MODULE

OCT 22 1990

MEMORANDUM FOR: Joseph O. Bunting, Chief
Engineering Branch, DHLWM

FROM: Ronald L. Ballard, Chief
Geosciences and Systems Performance Branch, DHLWM

SUBJECT: REQUIREMENTS FOR A SOURCE TERM MODULE

You recently requested that I provide to you a description of the requirements for a source term module that would be compatible with and sufficient for the purposes of total system performance assessment. The desired objective, as expressed by Mr. Browning, is that the source term code developed to evaluate compliance with subsystem requirements be, to the greatest extent practicable, directly compatible with the source term component of the total systems code. Such an arrangement would optimize usage of resources allocated to code development.

Although a modular source term code capable of fulfilling the needs for total systems performance assessment and waste package performance assessment is desired, it is apparent from the nature of various components of the module (e.g., geochemical and hydrologic computational components) that the code development will require substantial work by a multi-disciplinary staff. An effective way to assure proper coordination of this interdisciplinary effort is within the context of the ongoing iterative performance assessment activities. In order to meet this objective, HLEN should take the technical lead for the waste package failure model, the waste form dissolution model, and the thermal-mechanical model (which may have considerable input from hydrogeology, especially if coupled heat transfer processes are significant). HLGP will provide the technical lead for nearfield transport (because the principal activities involve hydrology, geochemistry, transport, and performance assessment modeling) and will provide some of the inputs for the waste package failure and dissolution models.

Input and output parameters for the various models have not yet been definitively established. Meetings between our technical staffs will be necessary to formulate the technical details of the module interfaces. An enclosure is included however, which provides a preliminary description of the expected source term interactions and information requirements for the total system modeling exercise.

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I would like to obtain your views on the degree to which the source term module work identified herein can be supported by your staff. The Phase-2 modeling work is scheduled to be discussed at Wednesday's Branch Chief meeting, at which time we can discuss HLEN support. Also, a final draft of the Iterative Performance Assessment Phase-2 Plan will be forwarded to you shortly. As you are aware, substantial staff and contractor resources are included in the FY-91 budget for this work.

/s/

Ronald L. Ballard, Chief
Geosciences and Systems Performance Branch, DHLWM

Enclosure:
As stated

cc: R.E.Browning
B.J.Youngblood
J.J.Linehan

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Ronald L. Ballard, Chief
Geosciences and Systems Performance Branch, DHLWM

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REQUIREMENTS FOR THE PROPOSED SOURCE TERM CODE

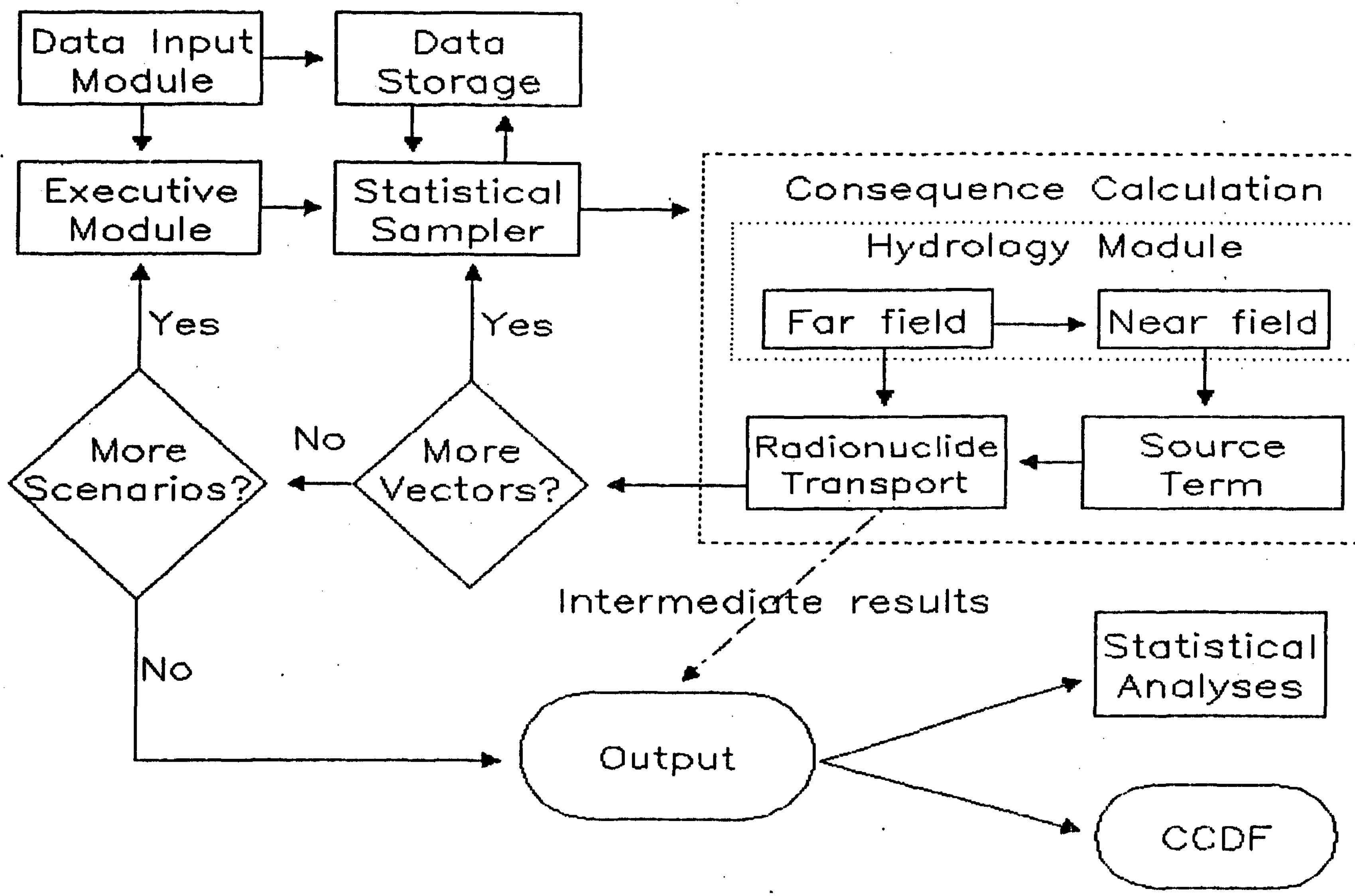
INTRODUCTION

Phase 1 of Iterative Performance Assessment (IPA) was completed by NRC staff in April 1990. The objective of Phase 1 of IPA was to demonstrate NRC's capability to conduct a performance assessment for a HLW repository (NRC, 1990). As indicated in the NRC Phase 1 report, a number of assumptions and simplifications were made to complete the work in Phase 1. In future iterations of the IPA, more realistic models will be used and some of the assumptions of Phase 1 relaxed. One of the conclusions reached at the completion of Phase 1 work was that inclusion of a realistic source term in subsequent IPA iterations was of high priority. In response to that conclusion, it is proposed that work on development of a "Source Term Code" be undertaken such that an improved source term code is available for the second iteration.

The proposed source term code would eventually become a part of the "Total System Simulator (TOSS)." Some components of TOSS were available at the time the first iteration of IPA was done. Other components, such as the Source Term Code, were available only in a very rudimentary form. Still others are yet to be developed. A source term type of code is also needed to investigate the provisions of 10 CFR Part 60.113 that relate to the performance of the engineered barrier subsystem i.e., containment and gradual release. In general, the code for investigating gradual release provisions of 10 CFR Part 60.113 may be required to have much finer detail built into it than is required for a source term code that will become a component of the total system simulator. Therefore, one may think of developing two models, one a detailed one and the other in which some processes are either omitted or treated in a simpler fashion or lumped together. One the other hand, the simpler model can not omit important detail and an effort to develop two models independently does seem to be duplicative. For one code to fulfill the twin needs of investigating provisions of 10 CFR Part 60.113 and to be a component of total system simulator, flexibility should be built into the source term code so that it can operate at various levels of complexity. The requirements in the following can be adapted for either approach (i.e., one or two codes), but are, in general, suited to the total system simulator.

A flow diagram of TOSS, Figure 1, shows how the source term code is intended to interface with the total system performance assessment code (TOSS). Two very important points made in the flow diagram are worth emphasizing: (1) the sequencing over scenarios must be performed external to the source term code and (2) the stabilized sampling of model parameters must be performed external to the source term code. In both cases the motivation for this arrangement is to assure that the source term and other consequence modules

General Flow Diagram for NRC/CNWRA Total System Performance Assessment Code



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(hydrology and radionuclide transport) are all operating with a consistent set of inputs. Of course, for applications of the source term code to assess compliance with quantitative subsystem performance standards, a separate (but similar) arrangement for sampling scenarios and parameters will be needed. Since the subsystem standards are for anticipated conditions and the total system standard is for anticipated and unanticipated conditions, the set of scenarios for the total system application will be larger and usually contain all the scenarios used for the subsystem application.

OBJECTIVE OF THE PROPOSED SOURCE TERM CODE

The objective of the source term code is to simulate the near-field environment in the repository and the behavior of the ensemble of waste and waste packages in the repository so that the rate at which radionuclides are released to the geosphere (site) can be estimated.

The proposed source term code will eventually become a part of the Total System Simulator. Because of the probabilistic nature of the total system performance criteria (40 CFR Part 191), it is expected that the code will be used to make a large number of simulations (rather than a single simulation, if the criteria were deterministic in nature). Therefore, in deciding on a structure of the proposed code, some trade off between amount of detail (and hence complexity) to be included in the model and the computational efficiency will be necessary. While we shall make judgments initially about the details to be included in the model, there may be several iterations of development before a sufficiently complete, accurate and workable model will emerge.

NAME OF MODEL

Tentatively (until a better name comes forth), the model is named REFRE (Release From Repository). A name may not be needed if it is decided to have one source code, since EBSPAC (see below) may be that code.

COUPLING TO EBSPAC

The Center is developing a waste package failure (containment) model which has been named EBSPAC. There are plans to include the modeling of release into EBSPAC also. However, at present the stress in EBSPAC is on the modeling of waste package failure mechanisms including various corrosion modes for the container. The early version of this model is expected to produce the time to failure of a waste package and the failure rate (number of packages per year) of the waste packages. Output from this early version of EBSPAC will become an input to REFRE. Provisions may need to be made to allow the output of EBSPAC to be correlated with variables affecting REFRE. This view is reflected in the schematic of REFRE and no further discussion on waste package failure is included in this document.

DESCRIPTION OF TECHNICAL REQUIREMENTS ON REFRE

The possible modules to be included in REFRE are shown in Figure 2. In order to provide flexibility, the program should provide for switches so that one may execute any particular module or may elect not to. For example, the code user

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should be able to read in a water flow rate instead of actually executing the hydrogeologic module. If the water flow rate is directly input, it should be possible to have this rate read in as time- and space-dependent, possibly in a table format. In addition, a probability distribution or some other statistical measures describing the uncertainties of the flow rate should be read. As an alternative, the hydrogeological module may provide for a solution of a two-dimensional Richard's equation which is collapsible to one-dimensional. Similar comments apply to the other modules identified in the figure.

For modeling of source term, it is expected that the repository will be divided into a small number of compartments (possibly no more than 20). Each compartment will have one or more of its attributes different from others, e.g., type of waste form, age of waste, inventory, chemical environment, hydrogeologic characteristics, location in space, etc. The source term calculation will then proceed for each of these compartments. In effect, as many source terms will be calculated as there are compartments.

Effort should be made to include the following items in the proposed model:

(a) Liquid and gaseous pathways.

(b) Spent fuel and glass waste form.

(c) Inventories in matrix, grain boundaries and gap.

(d) Congruent and preferential leaching models.

(e) Dependence on geochemistry.

(f) Waste package failure distributed in time.

(g) Uncertainties in the form of probability distributions.

(h) Diffusive and convective mass transport.

(i) Temperature-dependent geochemistry.

(j) Kinetics of gas formation.

(k) Distribution of waste, properties, and mass transfer in space.

The level of detail included in the model on each of the topics listed above may vary depending upon the importance of the topic to release and computability. The basic principle to be followed in including the level of detail is to include a 'state of the art' formulation, and to provide, through user selectable switches, a simpler formulation if one exists.

Two methods of uncertainty analysis should be allowed for: 1) Monte Carlo through either Latin Hypercube Sampling, Random Sampling, or both, and 2) The Fast Probability Analysis Technique coupled to Importance Sampling. The

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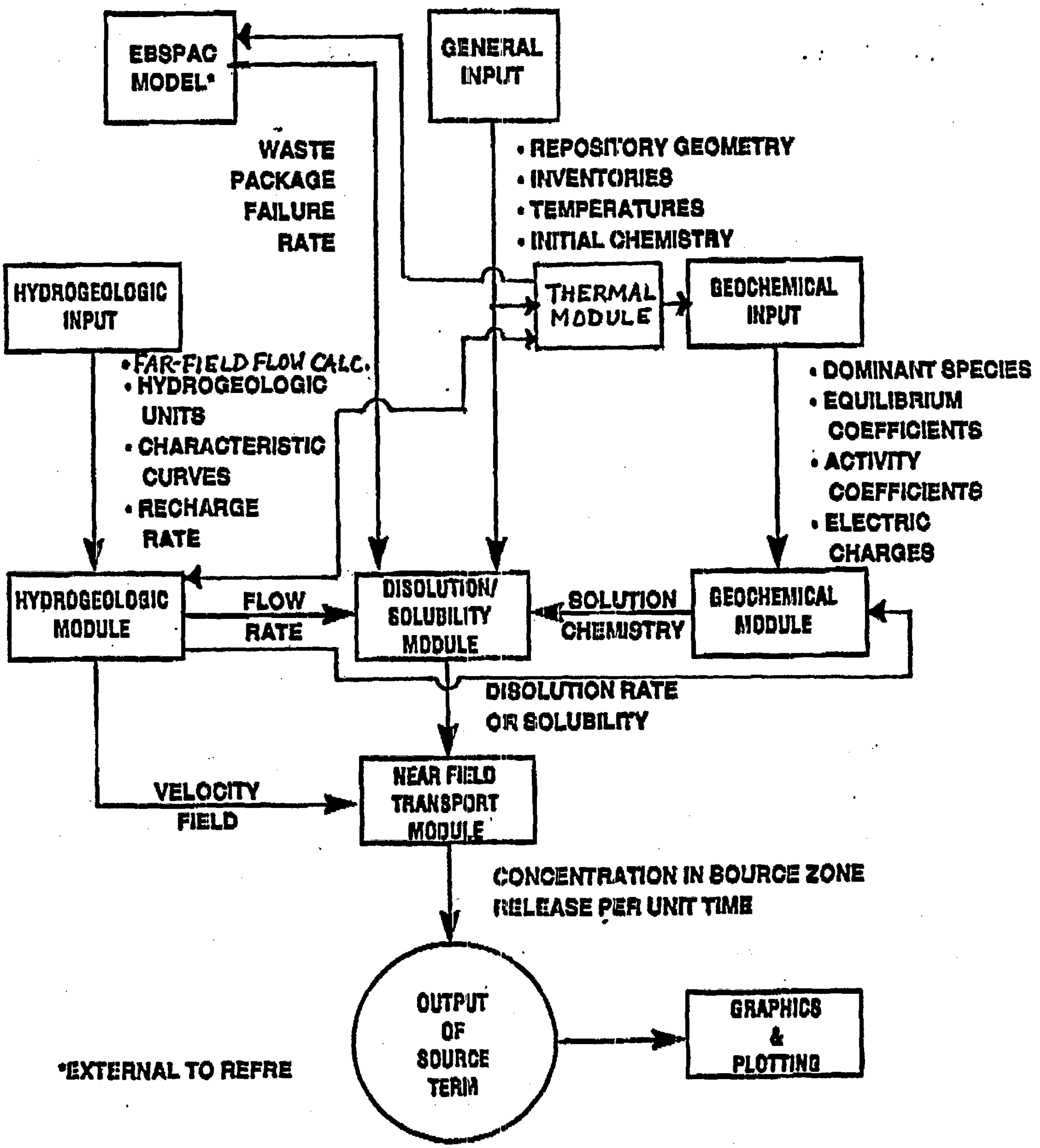

PROPOSED STRUCTURE OF REFRE — THE SOURCE TERM CODE

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statistical sampling driver will be assumed to be external to REFRE (e.g., part of the total system code).

A brief description of each module indicated on the schematic diagram is provided below.

1. EBSPAC MODEL: In the initial design of REFRE, EBSPAC may be assumed to be an external model which provides data on waste package failures. At some stage, we shall have to make sure that data common to EBSPAC and REFRE is the same.

2. HYDROGEOLOGIC MODULE: This module should be designed to provide information on liquid and gas flow rates through the repository. If properly designed, it may be possible to treat both the saturated and unsaturated flow . Although, primarily the unsaturated flow part would be used for the Yucca Mountain site, some of the scenarios to be dealt in the TOSS may require analyses with a saturated environment. It should be possible to solve either a one- or two-dimensional flow problem. It is anticipated that a steady state solution would be of interest in many simulations; however, consideration should be given to providing for unsteady simulations. As indicated earlier, a provision should be made in the driver module to omit execution of the hydrogeologic module if the flow rate and velocities can be read directly into the REFRE.

3. GEOCHEMICAL MODULE: The chemical nature of the solution that comes into contact is anticipated to be the main determining factor in estimating the release rate. The geochemical module will provide for the estimation of this water chemistry. For using the geochemistry module, the user of REFRE will be required to know the dominant species that will play the major role in determining the solution chemistry. Thus, while this module will have the basic principles (mass conservation and reaction equilibrium) of the static speciation built into it, it will not be as general as the available detailed speciation computer codes such as the EQ3/6. Again, a provision should be made to omit execution of this module, if the user so desires.

4. DISSOLUTION/SOLUBILITY MODULE: This module in REFRE will always be executed. Given the chemistry of the solution and the flow rates, this module will determine the rate at which dissolution occurs. As much as possible , a general dissolution rate expression should be coded. The dependence of various coefficients (rate constant, chemical affinity) in this expression on thermodynamic properties of the bulk phase should be included. Eventually the dissolution/solubility module should simulate the interactions among the waste, waste package components, and groundwater.

5. NEAR-FIELD TRANSPORT MODULE: Once a release rate or concentration of a species is estimated, this module will deal with the transport of the species in the near field. Transport primarily by diffusion and convection will be considered. Precipitation and formation of colloids will be included as source/sink terms in the transport equation. The convective velocities will either be read as input data or be obtained from the hydrogeologic module.

6. GRAPHICS AND PLOTTING MODULE: This may be written as a post-processor. The aim would be to display the source term.

7. OTHER CONSIDERATIONS: At the moment, a thermal module is not included. It is expected that the temperatures will be either read directly or provided by the EBSPAC model.

DESCRIPTION OF PROGRAMMING REQUIREMENTS

The program should be written in ANSI standard Fortran F77. If possible, the input should be format free. The program should be modular. An effort should be made to make it compatible with the EBSPAC and the proposed TOSS codes.

SCHEDULE

The basic approach should be completed by October 1990.

The model for waste package failure should be completed by August 1991. The model of groundwater contact with waste should be completed by July 1991. Spatial and temporal modeling should be completed by June 1991.

A finished module, including testing and benchmarking, should be completed by the end of August 1991.