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Center for Nuclear Waste Regulatory Analyses

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January 9, 1997
Contract No. NRC-02-93-005
Project No. 20-5708-572

U.S. NUCLEAR REGULATORY COMMISSION
ATTN: Dr. Kien C. Chang
Program Element Manager
Division of Waste Management
Mail Stop T7C-6
Washington, DC 20555

SUBJECT: Response to NRC staff comments on Intermediate Milestone 20-5708-572-640, Engineered Barrier System Performance Assessment Code: EBSPAC Version 1.0β, Technical Description and User's Manual, CNWRA 96-011

Dear Dr. Chang:

We have received your letter dated October 8, 1996, regarding the above referenced subject, accompanied by some general and specific comments (Enclosure 1 of your letter), as well as comments from Richard Codell (Enclosure 2 of your letter). The purpose of this letter is to respond to the comments attached to your letter. Enclosed are the responses prepared by Gustavo Cragnolino and Sitakanta Mohanty. The responses are provided as two attachments: (i) Attachment 1 addresses comments in Enclosure 1 of your letter and (ii) Attachment 2 addresses comments in Enclosure 2 of your letter.

Specific comments and changes suggested in your review comments as well as others provided by NRC staff during the training workshop on EBSPAC held at the NRC on December 11-12, 1996, will be incorporated in a revised version of the report to be issued following the delivery of EBSPAC Version 1.0 to the NRC.

I believe that the workshop on EBSPAC was very valuable, and I would like to take this opportunity to thank you and other NRC staff in helping to set up the workshop.

Sincerely,

N Sridhar

Narasi Sridhar
Element Manager
Engineered Barrier System

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NS/blg
Enclosure

cc: J. Linehan, S. Fortuna, B. Stiltenpole, B. Meehan, J. Greeves, M. Federline, J. Austin, M. Bell, J. Thoma, R. Weller, R. Codell, T. Ahn, D. Dancer, W. Patrick, CNWRA Directors, CNWRA Element Mgrs., S. Mohanty, G. Cragnolino, D. Dunn, P. Lichtner, R. Manteufel, S. Rowe (SwRI)

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ATTACHMENT 1

RESPONSE TO REVIEW COMMENTS ON EBSPAC VERSION 1.0β, TECHNICAL DESCRIPTION AND USER'S MANUAL (ENCLOSURE 1 OF NRC LETTER)

1. Addition to future work on page 6-1

The comments can be classified in two groups. The first group (bullets 1, 3, 4, and 5) includes the consideration of models for cladding failure, glass leaching, the effect of partially failed container, canister, and cladding on radionuclide release, and the effect of waste package degradation on criticality. These models should be considered a part of future enhancement of the Engineered Barrier System Performance Assessment Code (EBSPAC) development. This was stated in the plan for the development of detailed models for EBSPAC that was presented to the Nuclear Regulatory Commission (NRC) in fiscal year (FY)95. Although Center for Nuclear Waste Regulatory Analyses (CNWRA) staff will not be involved in this development as a result of lack of funding for the Container Life and Source Term KTI during FY97, these models should be incorporated in the list of future developments suggested on page 6-1 of the CNWRA 96-011 report following an adequate prioritization. It should be noted that any future development of EBSPAC should comply with the software control requirements in TOP-018.

Comments under bullets 2 and 6, belong to a different group. Probabilistic assessment of container life and source term, as clearly stated in the report, will be done by the NRC/CNWRA TPA code within which EBSPAC will serve as the source term module. Disruptive events are already considered in EBSPAC Version 1.0β, as noted on page 3-1 of the report, in terms of the time of occurrence, but the specific effect on the source term will be considered as part of the overall development of the TPA code.

2. Other comments and questions

Specific comments included as bullets in this item will be addressed and incorporated in the revised issue of the user's manual for EBSPAC Version 1.0.

(ii) A more realistic model for matrix dissolution of SF (i.e., based on short-term experimental data) that considers dissolution as a time varying function through the variation of temperature with time was incorporated to EBSPAC as opposed to a fixed value used in SOTEC.

(iii) EBSPAC allows for gaseous release from the unwetted part of the SF, whereas liquid release occurs on the wetted part up to the maximum allowed release time.

From the computational point of view, it should be noted that the variable time stepping of EBSPAC integration algorithm eliminates the need for an arbitrarily chosen time constant except when the flow rate used is too high or too low. The "time constant" is interpreted as the time taken by the water to fill up the empty space inside a WP before water flows out. A time constant of 5 years is used in EBSPAC instead of 50 years as used in SOTEC so that the code can handle very high flow rates. Additionally, the use of variable time stepping helps to some extent in the adjustment to either faster or slower decay of radionuclides. Other approaches such as simplifying or eliminating stiff equations or using a closed-form solution for the filling rate of WP as a function of time can be implemented to improve the efficiency of the code as suggested by R. Codell (Enclosure 2). These modifications can be considered for further development of EBSPAC.

It should be noted, however, that EBSPAC runs simulations up to a million years and the run time appears to scale linearly from 10,000 to 100,000 to 1,000,000 years, as shown below as approximate cpu times.

Simulation Time (yr)	SUN IPX/cell	SPARC20/cell
10,000	73 s	12 s
100,000	602 s	115 s
1,000,000	4345 s	811 s

The code, however, exhibits the same limitations as NEFTRAN with regard to the times at which temperature and relative humidity are provided in the output table of the thermal model to be used in the TPA code.

Distribution of failures and release

EBSPAC focuses on a single WP for determining the failure time due to corrosion (or mechanical failure) and then for release calculations assumes that all WP in a cell that have not failed prior to the failure time due to corrosion fail simultaneously. The best approach to capture the variabilities in the repository is to divide the repository in many cells. This approach will significantly increase the run time, but improvements in the efficiency of EBSPAC will not significantly reduce the execution time as long as the time required for NEFTRAN to calculate unsaturated zone transport is not reduced significantly.

Thermal Models

Calculations used in EBSPAC were based on representative WP in the center of the repository (far from the edge) corresponding to the highest temperature expected. Temperature calculations based on subarea location in the repository will be performed as part of TPA 3.0 in the future.

ATTACHMENT 2

RESPONSE TO RICHARD CODELL'S COMMENTS ON EBSPAC VERSION 1.0β, TECHNICAL DESCRIPTION AND USER'S MANUAL (ENCLOSURE 2 OF NRC LETTER)

The response to these comments is organized following the format used in the NRC Enclosure 2.

Introduction

The new waste package (WP) design proposed by the DOE as well as modifications in the design of the engineered barrier system (EBS), including high thermal loadings, horizontal emplacement of the WPs in drifts, and use of backfill, were taken into consideration in the WP failure and radionuclide release models used in Engineered Barrier System Performance Assessment Code (EBSPAC) Version 1.0β. Possible changes in the Nuclear Regulatory Commission (NRC) regulations regarding the elimination of the subsystem requirements contained in 10 CFR 60.113 were also taken into consideration and the simulation period was extended to 10,000 years from the 1,000 years used in SCCEX, with an option for longer simulation times. Because EBSPAC will be incorporated as a source term module to the TPA code, many simplifying assumptions are used to reduce code execution time such that it becomes comparable to that of other modules in the TPA code. This is the rationale for the use of steady state models for the description of several processes.

Finally, as in the case of any other code, it is obvious that ". . . the model results are highly dependent on assumptions made." In this regard, the relevant questions can be summarized as: (i) are the assumptions reasonable on the basis of the existing knowledge, and (ii) are the results conservative and can sensitivity analyses be performed in a simple manner to assess the significance of certain parameters to WP failure and radionuclide release? These questions are answered below in response to R. Codell's comments.

Gaseous release model

It is recognized that experimental data published in the literature and used in EBSPAC were obtained for a limited range of temperatures. The model presented in Eqs. (2-36) and (2-37) of the user's manual takes temperature into account through the temperature-dependent diffusion coefficient (D_m). EBSPAC sums the gaseous releases from all time intervals assuming isothermal conditions in each time interval. However, no adjustable time step-based integration is used to determine gaseous release due to spent fuel (SF) oxidation. In addition, the initial condition for computations in each time interval is such that the gaseous releases are conservatively estimated.

Liquid release model

The basic models of the liquid release part of the code were not changed because the intention was to use those presented in SOTEC as far as they were applicable. The new WP design does not seem to require, with the exception of certain geometric considerations, any substantial change in the model for liquid release. Regarding the conceptual models for release, the following points can be made:

(i) The effect of the horizontal emplacement of WPs in drifts and its influence on release is accounted for in EBSPAC through appropriate consideration of the rise of the water level inside the WP.

Waste Dissolution Rate

The model for waste dissolution is based on experimental data under flow-through conditions and represents the intrinsic rate of dissolution which may lead to conservative calculations. However, it is commonly accepted that radionuclides such as C-14, Tc-99, I-129, and Cs-135, which have long half-life times, also exhibited high solubility limits. Under near-stagnant flowing conditions, these radionuclides are released congruently from the UO_2 matrix. Whereas UO^{2+} ions can be redeposited as secondary minerals on SF surfaces, these long-lived radionuclides could be released without being limited by the leachate concentration as long as secondary minerals do not act as effective diffusion barriers. Our calculation in the example problem shows that the leaching time is about 250 to 3,000 years (depending on how the SF surface area is computed) which is substantially shorter than the period estimated in SOTEC. However, different approaches can be easily implemented to take into consideration decreases in the rate of dissolution associated to the precipitation of secondary uranyl silicate minerals and the presence of Ca^{2+} ions and Si species in the groundwater. A factor could be introduced into the input file that can be modified by the user to specify the desired surface area until a resolution is reached regarding an acceptable value of surface area for SF dissolution. This approximate approach can be easily implemented.

Water Infiltration

The data used in EBSPAC is only presented as an example. The composition of the water contacting the WP is derived from J-13 water but modified by the effect of heat and reactive transport as calculated by MULTIFLO. Alternate calculations of the near field environment using pore water composition as the starting point can be easily incorporated as input to EBSPAC since these calculations are performed externally. Both in TSPA-95 as in NRC-IPA it is assumed that all waste forms are exposed to aqueous environments. The experimental basis for this assumption is not solid enough although limited data obtained at Argonne National Laboratory suggested that it is valid at high relative humidities (e.g., close to 100 percent). In case of full or partial wetting, the current version of EBSPAC can be easily modified by introducing parameters to account for the fraction of SF surface that is wetted.

Model dependence and assumptions

Although predictive models ideally should be based on first principles, this is not always possible for the description of complex phenomena. Whenever possible, models or equations based on fundamental principles were used. However, one of the main purposes of the models used in EBSPAC is to investigate the sensitivity of predictions on model parameters that cannot be completely determined experimentally or indirectly estimated from other measurements. For example, to determine the amount of water contacting the WP, it is necessary to predict infiltration rates. To be able to predict infiltration rates would require knowing rainfall which, in turn, would require being able to predict the weather. As indicated by R. Codell, this is less critical in the case of repositories located in the saturated zone where it is assumed that WPs are always in contact with groundwater. Whenever necessary and possible, the simplified models used in EBSPAC could be confirmed by more detailed mechanistic models developed as auxiliary analyses.

We agree that if time and resources are available, it would be desirable to improve the models dealing with radionuclide release, to consider particularly peak releases, and accordingly implementing more sophisticated numerical algorithms to deal with these cases.

UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555-0001

October 8, 1996

Dr. Narasi Sridhar, Manager
Engineered Barrier System Program Element
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road
San Antonio, TX 78228-0510

SUBJECT: ACCEPTANCE OF A DELIVERABLE FOR INTERMEDIATE MILESTONE 20-5708-572-640, ENGINEERED BARRIER SYSTEM PERFORMANCE ASSESSMENT CODE: EBSPAC VERSION 1.0B, TECHNICAL DESCRIPTION AND USER'S MANUAL, CNWRA 96-011

Dear Dr. Sridhar:

We have received the subject manual and find it acceptable in fulfillment of the requirements of Intermediate Milestone 20-5708-572-620. This manual documents NRC's assumptions and understanding of the processes included in EBSPAC Version 1.0B, code description, and sample problems. We consider that this work, along with the future developments recommended by this manual, will contribute to the resolution of many issues regarding long-term performance of waste packages for the geologic repository.

Enclosed are some general and specific comments we have on the manual. Please consider them in any future work we may have on EBSPAC development. We understand that you are in the process of transferring the Code to NRC with a plan for a workshop on EBSPAC application, and we shall have an opportunity to address details of the Code regarding its use in NRC's computer facility. We are looking forward to participate in these activities.

The action taken by the above direction is considered to be within the scope of the current contract. No change to cost or delivery or contracted products is authorized. CNWRA should review the direction and identify any resulting impact on scope, schedule, or cost. If you have any questions regarding this matter, please call me on (301) 415-6612.

Sincerely,

Kien C. Chang
EBS Program Element Manager
Engineering and Geosciences Branch
Division of Waste Management
Office of Nuclear Material Safety
and Safeguards

Enclosures: As stated

cc: J. Linehan, NMSS/PMDA
B. Meehan, ADM/CAB

EMs
Dirs
EBS staff

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REVIEW COMMENTS ON EBSPAC VERSION 1.0B, TECHNICAL DESCRIPTION AND USER'S MANUAL, SEPTEMBER 1966

(1) Addition to future work on page 6-1

- Incorporation of the cladding failure models. The cladding failure models include creep, localized corrosion, and hydride reorientation.
- Consideration of disruptive events in source term. The disruptive events include volcanism and seismicity.
- Consideration of partially failed container, canister, and cladding in radionuclide release.
- Consideration of HLW glass leaching.
- Consideration of criticality during the degradation of waste package. For instance, water intrusion and geometry change are events under which criticality needs to be considered.
- Probabilistic assessment of container life and source term.

(2) Other comments and questions

- Please provide units for the parameters of equations, e.g., Equations 2-10, 2-18, 2-41, 2-48, and 3-1.
- Page 2-9. Why can the local vapor partial pressure not exceed the atmospheric pressure?
- Section 2.5.1. At a given temperature T and corrosion potential E_{corr} only constant passive currents are considered. Does passive current change as the oxide grows in thickness?
- Page 2-29. Change the title of Section 2.7.1.3 to "Oxidation of Spent Fuel."
- Page 2-34. In Equation 2-45, should "λKC" be "λC"?
- Page 2-37. The reference to (Manaktala, et al., 1996) should be (Manaktala, et al., 1995).
- Page 3-3, Section 3.1.2. Include a statement to explain that for EBSPAC Version 1.0 β radionuclide release calculations, unlike waste package life-time calculations, only Type 1 (anticipated) scenarios are addressed, and that Type 2 (disruptive) scenarios are not treated.

Enclosure 1

- Page 3-5, second paragraph from the bottom. Porosity does not increase the surface area exposed to leachates or air because it is isolated from the external surface. The exposed surface area from transgranular fractured subgrains is the largest, followed sequentially by that from individual grains, particles, and pellets. If fuel was not crumbled by oxidation, the particle size (≈ mm) can be used. If individual grains or subgrains are exposed, the grain size (≈ 10 micrometer) or the subgrain size (≈ 1 micrometer) can be used, respectively. Fragmentation resulting from intergranular and transgranular oxidation could increase the surface area by a factor from 100 to 1,000 respectively, in reference to particles.

- Page 7-6, please add:
  Rothman, A. J. 1984. *Potential Corrosion and Degradation Mechanisms of Zircaloy Cladding on Spent Nuclear Fuel in a Tuff Repository*. UCID-20172, Livermore, CA: Lawrence Livermore National Laboratory.

Note to: Kien Chang

From: Richard Codell

Subject: Review of EBSPAC Version 1.0 Beta

Introduction

The authors of this report have incorporated several important improvements over SOTEC into EBSPAC, but the EBSPAC code is deficient in a number of ways. Among these deficiencies are possible misapplication of steady state models to transient analyses and lack of recognition of changes to the operating paradigm for the Yucca Mountain repository, in light of new waste package designs and changes to the regulations. Furthermore, the model results are highly dependent on assumptions made.

Gas release model

The solution for diffusion of gaseous radionuclides out of the fuel is for the isothermal case. It does not recognize that the temperature is varying with time. There is practically no acknowledgement of how EBSPAC copes with this problem. They only admit that "Simple analytical solutions are used in gaseous release calculations, avoiding the use of time consuming numerical integrations." (page 3-4, second paragraph). I discussed this question with Tae Ahn and he assured me that the code handles the problem of transient temperature. I would just like to see the explanation for myself.

Liquid release model

The developers incorporate the different waste package design into the liquid release model, but did not change the basic structure of the release and transport model. They improved the solution somewhat by incorporating a better numerical integration algorithm, but I believe that the program could be greatly improved by a basic restructuring of the computations. The numerical inefficiencies in the Phase 2 SOTEC code were tolerable because the calculations were restricted to 10,000 years. For calculation times on the order of 100,000 to a million years, the calculations become burdensome. The biggest obstacle to efficiency is the numerical integration of the differential equations. A slightly improved algorithm like the 5th order Runge-Kutta incorporated in EBSPAC does not overcome the necessity to take small time steps, which are controlled by the time constants of the model.

I feel that the best way to cope with this problem is to restructure the code to reduce dependence on numerical integration, and choose alternative methods that allow large time steps. I have dealt with similar problems successfully before. I would look at several possibilities:

1. Inspect the equations in EBSPAC with the view of simplifying or eliminating those parts likely to be adding to the computational burden or that make the equation set "stiff", i.e., possessing widely separated eigenvalues.

For example, I had programmed SOTEC to numerically integrate the flow input and output to the failed container. This could easily be replaced with a closed-form solution that gives the volume of water in the container versus time. Another possible simplification would be to the diffusive transport part. I believe that in most cases this part of the model contributed relatively little to the release for those cases that had finite advective flux, and the cases that had no advective flux had inconsequential results anyway. It may be possible therefore to eliminate the numerical solution and replace it with a simpler analytical solution.

2. Employ numerical algorithms specially designed for stiff equations. There is a voluminous literature on stiff equation solvers and many computer codes available from sources on the Internet. I have used such solvers successfully in the past.

Distribution of failures and release

I think an increasingly important problem in the source term model is the distribution of the failure rate for the waste packages and the release rate. This takes on more importance because the new regulations will likely be based on peak dose, and a spread-out distribution would have a lower peak. Cumulative release over 10,000 years is much less sensitive to the peak release rate from the repository.

In light of this concern, there should be more consideration in EBSPAC to the distribution of failures. This could be handled in at least two ways:

1. Run more waste packages. The current analysis is patterned after 7 repository zones, with one "representative" waste package per zone. Determining what is "representative" is a challenging problem, which doesn't capture the variability in the makeup and environment of the containers in different parts of the repository, or the random nature of the phenomena governing failure of the packages and releases from them. This problem can be alleviated by taking more than one waste package, perhaps ten or one hundred per repository zone. Of course, this would lead to greater run times, and without greatly improved efficiency in the calculations, could be impractical for production runs with many vectors. It might still be reasonable for auxiliary analysis, however.

2. Determine how uncertainty and variability propagates through the calculations. This is an alternative to running more waste packages that tries to determine analytically how variability propagates through a calculation. I touched on this thought only briefly in the Phase 2 analysis. See Appendix M in that report.

   The basic principal of this kind of analysis, usually called "stochastic analysis" is common in physics and more recently in hydrology and other sciences. The coefficients of the equations representing the model are treated as uncertain, or at least variable, represented as distributions.

These distributions can be correlated. The resulting differential equations cannot be solved directly, but can be solved in terms of their moments, e.g., the mean and the variance. This is not always so easy, but I believe that it would be tractable in this case, since the model consists mostly of ordinary differential equations. The results of this modeling would be directly useful; we would be able to express the mean and variance of the release rate from the waste packages. I believe that this would be a fruitful approach. I recommended that the work in Appendix M be expanded. Since no one picked it up, I am proposing to expand it myself.

Thermal Models

It isn't clear to me from reading Section 2.0 how the overall repository temperature is calculated. The analysis talks only about the calculation for a single waste package in an array of equally space waste packages. The waste packages in the center of the repository will be hotter than those on the edge. Are the temperatures superimposed to get this effect? Has it even been taken into account?

Waste Dissolution Rate (Section 2.7.2.4)

The waste dissolution model is based on data from the flow-though experiments of Grey and Wilson, which is likely to overestimate the rate of dissolution. It seems unlikely that the waste would be exposed to flow-through conditions, which may indicate that the model is unnecessarily conservative in this place.

Water Infiltration

The water coming into contact with the fuel is assumed to have the composition of J-13 water. We have known for a number of years that this is a bad assumption. Isn't it possible to do any better than the J-13 assumption? I believe there are data on water squeezed out of rock, and also water in equilibrium with tuff at various temperatures, both experimentally and from geochemical models.

Model dependence on assumptions

Predictive models ideally should be based on first principles, and not depend on assumed values of unmeasured coefficient. Unfortunately, EBSPAC, and SOTEC before it, are extremely dependent on such assumptions; e.g., mechanisms for wetting the fuel with liquid water, the fraction of the fuel getting wet, and the flow rate of liquid water through the container. I believe that the uncertainty in a single parameter, "flow rate of water coming into contact with the waste", could easily dominate the model results. Its worth pointing out that source term models for repositories in the saturated zone generally are not so dependent on the above parameters, since they assume the waste packages to be bathed in water anyway (although there are undoubtably other sensitive modeling assumptions for their cases).

I am not sure what to do about this problem except to acknowledge them, and use the fact to give perspective to other parts of the model. Until we get a handle on these critical parameters, other model improvements might not be worth the trouble.

If you have any further questions, do not hesitate to call me at 415-8167

Richard Codell