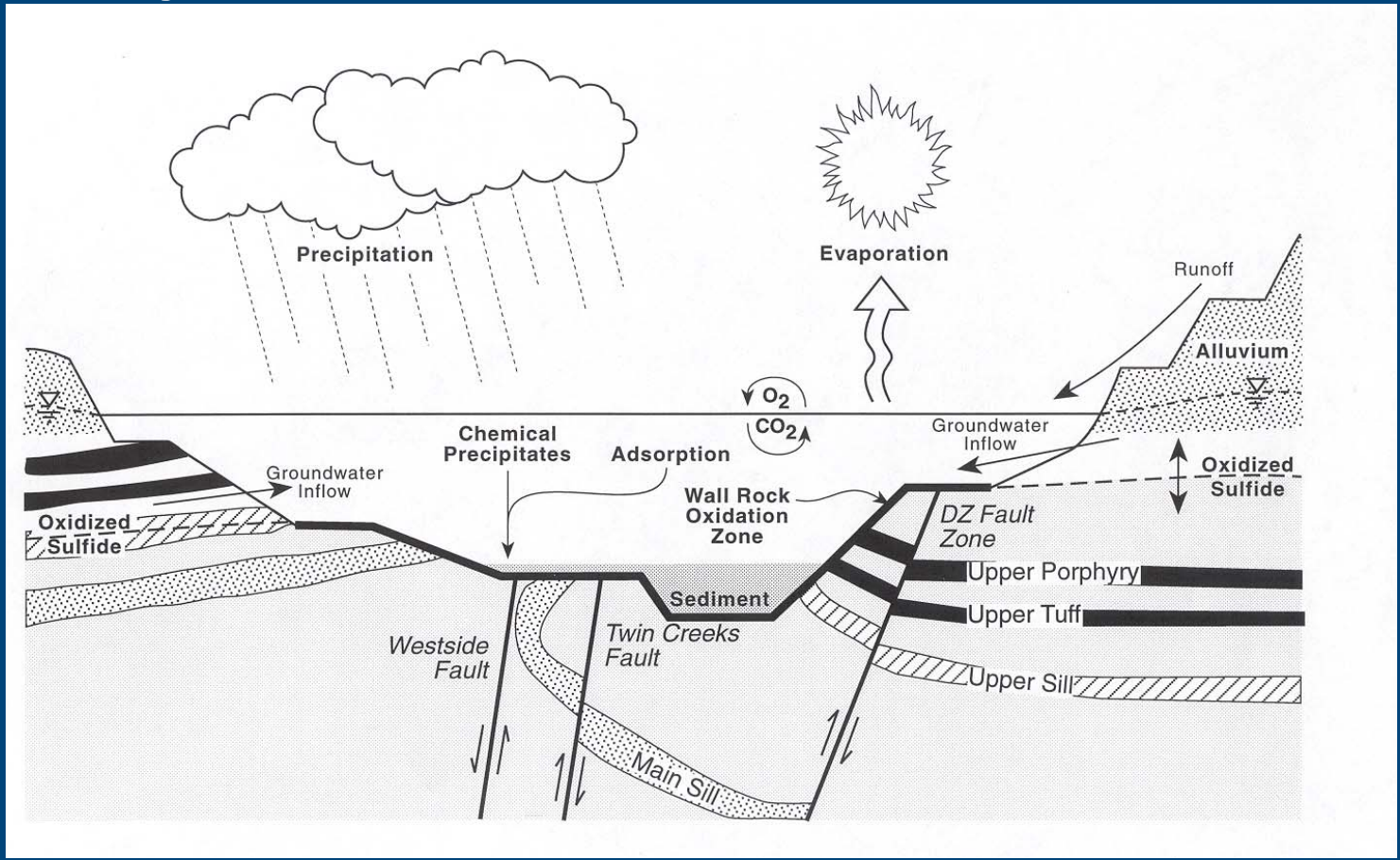
Source: Exponent 1998

Conceptual Model Example: Tailings Impoundment



Source: Vick 1990

Conceptual Model Example: Pit Lake Water Quality Twin Creeks Pit Lake



Source: PTI 1994.

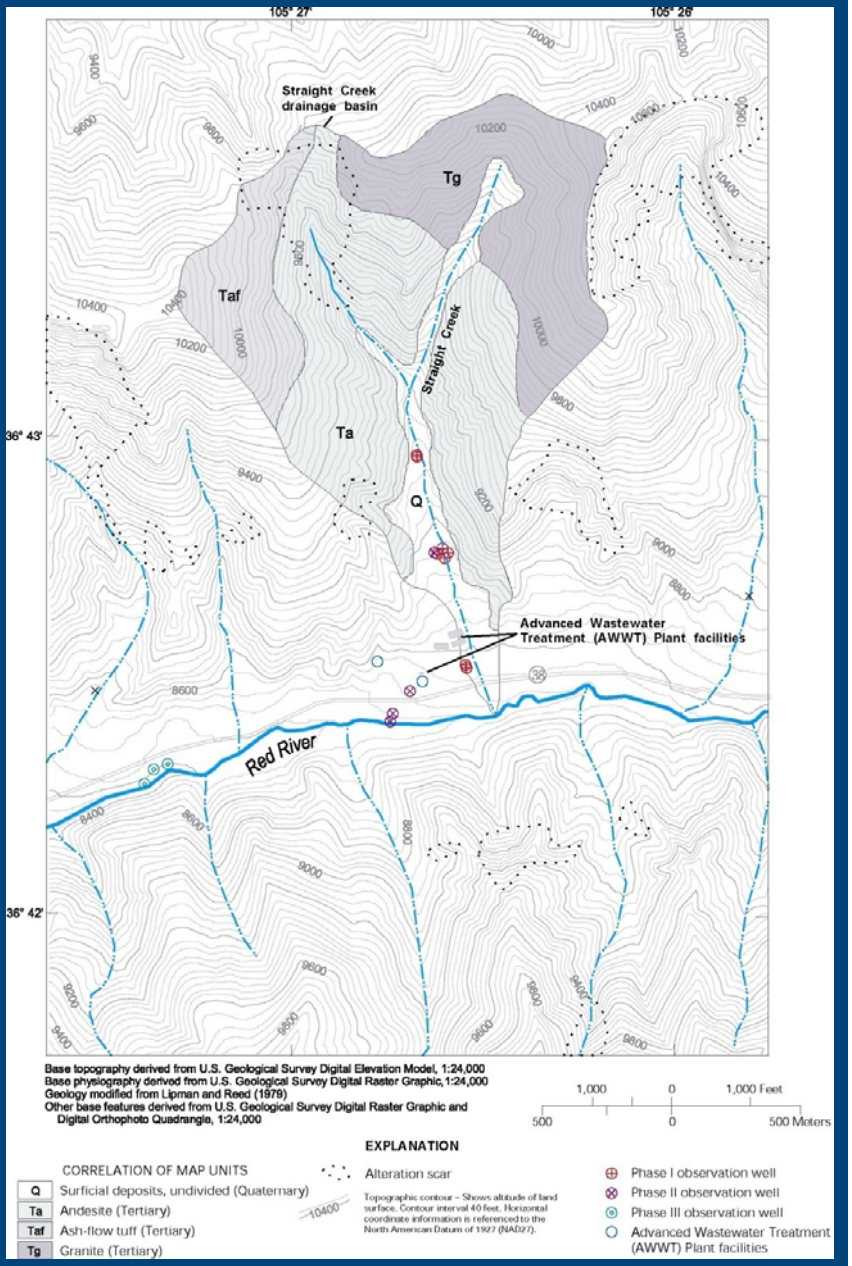
Flawed Conceptual Models: Questa and the Red River, NM

1. Pathway for groundwater flow from mountain catchment into main stem related to topography

2. All elevated sulfate and metals in downstream alluvial groundwater at mine site is derived from natural sources upstream

3. Soil/sediment leach tests = groundwater composition

Pathway for groundwater flow from mountain catchment into main stem related to topography? No



Acid rock drainage hugs north bank in the alluvium until it reaches a narrowing of the canyon where the groundwater is forced out and mixes with both the groundwater in the alluvial aquifer and with the water column (at the red circle).

Flawed Conceptual Models: Questa and the Red River, NM

All elevated sulfate and metals in downstream alluvial groundwater at mine site is derived from natural sources upstream

No – about 30% of the alluvial groundwater carrying natural acid rock drainage emerges into the Red River before reaching the mine site

– 20-40% of the sulfate load emerges into the RR before reaching the mine site

– additional sulfate loading enters the RR alluvial groundwater along the mine site

3. From Concept to Quantification

a. Computer codes as conveyors of models

b. Geochemical databases

c. Types of models and popular codes
   - Physical (hydrologic)
   - Geochemical
   - Coupled

Computer Codes as Conveyors of Models Geochemical Site-specific Data Input

1. Speciation: (1) charge balance, (2) toxicity and bioavailability, (3) conductivity check, and (4) saturation index calculations

1. Virtual mineral and water compositions for unconstrained forward modeling (or future scenario simulations) of water-rock interactions

2. Actual mineral and water compositions for constrained inverse modeling of water-rock interactions

Importance of Reliable Water Sampling and Accurate and Precise Analyses

- On site parameters: pH, T, specific conductance, DO, EMF need to be measured carefully. Water must be filtered, preferably through < 0.45µm to (a) remove iron-oxidizing bacteria, (b) remove solid particles. Speciation computations are very sensitive to pH and only a professional or carefully trained individual should be making these measurements. Measurements can be good to ±0.05 units under the best of conditions but no better. Goal should be to get to ±0.1

Geochemical Databases

1. Thermodynamic and kinetic
2. Numerous thermodynamic data sources and types
   - NIST (National Institute of Standards and Technology)
   - IUPAC (International Union of Pure and Applied Chemistry)
   - SUPCRT (Helgeson and others)
   - USGS
   - JANAF Tables (Joint Army-Navy-AirForce)
   - Groups in several foreign countries
   - OECD/NEA (focused on radionuclides from waste)
3. Problem of internal consistency

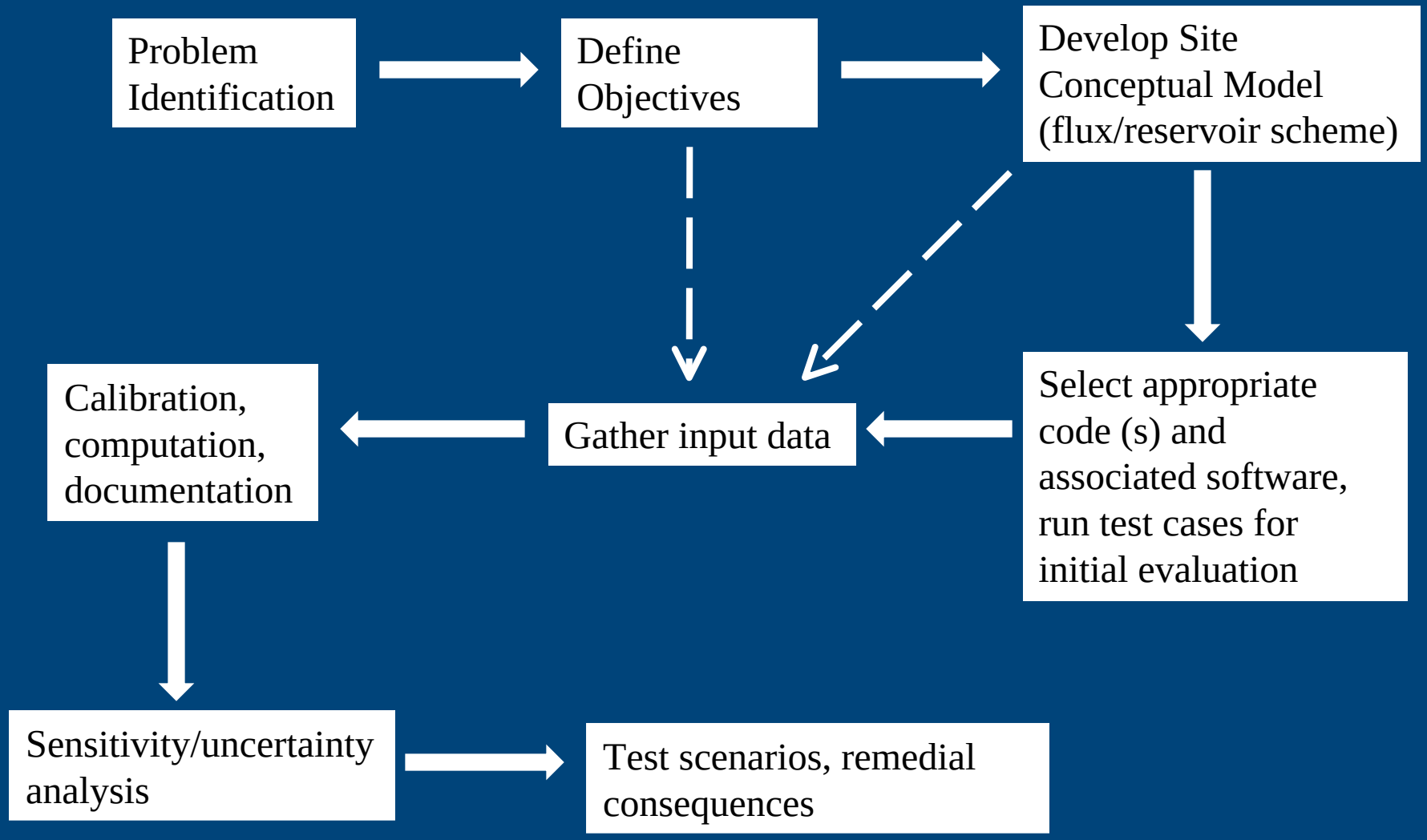
Most databases are compiled without strict adherence to maintaining internal consistency and may be an important source of error

Geochemical Databases

Problem of internal consistency

1. Consistency with the fundamental laws of thermodynamics and their consequences
2. Common scales for T, P, energy, mass, physical constants
3. Resolution of measurement conflicts
4. Same mathematical model is used for temperature or pressure dependence.
5. Same (and appropriate) chemical model is used finding standard states

General Modeling Steps



Conceptual Model to Mathematical Model: Code Selection

- Questions to ask:
  - What are the objectives and endpoints of the modeling
  - What processes will influence water quality, and what codes can simulate them
  - Use of coupled or separate water quantity/quality codes
  - The type and quality of data available (or that could be collected) versus the type of data needed for the code
  - Ease of use, graphical interfaces
  - Availability of the code to others

Code Evolution

- Model complexity grew with computing power (faster now)
- Many codes built in 1980s
- Interfaces have made modeling easier: inputs and outputs
- Visual output

Use of Proprietary Codes

- Prevents independent examination by other consultants, regulators, and public interests; creates uncertainty about legitimacy of results; less use = fewer bugs worked out
- Many public-domain or reasonably priced codes are available
- Avoid use of proprietary and expensive codes for predictive modeling
- Consider any added value v. lost transparency

Mathematical Models – Need Solutions to Partial Differential Equations

- Flow in saturated, anisotropic porous media

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial h}{\partial z}\right)=S_s\frac{\partial h}{\partial t}$$

- Contaminant transport (advection-dispersion equation, for transport in saturated, porous media, nonreactive chemical)

$$\left[\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)\right]$$

$$-\left[\frac{\partial}{\partial x}(\bar{v}_xC)+\frac{\partial}{\partial y}(\bar{v}_yC)+\frac{\partial}{\partial z}(\bar{v}_zC)\right]=\frac{\partial C}{\partial t}$$

Freeze and Cherry 1979

Types of Solutions to Mathematical Models

- Analytical model: Uses classical mathematical techniques for solving differential equations. Typically requires simplifying assumptions for boundaries, initial conditions, homogeneity of system etc. H = f(x,y,z,t)

- Numerical model: Solves a system of equations by dividing the area of interest into pieces (grid cells or elements). Allows for more complex conditions in the system (parameters can vary in space and time)

  (e.g., Finite difference, finite element)

Hydrologic Codes

Near-surface hydrologic processes

- Example question:

  How much of the precipitation that falls on this waste rock pile will infiltrate into the pile (and later transport sulfate and metals into this lake)?

Yanacocha Mine, Peru

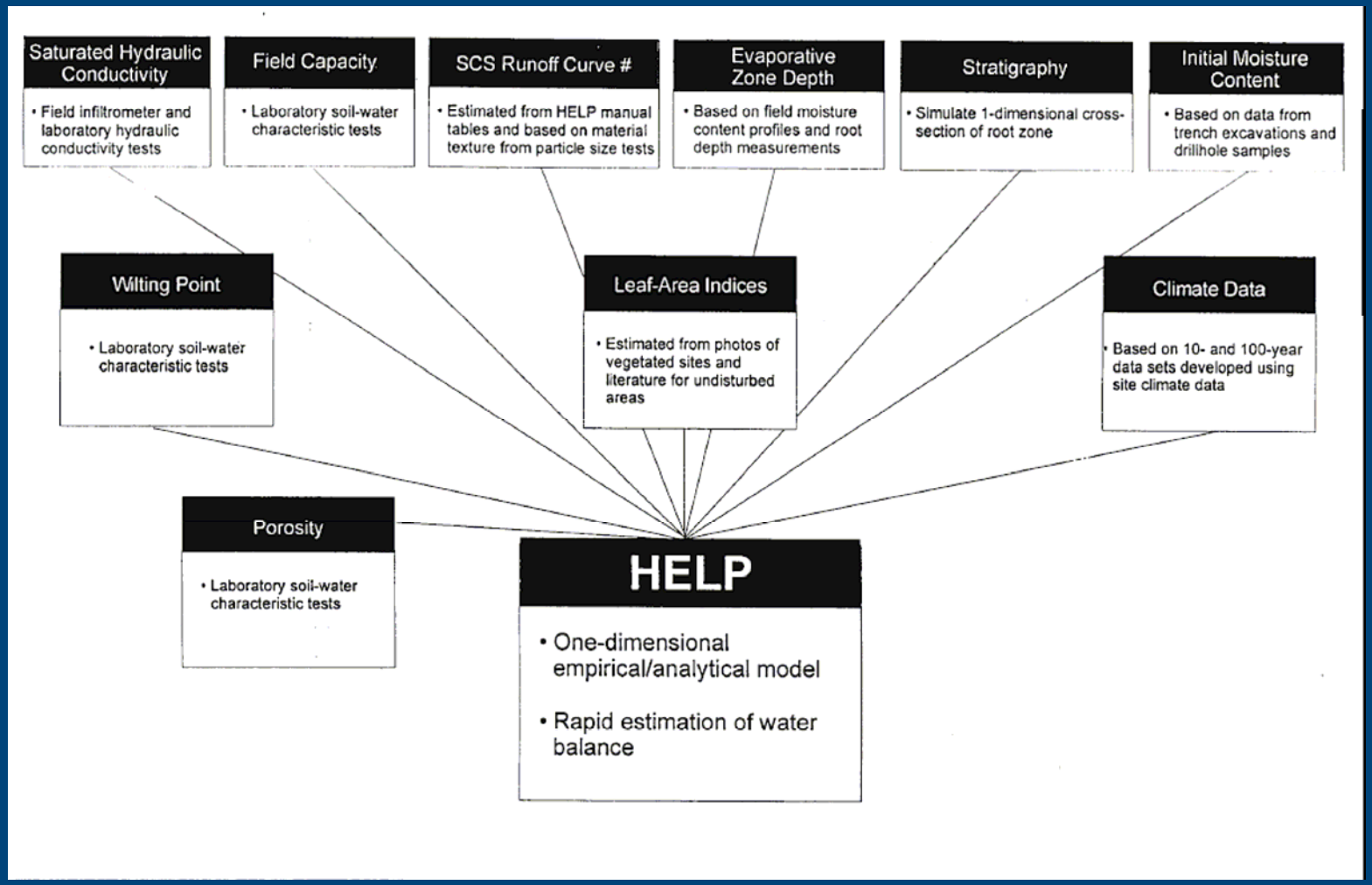
Hydrologic Codes

- Near-surface hydrologic processes
  - Used to estimate runoff, infiltration, evaporation rates through/from mine units
  - Water balance (infiltration, runoff, evapotranspiration)
    - HELP (US EPA), HEC-HMS (US ACOE)
  - Water balance + contaminant transport
    - HSPF (US EPA), PRZM 3 (US EPA)

Inputs – Hydrologic Codes

- Near-surface hydrologic process
  - Water balance: Precipitation, temperature, wind speed, incident solar radiation, vegetative cover (for evapotranspiration); hydraulic conductivity/permeability of soil/geologic material; soil moisture storage and transmission requirements
  - Water balance + contaminant transport: Same as above + source concentrations/loads, initial soil concentrations, contaminant fate/transport parameters (e.g., adsorption, precipitation)

Example of Input for near-surface Process Model Using HELP Code



Exponent 2001

Hydrologic Codes

Vadose zone

- Example question:

  How will the creation of waste rock piles, open pits, and other disturbances affect timing of recharge to groundwater and base flow in streams? How will wetting front migrate through waste rock?

Yanacocha Mine, Peru

Hydrologic Codes
Vadose zone (cont.)

- Example question:

  Will tailings water from this impoundment infiltrate to groundwater and impact surface water?

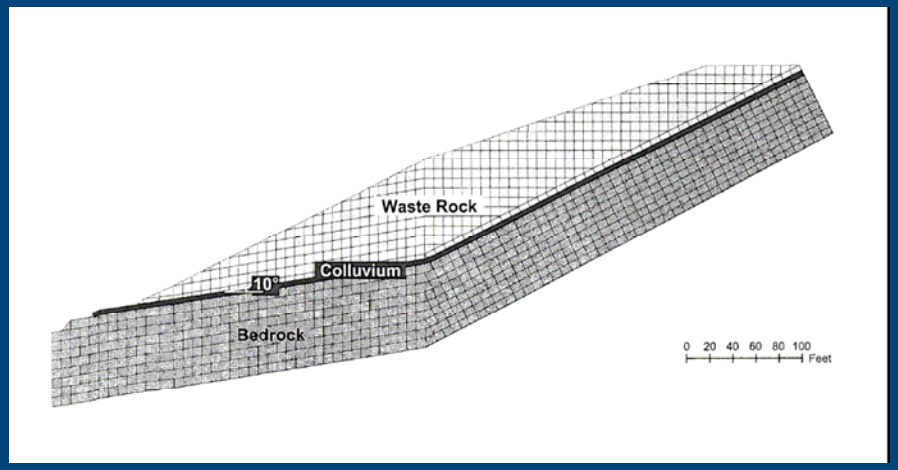
Hydrologic Codes

Vadose zone

- Richards' equation describes vertical unsaturated flow.
- Solutions to Richards' equation:
  - Analytical solutions can be used with specific assumptions
  - Numerical codes need to be used in more complex situations

Hydrologic Codes

Vadose zone



Exponent 2001

- Used to estimate seepage amounts and quality through unsaturated areas of mine units and underlying unsaturated zone
- Vadose zone percolation
  - 1D: Hydrus-1D (US Salinity Lab), Unsat-H (PNWL)
  - 2D: Hydrus-2D, VS2D (USSG), SEEP/W (Waterloo)
  - 3D: T2VOC (based on TOUGH codes, LBL)
- Vadose zone percolation and contaminant transport
  - SUTRA (USGS), VS2D/T (USGS), FEFLOW (Waterloo Hydrogeologic), T2VOC

Inputs – Hydrologic Codes

- Vadose zone codes
  - Percolation: Infiltration rates; any layering or heterogeneity in geologic materials; hydraulic properties of soils/geologic units, such as moisture retention properties
  - Percolation + contaminant transport: Quality of water entering the vadose zone and initial concentrations of constituents in vadose zone; parameters describing partitioning between soil/rock and water

Hydrologic Codes
Groundwater

- Example question:

  If the mine pumps groundwater to keep this open pit dry, will that affect flow in springs and creeks near the mine?

Hydrologic Codes
Groundwater (cont.)

- Used to simulate mine dewatering and reflooding, and flow and contaminant transport in groundwater to receptor (well, stream, lake)
- Groundwater flow
  - MODFLOW (USGS), FEFLOW (Waterloo Hydrogeologic)
- Groundwater flow and contaminant transport
  - MODFLOW-MT3D, MODFLOW-SURFACT; SUTRA (USGS); FEFLOW, FEMWATER (EPA)
  - Fracture Flow: FRACTRAN (Waterloo), TRAFRAP-WT (Hydrogeologic, Inc.)

Inputs – Hydrologic Codes

Groundwater

- Groundwater flow: Hydraulic conductivity, porosity, storage characteristics, thickness of geologic units, areal recharge, surface water recharge, pumping or re-injection of water from wells, discharge to surface water; model boundaries (streams, flow barriers, etc.). For fracture flow/transport: Also need fracture spacing, orientation, aperture.
- Groundwater flow + contaminant transport: Same as above plus contaminant input concentrations; dispersion properties of aquifer, retardation characteristics of contaminant (Kd).

Hydrologic Codes

Limnologic codes

- Example question:

  Will this pit lake be eutrophic? Will it turn over once, or twice a year or will it be stratified?

Hydrologic Codes

Limnologic codes (cont.)

- Used to simulate mixing, nutrient/primary productivity of lakes (pits), sediment, eutrophication, kinetics, metal cycling, changes in biomass
  - CE-QUAL-W2 (2D, hydrodynamic, water quality; US Army Engineer Waterways Experiment Station)
  - DYRESM (1D) or ELCOM (3D) (Univ. W. Australia)
  - CAEDYM (aquatic ecological; Fe, Mn, Al cycling; Univ. Western Australia)

Hydrologic Codes
Stream/river

- Example question:

  Will upstream mining cause metals concentrations in this river exceed water quality criteria for aquatic life?

Hydrologic Codes
Stream/river (cont.)

- Simulate flood hydrograph, continuous streamflow, effect of transient runoff events on streamflow,
- Streamflow quantity
  - HEC-HMS (single event rainfall-runoff, US ACOE)
  - SWRRB (USDA), PRMS (USGS), MD_SWMS (USGS), MIKE-SHE (continuous streamflow)
- Streamflow quantity and quality
  - WASP4 (US EPA)
  - OTIS-OTEC (USGS)

Inputs – Hydrologic Codes

- Stream/river codes
  - Stream flow/quantity: Channel geometry, flow data, tributary flow data
  - Stream water quality and quantity: Point and non-point contaminant source data; concentrations in stream and tributary inputs, temporal streamflow data; channel geometry; sediment/water contaminant partitioning (Kd)

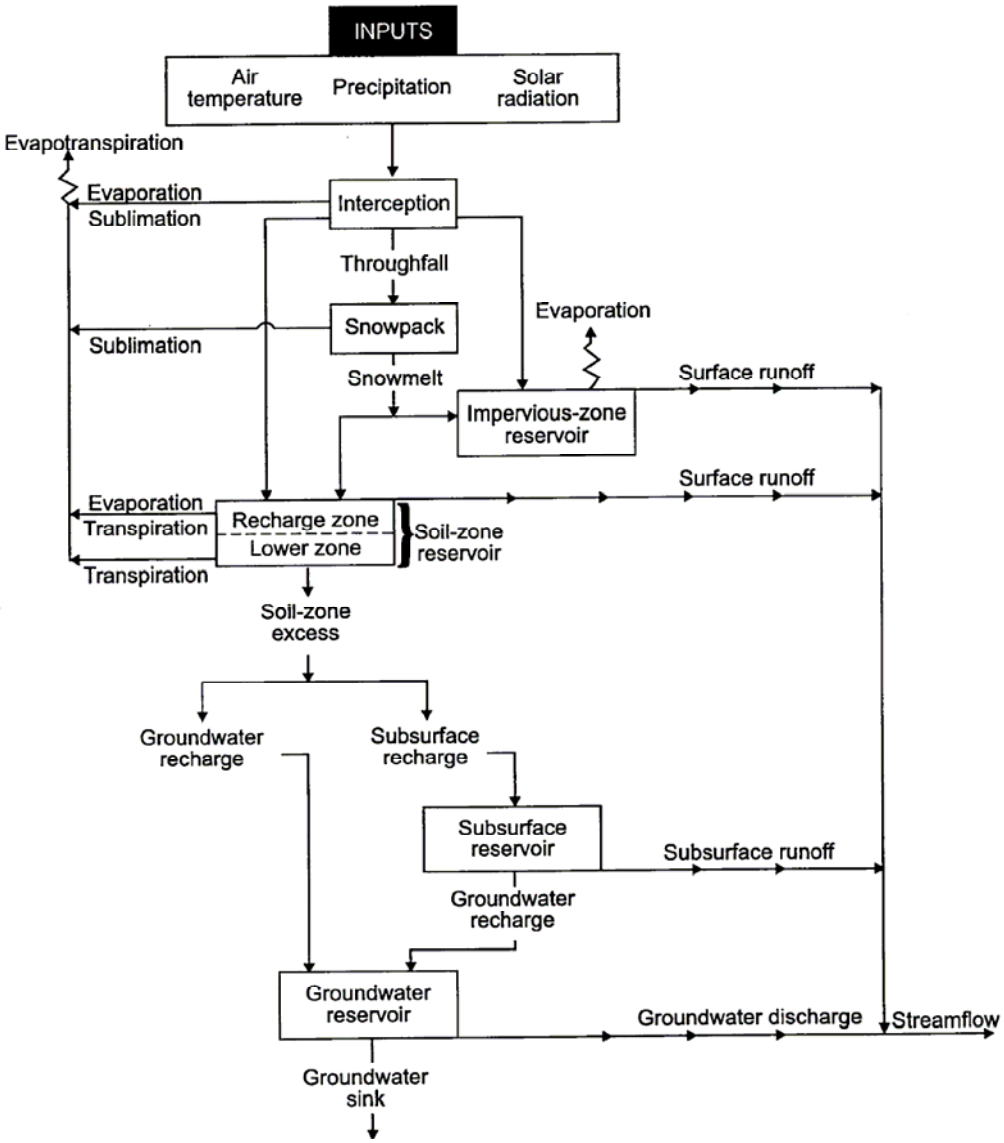
Hydrologic Codes

Integrated hydrologic/watershed codes

- Simulate all components of hydrologic flow regime and interaction between components
  - MIKE SHE (British Institute of Hydrology, Danish Hydraulic Institutes)
  - PRMS/MMS (USGS)
  - HSPF (US EPA)

Watershed Code Example

PRMS (Leavesley et al. 1983)



Types of Geochemical Models and Codes:

- Types of models
- Available codes in common use

Reactive-transport (coupled) Codes

1. Surface-water codes
    1. OTIS and OTEQ (USGS-supported)
    2. WASP (EPA supported)
2. Groundwater codes
    1. MT3DMS (University of Alabama)
    2. PHAST (USGS-supported)
    3. PHT3D (CSIRO-supported; PHREEQC-2 + MT3DMS)
    4. TOUGH-AMD (originally LBL-supported)
    5. MIN3P (University of Waterloo/UBC)
    6. RETRASO (Barcelona, CSIC)
    7. SULFIDOX (ANSTO)

Reactive-transport (coupled) Models and Codes

2 approaches:

global-implicit formulation (one-step approach, or simultaneous)
or
operator-splitting formulation (two-step approach, or sequential)

The mathematical problem is that of combining nonlinear mass-action mass-balance thermodynamic and kinetic equations with the differential equations of advection-dispersion. They have been directly substituted in the simultaneous approach but computing times can be laborious. The sequential approach is more efficient. Most modelers preferred the sequential formulation in the past but now with more computing power, there is increasing use of the simultaneous formulation.

Hydrologic and Geochemical Modeling

- Example question:

  What will be the water quality in this pit lake? Will it sustain a fish population? Will it pose an unacceptable ecological risk?

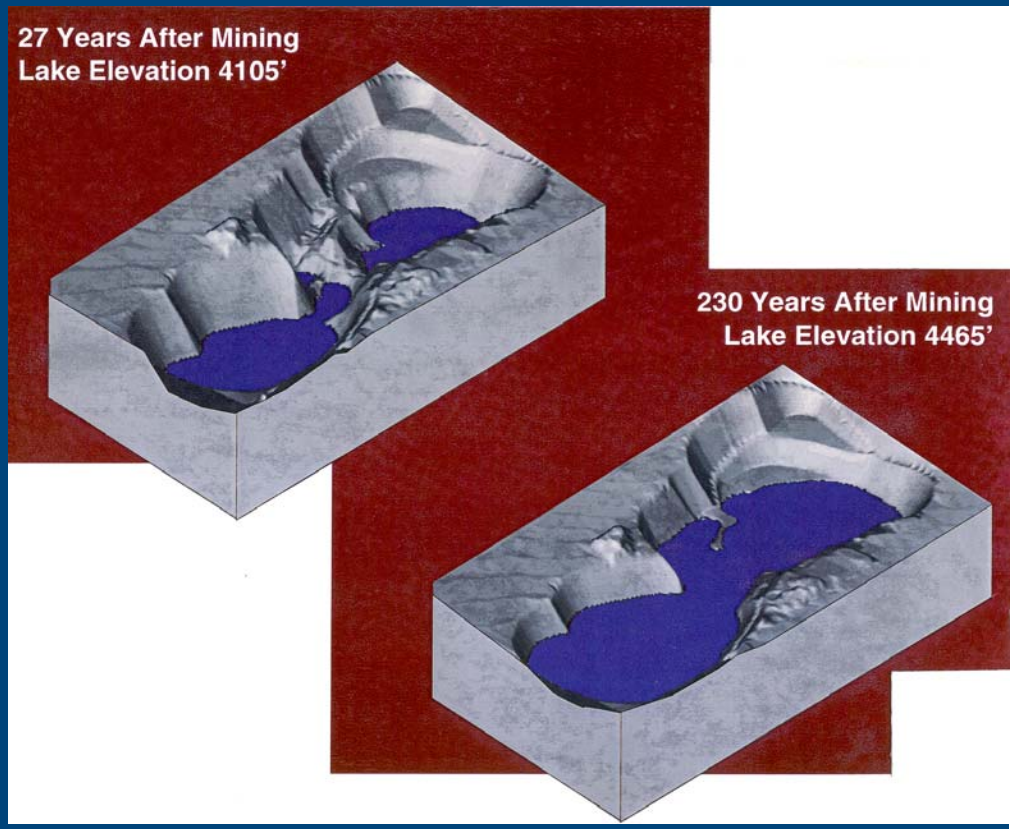
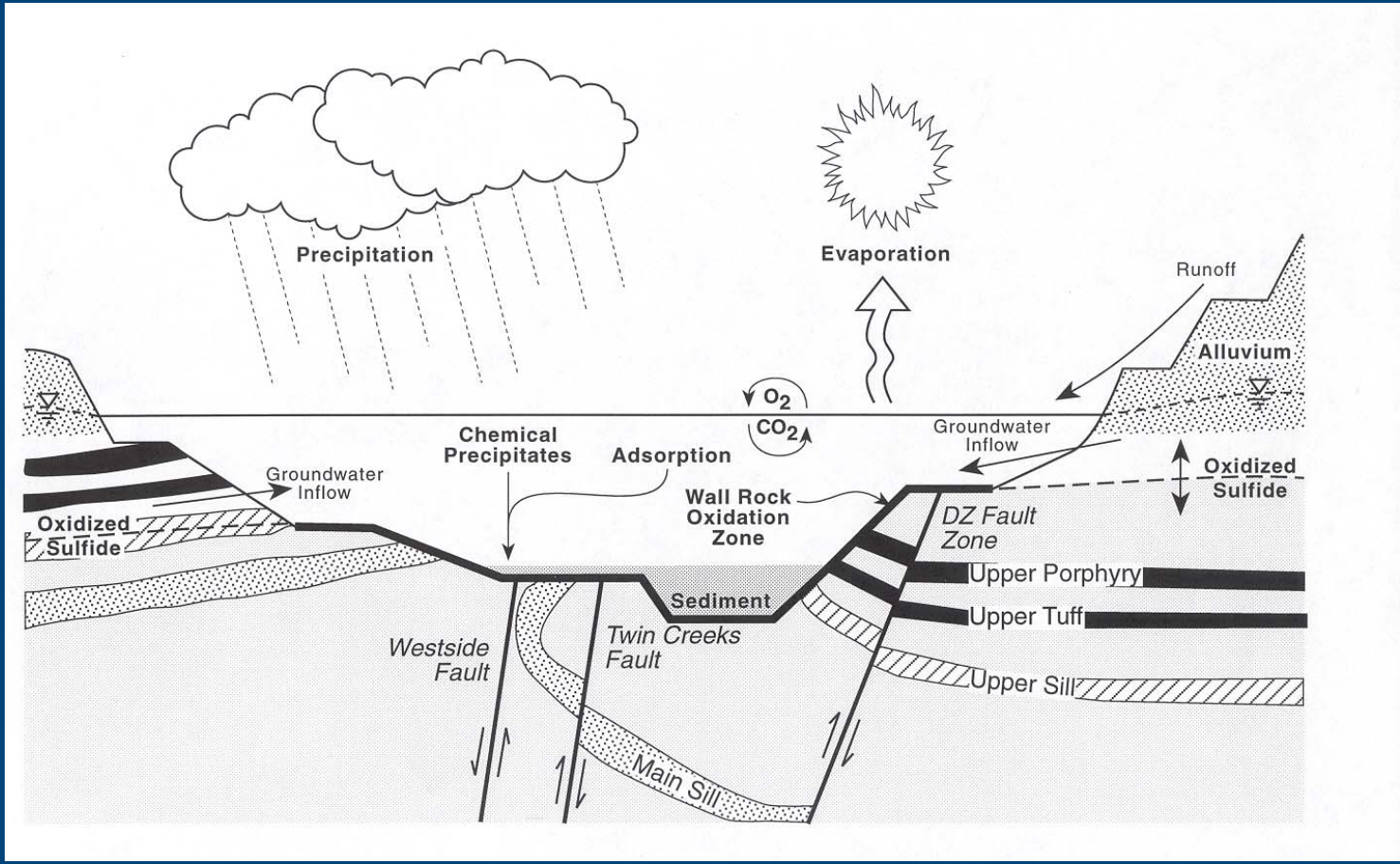


Image from PTI Environmental Services 1996

Pit Lake Water Quality Model



PTI Environmental Services 1996

Hydrologic and Geochemical Modeling

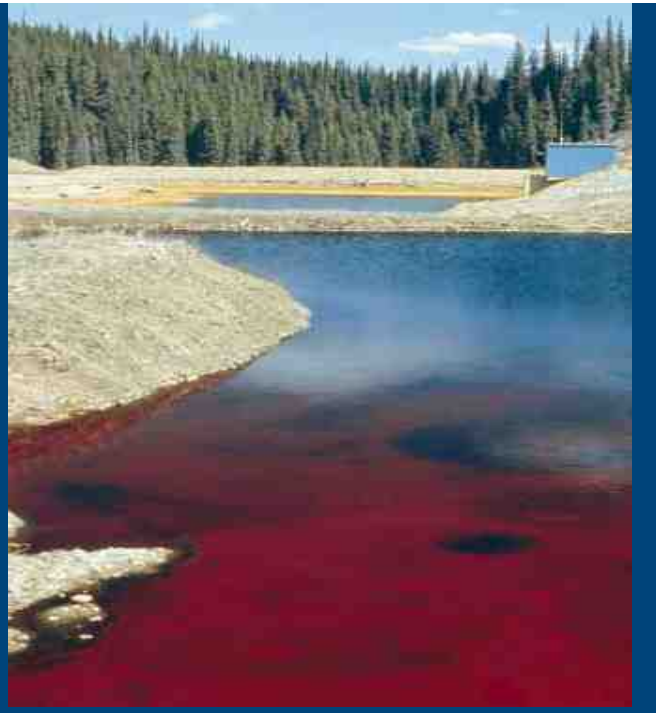
- Pit lake water quality modeling considerations
- Water balance for lake: Groundwater inflow/outflow, precipitation, runoff from high walls, evaporation from pit lake surface, any surface water inflow (groundwater flow code, near-surface process code)
- Sources of metals/acid to the lake from oxidizing wall rock, inflowing groundwater, runoff over high walls (pyrite oxidation model, chemistry data)

Hydrologic and Geochemical Modeling (cont.)

- Geochemical reactions within the lake (geochemical models)
- Limnology of the lake, stratification? (limnological models)
- Potential ecological receptors? Fish? Humans? (food web models)

Modeling Process: Evaluation; Documentation; Calibration; Sensitivity Uncertainty

How Confident Are We in Model Results?



- Model calibration
- Sensitivity analysis
- Uncertainty
- Model documentation
- Model evaluation

Model Calibration

- Calibration – comparing site-specific observations (e.g., stream flows, groundwater elevations, or pit lake concentrations) with model simulations. Calibration includes adjusting model parameters (e.g., hydraulic conductivity or porosity) so that the output from the model reproduces observed field conditions (see Hill, 1998).
- Environmental models can be calibrated but never validated (Oreskes and Belitz, 2001).

Forward Modeling and Calibration

- Most mine-site modeling is forward modeling (predicts conditions far into future)
- Models may also be used to “hind cast” (e.g., reconstruct historical concentrations for exposure)
- Are data available to describe existing conditions for calibration?
- Can use existing analogs, e.g., pit lakes in similar geology/of similar dimensions, etc. or existing waste rock
- Can model reproduce observed conditions? If not, we can have no confidence in ability to predict

Forward Modeling and Calibration

- In general, more data for calibration and better fit = increasing confidence in predictive results
- BUT perfect calibration does not necessarily equal good predictive capability
  - Good calibration to poor conceptual model?
  - Tweaking of model parameters locally, missing larger scale properties (Freyburg 1988)

- As more field data are gathered, conceptual model should be reevaluated, may need to change model and recalibrate

Sensitivity Analysis

- Addresses inherent variability in some input parameters
- Do sensitivity analysis and see what controls variability and if more data are needed
- Use ranges of values that are representative of site conditions
  - Example: Hydraulic conductivity
  - Example: Concentrations in effluents or streams, groundwaters

Sensitivity Analysis (cont.)

- How representative are the input values of actual conditions?
- How much can the values vary?
- What is the cumulative effect of uncertainty on the variable of interest (e.g., metal concentration in a stream)?

- Sensitivity analysis may not bound uncertainty

Uncertainty Analysis/Predictive Error

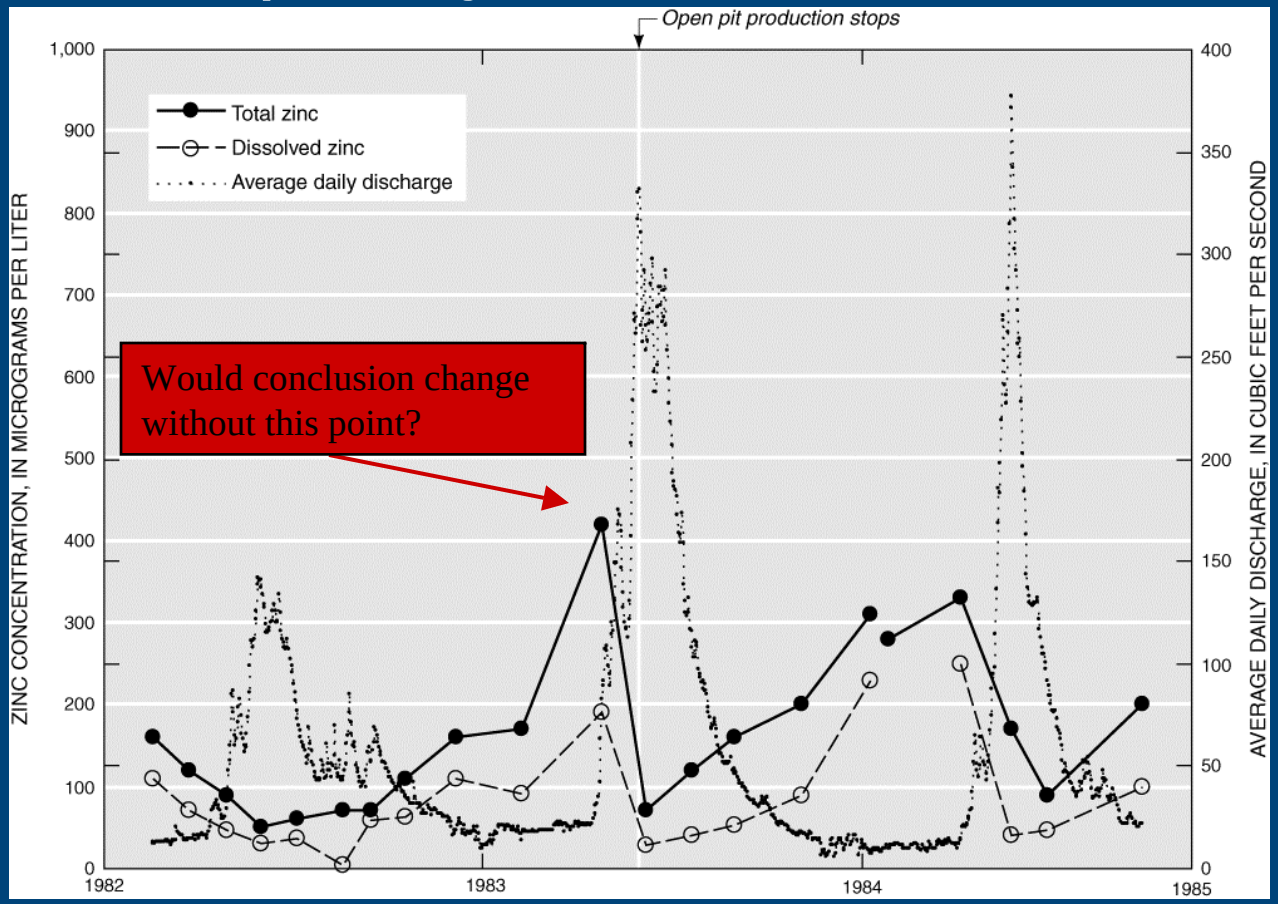
- Rarely stated/recognized in modeling
- Sources
  - Incorrect conceptual model
  - Key processes overlooked
  - Incomplete characterization
  - Incomplete knowledge of geochemical/hydrologic conditions
  - Inappropriate timeframe for predictions

Sources of Uncertainty

- Modeling inputs – Incomplete characterization
  - Large natural variability in hydrologic and geochemical parameters; seasonal variability in flow and chemistry
  - Inability to sample “all” of the material of interest – characterization must infer from limited number of samples
  - Measured parameters at points, or in lab, may not represent larger field-scale processes
  - Mine facilities (e.g., waste rock piles, tailings impoundments, open pit geometry) can change with changing mine plan
  - Extrapolation to future (e.g., changing climatic conditions)

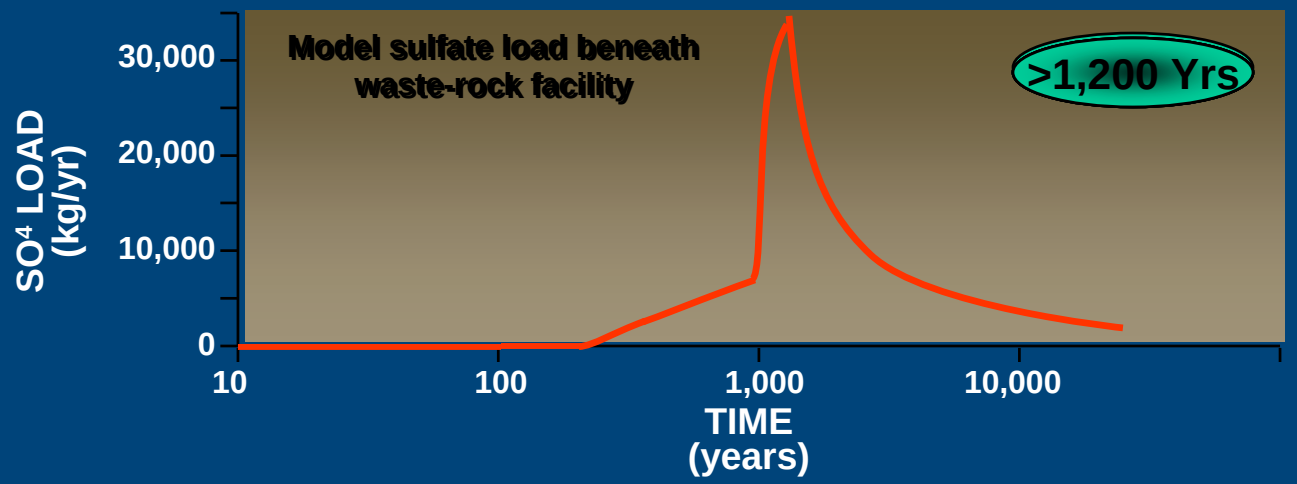
Incomplete Characterization: Boreholes Can Not Give You the Whole Picture

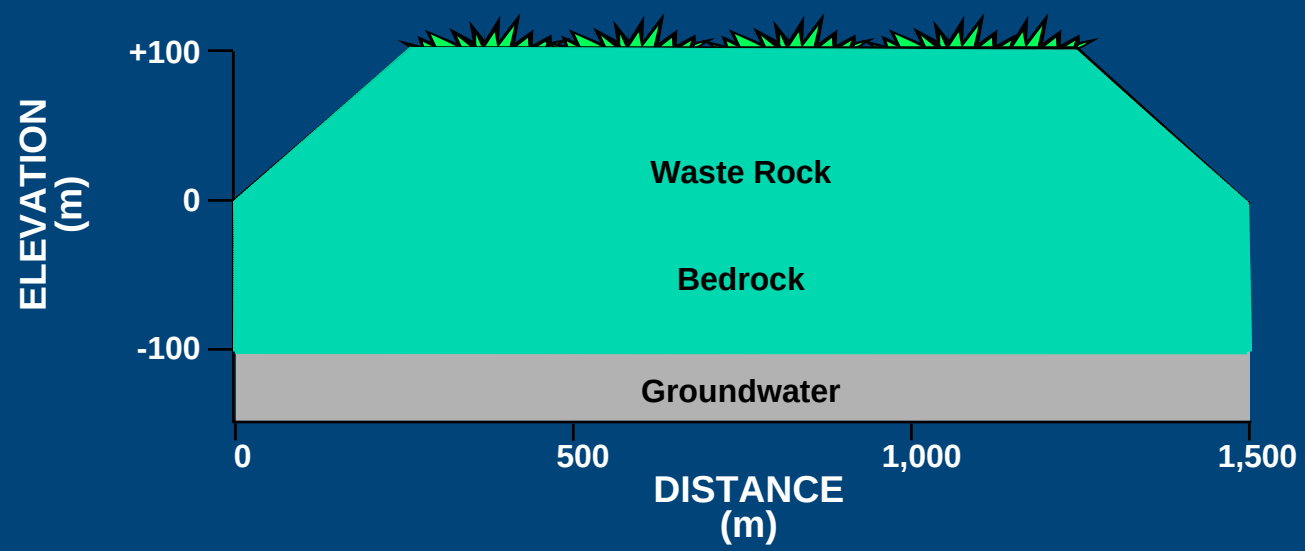
Uncertainty Due to Seasonal Variability/ Sample Frequency



Red River, Near Questa Molybdenum Mine, New Mexico: Zinc and Flow (Maest et al., 2004).

Timeframe for Predictions: Example of Waste Rock Loading in Arid Environment





Graphics from Kempton 2000

Sources of Uncertainty – Modeling

Acknowledge and evaluate effect on model outputs; test multiple conceptual models

- "…there is considerable uncertainty associated with long-term predictions of potential impacts to groundwater quality from infiltration through waste rock...for these reasons, predictions should be viewed as indicators of long-term trends rather than absolute values."

Sources of Uncertainty – Modeling (cont.)

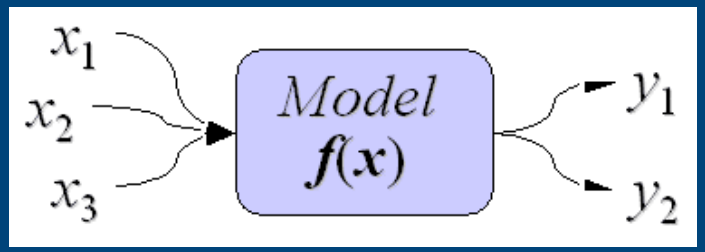
- Timeframe for predictions
  - Modeling results can depend on timeframe chosen (e.g., time for solutes to move through waste rock pile or concentrate in pit lake; availability of neutralizing material; climate change).
  - While recognizing the uncertainty, extend predictions to the timeframe required (regulatory), but don't chose arbitrary cutoff point
  - Base timeframe on the physical conditions (e.g., pit lake chemistry to steady state or exceedence of ecological thresholds). Predict timing/magnitude of waste rock impacts, even if far in the future.

Uncertainty Analysis

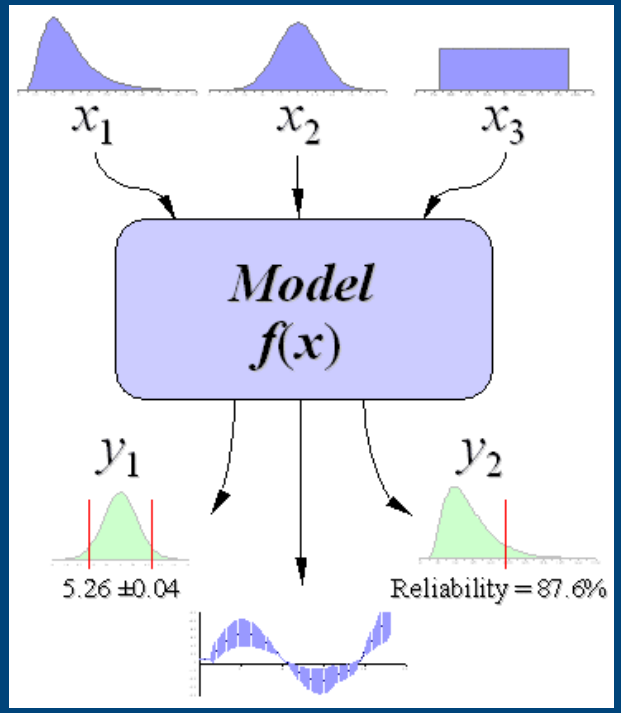
- Methods for estimating
  - Monte Carlo analysis
  - Stochastic methods
  - Sensitivity analysis
- Analyses indicate uncertainty in site parameters, but will not address uncertainty/errors in conceptual model

Monte Carlo vs. Deterministic

Deterministic model:



Monte Carlo model:



Wittwer, J.W., "Monte Carlo Simulation Basics" From *Vertex42.com*, June 1, 2004

Summary – Modeling Process

- Sound conceptual model is critical, should be willing to change if additional information suggests need
- Select codes based on important processes to be simulated and modeling objectives – no “one size fits all”
- Using a more complex/sophisticated code does not guarantee a “better” answer; code should be selected based on conceptual model and the extent to which it can be supported by available data

Documentation

- Models must be adequately documented so they can be evaluated
- Documentation should include
  - Conceptual model description, including important processes that affect results
  - Code selection
  - Model input and estimation of all parameters – data used, analyses conducted
  - Model calibration
  - Mass balance/error checks
  - Model results
  - Evaluation of model uncertainty
  - Documentation sufficient to reproduce modeling study

Summary – Modeling Process (cont.)

- Models must be well documented and “transparent” – no black boxes
- Uncertainty in model results needs to be stated and defined
- Limits to reliability of modeling – use ranges rather than absolute values
- Need for more long-term case studies (“post-audits”)
- Hardrock mine sites typically involve complex hydrologic and geochemical processes, and if applied appropriately, models can help us to understand these systems

Model Evaluation

- How does one judge whether a model or a set of models and their results are adequate for supporting regulatory decision making? The essence of the problem is whether the behavior of a model matches the behavior of the (real) system sufficiently for the regulatory context.

Excerpts from NAP (National Academies Press)
Models in Environmental Regulatory Decision Making (2007), chap. 4, Model Evaluation

Major problem: If model results agree with independent observational data does that mean that the model is correct?

Alternatively, if the model results don't agree with independent observations data does that mean that model is incorrect?

Model Evaluation

3 basic goals:

- the need to get the right answer

- the need to get the right answer for the right reason

- transparency

Model Evaluation; Nordstrom's Guidelines on the Use of Models

1. Modeling cannot give an exact answer, only an approximation.
2. Modeling can never substitute for reliable and relevant field data.
3. The biggest weaknesses of any model computation are the quality of the input data and the adequacy of the assumptions (implicit and explicit).
4. Model computations are not unique.
5. Model and code reliability can be tested in some limited ways.

Model Evaluation: Nordstrom's rules (cont.)

6. The main conclusion or argument based on model computation should be reproducible in a simpler manner by hand calculation.

7. Model computations must be explicable to non-modelers.

8. No matter how much data is acquired, no matter how sophisticated the modeling, there are always factors one cannot know that prevent our ability to predict the future.

9. The more sophisticated the modeling, the less we know about how well the model performs or how it works (the "complexity paradox").

10. Is it necessary to predict?

Model Evaluation

Many of these [environmental] models have a dangerous sophistication for computing almost any type of possibility without adequately constraining what is probable.

WHAT ARE MODELS AND MODEL VALIDATION? THE REGULATORY VIEWPOINT

"model - an assembly of concepts in the form of mathematical equations that portray understanding of a natural phenomenon."

ASTM (1984) "Standard Practice for Evaluating Environmental Fate Models or Chemicals"

"Model validation is the process of assuring that the models used adequately represent the real system behavior . . ."

OECD/NEA (1991)

". . assurance that a model, as embodied, in a computer code, is a correct representation of the process or system for which it is intended."

Nuclear Regulatory Commission

". . a process whose objective is to ascertain that the code or model indeed reflects the behavior of the real world."

USDOE

"Providing confidence that a computer code used in safety analysis is applicable for the specific repository system."

HSK (Swiss equiv. to USNRC,1993)

Evaluation Issues

Problem Identification	What is the goal of the model? Who will use it? What types of decisions will it support? What data are available to support the model?
Conceptual Model	Available and alternative theories Assumptions Uncertainties Peer Review
Constructed Model	Spatial/temporal resolution Algorithm choices Assumptions Data availability/software tools Quality assurance/quality control Test scenarios Corroboration with observation Uncertainty/Sensitivity Peer review
Model Use	Appropriateness of model for problem Assumptions Model extrapolation Input data quality Comparison with observation Uncertainty/Sensitivity analysis Peer review

"Providing confidence that a computer code used in safety analysis is applicable for the specific repository system."

HSK (Swiss equiv. to USNRC,1993)

WHAT IS PREDICTION?

Two meanings of this word are in usage:

LOGICAL PREDICTION

the deduced consequences of a model (scientific usage)

TEMPORAL PREDICTION

actual prediction of a future event in time (popular usage)

CONCLUSIONS

- No agreement on definition of model validation
- Model validation can be misleading
- Model validation can be always attainable
- Model validation can be always unattainable
- Philosophers argue against validation
- Scientists argue against validation