A COMPUTER SIMULATION PROBABILITY MODEL FOR GEOCHEMICAL PARAMETERS ASSOCIATED WITH COAL MINING OPERATIONS

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Abstract.--There have been many attempts to empirically model the environmental effects of various geochemical parameters associated with mining. Each of these attempts has encountered the single greatest barrier of any empirical approach; the randomness of data. Randomness manifests itself in many forms from the degree of variability within a specific dataset to the degree of intrinsic error associated with the measurement of certain variables. There are simply too many random processes, variables, and interrelations associated with a coal mine site to allow the depiction of any environmental response within reasonable certainty using only basic scientific principles, equations, and empirical formulae. Computer simulation modeling provides an effective mode of evaluating the intrinsics of such a random system. In order to generate a random probability simulation model, it is necessary to isolate pertinent elements of the system, which in this case are sulfate concentration, effluent flow, and kinetic rock properties. Some logistical set of formulated interactive governing rules must be then devised whereby the model can be limited to those aspects of the system which are deemed to be pertinent to the analysis and types of solutions for which answers are sought, which in this case is simultaneous pyrite oxidation-sulfate elimination. Within the context of this logic, a quantifiable ratio between the rate of acid generation within a mining system and the rate of acid elimination from the system has been derived. With this information in hand it is now possible to project the longevity of acid effluent from a mining operation, develop better treatment or ameiloration strategies, and determine the chemical impact of these mining operations on the immediate localized watershed.

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INTRODUCTION

A mathematical model is an attempt to quantify a specific parameter associated with a system on the basis of other measurable variables. The majority of such models deal with limited aspects of mining such as hydrological predictions, level of acid generation, or acid amelioration. Most of the models can be classified as being empirical; that is, a model dealing with variables simplified to standard regression formulae which usually have a basis in some standard chemical or engineering principle. A macromodel on the other hand, is a model which draws conclusions or predictions based on the entire mine operation with all of its interrelations and interactions.

Two important criteria exist concerning error and randomness and how these factors can effect the success of an empirical model:

1) THE MODEL MUST BE ABLE TO ABSORB THE INTRINSIC AND INHERENT ERROR OF THE SYSTEM

The model cannot be so filled with variables, constants, and complexities that the sum total of intrinsic error encountered in the measurement of the individual component variables and the error inherent in any subsequently predicted parameters becomes disguised in the form of high uncertainty. The inclusion into the model of any single variable or group of variables for which there exists a potentially high intrinsic error of measurement for the sake of higher statistical significance cannot be justified.

2) IT MUST BE ABLE TO MINIMIZE RANDOMNESS

The model may be highly dependent on variables which are random by their own nature. This randomness must be absorbed into the model and thus be reduced rather than subtly concealed in a region of high uncertainty brought about by the randomness.

A large-scale macromodel for mining operations seems to have eluded empirical modeling attempts. One need look no further than the two model qualifiers previously listed to discover the reasons; namely randomness and variable error.

Randomness and Mining Operations

Sources of randomness in an acid producing mining system can be found everywhere. Some of the sources show high levels of randomness while others will show low levels of randomness. A few of the highly variable parameters are summarized below:

1) THE VARIABILITY FOUND IN THE PERCENT TOTAL SULFUR OF INDIVIDUAL OVERBURDEN LITHOTYPES
2) EFFLUENT FLOW MEASUREMENT
3) CHEMICAL CONCENTRATION VS EFFLUENT FLOW The plot shown in figure 1 illustrates a mathematically random relationship between effluent sulfate concentration and flow
4) CLIMATIC FACTORS
5) TURBIDIMETRIC SULFATE ANALYSIS used as the measure of a acid generated
6) VARIABILITY OF PYRITE AS DETERMINED BY X-RAY DIFFRACTION ANALYSIS
7) VARIABILITY OF THE KINETIC RATE CONSTANT FOR PYRITE OXIDATION
8) VARIABILITY IN THE ACTUAL CHEMICAL MODEL

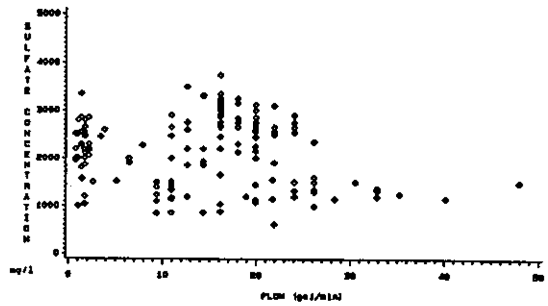

Figure 1. Random nature of sulfate concentration vs flow. Data from site DLM 133-78.

DESCRIPTION OF RESEARCH

A Random Probability Simulation Model

An alternative solution to the problems synonomous with empirical modeling is to develop a logical, quantifiable model that absorbs both randomness and error. Such a modeling scheme exists in Probability Simulation Modeling (PSM). In this type of predictive modeling, the randomness of the data itself and the error associated with individual measurements are both absorbed into the probability distribution of the data. The difference between the PSM approach and empirical modeling is that in PSM modeling the DISTRIBUTION of the data rather than the magnitude of INDIVIDUAL data points form the working data set.

One needs then to develop a logical set of rules to govern the relationship of the data distribution and any experimental parameter of interest. It is therefore possible to evaluate the effects of numerous possible combinations of parameter values (data randomness) that exist in their respective distributions.

Two important properties of a PSM are:

1) the scientific or mathematical principles governing the system have been obeyed and,
2) the statistical integrity of the original data is upheld.

The objective of this work was to develop a model which would focus on the two basic processes: 1) the production of acid within a minesite and 2) the elimination of the acid from the system. A well-established mathematical formulation known as Simultaneous Species Production-Elimination (SSPE) exists that logically describes a system. In essence, this principle states that the change in the rate of the appearance and disappearance of any species from a system is given by the differential.

$$\frac{dS}{dt} = aS(t) - bS(t) \qquad \text{(EQUATION 1)}$$

This mathematical relationship states that the rate of change with time of any chemical parameter, (S), is equal to the rate of production of S, (a), times the amount of S present at some time (t), minus the rate of elimination of S, (b), times the amount of S present at the same time, t.

This differential equation is then solved to yield a working mathematical relation:

$$S(t) = \frac{a S_0}{(b - a)} \left(e^{-at} - e^{-bt} \right) \qquad \text{(EQUATION 2)}$$

This is a member of a series of differential equations called the "Bateman Equations', after the man who derived them.

The rate constants a and b will subsequently be referred to as alpha and beta, respectively.

The SSPE model is utilized quite frequently in the study of natural systems such as the determination of the abundance of an intermediate radioactive isotope in a breakdown sequence, biochemical assimilation of hormones, and in the study of the potential effects of toxic wastes on biological systems.

The SSPE equation offers an excellent governing principle for a systems model that will allow the monitoring of pyrite oxidation products (including acid effluent) associated with a mining operation. The analogies to radioactive decay and biochemical production assimilations are parallel. In a mining operation, acid is formed as pyrite oxidizes to sulfate at a rate alpha. As a result of ground water movements, the sulfate is removed from the minesite at a rate beta. The overall process can be written:

$$FeS_2 \xrightarrow{\text{alpha}} SO_4^{-2} \text{ (in site)} \xrightarrow{\text{beta}} SO_4^{-2} \text{ (effluent)}$$

Once the values of alpha and beta (production and elimination) of the sulfate species are known, questions concerning the products of pyrite oxidation that can be answered include:

1. How fast are they being formed?
2. How fast are they being eliminated?
3. How long will the acid-producing process last?
4. What will be the effect on the system of a reduction in the magnitude of alpha as a result of the incorporation of an ameliorant?

These are questions that need to be addressed in order to solve the problems of acid mine drainage (AMD), but are questions that cannot be answered using empirical models without the introduction of large uncertainties. However, through a probability simulation analysis, solutions to such problems can be found.

The Generalized Concept of AMD as a SSPE System

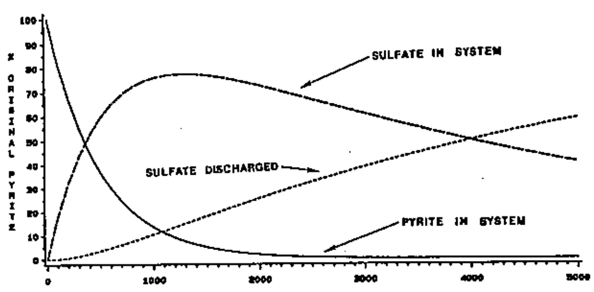

Figure 2. The pyrite-sulfate system showing the three prominent stages of sulfur species according to SSPE.

Figure 2 shows the percentage of original pyritic sulfur available in a mining system that through time exists as either unreacted pyrite, sulfate built up in the minesite, or discharged from the minesite as effluent. Note that there is a buildup of the products of oxidation (sulfate) in the system from the outset. The magnitude of alpha will determine the rate at which these oxidation products are generated. Conversely, beta is the prime indicator of the extent to which these products are being flushed from the system. It is, therefore, the ratio of alpha to beta that provides a complete insight into the buildup of oxidation products in the system. The equation tends to show that the time required for pyrite oxidation is short compared to the time required to flush the oxidation products from the system. The PSM provides a means to quantify these observations.

The Development of a Simulation Model

The goal of a simulation is to provide a mathematical procedure that will:

1) be able to utilize analytical data to predict parameters of an acid-producing system,
2) be as unaffected as possible by data randomness,
3) adhere to sound scientific principles, and
4) reproduce the statistical distribution observed in actual field data.

In order to develop such a simulation, it is necessary to know:

1) mine size and geometry,
2) field sulfate concentration and flow measurements of the effluents, the date and the discharge point where these measurements were made, and
3) geochemical and chemical kinetic rock properties (Sulfur content and Alpha values associated with the strata encountered in the minesite).

The water quality and flow data used in this study were obtained from three sources: 1) Data from samples collected at the actual field sites and analyzed by the Analytical Section of the West Virginia Geological Survey. Effluent flow measurements were made at the time of sample collection. 2) Data compiled in the Office of Surface Mining and the West Virginia Department of Energy, and 3) Information available on CRIS (Coal Reclamation Information System) DATABASE. The CRIS DATABASE includes a suite of water quality, overburden analyses, and general mine information for more than 300 minesites in the 12 northern coal producing counties of West Virginia. In addition, a complete suite of lithotypes associated with coal representing five different coal beds over a five-county area were collected and analyzed for numerous chemical properties, among which were the kinetic rate constant, alpha using a method developed and reported by the authors, and the total percent sulfur. These data are contained in a formatted form identified as the "WRI DATABASE OF CHEMICAL CHARACTERISTICS OF TOXIC ROCK MATERIALS". A compilation of the alpha value and the total percent sulfur ranges for different lithologies is shown in Tables 1 and 2 respectively.

Table 1 Range of alpha values for specific lithotypes from WRI database

TYPE	HIGH RANGE ALPHA	LOW RANGE ALPHA
BONE COAL	0.003428	0.000274
OVERBURDEN SHALE	0.009978	0.000073
PIT REFUSE	0.010681	0.001020
PREP REFUSE	0.030556	0.001074
ROOF SHALE	0.026499	0.000165
SANDSTONE	0.131424	0.000271
SEATEARTH	0.167421	0.001428
SHALE PARTING	0.105798	0.000676
SILTSTONE	0.021484	0.006730

TABLE 2. Range of sulfur values for specific lithotypes from WRI database

TYPE	LOW RANGE SULFUR	HIGH RANGE SULFUR
BONE COAL	0.195	5.040
OVERBURDEN SHALE	0.221	9.736
PIT REFUSE	0.080	4.242
PREP REFUSE	0.032	9.572
ROOF SHALE	0.030	7.010
SANDSTONE	0.004	10.063
SEATEARTH	0.037	9.144
SHALE PARTING	0.047	6.334
SILTSTONE	0.046	0.374

The Simulation

Following is a brief description of an actual computer simulation defining what the computer is doing and what decisions the computer is expected to make.

1. The computer reads into memory the following minesite data:
   a. The permit number
   b. Dates of active mining
   c. Present mine status
   d. Type of surface mine
   e. The disturbance acreage
2. The computer reads into memory the following field data:
   a. The date of sampling
   b. The location of sampling
   c. The sulfate concentration of the effluent
   d. The effluent flow measurement
3. The computer then determines the statistical relationship between the sulfate concentration data and the flow data for each sampling location. This is done for each season of the year. It is at this point that the computer is programmed to decide whether the sulfate-flow relationship for each discharge point and each annual season is:
   a. A completely random number (Figure 8)

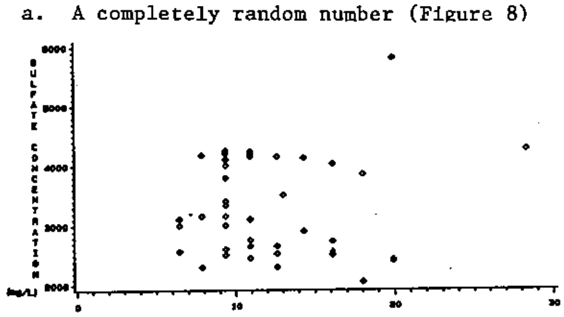

Figure 8. Random nature of sulfate concentration vs flow. Data from site DLM 71-75.

   b. A statistically significant inverse curve (Figure 9)

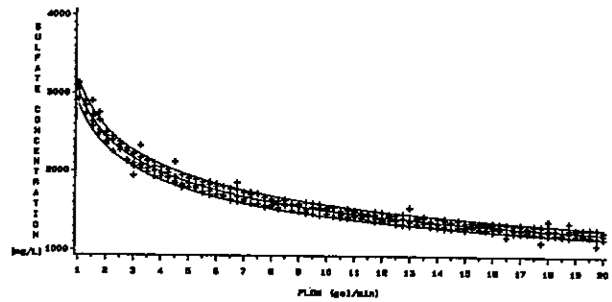

Figure 9. A computer generated statistically significant inverse relationship for sulfate concentration vs flow. No such relationship was encountered during the study.

   c. A multimodal random number (Figure 10)

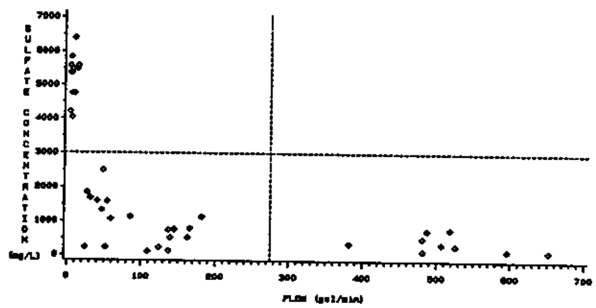

Figure 10. A multimodal random relationship between sulfate concentration vs flow. Data from site Bethel Road Refuse Pile.

These are the three relationships that have been shown to exist between sulfate concentration in the effluent and the flow measurement of the effluent. The criteria on which the computer makes this decision can be seen in table 3.

Table 3. Determination of data distribution type based on flow and sulfate concentration data.

TYPE OF DATA DISTRIBUTION	TYPE OF CORRELATION	CORRELATION COEFFICIENT	REMARKS
TOTALLY RANDOM	PEARSON	< 0.20	(SEE FIG. 8)
	40%-60% OF 10 RANDOM POINTS SHOW NEGATIVE SLOPES IN 1000 TRIALS	-----	
INVERSE	POWER TRANSFORMATION	> 0.90	(SEE FIG. 9)
MULTIMODAL RANDOM	CANONICAL GROUP CLUSTER	------	DEFAULTS IF OTHER DISTRIBUTIONS FALL (SEE FIG. 10)

4. The computer will then read available stratigraphic information, determine the volume percent of each significant stratigraphic layer, and will then determine an operational alpha value for the minesite based upon the compilation of alpha values in the "WRI DATABASE" and the geologic cross section or drill core log.

When all of the aforementioned information has been generated, the computer enters "RANDOM SIMULATION MODE", which is the portion of the software that determines the BETA value associated with the minesite.

RESULTS AND CONCLUSIONS

Results of the Simulation

Figure 3 is a histogram of beta values generated by 1 million computer simulations and beta

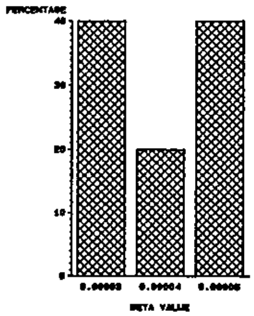

Figure 3. Histogram showing the range of beta values for site DLM 135-78 obtained from SSPE/PSM.

generations for a particular minesite. The field data for this graph are from the DLM permit 135-78 in Upshur County, WV. This distribution of beta is quite acceptable based on the narrow range of potential beta values that were generated.

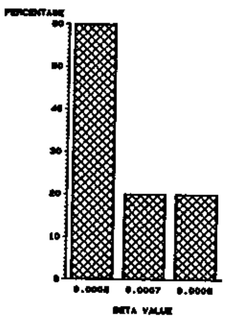

Figure 4. Histogram showing the range of beta values for site Bethel Road Refuse Pile obtained from SSPE/PSM.

Figure 4 shows a histogram for 1 million computer-generated beta values that correspond to field data on the Bethel Road gobpile, Monongalia, Co., WV. Note that the range of beta values calculated for the gobpile is smaller than the range of beta values for the DLM 135-78 site. The reason for the difference lies mainly in the characteristics of the materials of which the two sites are constituted. In a gobpile the material is essentially a single, relatively homogeneous lithology, namely prep plant refuse, while in a reclaimed surface mine, there is a diversity of lithologies. As a result, the number of combinations of possible sulfur and alpha values associated with the diverse lithologies found in a reclaimed surface mine are considerably greater than in the monolithologic gobpile.

This successful simulation was accomplished with a minimum number of empirical formulae. The simulation has completely absorbed all of the randomness associated with the measurement and distribution of these data. As can be seen in Table 4,

Table 4. DLM 135-78 sulfate and flow, actual (field) and simulation statistics.

VARIABLE[1]	MEAN	STANDARD DEVIATION
----------------	DISCHARGE PT = 1	--------------
FIELD SULFATE	1,272.4	234.1
SIMULATION SULFATE	1,274.4	230.8
FIELD FLOW	19.7	9.8
SIMULATION FLOW	19.8	9.5
----------------	DISCHARGE PT = 2	--------------
FIELD SULFATE	2,589.7	633.3
SIMULATION SULFATE	2,587.8	638.0
FIELD FLOW	17.1	4.7
SIMULATION FLOW	17.3	4.5
----------------	DISCHARGE PT = 2A	--------------
FIELD SULFATE	2,244.1	507.7
SIMULATION SULFATE	2,238.8	504.8
FIELD FLOW	1.5	0.59
SIMULATION FLOW	1.5	0.57
----------------	DISCHARGE PT = 2B	--------------
FIELD SULFATE	2,633.1	443.5
SIMULATION SULFATE	2,599.9	448.8
FIELD FLOW	15.3	5.7
SIMULATION FLOW	15.2	5.4

[1] Sulfate measurements in mg/L and flow measurements in gal/min.

the statistical distribution of the sulfate concentration and flow values generated in the random simulation matches the statistical distribution of the original data set very closely. In other words, the mining system has been found to adhere to the Simultaneous Species Production-Elimination principle.

With the computer generation of a beta value, all the data needed to analyze the pyrite oxidation and oxidation product elimination associated with the system are available. Using EQUATION 2, sulfate concentrations of effluents were calculated using a time-series algorithm.

Figure 5 shows the computer-projected sulfate

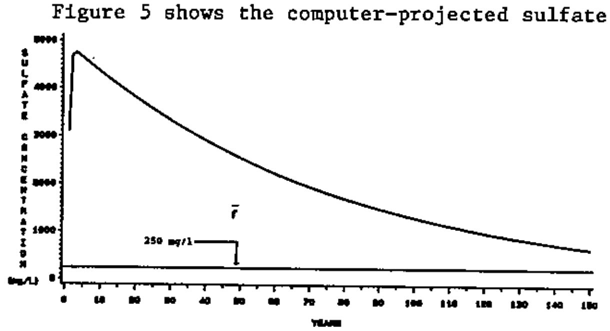

Figure 5. Curve showing the longevity for site DLM 135-78.

concentration of the minesite discharge of DLM permit 135-78. The discharge is projected to 250 mg/L sulfate concentration (drinking water standard). From this plot it is possible to make an estimate of the acid-producing lifetime of the minesite. The computer-generated curve is based on all of the sulfate and effluent discharging from a single point. Figure 6 displays a significant break that

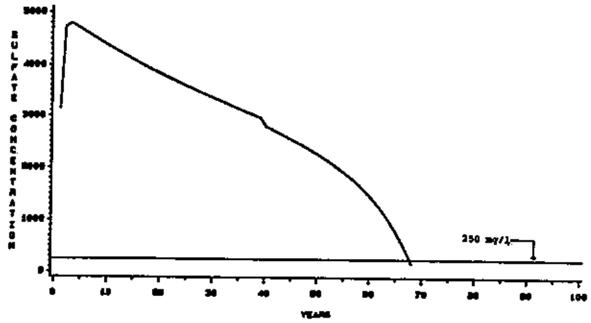

Figure 6. Longevity curve for DLM 135-78 with a 'hypothetical break' point.

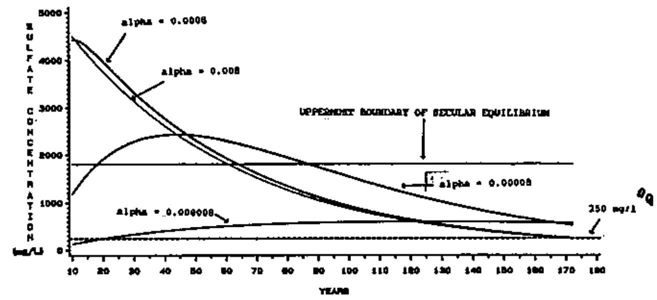

Figure 7. Effect of amelioration on the alpha value of a mining system.

occurs when alpha no longer plays a significant role in the system. It is at this point that the amount of reactive material has been reduced to a negligible level. This break point is arrived at using the laws of chemical kinetics and the mean-lifetime concept of reactive substances. This estimation is preliminary and further study is necessary to ascertain a more exact break point. Table 5 gives the beta and longevity information,

Table 5. Beta values and projected longevities of various studied minesites.

MINE SITE	BETA (1/days)	ACTIVE LONGEVITY (years)
BETHEL ROAD GOBPILE	5×10^{-3}	30-40
DLM 135-75 MT. TOP REMOVAL	5×10^{-4}	45 +
DLM 23-76 MT. TOP REMOVAL	2×10^{-4}	45 +
DLM 71-75 MT. TOP REMOVAL	5×10^{-4}	45 +
DLM 58-77 MT. TOP REMOVAL	5×10^{-4}	45 +
EVERETTSVILLE GOBPILE	5×10^{-3}	25-30
PIERCE SITE	2×10^{-4}	50 +
WALNUT HILL GOBPILE	1.5×10^{-3}	28 +

the time required before the level of oxidation products released from the system is environmentally acceptable within the context of existing regulations, for the sites studied. The time (years) axis corresponds to the elapsed time from the initiation of mining.

Amelioration and the SSPE/PSM Model

The amelioration production-elimination model allows the development of an amelioration strategy. Beta values, being related to physical parameters, do not change with amelioration. Alpha, on the other hand being related to chemical parameter values do change. The purpose of amelioration is to reduce the alpha value (the rate of pyrite oxidation) to a level where the mine system will approach a condition known as 'secular equilibrium'. When a system has achieved secular equilibirum, the build-up of oxidation products is drastically reduced. At this point, the concentration of oxidation products being generated approaches zero. Figure 7 shows the theoretical effect on the sulfate concentration of a mine discharge existing at various alpha levels. The alpha and beta values chosen to generate this graph are those associated with the DLM permit 135-78. The curve is denoted as 'control'. This graph does NOT show the existing effect of amelioration on this particular minesite, but what the effect would have been had proper amelioration of pyrite oxidation been carried out as part of the overall mining operation while the minesite was active. The lowest curve represents an alpha reduction of 1000 times. The curve (alpha = 0.000008) is the upper boundary of 'secular equilibrium'. The mathematics dictate that the sulfate concentration must gradually increase, but it can be easily seen that below the curve corresponding to alpha = 0.000008, in the region of 'secular equilibrium', the concentration of pyrite oxidation products in the discharge are quite manageable. Not only are the concentrations of oxidation products being generated very low, but the build up of oxidation products in the system is also low.

Hydrological Impact Assessment and the SSPE/PSM Model

The proposed model can also be used to evaluate the hydrological impact assessment potential of a proposed minesite. Knowing the alpha, beta and discharge distribution for a particular mining operation, a discharge simulation is possible. When this discharge simulation is added to existing stream quality data and principles of mass balance, a hydrological impact simulation (assessment) is possible.

Data were extracted from the CRIS DATABASE. Search of the data base located an area where water quality and flow data existed prior to the 1982 initiation of a proposed downstream mining operation. This particular mine site was chosen for three reasons: 1) the isolated nature of the proposed site provided an excellent proving ground for the simulation, 2) the proposed site was to be a mountaintop removal operation; a mine type for which the beta (chemical elimination) constants for the pyrite-sulfate system were reasonably well established during the course of this current research endeavor, and 3) stream quality data for a downstream area were compiled in 1985. Using the pre-1982 water quality data and the available general mine information data, a new prototype model was developed for the purpose of simulating the mine discharge into the stream from a minesite exhibiting the chemical patterns reflective of the pre-1982 data. The model included the development of alpha and beta values that could be expected for species other than sulfate ion. The simulation was used to project the change in basic water quality parameters that would result from the mining operation and predict the water quality that would be seen by the year 1985. These predicted data were then compared to the actual 1985 data taken downstream from the 1982 mining operation. Using beta values found to be common to mountain top removal operations for the respective ions in question, this new prototype computer simulation package and a system now comprised of the mining operation and the receiving stream, the results shown by the 1985 water quality study were accurately projected (See table 6).

Table 6. CHIA predictive capabilities of PSM modeling technique for a selected mining operation.

CHEMICAL SPECIES	1982 ANALYSIS (mg/L)	2-YEAR PROJECTON	1985 ANALYSIS (mg/L)
SULPATE	940	slight increase to 1,020 mg/l	1,030
IRON	58	very slight increase; estimate should be (statistically) about equal	48
ACIDITY	510	moderate increase (15%)	575
MANGANESE	.05	no statistical change	.04

CONCLUSIONS

This research has established several important points: 1) the nature of the data associated with a mining operation is too randomly distributed and too high in intrinsic error of measurement to be used in a reliable empirical model. 2) the distribution of this randomness and error can be incorporated into a viable model provided this model is designed to deal with distributions of data, rather than discrete data points or statistical averages assumed to be Gaussian distributions. Such modeling technique is called a "RANDOM PROBABILITY SIMULATION" or PSM. In order to utilize a PSM one must first find a logical, scientifically sound principle that governs the system in question. The mathematical concept of Simultaneous Species Production-Elimination meets all logistical and scientific criteria as a governing principle for the generation and discharge of geochemical parameters associated with pyrite oxidation in a mining operation. 3) this mathematical principle incorporated into a PSM allows the critical evaluation of the pyrite oxidation-acid elimination relationship that exists in a mine. Knowing this relationship allows scientifically sound amelioration planning and with modification, will allow the development of a viable hydrological impact assessment procedure that will be relatively free from guesswork and random error. The relationship between pyrite oxidation and effluent discharge for a particular mining operation can be quickly established using existing field data, making the model quite useful in reclamation planning with abandoned mine lands.

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