NOTES ON THE NEXT GENERATION MACROMODEL
A UNIFIED COMPUTATIONS SYSTEM FOR PREDICTING
POST SEALING WASTE DEPOSITORY PERFORMANCE

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MASTER

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1. INTRODUCTION AND PURPOSE

At the current time development and improvement activities are underway on computer software and on several analytical ideas related to the calculation of the risk from waste migration after sealing of a depository. These ideas and software modules may be viewed as components of a total system model for such risk calculations. This total model has been dubbed "The Macromodel" and is so referred to among project personnel. The set of component improvements now underway can be viewed thus as a round of improvements to, or as a new generation of the macromodel that now exists and has been used up till this time.

The purpose of the present notes is to pull together these software and analytical ideas into an overall portrayal or blueprint of the new macromodel that is evolving. The purpose of the blueprint is to clarify the relationship of the components and the interfaces required, to facilitate the alignment of all parties concerned and to allow a definitive specification of the work remaining to be done.

It is intended that this unified macromodel will be resident on the LLL computer and will be used there to evaluate the suitability of various proposed depository designs and depository site location concepts. The knowledge of suitability that results from this usage will contribute towards the writing of regulations governing design and location of depositories.

It is recognized that the blueprint outlined in these notes may not be the "final" version. It is intended however that this attempt at a unified presentation provide a framework for the gathering of ideas and information so that when all the corrections, additions, criticisms and clarifications have been input, we will have an agreed upon product definition and action plan to achieve it.

We note again that the macromodel as used in these notes is aimed at calculating only the post emplacement risk of a depository stemming from possible waste migration to the biosphere. The regulations will consider as well the risks involved in pre-sealing, processing and transportation activities.

2. NOTATION

We shall use a notation based upon the following diagram:

Figure 1.

in which we have for later convenience defined a local vicinity V around the repository and labeled by L the interface between this local region and the geosphere, G , as a whole. Similarly we denote by S the boundary between the geosphere and the biosphere, i.e., the boundary separating the domain where biological transport processes are active from that of purely physical/chemical processes. S thus is roughly a few meters below the earth's surface.

To carry the notation further, let:

- σ denote a complete set of site descriptors, i.e., depth, geology, permeability, etc., including a description of the geometry of the site, its location, the materials properties, hydrology, and all numbers and facts necessary to characterize the site.
- ζ denote the set of parameters and descriptors necessary to characterize a particular repository design, including the quantities of waste, by isotope, stored there.
- ϕ denote the set of parameters and descriptors necessary to define the waste form, its packaging, and the container in which it is placed in the earth.

Then, for our purposes the set

$$\{\sigma, \zeta, \phi\} \equiv \omega$$

defines a waste disposal system.

In addition, we shall find it convenient to look at a depository at four different "scales" or "levels of magnification." The first scale, shown in Figure 2, is a perspective drawing of a representative view of the region surrounding a proposed depository site. We refer to this scale as the "region" or the "basin."

Figure 2. Site Geometry

The second scale is that of the local vicinity of the depository, represented in Figure 3. The third scale is that of a typical tunnel shown in Figure 4. The final scale is that of the waste canister itself, the vault in which it sits, and the immediate rock surroundings, represented in Figure 5.

3. MACROMODEL OVERVIEW

Conceptual Calculation Sequence

Conceptually the macromodel, any overall model, must go through the sequence of steps shown in Figure 6A. Beginning with a description $\omega = \{\sigma, \zeta, \phi\}$ of the waste disposal system, we must compute the hydrology, that is the water flow patterns in the basin, in the repository itself and in the vicinity of the canisters in particular. From this, in principle we can determine the performance of the waste containers and vaults, i.e., whether radioisotopes are released from the containers and if so, when and how much. If such isotopes are released, we can determine their motion through the ground until the points of entry into the biosphere. Similarly, in principle we can next follow their motion within the biosphere and compute the amount and type of damaging effects on man. This damage is the final output of the calculations.

Since the transport part of the problem is linear (if twice as many curies are released, twice as many enter the biosphere), it is convenient to reformulate this part of the problem in terms of a "Green's Function approach" as shown in Figure 6B. What we call the ground transport Green's Function expresses the amounts and types of radioisotopes reaching the

Figure 3. Depository Geometry

Figure 4. Tunnel Configuration

Figure 5. Representative Canister and Vault

Figure 6A. Calculation Flow Diagram

Figure 6B. Flow Diagram with Greens Functions Delineated.

Figure 6C. Symbolic Handling of Probabilistic Calculations.

biosphere per unit amount of each isotope released. Similarly, the bio-transport Green's Function expresses the strength of the resulting radiation dose field per unit isotope reaching the biosphere. The actual radiation field is then calculated by simply multiplying the combined Green's Function by the actual quantities of radioisotopes released.

The "strength" of the radiation field at any point and time, i.e., the effect of entry of radioisotopes entering the biosphere, is most usefully measured in terms of the dosage delivered by those isotopes to a so-called "standard man" living at that point at that time. The definition of the "standard man" includes a standard weight, diet, metabolism, length of life, etc. The standard man concept thus serves essentially as a field detecting instrument which measures the radioisotope concentrations in the environment in terms of a convenient unit. Actually, when we consider dose to the various organs, the instrument becomes a "vector valued" field detector--characterizing the radiation field at any point and time, in terms of a vector, the i^{th} component of which gives the lifetime dose to the i^{th} organ of a standard man who lives at that space point, at that time after sealing of the repository.

The strength of the field itself is one measure of the "damage" associated with the release of radioisotopes. It is useful also to measure damage in terms of the biological effects of the dosage to the standard man and, to the entire population assumed present.

Probabilistic Aspects

The calculation outlined above is "deterministic" in that given the system description the measures of damage are determined. In actual fact we will not know the system description fully. Porosities, permeabilities, rainfall rates, corrosion rates, etc., will not be known with certainty. Our state of knowledge of each parameter however can be described in the form of a finite probability distribution (FPD). Thus, for example, the system description, ω , can be written:

$$\omega = \{ \langle p_i, \omega_i \rangle \} \quad (3.1)$$

as a set, $\{ \}$, of doublets $\langle, \rangle$, each doublet containing a set, ω_i , of system description parameters and an associated probability p_i .

For each parameter set ω_i , we then do a deterministic calculation and obtain a corresponding measure of damage, d_i , which thus also has the probability p_i . Repeating this for all the ω_i gives then an FPD for the damages

$$d = \{ \langle p_i, d_i \rangle \} \quad (3.2)$$

which we can now plot cumulatively in the form of a Risk Curve

where the ordinate at any point, d , is the probability of damage exceeding that value.

This process may be thought of as placing a "probabilistic wraparound" on the deterministic calculations as represented by Figure 6C.

It is important to note however, that Figure 5C is meant to be symbolic of the principle involved. It is not meant to suggest that the actual computational procedure will be to do an entire beginning-to-end deterministic calculation for each combination of system parameters. This would clearly be prohibitive computationally. The actual process will be to segregate the overall deterministic model into pieces. Each piece is treated probabilistically, with probabilistic output passing from one piece to the next. (More details on this procedure are given in References (1) and (2). In particular, note the Condensation Operation, Section 9 of Reference (2), and note that the basic operation of adding FPD's may be viewed as a deterministic addition with a probabilistic wraparound.)

4. MACROMODEL FLOW DIAGRAM

The basic ideas of the previous section are put forth again in the flow diagram of Figure 7, now in a more detailed presentation which more closely reflects the structure of the computational system we are proposing.

The process begins with descriptions of the region, depository, vault, canister, and population parameters any or all of which may be probabilistic as shown. The hydrology portion of the calculation is broken into four stages as shown corresponding to the four levels of magnification of Section 2.

Within the dashed lines is the overall Green's Function calculation, now broken into three parts representing the motion of waste through the local vicinity V , the geosphere G , and the biosphere B .

The amount of waste released is calculated from a knowledge of what isotopes are present as a function of time (ORIGEN) and from a model of the corrosion/

*Note: Probabilistic wraparound shown is symbolic. Actually each module has its own wraparound.

Figure 7. Macro Model Flow Diagram

dissolution behavior of the canister and vault as influenced by the flow of water in the immediate vicinity.

We next describe these component modules individually.

5. SITE HYDROLOGY

The first step is to compute the overall ground water flow pattern in the repository region including all the possible paths to surface waters and to man. We feel it essential that this calculation be done within the context of a three-dimensional model, that is a three-dimensional representation of the surface and subsurface structure pictured in Figure 2.

We recognize of course that a detailed, three-dimensional hydrology calculations code is very expensive in computer time, so that some approximation must be made. We feel it important however that such approximate treatment be in the form of an "approximate 3-D model" rather than as a two- or one-dimensional approximation to a 3-D model. The latter we feel, have low confidence factor and low intuitive appeal whereas the 3-D model, if there is doubt, can always be run again with more mesh points or an improved difference equation, etc.

An existing 3-D model of the type we are talking about is contained in the hydrology program AFPM written by Ian Miller of Golder Associates.⁽³⁾ This program is organized on a layer cake principle with two-dimensional sheets of points representing the strata, and vertical pipe flow allowed between the strata. The sheets can be curved and contoured as are real strata and can be discontinuous to represent fault planes.

It seems to us that this program strikes a good balance between accuracy and economy. We recommend that it serve as the site hydrology module in Figure 7.

The input to this module would be the geometry of the basin. This is set up once and for all for any given basin. Properties and dimensions of strata, and climatology can then be varied to explore the effect of uncertainties.

The output of the program is the flow volume, speed, direction and hydrostatic pressure at each point in the basin. These pressures become part of the input for a closer look at the hydrology in the local vicinity of the depository itself.

6. DEPOSITORY HYDROLOGY

The hydrology in the local vicinity of the depository is studied using the code REPFL0. In this code, the picture is typically something like Figure 8. The depository tunnels are represented as one dimensional pipes and flow is allowed in the tunnels and shafts. Outside the depository itself flow is assumed to be strictly vertical, from the lower aquifer to the upper with a certain amount intercepted by the tunnels and thence conveyed to the upper aquifer through the depository.

The hydrostatic pressures $H_u(x,y)$, $H_l(x,y)$ in the upper and lower aquifers are known from the regional hydrology studies. The pressures in the tunnels depend upon the flow rates in the tunnels and the hydraulic properties of the backfill. The flow rates in the tunnels are related to the flow rates into the tunnels from the immediate surrounding rock. These in turn must be consistent with the vertical flow between the two aquifers.

Figure 8. Typical Representative REPFLO Model

REPFL0 iterates all these flows to consistency with each other and with the corresponding pressures. In order to do this on the scale of Figure 8, however, it needs to know something about the relation of the hydrostatic heads in the tunnel to those in the surrounding rock. This relation is established through a detailed look at the two-dimensional flow field in the immediate neighborhood of the tunnel.

7. TUNNEL HYDROLOGY

At this level the picture is something like Figure 9. We wish to know the relation between the flow into the tunnel, q_T , and the pressures. To first order this relationship will be of the form

$$q_T = C_1[H_1 - H_T] + C_2[H_2 - H_T]$$

where C_1 and C_2 depend upon the specific geometry of the tunnel and the fracture zone if any. By studying this 2-dimensional flow field for various pressures, we can find C_1 , C_2 which are then used as part of the input to REPFL0.

8. LOCAL WASTE TRANSPORT

After the REPFL0 calculation has been done, we are in position to establish a "Local Pipe Model" to represent the transport of waste from various points in the depository to the points of entry into the geosphere G.

It is a good idea at this time to aggregate the depository into a small number (≤ 10 say) of "source points" representing points close to the shaft far from the shaft, etc.

Figure 9. Tunnel Hydrology

Each source point is now connected to one or more points of entry by one or more flow "paths." Each path consists of a series of "pipes" in which the water flow rate and velocity are known as well as the porosity, permeability and retardation.*

We now wish to establish the "Local Transport Green's Function."

$$L(\underline{r}, t; \underline{r}_0, t_0) \quad (8.1)$$

which contains the information on the transport between the source points $\underline{r}_0$, and the points of entry, $\underline{r}$, between V and G .

More specifically, L is matrix, the i, j^{th} element of which is defined as:

$$L_{ij}(\underline{r}, t; \underline{r}_0, t_0) \equiv \begin{array}{l} \text{the flow rate of isotope } i, \text{ at time } t, \\ \text{through the point } \underline{r} \text{ in consequence} \\ \text{of a unit release of isotope } j \text{ at point} \\ \underline{r}_0, \text{ time } t_0 \end{array} \quad (8.2)$$

Here $\underline{r}_0$ ranges over the source points, and $\underline{r}$ over the points of entry between V and G . We write this concisely as

$$\underline{r}_0 \in \mathcal{D} \quad (8.3a)$$

$$\underline{r} \in L \quad (8.3b)$$

and we understand that $\mathcal{D}$ and L now represent finite sets of points we have specified.

With respect to the methodology for computing L , we recommend a procedure along the lines of that described in Reference (4), Appendix J. In this approach the time dependence of L_{ij} will be expressed

*The retardation will be estimated in light of what is known about the water chemistry at each point; this in turn estimated from the flow patterns identified in the regional and local hydrology calculations.

in terms of a known analytic form, which we shall label by $X(t)$ (for transport). This form will have in it two parameters,

$$\begin{aligned}\mu &\equiv \text{the flow time} \\ \sigma &\equiv \text{the dispersion time.}\end{aligned}\tag{8.4}$$

These parameters in turn are functions of the path between $\underline{r}_0$ and $\underline{r}$, i.e., the number of pipes, the properties of the pipes, and also on the isotopes in question, i, j .

$$L_{ij}(\underline{r}, t, \circ \underline{r}_0, t_0) = X(t - t_0, \mu_{ij}(\underline{r}, \underline{r}_0), \sigma_{ij}(\underline{r}, \underline{r}_0)).\tag{8.5}$$

If there is more than one path between $\underline{r}$ and $\underline{r}_0$, L_{ij} will be a sum over the paths:

$$L_{ij} = \sum_{\substack{\text{paths} \\ k}} X(t - t_0, \mu_{ij}^k, \sigma_{ij}^k)\tag{8.6}$$

Thus, the local transport function L_{ij} is specified by simply specifying the two parameters μ_{ij} , σ_{ij} for each path. The details of how this is to be done are spelled out in a forthcoming note by A. Kaufman.⁽⁶⁾

9. REGIONAL WASTE TRANSPORT

Next, based on the regional hydrology, we establish a "Regional Pipe Model" representing the transport from the local surface L , to the points of entry, S , into the biosphere. And in the same way, we compute:

$$G_{ij}(\underline{r}, t; \underline{r}_0, t_0) \equiv \text{the flow rate of isotope } i \text{ at time } t, \\ \text{into } B \text{ through the point } \underline{r} \text{ in consequence} \\ \text{of a unit quantity of isotope } j \text{ entering } G \\ \text{at } \underline{r}_0, t_0.$$

where now $\underline{r}$ and $\underline{r}_0$ range over the interface surfaces

$$\underline{r}_0 \in L$$

$$\underline{r} \in S.$$

To find G_{ij} , we recommend here using the same process as for L_{ij} . Thus

$$G_{ij} = \sum_{\substack{\text{paths} \\ k}} X(t - t_0, \mu_{ij}^k, \sigma_{ij}^k)$$

where the parameters $\mu_{ij}^k, \sigma_{ij}^k$ characterize the set of pipes constituting the k^{th} path between $\underline{r}_0$ and $\underline{r}$.

Comment

The L and G functions can now be convoluted to produce a single Green's Function from the depository source points to the points of entry into the biosphere.

The same computer module that produces the L and G functions can be used to convolve them since this operation simply amounts to putting two series of pipes together into a longer path.

The combined Green's Function is useful, and so also are the L and G functions individually. Thus L can be used separately to explore the effectiveness of various depository designs and tunnel designs. G of course can be used to compare various siting proposals.

10. WASTE TRANSPORT IN THE BIOSPHERE

The initial module addressing the biosphere portion of the model should be the TASC program BIODOSE. Under this treatment, a given rate of isotope input to the biosphere disperses itself into an equilibrium distribution in the various compartments of the biosphere. The lifetime dose to a standard man living in the environment of these compartments can then be calculated.

Results of this kind of calculation are shown in Reference (5), Figures 3.1-2, 3.2-1, 3.2-3. These curves give the dose to standard man per KWe-Yr worth of waste entering the biosphere as a function of the age of the waste at the time of entry. For example, in Figure 10,

Figure 10. Dose to standard man per MWe-Yr worth of waste reaching the biosphere per year at time T after removal from reactor.

Let $B(T)$ be the standard dose from one MWe-Yr waste of age T . From the release and ground transport parts of the calculation we will have, $q_B(t)$, the amount of waste reaching the biosphere at time t after sealing of the repository. Let us measure $q_B(t)$ in MWe-Yr of waste entering the biosphere each year. Presumably this function will have a shape something like:

and will be slowly varying so that the distribution in the environmental compartments may be taken to be the equilibrium distribution at any time. The dose to standard man then at time t is:

$$s(t) = \text{Dose at } t = B(t)q_B(t) \quad (10.1)$$

(since on our time scale $T \approx t$).

It may be that there is more than one space point of interest in the biosphere. In this case, BIDDOSE is run for each point giving

$B(\underline{r}, \underline{r}_0, T) \equiv$ Lifetime dose for a standard man living
at point $\underline{r} \in B$ in consequence of the entry
into the biosphere at point $\underline{r}_0$ of one
MWe-Yrs worth of waste of age T .

$$\underline{r} \in B, \underline{r}_0 \in S \quad (10.2)$$

which we can regard as the Green's Function for biotransport. The actual dose to a standard man at $\underline{r}$ then is:

$$s(\underline{r}, t) = \int_S B(\underline{r}, \underline{r}_0, t) q_B(\underline{r}_0, t) d\underline{r}_0 \quad (10.3)$$

where $q_B(\underline{r}_0, t)$ is the flow rate of waste into the biosphere through point $\underline{r}_0$ at time t .

If we now explicitly recognize in our notation that the dose depends upon the parameters, ω , of the waste disposal system, we write

$$s(\underline{r}, t | \omega) \quad (10.4)$$

The maximum of this over $\underline{r}$, t

$$s(\omega) \equiv \max_{\underline{r} \in B} \max_t s(\underline{r}, t | \omega) \quad (10.5)$$

can serve as a convenient measure of the damage resulting from the waste disposal system ω . Thus, recognizing that ω is probabilistic (3.1), and identifying $s(\omega_i)$ with d_i , we obtain the risk curve (3.2).

We note also that assuming a population distribution $P(\underline{r}, t)$, we can calculate the population dose as another damage measure

$$d_i \equiv \int_{\underline{r} \in B} \int_0^\infty P(\underline{r}, t) s(\underline{r}, t | \omega_i) dt d\underline{r} \quad (10.6)$$

11. THE WASTE SOURCE

The waste migration process starts of course with its release from the waste container, by which we refer to the canister and vault combination. We think it should be possible to design these containers to isolate waste for at least thousands of years, perhaps indefinitely. We feel that irrespective of the expected efficacy of the geological isolation from the biosphere it is desirable to have yet another very secure barrier in the container itself, and that the cost of this extra assurance will be minor compared to the peace of mind and decrease in obstruction and litigation stemming from lack of confidence in waste isolation...

Accordingly within our macromodel there will need to be some sort of model to represent the performance of the waste containers. A vital input to this model of course will be the flow speeds, volumes and the water chemistry in the immediate vicinity of the canisters. For this purpose, we will need another 2 or 3 dimensional hydrology program at the level of the vault. This program will be fed by results of the tunnel level and depository level hydrology calculations.

The output of the canister program will be the function

$$q(\underline{r}, t) = \text{waste released of point } \underline{r}, \text{ time } t. \quad \underline{r} \in \mathcal{D} \quad (11.1)$$

where $\mathcal{D}$ represents the depository itself.

This release can be expressed in MWe-Yr equivalent, or reactor year equivalent or whatever is convenient, and if appropriate can be broken down by isotope, so that q becomes a vector

$$q(\underline{r}, t) = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ \vdots \end{bmatrix} . \quad (11.2)$$

Combining $q(r,t)$ with the L and G functions, we obtain $q_b(r,t)$ the release into the biosphere, which combines with the biotransport function B to give the damage measures as described in Section 10.

12. CONCLUSION AND RECOMMENDATIONS

Implementation of the Macromodel

What we have described so far is an outline or overall blueprint of the Macromodel. A multitude of detail will need to be filled in before an integrated operational package along this line exists at LLL. Not all these details can be foreseen at this time. Nor is it wise or fruitful to try overly hard to foresee them in the abstract. Accordingly, we recommend an implementation action plan consisting of two main thrusts in parallel:

- (1) Continue development of individual modules and getting these upon the LLL computer as currently being done.
- (2) Pretend that the new Macromodel already exists and begin using it to generate the regulatory information desired.

In this second action since the unified program does not exist, we shall have to use it piecemeal; some modules on the LLL machine, some elsewhere. Some calculations will have to be done by hand. Some will be done by guess. Approximations will be made, there will be a lot of patchwork and back and forth. We consider this an essential stage in the development of the Macromodel and cannot stress this too highly.

It is essential to begin doing the calculations desired by Regulatory "as if" the Macromodel existed. This will clarify for us and NRC the details of the questions we wish to ask of the model and the details of the design and interconnections of the modules.

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