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MACRO1: A CODE TO TEST A METHODOLOGY FOR ANALYZING NUCLEAR-WASTE MANAGEMENT SYSTEMS

ABSTRACT

The MACRO1 computer code has been written to test a methodology for analyzing nuclear-waste management systems. The code is primarily a manager of probabilistic data and deterministic mathematical models. The user determines the desired aggregation of the available models into a composite model of a physical system. MACRO1 then propagates the finite probability distributions of the inputs to the model to finite probability distributions over the outputs. MACRO1 has been applied to a sample analysis of a nuclear-waste repository, and its results compared satisfactorily with previously obtained Monte Carlo statistics. A more refined and extensive version of the code, MACRO2, is currently being prepared.

INTRODUCTION

Lawrence Livermore Laboratory is engaged in a study of the performance of deep geologic repositories for high-level nuclear wastes. The purpose of the study is to aid the U.S. Nuclear Regulatory Commission in making decisions about waste-repository regulations and licensing applications.

The following paragraphs, from a report prepared in 1978,[1] describe the ramifications involved in such a study.

> "Evaluating the hazards associated with the disposal of high-level radioactive wastes in deep geologic strata demands that we acknowledge the uncertainties implicit in our predictions. These uncertainties by no means invalidate the findings of waste disposal studies, but only by properly accounting for the uncertainties can we assure that conclusions and forecasts will stand up to criticism. And only if the uncertainties are dealt with quantitatively is it likely that some disposal sites can be confidently evaluated as safe and that the sites with the greatest

margins of safety can be identified. In addition, by identifying the sources of the uncertainties we can separate disposal sites that are merely unacceptable today (but that might become acceptable as technology improves and uncertainties diminish) from those that are clearly inappropriate for waste disposal. Identifying those same sources of uncertainty also provides direction for future research. Prediction uncertainties in this scheme arise from three sources, which can be described as follows:

"● Descriptive uncertainties. These include uncertainties in all the parameters used to describe the disposal site, for example, the dimensions of aquifers, the porosity of surrounding rock, the thickness of rock layers, and the temperature.

"● Dynamic uncertainties. These are the uncertainties in the mathematical model used to predict the future dispersion of the waste. They include, for example, uncertainties in the dynamical laws that govern the interactions between the waste and the geologic environments.

"● Random-event uncertainties. Events such as meteor strikes and earthquakes cannot be predicted, but they can be dealt with statistically. They form a third group of uncertainties.

"If we were to take these sources of uncertainty to be independent, the total uncertainty in the predicted hazard from the buried waste could be written as

$$\sigma_{TOT} = \sqrt{\sigma_D^2 + \sigma_M^2 + \sigma_R^2} \quad ,$$

where σ_D, σ_M, and σ_R are the uncertainties in the hazard due respectively to descriptive, dynamic, and random-event uncertainties. The total uncertainty is a reflection of the state of current technology--which determines how accurately we can describe the site and how accurately we can model future behavior--and is a measure of how confidently decisions and predictions can be made. Thus one of the obvious aims of residual uncertainty analysis is suggesting ways to reduce the size of σ_{TOT} by pointing to the sources of uncertainty most likely to yield to further work."

We wrote the MACRO1 computer code to test the implementation of the probabilistic arithmetic methodology proposed by Kaplan.[2] Because it is a test code, MACRO1's primary purpose is to aid in the design and development of MACRO2, a more extensive and refined code for analyzing uncertainty in nuclear-waste disposal systems.

MACRO1 is primarily aimed at the propagation of descriptive uncertainties through dynamic models. It does not provide for the rigorous correlations and constraints necessary to describe accurately the physics of the system. Input variables and portions of the system are treated as if they were statistically independent.

This assumption of independence has the effect of overstating the degree of uncertainty concerning system parameters and system performance. For example, measurements of permeability and porosity for a particular formation indicate a relatively strong correlation.[3] Ignoring this correlation results in computation of unrealistically large spreads in water velocities.

The simple physics models available in MACRO1 are nuclide transport models and one-dimensional hydrology models.[4,5] Since physical constraints, correlations between variables, and laws of conservation are not rigorously satisfied, any probabilistic results must be interpreted with great care.

PROBLEM DESCRIPTION AND SOLUTION

MACRO1 solves a class of problems that determine the probability distribution on a set of output variables, given the probability distribution on a set of input variables and a deterministic function from the input variables to the output variables.

This transformation problem is expressed as

$$p(\bar{Y}) = \int_{S_I} p(\bar{x})\,\delta(f(\bar{x}) - \bar{Y})\,d\bar{x} \tag{1}$$

where

$\bar{Y}$ is a vector of output variables, $\bar{Y} = (y_1, y_2, \ldots, y_n)$

$\bar{x}$ is a vector of input variables, $\bar{x} = (x_1, x_2, \ldots, x_m)$

S_I is the m-dimensional input sample space = $\left\{\bar{x} \mid \bar{x} \text{ is an input}\right\}$

S_O is the n-dimensional output sample space = $\left\{\bar{Y} \mid \bar{Y} = f(\bar{x}),\ \bar{x} \epsilon S_I\right\}$

f is the deterministic function from S_I to S_O

$p(\bar{x})$ is the probability density function over S_I

$p(\bar{Y})$ is the probability density function over S_O

$\delta(f(\bar{x}) - \bar{Y})$ is the Dirac delta function.

The MACRO1 computer code approximates the probability density functions over S_I and S_O by partitioning S_I and S_O into a union of disjoint subsets I_i and O_j:

$$S_I \equiv \bigcup_{i=1}^{I} I_i\ ,\ I_i \cap I_j = \emptyset \text{ if } i \neq j \tag{2}$$

$$S_O \equiv \bigcup_{j=0}^{J} O_j\ ,\ O_i \cap O_j = \emptyset \text{ if } i \neq j \tag{3}$$

and

$$p(\bar{x} \epsilon I_i) = \int_{I_i} p(\bar{x})\ d\bar{x},\ i = 1,2,\ldots, I \tag{4}$$

$$p(\bar{y}\epsilon O_j) = \int_{O_j} p(\bar{y})\, d\bar{y},\ j = 1,2,\ldots, J\ . \tag{5}$$

MACRO1 then approximates the integrals of Eqs. (1) and (5), given the discretization of Eqs. (2) and (3), the input distribution, Eq. (4), and the deterministic model f. This approximation uses the probabilistic arithmetic described by Kaplan.[2]

FINITE PROBABILITY DISTRIBUTIONS

Since we are interested in computer calculations, we define finite probability distributions as sets of doublets,

$$\left\{<\bar{x}_i, P_i>;\ i = 1,2,\ldots, I\right\}\ , \tag{6}$$

where

$\bar{x}_i$ is a representative value denoting neighborhood (some I_j of Eq. 2)

P_i is the probability that $\bar{x}$ is in the neighborhood of Eq. (4).

For example, in MACRO1, if x is a scalar variable, we may define

$$x_i = 10^{i/M},\quad i = 0,\pm1,\pm2,\ldots\ ,$$

where M is some fixed number per decade (say $M \approx 5$). We then define the neighborhoods as the half-open intervals

$$N(x_i) = (x_{i-1/2}, x_{i+1/2}] = \left(10^{\frac{2i-1}{2M}}, 10^{\frac{2i+1}{2M}}\right] \tag{7}$$

and let P_i be the probability that variable $x\epsilon N(x_i)$.

Now, if we truncate and normalize, we say that

$$\left\{<x_i, P_i>\,|\, i = \underline{i}, \underline{i}+1,\ldots, \bar{i}-1, \bar{i}\ ;\ \sum_{i=\underline{i}}^{i=\bar{i}} P_i = 1\right\} \tag{8}$$

is a finite probability distribution (FPD) and may be thought of as a discrete approximation to the continuous probability density function, $p(x)$, of the variable x.

The generalization to vector-valued x is straightforward. We need only decide on neighborhood and truncations to reduce the continuous density function to a discrete approximation. For example, in MACRO1, we consider that, if $\bar{x} = (x,y)$, then

$$N(x_i y_j) \equiv \left(x \frac{2i-1}{2M}, x \frac{2i+1}{2M}\right] \oplus \left(y \frac{2j-1}{2N}, y \frac{2j+1}{2N}\right] , \tag{9}$$

where, as before, M and N describe the number per decade. The joint FPD then is described by the set

$$\left\{ \langle x_i y_j, P_{ij} \rangle \,|\, i=\underline{i},\underline{i}+1,\ldots,\bar{i};\, j=\underline{j},\underline{j}+1,\ldots,\bar{j} \;,\; \sum_{i=\underline{i}}^{\bar{i}} \sum_{j=\underline{j}}^{\bar{j}} P_{ij} = 1 \right\} \tag{10}$$

and P_{ij} is the probability that x and y are in the half-open rectangular neighborhood $N(x_i y_j)$.

PROBABILISTIC ARITHMETIC

Suppose x and y are independent, uncertain variables and suppose our states of knowledge with respect to x and y are expressed by the FPDs

$$\begin{aligned} x &= \left\{ \langle x_i, P_i \rangle \,|\, i=\underline{i},\underline{i}+1,\ldots,\bar{i}-1,\bar{i} \right\} \\ y &= \left\{ \langle y_j, Q_j \rangle \,|\, j=\underline{j},\underline{j}+1,\ldots,\bar{j}-1,\bar{j} \right\} . \end{aligned} \tag{11}$$

Let $\oplus$ stand for a deterministic combining of the inputs x and y to an output variable z:

$$z = x \oplus y ,$$

where $\oplus$ may be a simple arithmetic operator such as +, ×, -, ÷, or where $\oplus$ may, in fact, be a physics model. Then, following Kaplan's methodology, we use nested DO loops to compute the output FPD, first by

$$\left\{ \langle z_{ij}, R_{ij} \rangle \right\} = \left\{ \langle x_i \oplus y_j, P_i Q_j \rangle \,\middle|\, \begin{matrix} i=\underline{i},\underline{i}+1,\ldots,\bar{i}-1,\bar{i}, \\ j=\underline{j},\underline{j}+1,\ldots,\bar{j}-1,\bar{j} \end{matrix} \right\} \tag{12}$$

and then by applying a condensation to a previously discretized output space to obtain

$$\left\{\langle z_k, S_k\rangle \,|\, k=\underline{k},\underline{k}+1,\ldots,\overline{k}-1,\overline{k};\ \sum_k S_k=1\right\}, \tag{13}$$

where

$$S_k = \sum_{\left\{i,j \,|\, z_{ij} \in N(z_k)\right\}} P_i Q_j$$

and

$$\underline{k} = \text{minimum}\left\{k \,|\, S_k \neq 0\right\}$$
$$\overline{k} = \text{maximum}\left\{k \,|\, S_k \neq 0\right\}.$$

The extension to more than two independent input variables is the obvious one. However, if possible, we "factor" models using the condensation at intermediate steps (see the section on Factorization of Models).

If the inputs are mutually dependent, that is, are represented by a joint FPD, the procedure is essentially the same as above. We merely use $R_{ij} = P_{ij}$ = the probability that x and y are in the neighborhood represented by $N(x_i y_j)$ in the first step.

Some MACRO1 models allow for joint inputs of the form z = f(x,y). However, if, for example, y is jointly distributed with w and our model is to compute z = f(x,y), we require P(y) be extracted from the joint FPD to some new variable (say, a), and then we perform the function z = f(x,a).

MULTIPLE OUTPUT FUNCTIONS

Suppose we have a mathematical function from some input space to a two-dimensional output space:

$$(a,b) = f(x,y,z).$$

The MACRO1 methodology is then extended to produce an output joint FPD of the form of Eq. (10). MACRO1 does not make the general extension to more than two dimensions.

TRUNCATION OF FPDs

A large number of probability density functions, $p(x)$, have nonzero values for the full range $-\infty < x < \infty$, a range that is impractical for discrete computer usage. Hence, when we input an FPD, we allow for truncation of the tails. Further, FPDs that result from a model calculation may be truncated. MACRO1 offers the user several choices:

1. For input of normal or lognormal distributions, the user may specify some number N of standard deviations. The resultant FPD is truncated such that, if μ is the mean and σ the standard deviation, then

$$\text{if } x < \mu - N\sigma, \; p(x) = 0$$

or

$$\text{if } x > \mu + N\sigma, \; p(x) = 0.$$

2. FPDs may be nonsymmetrically truncated at the tails on the basis of the values of the accumulated probability, that is,

$$P_i \equiv 0 \text{ for all } i \text{ such that } \sum_{i<\underline{i}} P_i < (\text{input value 1})$$

and

$$P_i \equiv 0 \text{ for all } i \text{ such that } \sum_{i>\underline{i}} (1-P_i) < (\text{input value 2}).$$

3. MACRO1 includes a maximum value truncation. In this case, let $\hat{P}$ be the maximum probability in a generated FPD and let f be an input factor for which $0 < f < 1$. Then, for all i, where $\underline{i} \leq i \leq \overline{i}$, if $P_i < f\hat{P}$, P_i is set to zero.

In all the above truncations, the resultant FPD is normalized so that $\sum_i P_i = 1$.

Generally we use truncations not only on the tails of distributions, but also on relatively low values of probability. Thus, low values are not necessarily properly taken into account. For lognormal distributions in particular, truncation of the tails may result in highly incorrect values of the mean. The median is not significantly affected.

ACCURACY OF THE MATHEMATICAL METHODOLOGY

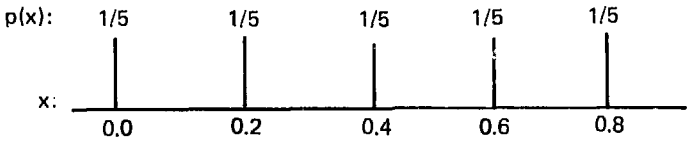
In MACRO1 we have not attempted to include the "mean preserving" discretizations as discussed in Refs. 2 and 6. In fact, in using MACRO1 as a test code, we have assumed that all variables are positive definite and that all variables can be reasonably discretized by Eqs. (7) and (9).

The default value for M, the number per decade, is 5. However, the user may choose different positive integer values for M, both for input variable discretization and for "prediscretization" of output variables.

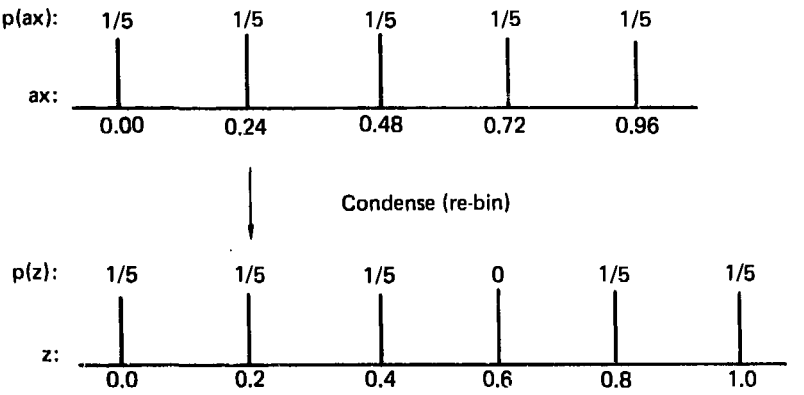
As with any discrete approximation to continuous (or even discontinuous) mathematics, the accuracy is highly dependent on the step-size chosen for the discretization. We consider two examples, both provided by W. J. O'Connell, Lawrence Livermore Laboratory.

Strobe Effect

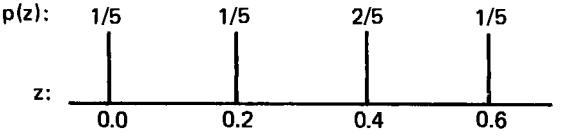
Consider an FPD for x as follows. The bins for x are centered on the values shown.



Now consider $z = a*x$, where $a = 1.2$ only. (a may be a constant, or $a = 1.2$ may be a value in a discretization of the $\bar{a}$ range.) The bin $z = 0.6$ is missed in the condensation operation. This pattern would be repeated regularly at $z = 1.8, 3.0, 4.2...$, because of the regular discretization of x.

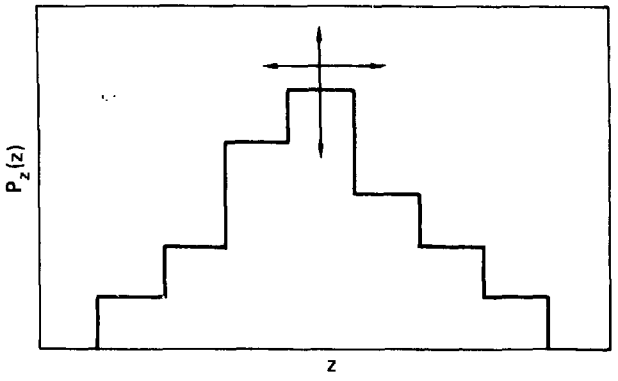


As the next example, consider z = a*x, where a = 0.8 only. For the same p(x) and discretizations as above, the result for z is:



Fuzziness Propagation

In the representation of $p_z(z)$ shown below, we define the uncertainty in $p_z(z)$ at z as the uncertainty in its value at z (the vertical arrow), and the fuzziness as the uncertainty in z as to which z bin an element of the total probability properly belongs. The total sum of $p_z(z)$ over z is fixed at 1.0.



If we discretize x at $\Delta x = 0.2$, the FPD's ability to represent the probability distribution of x is limited to intervals of $\Delta x = 0.2$.

Normally, when we add n variables, each having an uncertainty Δ, the result has an uncertainty $\Delta\sqrt{n}$. If we add the n variables pairwise with a condensation operation after each step, however, the error in the result will be larger.

If we have x and y with discretizations at Δx and Δy, $z = x \cdot y$ will have an error $\delta z^2 = x^2 \cdot \Delta y^2 + y^2 \cdot \Delta x^2 + \Delta x^2 \cdot \Delta y^2$. If this is followed by a condensation operation, the fuzziness δz is compounded by the discretization Δz and by the summing over bins in (x,y) that have different values for δz.

Improvements in Accuracy

It is possible to increase accuracy, at the cost of an increase in computer time. More finely discretized input parameters usually remove or reduce the strobe effect as well as the fuzziness. Smaller values for truncation factors and larger values for the number of standard-deviation truncations on input will reduce the truncation inaccuracies.

We have not presently developed algorithmic quantifiers for how much discretization and/or truncation is acceptable. Users of MACRO1 must consider each case, consider results in terms of "over several bins," and make decisions accordingly.

The MACRO1 computer code is a user-oriented manager of models and data. The data consist of both certain and uncertain variables (that is, FPDs); in the latter case, probabilities are propagated throughout the system as the models are executed. For readability, MACRO1 is coded in LRLTRAN in the form of subroutines. The MACRO1 code is highly interactive and contains an extensive HELP package, reproduced in Appendix A.

MACRO LANGUAGE

The MACRO language is a versatile one that allows the user--who will be an analyst--to choose, interactively, the models for his analysis and their order of execution. The commands are of the general form

TYPE MODEL [*input1,...,input10; output1,...output10*].

where *input* and *output* are either variable names or specifications of input-output devices.

The user names the variables, choosing names of up to 10 alphanumeric characters (for example, HEAD, LENGTH1, T1+T2). Since variable names primarily refer to the pointers to an FPD, its storage location, and its type, the FORTRAN conventions of decimal and integer naming have no meaning. Thus, K2 can refer to a floating-point variable.

The designated MODEL must be the name of a subroutine in MACRO1. These subroutines are the mathematics and physics models discussed in more detail in the next major section. They are listed in the HELP package (Appendix A).

MACRO recognizes four TYPEs of command:

1. INPUT - A series of models to input variable names and generate FPDs.

2. OUTPUT - A series of write and plot routines to display data numerically or graphically.

3. PROPAGATE - Executes the mathematics and physics models and propagates FPDs associated with uncertain inputs through these models to form output FPDs.

4. UTILITY - Executes a series of "housekeeping" routines; includes a set of commands that set up looping over a contiguous subset of commands for a prescribed number of times. The command set to be looped over may be altered by deleting or adding commands.

The amount of data to be generated during any analysis is never known in advance. The number of input and output variable names and their associated FPDs are specified by the user. To maintain the necessary flexibility and to conserve computer memory space, MACRO1 uses a data-naming and management methodology that is largely a set of pointers and attributes coupled with a dynamic linear memory allocation for FPD data.

MACRO1 memory consists of an expandable array, named DAT, in large-core memory. It contains the FPD probability values and

NNAM - pointer to next available pointer and attribute set.

NDA - pointer to next available location in DAT array. For each variable, N=1,2,..., NNAM-1.

NAME(N) - ASCII variable name.

NPD(N) - number of points per decade, M, where $x_i = 10^{i/M}$.

IMIN(N), IMAX(N) - lower and upper index for an FPD, $\{<x_i,P_i>;\ i = IMIN(N),\ldots,IMAX(N)\}$.

NDA(N) - pointer to the start of P_i in the DAT array.

JPD(N) - if part of a joint FPD, points to the name of the other variable.

NVC(N) - number of vector components if this is a vector variable.

NT1(N) - indicates origin of this variable, input, computed, etc.

NTS(N) - if input, member of standard deviations about the mean at which to truncate the FPD.

VM(N) - median value of the FPD.

SIG(N) - standard deviation of the FPD.

PSTL(N) - total amount of probability truncated because of NTS × SIG about the median.

PTFL(N) - total amount of probability truncated because of either accumulated truncation of tails or from $P_i < f \cdot P_{max}$ means set $P_i = 0$.

All FPDs are initially generated, condensed, and truncated in a temporary work space. The final values are normalized and then stored in the DAT array with appropriate values set for the pointers.

The UTILITY DISCARD routine allows any variable to be discarded when it is no longer needed. Pointers are reset and the DAT array is reduced in size.

INTERFACING WITH MODELS

In general, the interface to any particular mathematics or physics model requires

1. A check to see that the proper number of input variables has been specified and that each of these inputs has been previously defined.

2. A check to see that the proper number of output variables has been specified and that output names have not been previously used.

3. Proper sets of DO loops to compute the probability distributions.

4. Calls to the deterministic mathematics and physics subroutines.

5. Discretization of the output variables to complete the condensation operation.

6. Truncations (if desired) and storage of the resultant FPDs.

MODELS IN MACRO1

A model in MACRO1 is a set of computer algorithms that take given input parameters and by some combination produce output parameters. The models themselves are deterministic; however, uncertain inputs produce uncertain outputs. In general, we have models that are purely mathematical and models that are mathematical algorithms to compute physical processes.

The mathematics models are straightforward and virtually self-explanatory. The physics models are those required for the analysis of Mock Site A, a hypothetical waste-repository site that has also been modeled by other means. Appendix B discusses the validity and rationale of the physics models, and Refs. 3, 4, 5 and 7 augment the discussion.

FACTORIZATION OF MODELS

The computing speed of MACRO1 is greatly enhanced by using the condensation operation described in Eq. (13) at intermediate steps of "factored" models. The concept of factorization can be most readily described by a simple example.

Suppose our model is

$$w = xyz$$

and that each of x, y, and z are FPDs with 10^2 entries of nonzero probability. The straightforward three-deep DO loops of the methodology would then require 10^6 multiplications.

However, suppose that we "factor" the model to

$$u = xy$$

$$w = uz.$$

Then w = uz is mathematically equivalent to w = xyz by the associative law. In this case, u = xy requires 10^4 multiplications, and if u "condenses" to any number of neighborhoods less than $10^4 - 10^2$, we gain computationally. If, for example, u condenses to 10^2 neighborhoods, w = uz requires 10^4

multiplications. In that case, $w = uz = (xy)z$ requires a total of 2×10^4, still considerably less than 10^6.

Note that, if inputs are mutually dependent or if multiple outputs are generated, extreme care must be taken in the factorization. It may not be possible to factor some models readily or accurately. For example, suppose we wish to solve a one-dimensional hydrology and transport model. We are given

ΔH = head difference
L = length of flow path
K = hydraulic conductivity
η = effective porosity

and the equations

$$t = \frac{L}{v} \quad ,$$

where $v = \frac{q}{\eta}$ and $q = - \frac{k\Delta H}{L}$.

If we assume that ΔH, L, K, and η are all independent, we might compute, in a "factored" mode,

$$G = \frac{\Delta H}{L}$$

$$q = -GK$$

$$v = q/\eta$$

$$t = L/v,$$

which erroneously neglects the fact that the L in the last factor is identical with (and therefore dependent on) the L in the first factor.

If we now ignore the physics involved (that is, gradient, D'Arcy speed, velocity, time) and write

$$x = K/\eta$$

$$y = -\Delta H x$$

$$t = L^2/y,$$

the deterministic result is the same and we use the probability over L only once.

Suppose k and η are closely correlated (a "data" fact more than a "physics" fact, as described in Ref. 3), the computation of x in the above sequence can be readily accommodated and this factorization is acceptable. If, however, ΔH, K, and η were somehow correlated (a joint FPD), the above model would have to be factored differently or the basic methodology altered.

The primary point is that factorization can gain computing speed, but the user must factor consistent with the mathematics of the methodology rather than with physical constraints.

SAMPLE MACRO1 ANALYSIS OF A REPOSITORY

Mock Site A is a hypothetical site for a waste repository. It is based on actual geologic data and has been studied intensively[8] for the purpose of developing a methodology for evaluating nuclear waste repositories.

We used MACRO1 to analyze Mock Site A and compared our results with previously obtained Monte Carlo results.[7] The next section, which was virtually copied from Ref. 7, describes the Monte Carlo results.

MONTE CARLO ANALYSIS

Golder Associates devised the basic flow-path model of the preferred hydrology at Mock Site A. This model, containing five nodes and four flow paths, is shown in Fig. 1. The repository is located at node 1 in a layer of marlstone. Ground water leaving the repository flows downward to a lower aquifer (node 2), which at that point is at a lower hydraulic head than the upper aquifer. At the hinge line, the aquifer heads become equal. To the right of the hinge line, the lower aquifer is at a higher hydraulic head than the upper aquifer. Thus, at node 3 the ground water flows upward to the upper

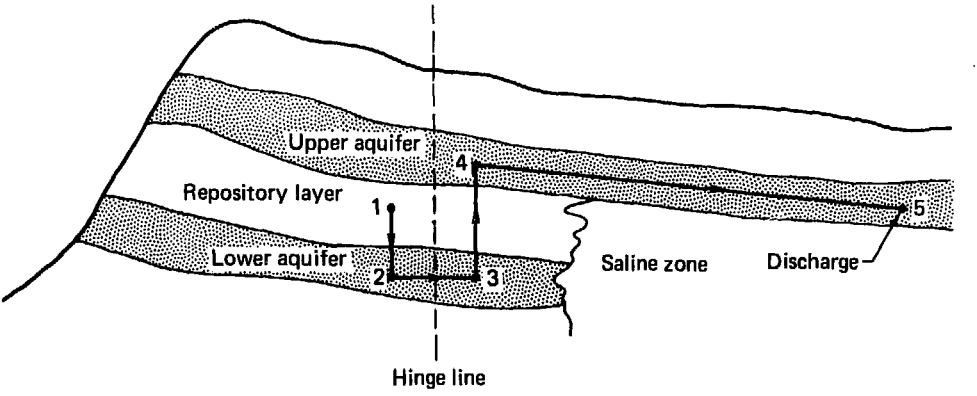


FIG. 1. Flow-path model for Monte Carlo calculation. The drawing is not to scale; the vertical scale has been exaggerated.

aquifer (node 4). The ground water then flows in the aquifer to a discharge at node 5. Note that the lower aquifer ends at a large saline zone.

This five-node model was analyzed by the Monte Carlo code NUTRAN, which simulates the flow of waste from the repository to the biosphere. Four types of inputs were used in NUTRAN: the properties of the flow paths, the head drops of the flow paths, the waste-dissolution properties, and the retardation factors.

Intrinsic Properties of Flow Paths

Table 1 presents the length, cross-sectional area, permeability, porosity, and dispersion of each flow path. All of these variables were assumed to be independent. All variables were bounded below by 0, and porosity was also bounded above by 1. The value used for the permeability of the pathway from the depository to the local aquifer was 10 times larger than actually found. This discrepancy causes only a very small change in results.

TABLE 1. Assumed statistics for pathway inputs.

		Pathway inputs				
Pathway	Parameter	Length, m	Cross section, m2	Permeability, cm/s	Porosity	Dispersion, m
Repository to lower aquifer	Distribution	Lognormal	Deterministic	Lognormal	Lognormal	Lognormal
	Median	59.50	2.82×10^{6}	8.56×10^{-7}	0.001	63
	Uncertainty	0.14		0.65	0.5	0.25
Lower aquifer	Distribution	Normal	Normal	Lognormal	Lognormal	Lognormal
	Median	4,835	1.25×10^{5}	2.39×10^{-3}	0.015	63
	Uncertainty	500	2.09×10^{4}	0.18	0.5	0.25
Lower to upper aquifer	Distribution	Lognormal	Deterministic	Lognormal	Lognormal	Lognormal
	Median	119	3.34×10^{6}	3.87×10^{-7}	0.001	63
	Uncertainty	0.14		0.5	0.5	0.25
Upper aquifer	Distribution	Lognormal	Normal	Lognormal	Lognormal	Lognormal
	Median	1.5×10^{4}	2.09×10^{5}	9.16×10^{-4}	0.012	63
	Uncertainty	0.05	4.10×10^{4}	0.44	0.5	0.25

Head Drop of the Flow Paths

NUTRAN determined the hydraulic pressure heads of each of the five nodes by a recursive process. The head of node 5 was arbitrarily set to 0 and the head drop between nodes 4 and 5 was randomly generated. The head of node 4 was then set equal to this head drop, and the process was repeated, with the head of each node set equal to the head of the succeeding node plus the head drop between the two nodes.

For the flow paths between the repository and the lower aquifer and between the lower and upper aquifers, the head drops at the location on which Mock Site A was based were actually measured and the NUTRAN results could be compared with those measurements. However, only gradients were measured for the two paths within the aquifers. For these two paths, therefore, NUTRAN generated the head drop as the product of the flow path length and gradient. These procedures are summarized in Table 2.

Waste-Dissolution Properties

The repository-resaturation time and waste-dissolution time control the time and rate of waste release to the geosphere. NUTRAN generated release time and rate randomly, using the parameters summarized in Table 3. Resaturation time is composed of a constant plus a random variable. The constant (32 years) is the sum of the average age of the waste in the repository and the time y required for the repository to refill with water. The random variable is the time required for the ground water to dissolve the canister, thereby making the waste available for dissolution. This variable was assumed to have a lognormal distribution with a median of 60 years. The dissolution time for the waste was assumed to be directly correlated with the dissolution time of the canister; that is, if the chemical composition of the ground water is such that the canister corrodes in a short period of time, the waste is also likely to dissolve in a correspondingly short time span. The dissolution time of the waste was assumed to have a lognormal distribution with a median of 2000 years and was calculated by scaling the randomly generated canister dissolution time.

TABLE 2. Assumed statistics for head drop inputs.

Pathway	Method of calculation	Parameter	Head drop	Gradient	Length
Repository to lower aquifer	Generate head drop	Distribution	Lognormal		Lognormal
		Median	42.90		59.50
		Uncertainty	0.10		0.14
Lower aquifer	Generate gradient (head drop = gradient × length)	Distribution		Lognormal	Normal
		Median		0.0015	4,830
		Uncertainty		0.2200	500
Lower to upper aquifer	Generate head drop	Distribution	Normal		Lognormal
		Median	16.0		119.00
		Uncertainty	1.6		0.14
Upper aquifer	Generate gradient (head drop = gradient × length)	Distribution		Lognormal	Lognormal
		Median		0.015	1.5×10^4
		Uncertainty		0.058	0.05

TABLE 3. Assumed statistics for variables controlling time and amount of waste release.

Variable	Method of calculation	Parameter	
Resaturation time (RT)	RT = 32 + y	Distribution of y	Lognormal
		Median	60.0
		Uncertainty	0.23
Dissolution time (DT)	$DT = 2000 \times (y/60)^{1.3}$	Distribution	Lognormal
		Median	2000
		Uncertainty	0.30

Retardation Factors

The retardation factors for the nuclides in the waste were established by dividing the isotopes into three groups (^{129}I and ^{99}Tc in group I, the other fission products in group II, and actinides in group III) and assigning a common retardation factor to all nuclides in the same group. The minimum, preferred, and maximum retardation factors for each group were estimated by LLL for water containing 1000 and 10,000 parts per million (ppm) of dissolved solids (Table 4). Golder provided estimates of the dissolved solids (in ppm) in the water in each flow path of the repository model (Table 5).

To produce probability density functions for the retardation factors requires an understanding of the terms "preferred", "maximum", and "minimum". "Preferred" is synonymous with "median". "Maximum" denotes a value of the quantity that is rarely exceeded. It is assumed that the "maximum" value lies two standard deviations above the mean; that is, 97.73% of all observations

TABLE 4. Retardation factors for selected particulate concentrations.

Concentration of dissolved solids, ppm	Nuclide Group I			Nuclide Group II			Nuclide Group III		
	Minimum	Preferred	Maximum	Minimum	Preferred	Maximum	Minimum	Preferred	Maximum
1,000	1	1	1	1	100	1000	1	100	10000
10,000	1	1	1	1	5	10	1	10	100

TABLE 5. Concentration of dissolved solids by pathway.

Pathway	Concentration of dissolved solids, ppm
Repository to lower aquifer	1,000
Lower aquifer	7,000
Lower to upper aquifer	10,000
Upper aquifer	1,500

will be below the maximum. "Minimum" refers to an absolute minimum since its value is always given as 1 (the smallest possible retardation). The minimum value is interpreted to lie two standard deviations below the median; that is, the distribution function will be constrained so that 2.27% of the observations are exactly 1.

Table 6 summarizes the probability distributions used for the retardation factors of each nuclide group in each flow path. The distribution of each retardation factor is either deterministic, in which case only the constant value is given; lognormal, in which case the median value and the uncertainty (the standard deviation of the logarithm) are given; or "log-linear," in which case the preferred and maximum values are given.

A repository has been modeled that corresponds to one of the random descriptions (except for retardation factors), and isotopes of only one of the nuclide groups have been placed in this repository. The retardation factors for that group in each flow path are independent of the repository and hence

TABLE 6. Probability distribution of retardation factors.

		Nuclide Group I	Nuclide Group II	Nuclide Group III
Repository to lower aquifer	Distribution	Deterministic	Log-linear	Lognormal
	Median (preferred)	1.0	(100.0)	100.0
	Uncertainty (maximum)	--	(1,000.0)	1.0
Lower aquifer	Distribution	Deterministic	Log-linear	Lognormal
	Median (preferred)	1.0	(7.83)	15.85
	Uncertainty (maximum)	--	(19.31)	0.60
Lower to upper aquifer	Distribution	Deterministic	Log-linear	Lognormal
	Median (preferred)	1.0	(5.0)	10.0
	Uncertainty (maximum)	--	(10.0)	0.5
Upper aquifer	Distribution	Deterministic	Log-linear	Lognormal
	Median (preferred)	1.0	(65.0)	78.48
	Uncertainty (maximum)	--	(501.2)	0.95

can be randomly generated according to the cumulative distribution functions in the flow paths. Such an experiment will accurately produce radioactivity release rates for that nuclide group. This experiment may also be repeated with each of the other two nuclide groups and will accurately produce results for each group separately. However, if all three groups are buried in a single repository, there should be some correlation between their respective retardation factors. No such correlation was included in producing the retardation factor for this study, since the precise nature of the dependence among the retardations is not completely understood.

MACRO1 ANALYSIS

In MACRO1 we systematically sample each value of each variable independently in each phase of the calculation. We further treat each of the four flow paths as independent entities. The resultant FPD histograms and statistics are then generated using every combination of mathematically possible (in view of the truncated input FPDs) repository and waste behavior pattern. Figures 2, 3, and 4 are MACRO1 histograms and probability plots for each of the three nuclide groups. Figure 5 gives histograms and plots for all three nuclide groups combined.

This methodology may lead to erroneous results because we have not properly considered the physics of the system in defining our models. For example, within any single flow path we have not taken into account the fact that permeability and porosity measurements generally show a correlation. Then, since

$$v = \frac{q}{\eta} = \frac{-\Delta H k}{\eta L} ,$$

if we choose independently the largest possible value of k and the smallest value of η, we can get water velocities that are orders of magnitude larger than those observed in nature. Even if the resultant probability on this high velocity is small and may not seriously affect our final statistics, we cannot ignore the fact that we have violated our physical model.

Treating each of the flow paths as independent entities, then "summing them up" with no regard for physical constraints can further introduce chances for erroneous results. For example, if we statistically choose the

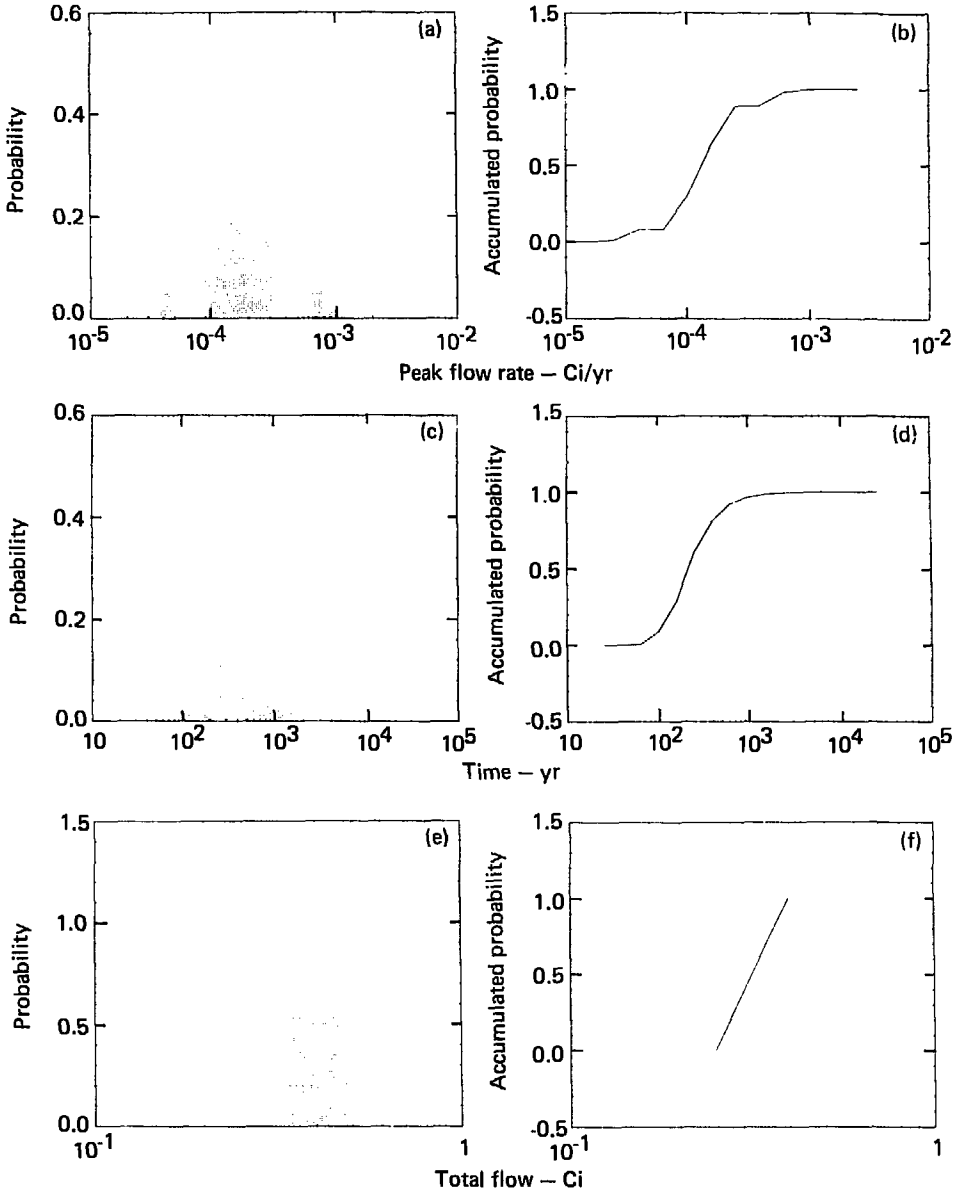


FIG. 2. For Nuclide Group I, MACRO1-produced FPD histograms and accumulated probability plots for peak flow rate (a and b, respectively), time of peak flow rate (c and d, respectively), and integrated flow (e and f, respectively).

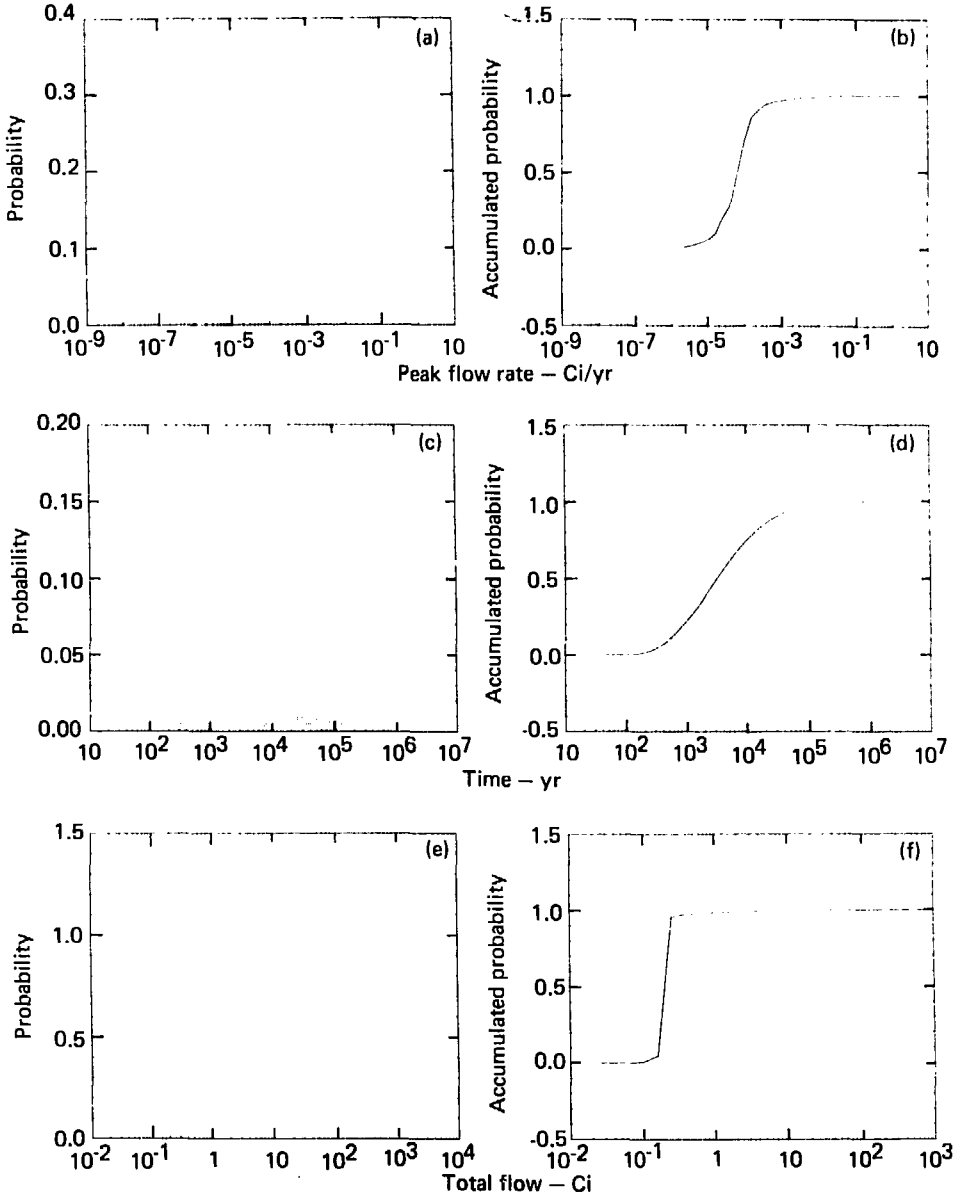


FIG. 3. For Nuclide Group II, MACRO1-produced FPD histograms and accumulated probability plots for peak flow rate (a and b, respectively), time of peak flow rate (c and d, respectively), and integrated flow (e and f, respectively).

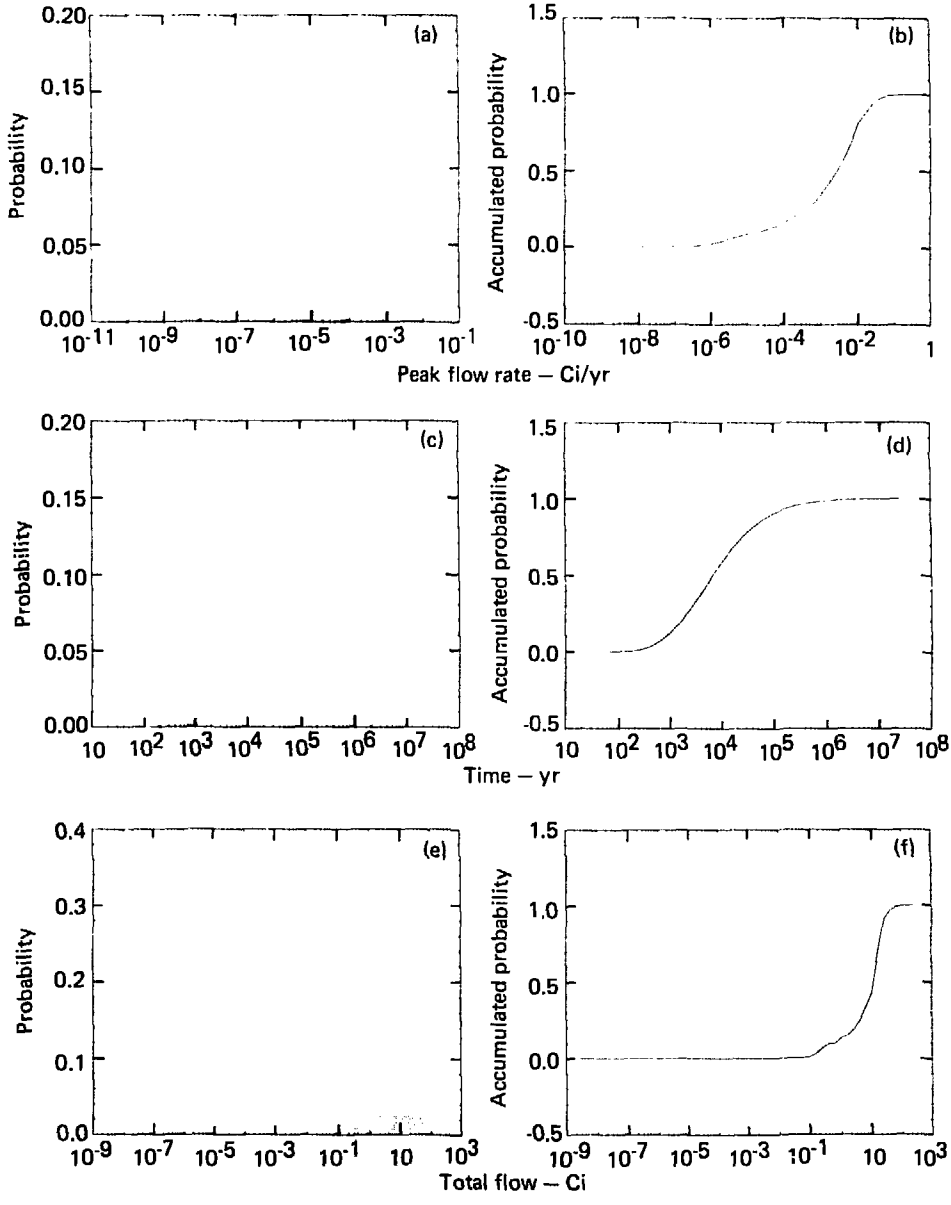


FIG. 4. For Nuclide Group III, MACROl-produced FPD histograms and accumulated probability plots for peak flow rate (a and b, respectively), time of peak flow rate (c and d, respectively), and integrated flow (e and f, respectively).

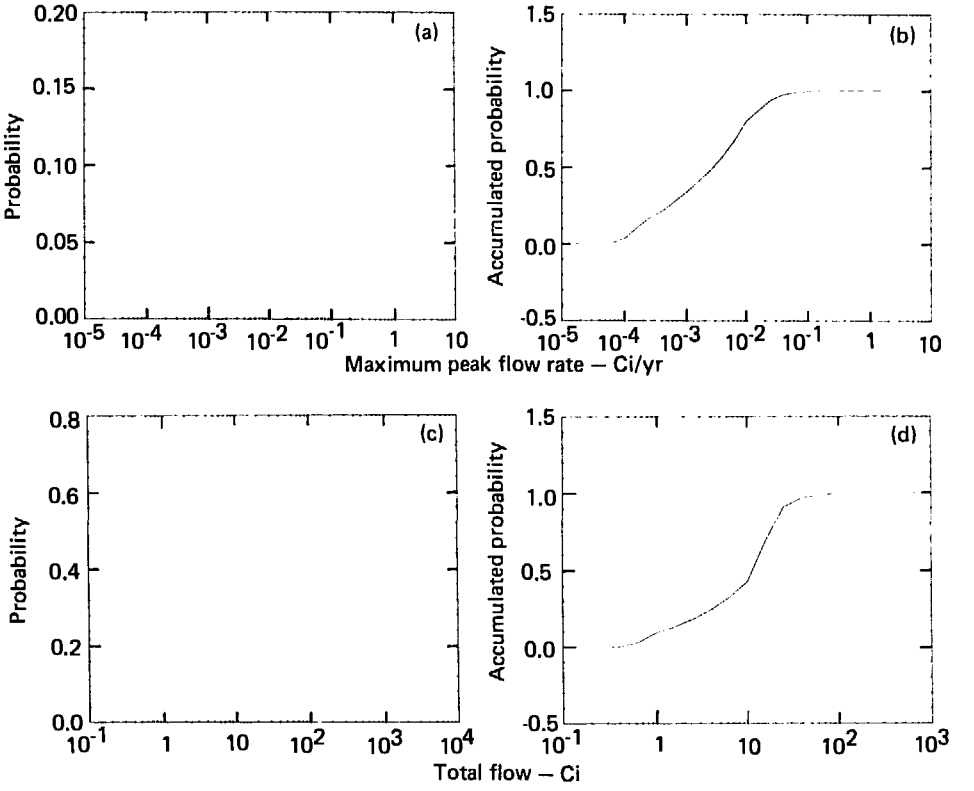


FIG. 5. For all three nuclide groups, MACRO1-produced histograms and accumulated probability plots for maximum peak flow (a and b, respectively) and total flow (c and d, respectively).

permeabilities of the aquifers to be smaller than the permeability of the aquitard, our flow path model may be totally incorrect.

As another example, if we choose the gradient of the upper aquifer (nodes 4-5) to be small and the remaining head differences and gradients to be large, an extrapolated head in the upper aquifer to a point directly over the repository might be lower than the head at the repository. This situation, though physically possible, does not satisfy our assumed flow-path model.

The point is, to produce results that are truly defensible, we must consider all of the model and physical constraints of the system as a whole. Implementation of constraints is a subject for further developmental work.

MACRO1 AND MONTE CARLO ANALYSIS COMPARED

Table 7 compares the "median" repository calculations of MACRO1 and NUTRAN. In this case, the calculation is purely deterministic and each variable is chosen to have its median value.

In general there is good agreement except for the time of peak flow. Here the MACRO1 model uses a square wave release function approximation whereas the NUTRAN model actually computes a convolution on the integral. The discrepancies are trivial, however, because the hazard curves are all nearly flat at the time of interest.[9]

Table 8 compares the statistical results of the MACRO1 calculations with those from NUTRAN. In comparing MACRO1 and NUTRAN results, we must remember that the MACRO1 output is discretized; that is, neighborhoods are represented by single values. With 5 points per decade, the neighborhoods are represented by

$$1. \times 10^{n}$$
$$1.58489 \times 10^{n}$$
$$2.51189 \times 10^{n}$$
$$3.98107 \times 10^{n}$$
$$6.30957 \times 10^{n}$$
$$1. \times 10^{n+1}$$

where $n = 0, \pm 1, \pm 2, \ldots$.

TABLE 7. Results of median repository run.

		Nuclide Group I	Nuclide Group II	Nuclide Group III
Peak flow rate, kCi/yr	NUTRAN	0.24	0.13	0.32
	MACRO1	0.22	0.13	0.35
Time of peak flow rate, yr	NUTRAN	610	4,400	5,400
	MACRO1	200	3,400	4,500
Integrated flow, MCi	NUTRAN	0.45	20.26	0.64
	MACRO1	0.45	0.26	0.65

TABLE 8. Statistical comparisons of Mock Site A analysis.

Variable		Statistics			
		Mean	Standard deviation	Median	Inter-quartile spread
Peak flow rate, kCi/yr					
Nuclide Group I	NUTRAN	0.36	0.28	0.27	0.13
	MACRO1	0.22	0.2	0.16	0.13
Nuclide Group II	NUTRAN	1.0	6.3	0.088	0.052
	MACRO1	1.2	19	0.1	0.12
Nuclide Group III	NUTRAN	0.35	0.72	0.1	0.15
	MACRO1	0.91	1.9	0.4	0.35
Time of peak flow rate, yr					
Nuclide Group I	NUTRAN	1,200	1,000	870	600
	MACRO1	394	509	251	151
Nuclide Group II	NUTRAN	16,000	27,000	6,300	6,600
	MACRO1	19,000	81,000	4,000	8,400
Nuclide Group III	NUTRAN	48,000	190,000	9,300	12,000
	MACRO1	99,500	699,000	10,000	22,600
Integrated flow, MCi					
Nuclide Group I	NUTRAN	0.44	0.0013	0.44	0.00071
	MACRO1	0.4	0.023	0.4	--
Nuclide Group II	NUTRAN	0.36	0.79	0.26	0.0088
	MACRO1	0.92	1.6	0.25	--
Nuclide Group III	NUTRAN	0.57	0.53	0.45	0.28
	MACRO1	0.61	0.68	0.63	0.38

Thus, for example, the interquartile spreads of integrated flow for groups I and II are not well defined because both the 25th and 75th percentiles fall in the same neighborhood.

Considering the discretizations, the comparisons with the Monte Carlo simulations are reasonably good. Thus, we could conclude that the 50 Monte Carlo samples give reasonable statistics, in terms of the 5-per-decade MACRO1. On the other hand, they both may be equally inaccurate.

CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE STUDY

We wrote MACR01 to test a methodology for analyzing proposed nuclear-waste management systems. The code is designed to accept uncertainties in the input parameters and propagate them over the sequence of models to produce probability distributions for the outputs. The discretized probability arithmetic in MACR01 produces results commensurate in accuracy with a Monte Carlo analysis.

MACR01's mathematical accuracy can be improved by decreasing the step sizes in the discretized input spaces and output spaces and by reducing the truncation factors. Each of these improvements requires increased amounts of computer time.

The present MACR01 code may be applicable to certain analysis problems; however, the physics models are highly simplified and may not produce sufficiently accurate results.

The major fault with the present methodology (and therefore with the code itself) is the lack of physical constraints and correlations that are necessary to produce credible results when the physics of the system model is considered as a whole. This is the primary area for future developmental work.

In its present form MACR01 should not be considered as a tool for either licensing or site-suitability analysis. In fact, each analysis performed should be carefully considered at each step. Further, at each step, the user should determine what decision questions are being considered and how MACR01 results will influence those decisions.

ACKNOWLEDGMENTS

The author expresses appreciation to those members of "Task X" with whom he had discussions that contributed to those efforts. In particular, the concepts have been discussed at length with A. M. Kaufman. K. G. Feller has contributed insight to the questions of accuracy and "factorization" of models. G. D. Duckworth and A. M. Kaufman contributed the dose models.

REFERENCES

1. T. Harvey, *Suggested Technical Scheme to Help Resolve Regulatory Issues*, Lawrence Livermore Laboratory, Livermore, CA, UCID-17858, July 1978.
2. S. Kaplan, "Notes on the LLL/NRC Waste Disposal Study II, Probabilistic Arithmetic," in *Notes for a Workshop on Risk Analysis and Decision Under Uncertainty*, Lawrence Livermore Laboratory, Livermore, CA, UCRL-15007 (1979).
3. Golder Associates, *Second Report, Development of Site Suitability Criteria for the High Level Waste Repository*, Lawrence Livermore Laboratory, Livermore, CA, UCRL-13793 (1977).
4. A. M. Kaufman, D. J. Isherwood, and B. Ross, *Calculated Radionuclide Migration From a Geologic High Level Waste Repository*, Lawrence Livermore Laboratory, Livermore, CA, UCRL-81148 (1978).
5. L. E. Berman, *et al.*, *Analysis of Some Nuclear Waste Management Options, Vols. I, II*, Lawrence Livermore Laboratory, Livermore, CA, UCRL-13917, (1978).
6. A. C. Miller III and T. R. Rice, *Discrete Approximations of Probability Distributions*, Applied Decision Analysis, Inc., Menlo Park, CA (1979).
7. M. S. Guiffre and M. F. Kaplan, *An Example of Monte Carlo Analysis Applied to Repository Siting*, The Analytical Sciences Corporation, Reading, MA, TR-1797-2 (1979).
8. W. J. O'Connell, *Mock Site "A" Assessment*, Lawrence Livermore Laboratory, Livermore, CA, UCRL-52718 (1980).
9. A. M. Kaufman and G. W. Pollack, Lawrence Livermore Laboratory, Livermore, CA, private communication (1979).

JMB/jvb

APPENDIX A. HELP PACKAGE FOR MACRO1

```
MACRO1A / 2 3
MACRO1 VERSION LOADED          01/21/80  17:07:22
ALL VARIABLES MUST HAVE POSITIVE VALUES
USE % TO ADD COMMENTS TO COMMAND STRINGS
COMMANDS ARE OF THE FORM
TYPE MODEL[INPUT1,...,INPUT10;OUTPUT1,...,OUTPUT10]
TYPE COMMAND OR END OR HELP
HELP
OPERATIONS ARE:
   TYPE       MODEL
INPUT
            LOGNORM
            LOGLIN
            CERTAIN
            COMPUTE
            VECTOR
            NORMAL
            UNIFORM
            TRIANGLE
            READDUMP
OUTPUT
            WRITE
            PLOTV
            PLOTLV
            PLOTCON
PROPAGATE
            PLUS
            MINUS
            TIMES
            DIVIDE
            SQRT
            EXP
            HYDROH
            HYDROG
            TRANSPORT
            DISSOL
            PDOSE
            TDOSE
            PCURIE
            TCURIE
            JADD
            JSUB
            JMUL
            JDIV
            JADDA1
            JADDA2
            WASTEDT
            CHYDRO
            HYTRANSH
            HYTRANSG
            POR\PERM
            E(L/K+X)
```

```
UTILITY
            EXTRACT
            LISTV
            TRUNCATE
            DUMP
            RESTART
            MAX
            MIN
            DISCARD
            LISTCSET
            %COMSETD
            %COMSETS
            ACOMSET
            SENS
FPD'S TRUNCATED AT FMAX*TRUNCATION FACTOR
DETAILS FOR MODELS ON NEXT CALL TO HELP
COMMANDS ARE OF THE FORM
TYPE MODEL[INPUT1;...;INPUT10;OUTPUT1;...;OUTPUT10]
TYPE COMMAND OR END OR HELP
BWLR\
HELP
HELP PACKAGE; LF OR END TO EXIT
TYPE OR ALL
ALL

**********************************************************
**********************************************************
INPUT - TTY INPUT OF VARIABLE NAMES AND VALUES
NAMES ARE ARBITRARY; UP TO 10 CHARACTERS
MODELS ARE LOGNORM LOGLIN CERTAIN COMPUTE
NORMAL;VECTOR;UNIFORM;TRIANGLE

**********************************************************
INPUT MODEL     LOGNORM
INPUT1=TTY
OUTPUT1=ARBITRARY VARIABLE NAME; I.LE.10
VARIABLE DISCRETIZED; NUMBER/DECADE=N MEANS
V=10.**I/N; I=IMIN;IMAX
TRUNCATED AT NS STD DEVS ABOUT MEAN
IF ACCUMULANT TO II.LT.TRUNCATION VALUE;
      THEN P(I)=0; I.LE.II;
OR IF ACCUMULANT TO JJ.GT.(1-TRUNC VAL);
      THEN P(J)=0; J.GE.JJ

**********************************************************
INPUT MODEL     LOGLIN
INPUT1=TTY
OUTPUT1=ARBITRARY VARIABLE NAME; I.LE.10
VARIABLE DISCRETIZED; NUMBER/DECADE=N MEANS
V=10.**I/N; I=IMIN;IMAX
REQUIRES MEDIAN AND MAXIMUM VALUES
IMIN=0; IMAX=(NR/DEC)*MAXIMUM+1
IF ACCUMULANT TO II.LT.TRUNCATION VALUE;
      THEN P(I)=0; I.LE.II;
OR IF ACCUMULANT TO JJ.GT.(1-TRUNC VAL);
      THEN P(J)=0; J.GE.JJ
```

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INPUT MODEL     CERTAIN
INPUT1=TTY
OUTPUTI=ARBITRARY VARIABLE NAME; I.LE.10
CERTAIN VALUE INPUT; NO DISCRETIZATION

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INPUT MODEL     COMPUTE
INPUT1=TTY
OUTPUTI=ARBITRARY VARIABLE NAME; I.LE.10
VARIABLE DISCRETIZED; NUMBER/DECADE=N MEANS
V=10.**I/N; I=IMIN;IMAX
COMPUTE MEANS BY PROPAGATE MODEL
DEFAULT NR/DEC=5 IF NOT INPUT

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INPUT MODEL     VECTOR
INPUT1=TTY
OUTPUTI=ARBITRARY VARIABLE NAME; I.LE.10
VARIABLE DISCRETIZED; NUMBER/DECADE=N MEANS
V=10.**I/N; I=IMIN;IMAX
VECTOR MEANS ALL COMPONENTS
DISCRETIZED WITH SAME NPD
EXPLICIT PROBABILITY FOR EACH VECTOR
INPUT INDIVIDUAL VECTOR COMPONENTS

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
INPUT MODEL     NORMAL
INPUT1=TTY
OUTPUTI=ARBITRARY VARIABLE NAME; I.LE.10
VARIABLE DISCRETIZED; NUMBER/DECADE=N MEANS
V=10.**I/N; I=IMIN;IMAX
TRUNCATED AT NS STD DEVS ABOUT MEAN
IF ACCUMULANT TO II.LT.TRUNCATION VALUE;
      THEN P(I)=0; I.LE.II;
OR IF ACCUMULANT TO JJ.GT.(1-TRUNC VAL);
      THEN P(J)=0; J.GE.JJ

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INPUT MODEL     UNIFORM
INPUT1=TTY
OUTPUTI=ARBITRARY VARIABLE NAME; I.LE.10
VARIABLE DISCRETIZED; NUMBER/DECADE=N MEANS
V=10.**I/N; I=IMIN;IMAX
REQUIRES MAXIMUM AND MINIMUM OF VARIABLE
MEDIAN SET TO AVERAGE TO GENERATE FPD
UNIFORM- P(K)=(LENGTH OF NBHD(K))/(MAX-MIN)

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
INPUT MODEL     TRIANGLE
INPUT1=TTY
OUTPUTI=ARBITRARY VARIABLE NAME; I.LE.10
VARIABLE DISCRETIZED; NUMBER/DECADE=N MEANS
V=10.**I/N; I=IMIN;IMAX
REQUIRES MAXIMUM AND MINIMUM OF VARIABLE
MEDIAN SET TO AVERAGE TO GENERATE FPD
TRIANGLE- P(K)=AREA UNDER TRIANGLE(S) FROM
   MIN TO MAX INCLUDED IN NBHD(K)
```

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INPUT MODEL     READDUMP
READ VARIABLES FROM EXISTING DUMP
    INPUT1=DUMP FILE NAME
    OUTPUT(I)=DUMP VARIABLE NAME, 1.LE.I.LE.10

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OUTPUT - WRITES VARIABLES TO TTY OR HSP-OUTPUT
         OR PLOTS TO TMDS AND FR80 FILE
MODELS ARE
      WRITE --TO TTY OR HSP
      PLOTV --PLOT PROBABILITY VS VARIABLE
      PLOTLV--PLOT PROBABILITY VS LOG OF VARIABLE
      PLOTCON--PLOTS PROBABILITY CONTOURS
      FOR INPUTI JOINT WITH INPUTI+1
INPUTI=VARIABLE NAME TO OUTPUT, I.LE.10
OUTPUT1=TTY OR HSP FOR WRITE
OUTPUT(I),I=1,10 TEXT LABEL FOR PLOT

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PROPAGATE - DOES LOOPS OVER UNCERTAIN INPUTS
            USES DETERMINISTIC MATH/PHYSICS
            MULTIPLIES PROBABILITIES AND SUMS
            TO DISCRETIZED OUTPUT

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     PLUS
INPUT1 PLUS        INPUT2=OUTPUT1

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     MINUS
INPUT1 MINUS       INPUT2=OUTPUT1

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     TIMES
INPUT1 TIMES       INPUT2=OUTPUT1

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     DIVIDE
INPUT1 DIVIDE      INPUT2=OUTPUT1

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     SQRT
SQRT(INPUT1)=OUTPUT1

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     EXP
(INPUT1)**INPUT2=OUTPUT1

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     HYDROH
1-D HYDROLOGY CALCULATION
HYDROH - INPUT1=HEAD DIFFERENCE
         INPUT2=LENGTH
         INPUT3=HYDRAULIC CONDUCTIVITY
         OUTPUT1=DARCY SPEED
COMPUTES TG=DH/L THEN D=TG*K
```

```
*************************************************
PROPAGATE MODEL     HYDROG
1-D HYDROLOGY CALCULATION
HYDROG - INPUT1=GRADIENT (DH/L)
         INPUT2=HYDRAULIC CONDUCTIVITY
         OUTPUT1=DARCY SPEED
COMPUTES D=G*K

*************************************************
PROPAGATE MODEL     TRANSPORT
1-D TRANSPORT FOR TIME AND PULSE WIDTH
INPUT1=LENGTH
INPUT2=DARCY SPEED
INPUT3=EFFECTIVE POROSITY
INPUT4=LONGITUDINAL DISPERSIVITY
OUTPUT1=TIME
OUTPUT2=PULSE WIDTH
FACTORED-COMPUTES V=D/P THEN
T=L/V AND S=SQRT(2*L*D)/V
PROB(T,S) JOINTLY DISTRIBUTED

*************************************************
PROPAGATE MODEL     DISSOL
RECHARGE AND CANISTER DISSOLUTION MODEL
   INPUT1=AVERAGE AGE OF WASTE(A)
   INPUT2=REFILL TIME(B)
   INPUT3=CANISTER DISSOLUTION TIME(C)
   OUTPUT1=TIME(T)
COMPUTES T=A+B+C

*************************************************
PROPAGATE MODEL     PDOSE
DOSE USES TASC - BIODOSE TABLES
     IN DISC LIBRARY DOS-ARS
     FOR TASC REFERENCE RIVER SYSTEM
INPUT1=1 FOR GROUP I ONLY
      =2 FOR GROUP II ONLY
      =3 FOR GROUP III ONLY
      =ALL FOR SUM OF THREE GROUPS
INPUT2=THREE DIGIT NUMBER WHERE
  FIRST DIGIT=0-HLW FROM U-RECYCLE,PU-STORAGE
             =1-SPENT FUEL
             =3-HLW FROM U-RECYCLE,PU-THROWAWAY
 SECOND DIGIT=0-AVE IND FROM SURFACE H20
             =1-MAX IND FROM SURFACE H20
             =2-POP FROM SURFACE H20
             =3-AVE IND FROM WELL H20
             =4-MAX IND FROM WELL H20
             =5-POP FROM WELL-I H20
             =6-POP FROM WELL-II H20
  THIRD DIGIT=0-WHOLE BODY EQUIVALENT
             =1-WHOLE BODY
             =2-GI -LLI
             =3-THYROID
             =4-BONE
             =5-LIVER
             =6-LUNG
             =7-KIDNEY
             =8-SKIN
```

```
INPUT3 - ARRIVAL TIME FOR NUCLIDE GROUP I
INPUT4 - PULSE WIDTH FOR GROUP I (TC,I)
INPUT5 - ARRIVAL TIME FOR NUCLIDE GROUP II
INPUT6 - PULSE WIDTH FOR GROUP II (FISS)
INPUT7 - ARRIVAL TIME FOR NUCLIDE GROUP III
INPUT8 - PULSE WIDTH FOR GROUP III (ACTS)
IGNORE INPUT5 THRU INPUT8 AND
USE INPUT3 AND INPUT4 FOR TIME,SIGMA
OF ANY GROUP IF INPUT1 IS NOT 'ALL'
INPUT5(OR 9)=CAN DISS TIME IF NON-ZERO
INPUT6(OR10)=WASTE DISS TIME IF NON-ZERO
MUST HAVE BOTH CDT AND WDT OR NEITHER
OUTPUT1=PEAK DOSE(PER MWE-YR OF WASTE
    IF ONLY ONE OUTPUT DEFINED
    IF TWO OUTPUTS DEFINED, THEN
          JOINT WITH
OUTPUT2= TIME OF PEAK IN YEARS

**************************************************
PROPAGATE MODEL     TDOSE
DOSE USES TASC - BIODOSE TABLES
      IN DISC LIBRARY DOS-RRS
      FOR TASC REFERENCE RIVER SYSTEM
INPUT1=1 FOR GROUP I ONLY
       =2 FOR GROUP II ONLY
       =3 FOR GROUP III ONLY
       =ALL FOR SUM OF THREE GROUPS
INPUT2=THREE DIGIT NUMBER WHERE
  FIRST DIGIT=0-HLW FROM U-RECYCLE,PU-STORAGE
             =1-SPENT FUEL
             =3-HLW FROM U-RECYCLE,PU-THROWAWAY
 SECOND DIGIT=0-AVE IND FROM SURFACE H20
             =1-MAX IND FROM SURFACE H20
             =2-POP FROM SURFACE H20
             =3-AVE IND FROM WELL H20
             =4-MAX IND FROM WELL H20
             =5-POP FROM WELL-I H20
             =6-POP FROM WELL-II H20
  THIRD DIGIT=0-WHOLE BODY EQUIVALENT
             =1-WHOLE BODY
             =2-GI -LLI
             =3-THYROID
             =4-BONE
             =5-LIVER
             =6-LUNG
             =7-KIDNEY
             =8-SKIN
INPUT3 - ARRIVAL TIME FOR NUCLIDE GROUP I
INPUT4 - PULSE WIDTH FOR GROUP I (TC,I)
INPUT5 - ARRIVAL TIME FOR NUCLIDE GROUP II
INPUT6 - PULSE WIDTH FOR GROUP II (FISS)
INPUT7 - ARRIVAL TIME FOR NUCLIDE GROUP III
INPUT8 - PULSE WIDTH FOR GROUP III (ACTS)
IGNORE INPUT5 THRU INPUT8 AND
USE INPUT3 AND INPUT4 FOR TIME,SIGMA
```

```
OF ANY GROUP IF INPUT1 IS NOT 'ALL'
INPUT5(OR 9)=CAN DISS TIME IF NON-ZERO
INPUT6(OR10)=WASTE DISS TIME IF NON-ZERO
MUST HAVE BOTH CDT AND WDT OR NEITHER
OUTPUT1=TOTAL DOSE(PER MWE-YR OF WASTE)

♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦
PROPAGATE MODEL     PCURIE
CURIES USES ORIGEN OUTPUT TABLES
      IN DISC LIBRARY CURIE-1
INPUT1=1 FOR GROUP I ONLY
      =2 FOR GROUP II ONLY
      =3 FOR GROUP III ONLY
      =ALL FOR SUM OF THREE GROUPS
INPUT2=1 FOR HLW-RRS CURIES
      =2 FOR SPENT FUEL - RRS CURIES
INPUT3 - ARRIVAL TIME FOR NUCLIDE GROUP I
INPUT4 - PULSE WIDTH FOR GROUP I (TC,I)
INPUT5 - ARRIVAL TIME FOR NUCLIDE GROUP II
INPUT6 - PULSE WIDTH FOR GROUP II (FISS)
INPUT7 - ARRIVAL TIME FOR NUCLIDE GROUP III
INPUT8 - PULSE WIDTH FOR GROUP III (ACTS)
IGNORE INPUT5 THRU INPUT8 AND
USE INPUT3 AND INPUT4 FOR TIME,SIGMA
OF ANY GROUP IF INPUT1 IS NOT 'ALL'
INPUT5(OR 9)=CAN DISS TIME IF NON-ZERO
INPUT6(OR10)=WASTE DISS TIME IF NON-ZERO
MUST HAVE BOTH CDT AND WDT OR NEITHER
OUTPUT1=PEAK CURIES/YR(PER MWE-YR OF WASTE)
   IF ONLY ONE OUTPUT DEF'NED
   IF TWO OUTPUTS DEFINED, THEN
          JOINT WITH
OUTPUT2= TIME OF PEAK IN YEARS

♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦♦
PROPAGATE MODEL     TCURIE
CURIES USES ORIGEN OUTPUT TABLES
      IN DISC LIBRARY CURIE-1
INPUT1=1 FOR GROUP I ONLY
      =2 FOR GROUP II ONLY
      =3 FOR GROUP III ONLY
      =ALL FOR SUM OF THREE GROUPS
INPUT2=1 FOR HLW-RRS CURIES
      =2 FOR SPENT FUEL - RRS CURIES
INPUT3 - ARRIVAL TIME FOR NUCLIDE GROUP I
INPUT4 - PULSE WIDTH FOR GROUP I (TC,I)
INPUT5 - ARRIVAL TIME FOR NUCLIDE GROUP II
INPUT6 - PULSE WIDTH FOR GROUP II (FISS)
INPUT7 - ARRIVAL TIME FOR NUCLIDE GROUP III
INPUT8 - PULSE WIDTH FOR GROUP III (ACTS)
IGNORE INPUT5 THRU INPUT8 AND
USE INPUT3 AND INPUT4 FOR TIME,SIGMA
OF ANY GROUP IF INPUT1 IS NOT 'ALL'
INPUT5(OR 9)=CAN DISS TIME IF NON-ZERO
INPUT6(OR10)=WASTE DISS TIME IF NON-ZERO
MUST HAVE BOTH CDT AND WDT OR NEITHER
OUTPUT1=TOTAL CURIES(PER MWE-YR OF WASTE)
```

```
************************************************
PROPAGATE MODEL     JADD
ARITHMETIC ON JOINTLY DISTRIBUTED VARIABLES
(IF NO JOINT INPUTS, USE SIMPLE ARITHMETIC
I.E., PLUS, MINUS, TIMES, DIVIDE)
JADD=+,JSUB=-,JMUL=*,JDIV=/
COMBINATIONS DEPEND ON NR OF INPUTS
INPUT1 JOINT WITH INPUT2 AND
INPUT3 JOINT WITH INPUT4
       MEANS
OUTPUT1=INPUT1 OPERATION INPUT3
       JOINT WITH
OUTPUT2=INPUT2 OPERATION INPUT4
INPUT1 JOINT WITH INPUT2
INPUT3 (NOT JOINT)
       MEANS
OUTPUT1=INPUT1 OPERATION INPUT3
       JOINT WITH
OUTPUT2=INPUT2 OPERATION INPUT3
INPUT1 ( NOT JOINT)
INPUT2 JOINT WITH INPUT3
       MEANS
OUTPUT1=INPUT1 OPERATION INPUT2
       JOINT WITH
OUTPUT2=INPUT1 OPERATION INPUT3
INPUT1 (JOINT OR NOT)
INPUT2 (NOT OR JOINT)
       MEANS
OUTPUT1=INPUT1 OPERATION INPUT2
       JOINT WITH
OUTPUT2=JOINT OF INPUT1(OR2)

************************************************
PROPAGATE MODEL     JADDA1
ARITHMETIC ON JOINTLY DISTRIBUTED VARIABLES
(IF NO JOINT INPUTS, USE SIMPLE ARITHMETIC
I.E., PLUS, MINUS, TIMES, DIVIDE)
OPERATION OF ADDITION BECOMES
OUTPUT1=SQRT( SUM OF SQUARES )
OUTPUT2=SUM
INPUT1 JOINT WITH INPUT2 AND
INPUT3 JOINT WITH INPUT4
       MEANS
OUTPUT1=INPUT1 OPERATION INPUT3
       JOINT WITH
OUTPUT2=INPUT2 OPERATION INPUT4

************************************************
PROPAGATE MODEL     JADDA2
ARITHMETIC ON JOINTLY DISTRIBUTED VARIABLES
(IF NO JOINT INPUTS, USE SIMPLE ARITHMETIC
I.E., PLUS, MINUS, TIMES, DIVIDE)
OPERATION OF ADDITION BECOMES
OUTPUT1=SUM
OUTPUT2=SQRT( SUM OF SQUARES )
INPUT1 JOINT WITH INPUT2 AND
INPUT3 JOINT WITH INPUT4
       MEANS
OUTPUT1=INPUT1 OPERATION INPUT3
```

```
       JOINT WITH
OUTPUT2=INPUT2 OPERATION INPUT4

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     WASTEDT
WASTE DISSOLUTION MODEL
INPUT1=CANISTER DISSOLUTION TIME(C)
INPUT2=CORRELATION EXPONENT(E)
INPUT3=MEAN WASTE DISSOLUTION TIME(D)
OUTPUT1=WASTE DISSOLUTION TIME
COMPUTES D◆(C/MEDIAN(C))◆◆E
SEE TASC 'MONTE CARLO-MOCK SITE A'

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     CHYDRO
CONSERVATION HYDROLOGY MODEL
INPUT1=HEAD DIFFERENCE
INPUT2=PERMIABILITY
INPUT3=PIPE LENGTH
INPUT4=PIPE AREA
OUTPUT1=TOTAL DARCY FLOW PER UNIT TIME
COMPUTES Q=H◆K◆A/L
H:K MAY BE JOINT

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     HYTRANSH
1-D HYDROLOGY AND TRANSPORT MODEL
COMPUTES MEAN ARRIVAL TIME AND PULSE WIDTH
INPUT1=HEAD DIFFERENCE
INPUT2=LENGTH
INPUT3=HYDRAULIC CONDUCTIVITY
INPUT4=EFFECTIVE POROSITY
INPUT5=LONGITUDINAL DISPERSIVITY
OUTPUT1=MEAN ARRIVAL TIME
     JOINT WITH
OUTPUT2=PULSE WIDTH
CALUCLATION FACTORED
COMPUTES X=P/K
          Y=H/X
          T=Y◆L◆◆2
          S=SQRT(2◆D)◆Y◆L◆◆(3/2)
P:K MAY BE JOINT

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
PROPAGATE MODEL     HYTRANSG
1-D HYDROLOGY AND TRANSPORT MODEL
COMPUTES MEAN ARRIVAL TIME AND PULSE WIDTH
INPUT1=GRADIENT
INPUT2=LENGTH
INPUT3=HYDRAULIC CONDUCTIVITY
INPUT4=EFFECTIVE POROSITY
INPUT5=LONGITUDINAL DISPERSIVITY
OUTPUT1=MEAN ARRIVAL TIME
     JOINT WITH
OUTPUT2=PULSE WIDTH
CALUCLATION FACTORED
COMPUTES X=P/K
          Y=G/X
```

```
          T=Y*L
          S=SQRT(2*D)*Y*L**(1/2)
P,K MAY BE JOINT

*********************************************************
PROPAGATE MODEL     POR\PERM
POROSITY-PERMEABILITY CORRELATION MODEL
REFERENCE - UCRL-13755-2
  INPUT1=I(INTERSTITIAL) OR F(FRACTURE)
  INPUT2=PERMEABILITY ,K
  INPUT3='SLOPE', A
  INPUT4='INTERCEPT', B
COMPUTES OUTPUT1=PERMEABILITY
           JOINT WITH
         OUTPUT2=POROSITY,PJ
BY PJ=A*LOG(K/B)  IF I,
  PJ=A*(K/B**2)**(1/3)  IF F
K,A,B MAY BE FPD'S

*********************************************************
PROPAGATE MODEL     E(L/K+X)
REF-SALT UTILITY MODEL
  INPUT1=POROSITY,P
  INPUT2=PERMIABILITY,
  INPUT3=LENGTH,L
  INPUT4=SUM(L/K),OTHER PATHS,
COMPUTES OUTPUT1=P*(L/K+X)
P,K MAY BE JOINT

*********************************************************

*********************************************************
UTILITY MODEL     EXTRACT
UTILITY EXTRACT - SUM SINGLE FPD FROM JOINT FPD

*********************************************************
UTILITY MODEL     LISTV
UTILITY LISTV - LISTS ALL NAMES, LENGTHS, ETC

*********************************************************
UTILITY MODEL     TRUNCATE
UTILITY TRUNCATE - TRUNCATE EXISTING FPD
INPUT(I) TO OUTPUT(I), I.LE.10
IF I IS JOINT, THEN MUST BE WITH I+1

*********************************************************
UTILITY MODEL     DUMP
UTILITY DUMP[FILE] - CREATES/WRITES DUMP

*********************************************************
UTILITY MODEL     RESTART
UTILITY RESTART[FILE] - READS RESTART DUMP

*********************************************************
UTILITY MODEL     MAX
UTILITY MAX[IN1,...,INN;IOUT] - GETS MAXIMUM
```

```
◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
UTILITY MODEL     MIN
UTILITY MIN[IN1;...;INN;IOUT] - GETS MINIMUM

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
UTILITY MODEL     DISCARD
UTILITY DISCARD[IN1;...;INN] - REMOVES VARIABLES

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
UTILITY MODEL     LISTCSET
UTILITY LISTCSET - LISTS COMMAND SET
      NUMBERED INPUT1 THROUGH INPUT2
            OR
      INPUT1=ALL

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
UTILITY MODEL     XCOMSETD
UTILITY XCOMSETD - EXECUTES COMMANDS
      NUMBERED INPUT1 THROUGH INPUT2
      FOR OUTPUT1 TIMES THROUGH THE SET
      DISCARDS PREVIOUSLY GENERATED OUTPUTS

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
UTILITY MODEL     XCOMSETS
UTILITY XCOMSETS - EXECUTES COMMANDS
      NUMBERED INPUT1 THROUGH INPUT2
      FOR OUTPUT1 TIMES THROUGH THE SET
      AND SAVES THE OUTPUT BY ADDING 1 TO
      THE NAMES ON EACH PASS THROUGH

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
UTILITY MODEL     ACOMSET
UTILITY ACOMSET - ALTERS COMMAND SET
      [D;OUTPUT1;...;OUTPUTN]; N.LE.10
            DELETES COMMANDS NUMBERED IN OUTPUTS
      [AA;OUTPUT1;OUTPUT2]
            ADDS OUTPUT2 COMMANDS AFTER OUTPUT1

◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆◆
UTILITY MODEL     SENS
AUTOMATED SENSITIVITY ANALYSIS
ASSUMES PREVIOUS DEFINITION OF COMMAND SET
ALLOWS LOOPS OVER ALL INPUT VARIABLES
WITHIN THE COMMAND SET THAT ARE
NOT OUTPUTS OF PRECEEDING COMMANDS
IN THE SENSITIVITY LOOP SET
ASKS FOR MEDIAN VALUES;MIN;MAX AND
NUMBER OF STEPS OVER SENSITIVE VARIABLES
FPD COMPUTED AS INITIALLY INPUT WITH NEW MEDIAN
ACTUALLY EXECUTES XCOMSETD
ASSUMES COMMAND SET INCLUDES OUTPUT
    INPUT1=NR OF FIRST COMMAND IN LOOP
    INPUT2=NR OF LAST COMMAND IN LOOP
COMMANDS ARE OF THE FORM
TYPE MODEL[INPUT1;...;INPUT10;OUTPUT1;...;OUTPUT10]
TYPE COMMAND OR END OR HELP
END
HARDCOPY OF HSP FILE? (YES OR NO)
```

```
NO
YOU MUST SAVE YOUR RESTART DUMPS
          AND
OUTPUT YOUR FR80 PLOT FILES

 ALL DONE
```

APPENDIX B. MODELS FOR MACRO1

G. D. Pollack

INTRODUCTION

MACRO1 was specifically designed to analyze the postemplacement phase of a nuclear-waste repository site. It explicitly includes the corrosion of the canister, the dissolution of the waste form, the regional hydrology and transport of the radionuclides, and the dose or curie commitment to an individual or population group (assuming a water use system). Each of the models represents only an approximate description of these phenomena, but each incorporates the most important features in a conservative manner.

The order in which the models are described reflects the temporal sequence in which they would occur in nature and, consequently, the order in which they are calculated in the code.

CANISTER CORROSION

The corrosion time of the canister will depend on the metallic form of the canister, the type and amount of ionic species in the water, the amount of oxidizing agent (such as ferric ion or dissolved oxygen) in the vicinity of the waste package, the temperature as a function of time, and, possibly, the flow rate of water past the canister. We have attempted to incorporate most of these factors into an *ab initio* model, but the model has not been validated against any experimental data and uses parameters whose experimental values are only poorly known. Therefore, we used best engineering judgment to obtain a median corrosion time (currently set at 60 years) and an associated variance. We added deterministic values for the age of the waste and the resaturation and repressurization time of the repository. When empirical data on corrosion rates, currently being sought at various institutions, become available, they should prove useful in developing phenomenological models for corrosion. Such models could be easily incorporated into MACRO1, to augment the current model, DISSOL.

WASTE-FORM DISSOLUTION

The dissolution of the waste form (currently spent-fuel assemblies) is a function of the same parameters that affect corrosion, as well as the radial distribution of the fission products within a fuel rod. Because fission products migrate in a fuel rod (for instance, iodine and technetium waste products move toward the surface in amounts determined by reactor temperature and residence time), we cannot assume that the predominant and relatively insoluble uranium in the rods will determine the rate of dissolution. Instead, we might expect differential dissolution rates for different species. MACRO1 allows such differential rates if desired, but assumes that the rates are constant in time. The dissolution time is assumed to be correlated to the corrosion time since they are both functions of the same set of factors. The current model (WASTEDT) uses a deterministic correlation, but this approach is not dictated by the structure of MACRO1 and may be easily changed.

REGIONAL HYDROLOGY

MACRO1's regional hydrology model can treat only very simple flow patterns and pathways. It assumes that one-dimensional flow paths will reasonably mimic the real hydrology even though the flow rate of water on a regional scale will in general be three-dimensional. We use this approach because the repository emplacement media currently being considered are all of very low permeability and porosity and are often layered, with very high horizontal-to-vertical anisotropy. These characteristics imply that the water flow will probably be through flaws of various types (either natural or induced by mining) or along bedding planes.

Our assumption is of least validity in the immediate vicinity of the repository, and more care must be taken to obtain meaningful results for near field flow. However, by taking the flow into or out of a repository as approximately one-dimensional, we can use a "resistor" network that contains both series and parallel path connections. Each segment of the flow path is characterized by permeability, porosity, cross-sectional area, and hydraulic gradient. For horizontal flow in aquifers or bedding planes, the hydraulic gradient is dictated by the angle of slope, but, in general, it will be a function of the geometrical structure of the network, the physical parameters

and gradients of the other path segments in the network, and the overall boundary conditions.

In most cases, it would be necessary to solve for some of the hydraulic gradients in a flow path by requiring conservation of water at each path connection point (node) and zero total head drop for any closed set of paths, while adding one or two boundary conditions on regional recharge rate or aquifer head. This approach would lead to a set of simultaneous linear equations which are straightforward to solve. MACRO2 will use this general procedure to obtain gradients, but MACRO1 does not. Instead, it makes the simplifying assumption that the only significant pathways of flow out of a repository will be all in series, with no branching of flow and no parallel connections. This assumption eliminates the need for solving simultaneous equations. However, MACRO1 does not assume conservation of flow at nodes and thus treats each path segment as independent of the other segments. All these simplifications are equivalent mathematically to allowing the gradient for a given path to be a free parameter, independent of any other segment's parameters, and with its own probability distribution.

In practice, the gradient in some pathways is considered to be the uncertain parameter, while in others both the head and the path length are unknown but have independent probability distributions. These two cases are handled by two distinct routines, HYDROG and HYDROH, respectively. The output of these routines are water velocity distributions computed according to D'Arcy's Law:

$$v_i = \frac{k_i}{\theta_i} g_i$$

or

$$v_i = \frac{k_i}{\theta_i} \frac{\Delta H_i}{L_i}$$

where

K = hydraulic conductivity
θ = effective porosity
g = hydraulic gradient
ΔH = head drop along a path
L = length of path
i = the various paths.

REGIONAL TRANSPORT

When a pulse of solute travels through a porous medium, the differential flow velocities (both magnitude and direction) associated with the various microscopic channels cause the pulse to be spread out, both in the direction of flow (longitudinal dispersion) and perpendicular to the flow (lateral dispersion). The amount of dispersion is assumed proportional to the average velocity of the water. Because of the one-dimensional nature of its hydrology model, MACRO1 must necessarily ignore lateral dispersion as a distinct phenomenon.

To model the effects of longitudinal dispersion, we make the fundamental assumption that the main features of the transport are adequately described by two quantities: the average time taken to traverse the sequence of path segments (note that the average time is not necessarily the transit time for the peak) and the variance of the pulse at its exit point into a large body of water. We use Laplace transform techniques to show rigorously that for a series of one-dimensional flow paths the following relationships hold:

$$t_T = t_0 + \sum_i t_i$$

$$\sigma_T^2 = \sigma_0^2 + \sum_i \sigma_i^2$$

where

t_i is the average transit time for the ith segment: $t_i = \frac{L_i}{v_i}$

t_T is the average total transit time

t_0 is the average dissolution time

σ_i^2 is the variance induced by transit through the ith pipe $\sigma_i^2 = \frac{2\alpha_i L_i}{v_i^2}$, α_i being the dispersivity of the ith path

σ_0^2 is the variance of the dissolution process

σ_T^2 is total variance.

A trivial generalization to a network of parallel and series paths exists and will be incorporated in MACRO2. The v_i's that appear in these formulas may be scaled from those produced in the hydrology computation by a factor of $1/R_{ij}$, where R_{ij} is the retardation of nuclide type j in path segment i. This retardation is due to a variety of ion-rock complexes and other factors. These retardation factors may have their own probability distributions that are dependent on groundwater chemistry and rock type, as well as nuclide type.

The output for the regional transport model in the code is then the probability distributions for the variables

$$\sum_i t_i$$

and

$$\sum_i \sigma_i^2 .$$

Hydrology and transport must be computed simultaneously when both the heads and lengths are uncertain variables, since L_i appears in both computations. MACRO1 actually combines hydrology and transport into one model, computed by HYTRANSG or HYTRANSH. Regional transport alone is calculated by TRANSPORT.

CURIE AND DOSE COMMITMENTS

To compute peak concentrations or fluxes of nuclides and associated doses, MACRO1 must translate the variance and transit times from the regional transport computation into statements about pulse heights. The fundamental assumption used is that, if the width of an input pulse into a series of flow paths is much less than the average transit time widths of any of the pipes, the spatial profile of the pulse at any given time will be approximately Gaussian. As it travels through the sequence of paths, the pulse will widen, but it is assumed to remain Gaussian. This approach implies that the peak value at any time is inversely proportional to the width. This Gaussian assumption is the rationale for computing only moments for the transport computation.

We consider the Gaussian approximation valid only when the input pulse width is small compared to the other time scales of the transport. In practice, the dissolution of the waste form will not necessarily be this rapid, so we have distinguished three cases for computational purposes. The first treats the case for which the dissolution time is sufficiently rapid that the pulse can be treated as spatially Gaussian. In this case, MACRO1 uses an analytic form for the flux that is a parametric function of t_T and σ_T:

$$J_0(t) = \frac{1}{\beta\sqrt{2\pi\eta^3}} \exp \frac{-(\eta - 1)^2}{2\beta^2\eta}$$

where

$$\eta = t/t_T$$

$$\beta = \sigma_T/t_T \quad .$$

This is the standard normalized solution to the transport equation (solved for flux rather than concentration) for a semi-infinite pipe with a δ-function input pulse. Similar expressions hold for concentration.

MACRO1 computes doses from this flux by taking into account that the potential hazard curves for the various nuclide groups (that is, the quantity, in curies, of a nuclide present as a function of time and waste form) will generally vary slowly compared to $J_0(t)$. The standard definition of peak individual dose,

$$D_{peak} = \max_t J(t)H(t) \quad ,$$

where H(t) is the potential hazard function, then becomes

$$D^{(1)}_{peak} = J_0(t_p)H(t_p) \quad ,$$

where t_p is the time at which $J_0(t)$ is a maximum. Similarly, the integrated population dose,

$$D_{pop} = \int_0^\infty dt\, J(t)H(t) \quad ,$$

becomes

$$D_{pop}^{(1)} = H(t_p) \int_0^\infty dt\, J_0(t) = H(t_p) \quad .$$

In the second case, the dissolution time of the waste is assumed to be of the same order of magnitude as the transit time widths (or path pulse width enlargements). Here, MACRO1 divides the input pulse (which currently is assumed to be a step function) into small step functions, each much narrower than the path transit times. Each of these short pulses is then propagated through the pipes so that the output of any individual pulse is given by $J_0(t_i)$, where t_i is the time when the ith short pulse arrives at the exit node. The total pulse is thus the sum of all these short pulses. MACRO1 then computes its maximum value and uses the formulas from the first case to compute doses.

In the third case, the dissolution time of the waste form is assumed much greater than the total transit time widths, so the final output is still a step function. In this case, the time dependence of the individual or population dose is given by the time dependence of the potential hazard curves,

$$D_{peak}^{(3)} = \max_t \left[H(t) \text{ for } \sum t_i \leq t \leq t_0 + \sum t_i \right]$$

and

$$D_{pop}^{(3)} = \int_{\Sigma t_i}^{t_0 + \Sigma t_i} dt'\, H(t') \quad .$$

In practice, MACRO1 uses a set discretization for both running time and for dividing up the input pulse for the second case. It then generates tables for peak curies, individual doses, and integrated population doses and thus can search tables during execution rather than computing.