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ENGINEERED BARRIER SYSTEMS PERFORMANCE ASSESSMENT CODE (EBSPAC) DEVELOPMENT PLAN — UPDATE 1

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ENGINEERED BARRIER SYSTEMS
PERFORMANCE ASSESSMENT CODE (EBSPAC)
DEVELOPMENT PLAN - UPDATE 1

1. INTRODUCTION

This document presents a development plan for the Engineered Barrier System Performance Assessment Code (EBSPAC). This initial plan is intended to serve as a guide for the early stages of EBSPAC development. Because of the complexity of EBS subsystem performance assessment, it would be impossible to define *a priori* the exact form each model and module would take. However, EBSPAC will have a modular design which will allow for ease of update as more complete models are developed. Also, it is understood that the model development within EBSPAC is an evolutionary process and that the final version of the code will involve an estimated three years of effort. Even though this is the case, two baseline models have been targeted for incorporation into EBSPAC during FY91. The overall development and implementation of EBSPAC will be in accordance with the Center for Nuclear Waste Regulatory Analyses' (Center) quality assurance and computer code control requirements.

This plan contains background material on performance requirements for the Engineered Barrier System with a discussion on two waste package performance assessment codes used by DOE. Also, included is an overview of the EBSPAC strategy and the mechanistic reasoning behind some of the model development. The model integration strategy is presented along with a plan for implementation.

The emphasis in the plan presented here is on the "containment" aspects of the EBSPAC development. The release rate modeling will be described in additional detail in a future plan update in early FY92.

2. BACKGROUND

The engineered barrier subsystem performance requirements consist of two parts:

1. a "containment" requirement for HLW packages, and

2. a radionuclide release rate limit from the engineered barrier system.

Together, these two parts are intended to control the release of radioactive materials to the geologic setting and to add confidence that the overall system performance objectives for the repository will be met. Specifically, 10 CFR 60.113 states the performance requirements for the EBS as follows:

> "The engineered barrier system shall be designed so that assuming anticipated processes and events: (A) containment of HLW will be substantially complete during the period when radiation and thermal conditions in the engineered barrier system are dominated by fission product decay; and (B) Any release of radionuclides from the engineered barrier system shall be a gradual process which results in small fractional releases to the geologic setting over long times...."

"In satisfying the preceding requirements, the engineered barrier system shall be designed, assuming anticipated processes and events, so that: (1) Containment of HLW within the waste packages will be substantially complete for a period to be determined by the Commission taking into account the factors specified in 60.113(b) provided, that such period shall be not less than 300 years nor more than 1,000 years after permanent closure of the geologic repository; and (2) The release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed one part of 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years following permanent closure, or such other fraction of the inventory as may be approved or specified by the Commission; provided, that this requirement does not apply to any radionuclide which is released at a rate less than 0.1% of the calculated total release rate limit. The calculated total release rate limit shall be taken to be one part in 100,000 per year of the inventory of radioactive waste originally emplaced in the underground facility, that remains after 1,000 years of radioactive decay."

In order to demonstrate compliance with 10 CFR 60.113, it is necessary to develop computer codes to simulate the key processes in the EBS. PANDORA and AREST are two computer codes developed and used by DOE as the major computational tools for EBS waste package design and performance assessment. The first version of PANDORA (PANDORA-1) has been developed and is undergoing testing. PANDORA-1, developed for the Yucca Mountain project, is based on a deterministic model evaluating the performance of one waste package at a time for a given set of initial and time-varying local conditions.

As described by Ramspott (Ramspott, 1988), PANDORA-1 is composed of seven coupled process modules. These are the radiation, thermal, mechanical, environmental (flow of water), corrosion, wasteform alteration, and radionuclide transport modules. The external process models which provide input to the internal modules include ORIGEN II, EQ3/6, TACO, and TOUGH. O'Connell, et. al (O'Connell, 1989) state that a model of diffusive contact and transport is deferred to the second phase, PANDORA-2.

The AREST Code, a probabilistic source-term code for waste package performance analysis, was originally developed by the Pacific Northwest Laboratory for the BWIP project (Liebetrau, 1987). The AREST code is divided into three parts:

1. Waste Package Containment,

2. Waste Package Release, and

3. Engineering System Release Components.

A computer Code User's Guide was published in May, 1989 (Engel, 1989). However, the version of the AREST Code documented in this User's Guide corresponds to the AREST model reported in 1987 by Liebetrau. In 1989, Engel reported that some new features have been incorporated into the AREST Code. The new features include a new release model for a partially saturated media and uranium precipitation. The new release model calculates steady-state release based on rates of matrix dissolution, diffusion, and convection. Engel also states that future developments for the AREST Code consist of a spatial variability of the repository and additional models for corrosion and release.

DOE has developed EBS subsystem assessment capabilities. However, the NRC has a requirement to determine DOE design compliance with the EBS subsystem regulatory requirements set forth in 10 CFR 60.113. To this end, the NRC has a need for a methodology suitable for independent assessment of the EBS subsystem performance. EBSPAC (coupled with a total system performance assessment code) is intended to provide the NRC with that needed methodology.

3. EBSPAC STRATEGY

Because of the complex nature of the processes affecting EBS performance, closed form analytical models may not be available for many processes. To evaluate DOE's design, it will be necessary to use credible embedded numerical models and numerical modeling codes (i.e., hydrology, radiation, geochemical, and thermal codes). Whenever feasible, the numerical models will embody the fundamental mechanisms which characterize the modeled system. However, when a model cannot be developed from first principles, empirical modifications to a theoretical model will be developed. The EBSPAC is designed with a modular structure in order to permit updating and modifications as new models and data are developed. A key element in the development of an adequate EBS compliance determination computer code is to have a probabilistic analysis framework that is accurate in the region of interest, provides a basis for sensitivity analysis, and is reasonably efficient. The Fast Probabilistic Performance Assessment (FPPA) methodology (Wu, 1988), developed at the CNWRA, meets these criteria and has been chosen as the probabilistic foundation for the EBSPAC. However, Monte Carlo-based schemes will also be retained within the code for both completeness and selective application purposes. Ultimately, the output from EBSPAC is expected to be compatible with the needs of a total system performance assessment code to assess the designed repository performance.

One of the key features of the FPPA methodology is its capability for providing sensitivity information on the uncertain variables. The sensitivity information is useful for compliance determination, particularly because the number of uncertain parameters involved in an EBS performance analysis is expected to be relatively large. The sensitivity ranking will be useful in determining if additional information should be gathered. The acquisition of additional information may demand significant effort, therefore, the optimum solution is to maximize the benefit of the new information relative to the added effort. The added effort may be justified if it eliminates a significant part of the uncertainty, thus leading to a higher confidence in the assessment result. A decision model may be established to investigate alternatives. Thus, the sensitivity information produced by the FPPA approach could provide the NRC with a decision-aiding tool to focus on critical parameters or models and to identify new research areas and guide experimental programs.

4. MODEL DEVELOPMENT CONSIDERATIONS

The material degradation models are at the heart of the EBSPAC system. These models allow one to extrapolate the performance of the waste package from relatively short-term test data or estimate the performance from input parameters. The models can be classified as:

1. material models,

2. environmental models, and

3. interaction models.

4.1 <u>Material Models</u>:

The waste package can undergo a variety of structural transformations under the repository thermal and environmental conditions. These transformations can affect the performance of the waste package materials either through degradation of their mechanical and physical properties or through a degradation of their corrosion resistance. For example, the container materials made out of type 304 stainless steel may be susceptible to the precipitation of carbides along grain boundaries and concurrent chromium depletion which can reduce its corrosion resistance. Other container materials may suffer from other structural changes including grain boundary segregation of deleterious elements in copper, order-disorder transformations in some nickel alloys, and agglomeration of iron-rich particles in some copper alloys. These structural transformations are material specific and their effects on material performance can be environment specific. For example, precipitation of chromium carbide at the grain boundary of a Ni-base alloy, alloy 600, can cause increased corrosion in acidic environments but may have no effect or even a beneficial effect in neutral or alkaline environments. Hence, the effort in this part of model development will focus on modeling the kinetics of structural change without considering its effects on performance. Performance will be considered in the interaction models. Some of the key processes and mechanisms that need to be evaluated for the materials stability models include:

1. The ability to predict structural transformations for various materials as a function of pertinent variables such as chemical composition and thermal history needs to be evaluated,

2. The kinetics of chromium-rich carbide precipitation needs to be studied and the effect of time and temperature on the development of chromium depletion zones needs to be assessed, and

3. The kinetics of segregation of metalloid elements such as phosphorus and sulfur to the grain boundaries needs to be evaluated.

Currently, no specific models have been chosen. However, structural changes as a function of chemical composition of a material can only be addressed by the use of empirical evidence. In some cases, semi-empirical calculations such as PHACOMP (Woodyatt, 1966) or other modifications can be used to predict the type of precipitation that can occur in a given material. Models, for specific materials, do exist to aide in assessing the effect of time and temperature on the development of chromium depletion zones. Some models that will be considered with respect to chromium depletion include DEPLETE which was developed by Was and Kruger (Was, 1985) and is specific to alloy 600, the model by Bruemmer (Bruemmer, 1990) which is specific to alloys such as Type 304 and 316 stainless steels precipitating $M_{23}C_6$, and the models by Mozhi, et. al (Mozhi, 1987) which pertain to various nitrogen-containing stainless steels. Phenomena such as segregation have to be quantified by extrapolation of experimental data from higher temperatures. These models will be assessed and appropriate models will be incorporated into EBSPAC. This assessment process will start in FY93.

4.2 Environmental Models:

Heat in the waste package and near-field environment is generated by radioactive decay of waste elements and their daughter products, and drives many hydrological, mechanical, and chemical processes. The heat generation rate depends on the quantity of waste material and its radionuclide inventory. Heat transfer through the waste package and near-field media can occur by convection, conduction, and radiation. The heat transfer rate is determined by the ambient conditions and the thermophysical properties of the media involved. Heat transmission and temperature in the waste package near-field are also affected by physical processes, particularly vaporization and condensation of water.

Elevated temperatures in the near-field environment at Yucca Mountain are expected to lead to a number of important geochemical variations. Rates of alkali feldspar dissolution and growth of secondary phases such as smectite, clinoptilolite, silica minerals and/or calcite would be accelerated. Volatilization of water will initially tend to purge the dissolved CO_2 affecting solution pH and will ultimately lead to precipitation of "salts" including silica in the near-field dehydration zone (Murphy, 1990). A heat-pipe is caused by nuclear waste heating which vaporizes pore water near the waste, releasing vapor into fractures. Driven by its pressure gradient, the vapor flows away from the waste and condenses where the rock is cooler. Because of capillary pressure gradient due to non-uniform liquid saturation, the condensate flows towards the waste surface through the porous rock (Pruess, 1988). These conditions may create a more corrosive environment for emplaced engineered materials.

Predicting the geochemical effects of the introduction of engineered materials in the near-field environment requires research that spans the engineering and geoscience disciplines. The geochemistry, hydrology, and thermal affects will be input to the EBSPAC through external code linkages. It is anticipated that EBSPAC will access these time-dependent data through a database module.

4.3 Interaction Models:

These models will be used to estimate the rate of material degradation and will use the output of the material stability and near-field environmental models. The primary models in this group will address localized corrosion (pitting, crevice, and intergranular corrosion), stress corrosion cracking, uniform corrosion/oxidation, leaching and dissolution of vitrified and spent fuel waste forms, and component mechanical instabilities due to fracture or yielding.

4.3.1 Crevice Corrosion

Crevice corrosion is considered to be the most important of the localized corrosion processes not only because crevices are unavoidable in engineering structures, but also because crevice corrosion can be a precursor to other degradation processes such as stress corrosion cracking. Crevices act to concentrate and acidify the environment within them because of poor mixing with the external environment, and electrochemical and chemical (e.g., hydrolysis) reactions within the crevices. In the case of the waste containers, crevices can also act to concentrate the environmental species due to purely thermal processes related to heat transfer from the radioactive decay. Such concentration mechanisms due to heat-transfer effects combined with flow disturbances have been observed in tube-tube sheet and tube-tube support plate crevices in nuclear steam generators. Thus, two types of crevice corrosion models need to be considered:

1. crevice corrosion under isothermal conditions, and

2. crevice corrosion under heat-transfer conditions.

In the steam generator crevices, the latter mechanism seems to prevail. In the waste containers, the predominance of one over the other is not established. It is the intent of the EBSPAC system to concentrate on the isothermal case first and then examine the heat-transfer case next. Some overlap between these two activities may also occur. For the isothermal case, although many models exist most of them applicable to relatively low temperatures (e.g., sea water at 25°C). The Watson and Postlethwaite model (Watson and Postlethwaite, 1990) has been chosen as the starting point for further development. This model is a finite difference based model that predicts changes in the chemical composition of the environment within the crevice as a function of time. Then a comparison is made at each time period between the calculated chemical composition and the critical chemical composition needed for the crevice to initiate active crevice corrosion. The time at which these two chemical compositions become approximately equal is the initiation time for crevice corrosion. This model and others of an equivalent nature are applicable only to aqueous solutions, which is considered to be an extreme condition in the repository with respect to corrosion. This model needs further improvement in terms of considering the effect of temperature, redox species, concentrated electrolytes, and anions other than chloride.

It must be noted that the above mentioned crevice corrosion models are relevant to chromium containing alloys. The copper-based alloys behave quite differently. In many cases, they exhibit higher corrosion outside the crevice because of easier access of cathodic species. However, copper-based materials may still be sensitive to the heat-transfer induced concentration of electrolytes within the crevice.

4.3.2 Pitting

Modeling of pitting is more difficult because the initiation stage is not well defined and initiation sites are often distributed at random on a given surface. Hence, pitting initiation has been modeled using stochastic methods. Extreme value statistical methods have been used to predict penetration of pipe walls by pitting, but these depend, for their time-extrapolation, on empirical, short-term data or ad-hoc assumptions of time dependance. Mechanistic models of pitting have been content with predicting the experimental observations of the dependence of pitting on environmental variables. Thus, no satisfactory methods exist for extrapolating short-term pitting corrosion data to long time periods. Because of this limitation and the greater engineering importance of

8

crevice corrosion, less effort will be made on pitting corrosion during the initial EBSPAC development. It must be noted that statistical predictions of pit penetration through the walls of a container can be done using experimental measurements of pit depths in long-term corrosion tests. However, these predictions are again limited to the time frame of the test and can only be used to scale-up in size scale (i.e., from a small sample to many containers).

4.3.3 Stress Corrosion Cracking

Stress corrosion cracking models also need considerable development from the current state of knowledge. Predicting stress corrosion cracking is made difficult by the lack of a single accepted mechanism which is unlike the case of crevice corrosion. The mechanism of SCC has been shown to vary with environment and material. Models, such as the Ford and Andresen model (Ford and Andresen, 1985), have been developed for crack propagation on stainless steels and nickel-base alloys in high temperature aqueous environments typical of nuclear power plants. However, it is not clear if the same underlying mechanism of stress corrosion cracking is operating for candidate container materials, such as alloy 825 or copper, in the repository environment. Hence, the development of stress corrosion cracking models will be initiated only after significant progress is made in crevice corrosion modeling. Other degradation modes such as uniform corrosion, oxidation, corrosion fatigue, and microbiologically-influenced corrosion may need to be considered in the eventual prediction of the EBS performance. In many of these cases, significant research needs to be performed to establish their importance before modeling can be undertaken.

4.3.4 Source Term

The source term model development is a key component of the EBSPAC release rate determination. This activity for FY91 is being conducted in conjunction with the Performance Assessment Element. A detailed source term development plan for EBSPAC will be presented in the EBSPAC Development Plan—Update 2 (Major Milestone No. 20-3702-013-210). This will enable the Center and NRC staff to evaluate the overall source term requirements pending the early results of the current source term effort.

A source term release rate model may be based on preferential leaching of certain chemical species or on the gross dissolution of the wasteform or both. The rate of mass transfer is affected by the chemical nature of the soluble material and the solvent, the temperature, and the flow rate of the solvent past the wasteform. The combination of leaching from the wasteform and the dissolution in the liquid phase determines the amount of material available for transport. In comparison to spent fuel, more data is available in the open literature on vitrified wasteform. Hence, as a first step, EBSPAC will contain a simple leaching model for vitrified wasteform. As stated earlier, part of the developmental activity for source term models is being conducted under the Performance Assessment Program Element. This activity is in support of the NRC'S Phase II Iterative Performance Assessment Program.

5. MODEL INTEGRATION APPROACH

Task 3 of the EBS program element activities is directed towards understanding and evaluating the performance of the various barriers within the EBS. EBSPAC will embody as completely as feasible the understanding and the evaluation techniques developed at the Center and through research by others.

5.1 Major Components of EBSPAC

The many lines of code, subroutines, and modules needed in EBSPAC can be divided into five major functional groups or components. The major components are the user interface, the material degradation models, the FPPA methodology, the external code linkages, and the database. These components are integrated through the EBSPAC Driver.

5.1.1 User Interface:

The EBSPAC user interface will have two forms. One form of the user interface will be an interactive preprocessor, which will guide the user through the input generation needed for a given analysis. All internal EBSPAC functions will be keyword driven and the preprocessor will construct the keyword-driven "USER" file. The ultimate form of the interactive preprocessor will allow the user to perform a fault-tree analysis in order to define the particular scenario to be analyzed. The other form of the user interface will allow the user to prepare the keyword-driven "USER" file in any editor or word processor and to submit that file through system commands directly to EBSPAC for data analysis. All EBSPAC data analysis are intended to run in a batch mode.

5.1.2 Material Degradation Module:

The material degradation models are the foundation of the EBSPAC system. These models which form the relationship between relatively short-term tests and long-term performance will be based on fundamental mechanisms, as described in Section 4. The material models, the environmental/mechanical models, and the interaction models are the three basic groups of models that will be included in the material degradation component of EBSPAC. Obviously, each of the aforementioned model groups will contain various models which allow the simulation of a number of possible analysis scenarios.

5.1.2.1 Material Models:

The material models will represent typical multiphase, multicomponent alloy systems. These models will attempt to capture the kinetic and thermodynamic quantities which affect the stability of a given material structure. The material behavior cannot be fully described from first principles, hence, empirical modifications to the theoretical models will be required. Material models will be expressed as equations or data points and will model the material mechanical properties, the material thermal properties, the material chemical composition, and key parameters (carbide precipitation, chromium depletion width, etc.) for determining the material degree of sensitization.

5.1.2.2 Environmental/Mechanical Models:

The environmental/mechanical models will embody the primary mechanisms in the near-field environment which can influence the rate of degradation and the subsequent failure mode of the waste package. The key environmental models will allow the simulation of the waste package radiation effects, thermal environment, the near-field hydrology (for determining whether the waste package is wet, dry or in steam), and the geochemistry. Corrosion of the waste package is very dependent on the geochemistry of the near-field environment. Also, the geochemistry of the water can affect the solubility of the radionuclides, thereby affecting the source term and the release rate from the EBS. The mechanical model will calculate the thermal and mechanical stresses at various locations in the waste package container.

5.1.2.3 Interaction Models:

The interaction models will couple the modeled conditions from the environmental/mechanical models with the material models in order to simulate the influence the environmental/mechanical loads will have on the modeled material systems. These models will be used to estimate the rate of material degradation and the potential failure mode of the waste package. The primary models in this group simulate pitting and crevice corrosion, stress corrosion cracking, uniform corrosion, component instabilities due to fracture or yielding, leaching and dissolution of vitrified wasteform. The chosen crevice corrosion model contains key parameters which incorporate the alloy composition, the critical crevice solution, the passive current density, ionic diffusion and migration, bulk solution, and crevice geometry.

5.1.3 FPPA Methodology:

The Fast Probabilistic Performance Assessment (FPPA) methodology is a powerful probabilistic tool developed by the Center. FPPA is believed to be a viable approach for addressing the assessment needs of the NRC in compliance determination of the EBS performance. FPPA is mainly used to perform sensitivity analyses. Based on these results, one can prioritize uncertain variables in an efficient way. Even though the FPPA methodology will be the foundation of the probabilistic analyses in EBSPAC, the Monte Carlo simulation will also be included for checking purposes.

5.1.4 External Code Linkages:

Because of the complexity of EBS performance assessment, EBSPAC will be required to accept data from major external computer codes. It is anticipated that hydrologic, radiation, geochemical, structural, and thermal computer codes will supply the time dependent boundary conditions to the internal EBSPAC material degradation models through external computer code linkages. These linkages will accept the data from the external computer codes and process it for acceptance by the appropriate model(s).

5.1.5 Database Module:

The mechanistic models within EBSPAC will integrate many different engineering and scientific disciplines. In order to effectively implement this integrated approach, EBSPAC needs ready access to a significant amount of technical data. This access will be provided through a relational database program contained as a separate module of EBSPAC. One will be able to add records to the database during an analysis run or use existing values. This will allow subsequent analyses to use some results and data generated by previous analyses.

5.1.6 EBSPAC Driver:

The major EBSPAC components and processes are integrated through the EBSPAC driver (Figure 1). The EBSPAC driver will control the simulation timing and the logic of module calling sequences. The planned waste package pre-failure interactions among the material degradation models, the external codes, and the database are shown as Figure 2. Subsequent to waste package failure, the planned interaction between the modeled wasteform and the modeled environment is shown as Figure 3.

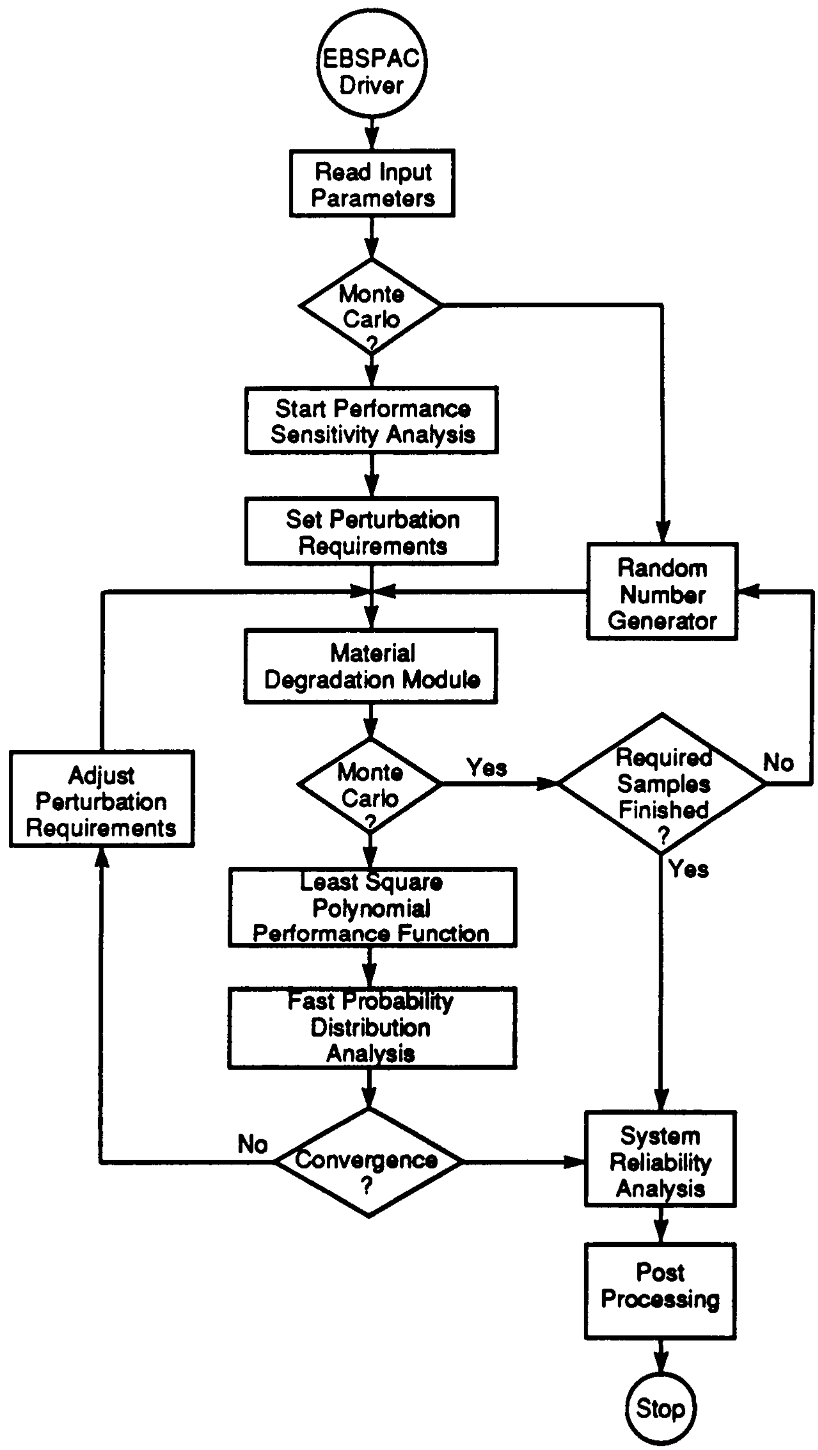

Figure 1. EBSPAC Driver Program

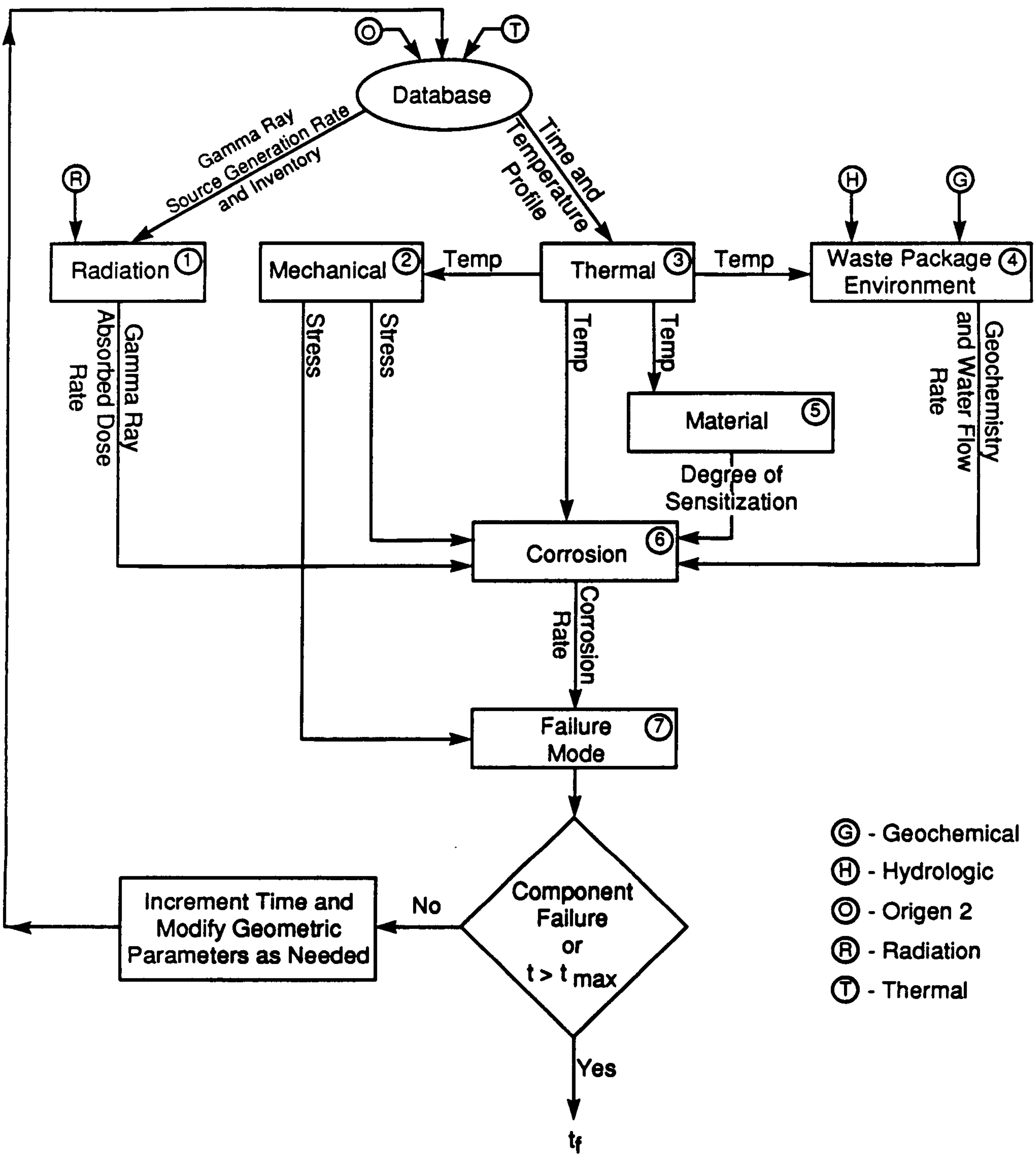

Figure 2. Interaction Diagram for Material Degradation Module-Containment

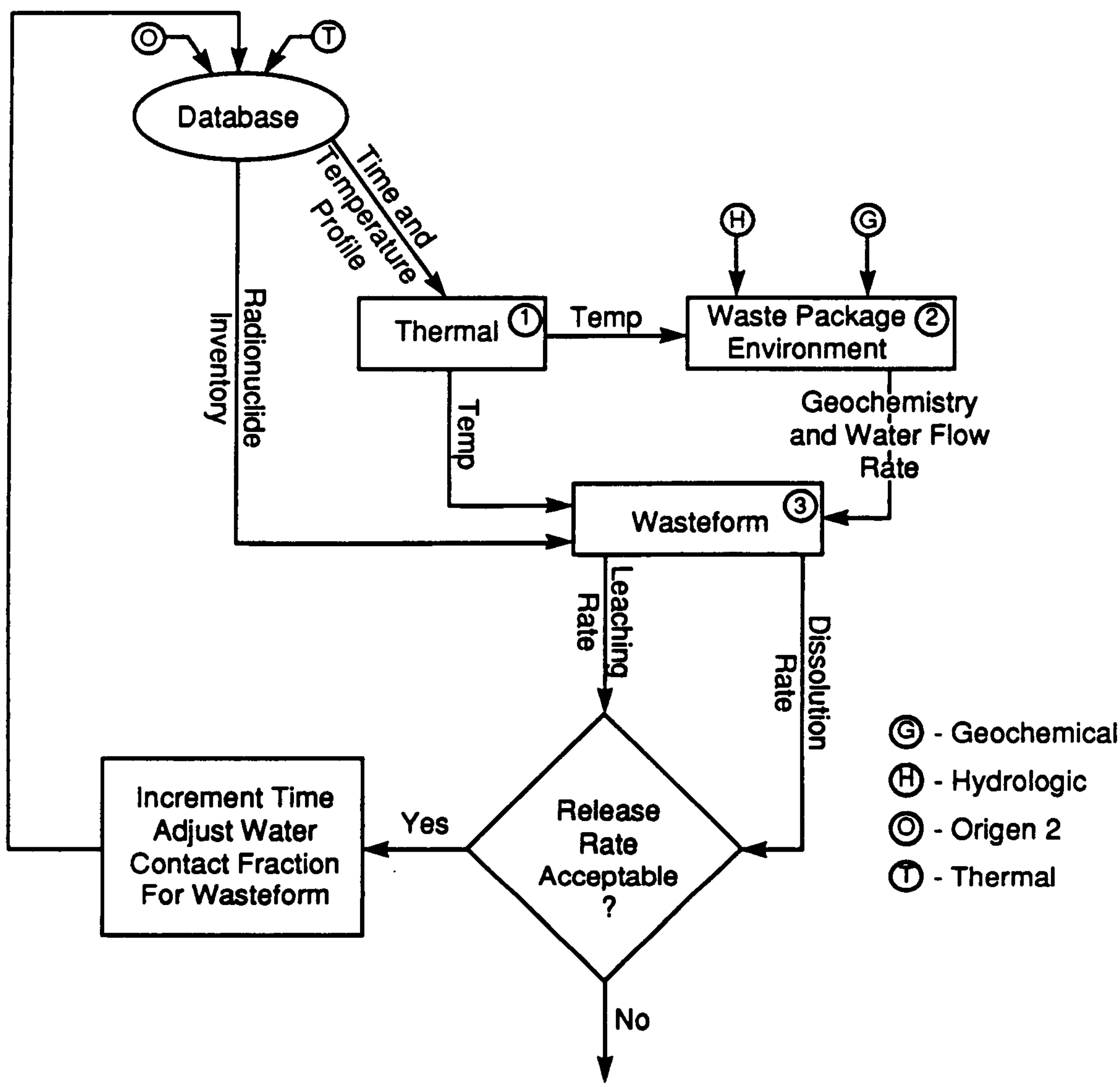

Figure 3. Interaction Diagram For Material Degradation Module-Release Rate

6. PLAN OF IMPLEMENTATION

The Center has, to date, developed and exercised the FPPA component of the EBSPAC. The FPPA code has been linked with CONVO and other subroutines in order to evaluate the FPPA methodology. In FY91, the FPPA methodology will be integrated into the EBSPAC structure through the development of the EBSPAC driver. The planned EBSPAC driver is shown as Figure 1.

Subsequent to the development of the main driver, work will begin on the coding of the thermal models for the waste package container and near-field region. It is envisioned that TOPAZ, a finite element heat transfer analysis computer code, will be used to calculate these detailed transient temperature distributions. Additionally, EBSPAC will contain a thermal module which will process the TOPAZ data and prepare it for use by other EBSPAC models. In FY91, customized subroutines will be developed for modeling the heat transfer boundary conditions applied to the TOPAZ (Shapiro, 1985) computational model. It is anticipated that the modeled heat transfer boundary conditions will include four possible models. They are as follows:

1. a decay heat generation rate model which will be based upon the waste material inventory, age and percent burnup. This condition will be modeled as a flux and applied to the inner surface of the waste container,

2. a thermal radiation model which will be applied at the outer surface of the container and at the borehole wall, and when appropriate,

3. a natural convection model which will be applied in the air gap between the container and the borehole wall, or

4. a conduction model which will be applied in the air gap between the container and the borehole wall.

In parallel with the implementation of the thermal models, work will commence on the development of the material degradation module framework. This framework will control the logic of the interactions among the material degradation models. The crevice corrosion model will be the first interaction model coded in this module. This model will include chemistry and thermal affects on crevice corrosion. A partially complete version of the crevice corrosion model will be developed in FY91.

Implementation of the mechanical model will commence during FY91. The mechanical model will calculate the mechanical and thermal stresses at various locations in the waste package. Initially, the primary locations for stress calculations will be the inner surface of the waste package container and the outer surface of the waste package container. The calculated stresses will be used in stress corrosion cracking models and in assessing container integrity and other potential failure modes.

A simple radionuclide leaching model for vitrified wasteform will be evaluated and incorporated during FY91. The final leaching model will ultimately include mechanistic understanding based on chemical, physical and loading characteristics of the vitrified wasteform. The leaching model will be the first of the wasteform alteration models integrated into the EBSPAC structure. The wasteform alteration models will calculate the amount of each radionuclide per year released into mobile form. The mobile form considered in FY91 will be solutes in water.

During FY91, an appropriate FORTRAN written database program will be located and integrated into the EBSPAC. The database design will allow the EBSPAC modules to access the needed data on a conceptual level. This database feature will eliminate data storage structure from module development consideration.

The coding and the implementation of the isothermal crevice corrosion and the uniform corrosion models will be completed during FY92. Models for crevice corrosion under heat-transfer conditions, stress corrosion cracking, and pitting corrosion will be initiated during FY92. These corrosion models will include chemical and thermal affects and where appropriate the effect of stress.

Subsequent to initiating the implementation of the stress corrosion and the pitting corrosion models, work on enhancing the radionuclide leaching model for vitrified wasteform will commence. The leaching model will be completed during FY92.

Also during FY92, evaluation and incorporation of the gamma ray dose model will commence. The attenuation and the absorbed dose rate from gamma rays are complex processes and cannot be modeled from first principles by a simple model. Hence, EBSPAC will contain a simplified model which interacts with a database of detailed calculations from an external computer code. The EBSPAC simplified model will, as a minimum, scale the calculated detail results (from the external code) over the time history of a waste package as the gamma source strength declines. Two types of data will be scaled. The absorbed dose rate at the wasteform surface will be scaled and the attenuation factors between the wasteform surface and the container outer surface will be scaled.

A hydrologic code will be used to calculate the rewetting time of the rock around the emplacement hole and the water flux during the earlier transient period. Hence, EBSPAC will contain a module which will use the results from the hydrologic code to help describe the waste package environment (i.e., air/steam, air/water vapor, or water). This module will describe how water will contact the container and the wasteform. This module will also describe the flow rate of the water that will contact the container and the wasteform. Implementation of this model will commence during FY92. A subsequent version of this module will contain the affect of geochemistry. Development of the external linkages for the thermal code and the hydrologic code will also commence during FY92. These activities will be accomplished by significant interaction with the Geosciences and System Performance Assessment staff at the Center.

The development of the interactive preprocessor will commence during FY92 and be completed during the subsequent fiscal year.

Activity Description, Related Milestones and Deliverables

The activity completion dates denoted below are target dates for use by the EBSPAC development team and they do not alter in any way the dates set forth in the FY91-92 EBS Program Element Operations Plan. Each activity mentioned below has the same leading 7-digit WBS [3702-013], only the last 6-digits are shown.

260000 - Design and Code EBSPAC Driver

Design of the EBSPAC driver started in FY90. The coding of this module should be complete at the end of February 1991. Documentation of the module development progress will be reported in the Program Manager's periodic report.

240005 - Customized Heat Transfer Boundary Condition Routines

Work on the customized heat transfer boundary conditions for the TOPAZ transient heat transfer analysis code will commence in March of 1991 and should be complete at the end of June 1991. Documentation of Task 2 progress will be reported in the Program Manager's periodic report.

260005 - Material Degradation Module Framework

The work on the material degradation module framework will begin in January 1991 and be complete at the end of July 1991. Documentation of the progress made in this task will be reported in the Program Manager's periodic report.

260010 - Interaction Models

Coding of the mathematical model for numerical simulation of crevice corrosion started in October 1990, and the base model should be complete at the end of July 1991. Work in this area will continue into subsequent years. Documentation of the progress made in this task will be reported in the Program Manager's periodic report.

240000 - Environmental/Mechanical Models

In April 1991, work will commence on the incorporation of a mechanical model to calculate mechanical and thermal stresses on the inner and outer surfaces of the waste package container. This work will continue into FY92. Work on additional E/M models will continue into subsequent years. Progress on this work will be reported in the Program Manager's periodic report.

230000 - Source Term Release Rate Models

During May 1991, work will begin on the coding for a release rate model simulating leaching of a vitrified wasteform. This work will continue into FY92. Development progress will be reported in the Program Manager's periodic report. This activity will be performed in conjunction with the System Performance Assessment Program Element schedules for FY91.

215001 - Database

In January 1991, efforts will commence towards obtaining a FORTRAN driven database for the EBSPAC. The database will be selected and integrated into the EBSPAC by the end of August 1991. Progress toward this effort will be reported in the Program Manager's periodic report.

18

7. CONCLUSIONS

Performance objectives set forth in 10 CFR 60.113 contains the requirements for the performance of particular engineered barriers after permanent closure of the repository. To evaluate the conformance of DOE'S EBS subsystem design and performance analyses of these designs to the regulations, the NRC needs a viable tool/methodology that is technically sound and is able to accommodate evaluation of alternate or extreme scenarios. Regulations in 10 CFR 60.113 contain numerical values of performance requirements in terms of times for containment and for gradual release rates. These numerical values dictate the use of computer programs that compute and manage diverse process models in addition to interacting with engineering and research databases. Faced with this challenge, the development of EBSPAC represents the solution for:

1. providing a credible tool for evaluating EBS performance of the DOE license application.

2. providing sensitivity analyses of critical parameters in a timely manner, especially when alternate modes or scenarios are proposed by any interested parties to the license application.

3. providing guidance to research areas and to assist in review of DOE submittals during the pre-licensing phase.

4. assisting the focus of EBS-related research for the NRC programs.

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