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To: Kien Chang

From: Loren Zaremba LZ

Subject: Activity Report, April 13 - May 3, 1987

This report covers a three week period (weeks 27 through 29 of my contract). However, I was unable to work during portions of week 28 and week 29 due to a death in my family. Consequently, this report summarizes my progress during approximately two working weeks.

PART II OF USER'S MANUAL

During weeks 27 through 29 I continued to work on Part II of the user's manual, which deals with the code called CONVO. This code was used to perform the probabilistic performance assessment of waste package lifetime in the FY86 methodology demonstration. The first three sections of Part II, the Introduction, General Features and Code Structure, have been completed and returned by the typist. The last section, entitled Code Use, was partially completed during week 27. The completed portion includes a description of the input parameters and formats. During week 28 I began to install some modifications into the program, including the ability to treat normal and lognormal distributions of the randomized input parameters. The version of the code used in the demonstration could only treat uniform distributions of these parameters. During weeks 30 and 31 I plan to complete the modifications and prepare a sample problem. I will then send the last section of Part II to the typist along with the corrections to the first three sections. I still hope to keep to my original schedule in which I have 10 working days left on my contract to incorporate comments and provide NRC with the final drafts of Parts I and II.

SANDIA COMMENTS ON DEMONSTRATION REPORT

I recieved Sandia's comments on our demonstration report toward the end of week 27. Unfortunately, I was called out of town shortly after that, and I was not able to prepare any written responses at that time. However, I discussed several of the comments with Ken Stephens on the phone, and the written comments he submitted to NRC on April 30 reflect this discussion. Since then I have had the opportunity to examine some of the Sandia comments more carefully. I have attached my responses to the comments of T. Bonano. I will respond to the comments of R. Guzowski when I submit my next activity report in approximately two weeks.

To: Kien Chang

From: Loren Zaremba LZ

Subject: Comments by T.Bonano on Aerospace Demonstration Report

I have read the comments by T. Bonano of Sandia on our draft Demonstration Report and have the following responses. I have limited these responses to those comments which relate to portions of the report for which I had some responsibility.

Section 4.3 - The comment states that the approach used to treat the temperature dependence of the diffusion coefficient is not really dependent on temperature, and concludes that this was done to be conservative. It is true that the approach does not treat the full temperature dependence, because this would require a solution to the diffusion equation with a diffusion coefficient which had an Arrhenius type temperature dependence. Carslaw and Jaeger address this in their book on heat flow and note that the problem has "not been fully discussed". I assume this means that a solution has not been found. This was the reason for the approach used in the report, rather than conservatism. However, the important point is that our analysis includes an approximate correction for the temperature dependence of the diffusion coefficient. This dependence has been overlooked by the DOE projects thusfar.

Section 4.5 - The comment states that experimental data is needed to determine the limitations of 1 and 2 dimensional transport models. This is not correct because the limitations are inherent. The dimensionality of the model effects the concentration gradient, which drives the transport process. Since the waste package system is 3 dimensional it is obvious that a three dimensional model will provide the best representation of the system.

Chapter 5 - The comment states that no mention is made of whether the modular and cascade methods were compared over a temperature range which is representative of that expected at a repository. However, this was clearly the case because the temperatures utilized in the calculations were obtained from the repository thermal model. Consequently, they are the expected temperatures to within the accuracy of the model.

Chapter 6 - The first comment on this chapter states that solutions to the transport problem which involve impulse and/or decaying sources are not complex, because analytical solutions exist. It also states that advection has been included with little increase in complexity. The fact that a solution is analytical does not mean it is not complex. Also, the complexity appears to increase rapidly with the degree of realism, e.g. dimensionality, number of media,and also decay chain length. The analytical solutions (e.g. BMI/OCRD-25) generally involve Laplace and Fourier transformations, and numerical integration. They can consume a fair amount of computer time and may not be appropriate for Monte Carlo calculations. However, some of the recent solutions such as those developed by A. Gureghian at Battelle should be tested to determine if they are suitable for use in probabilistic analysis.

The second comment indicates that SWIFT could not be used to simulate a waste package because the grid could not be made small enough. I believe this would depend on the size of the region included in the model. If symmetry were used to establish planes of zero flow, analogous to the manner in which adiabats have been used in finite element thermal analyses of waste packages, it may be possible to use a numerical code such as SWIFT.

The third comment states that a suggestion for including groundwater flow through the repository by combining it with diffusion-controlled release is not valid, because the flow could alter the nature of the transport. It appears that the suggested approach has been misunderstood. The intent of the suggestion was that the diffusive flow rate be used as a source term for a separate spatial region in which advection dominated. In solving the problem for the region where diffusion dominates, the flow region could probably be assigned a zero concentration boundary condition. The use of the diffusive flow rate in determining the advective source term would be similar to the use of the concentration in determing this source term, as is commonly done.

Section A.1 - The first comment states that the purpose of the methodology demonstration should not be to compare the results of different modeling approaches. However, I believe we were required to include such a comparison in our demonstration as part of our work statement.

The second comment states suprise that Simpson's rule ,rather than a more accurate technique such as Gaussian quadrature, was used to perform the numerical integration. Simpson's rule was chosen because it utilizes equally spaced basis points. The two functions which comprise the integrand of the convolution integral have different arguments (t' and t-t'). If the basis points are not equally spaced, as is the case with Gaussian quadradure, the values of the two functions, which are generally probability density functions, must be available for a very large number of points. This could have been done by using an interpolation scheme, but any increase in accuracy may have been lost in the process. Consequently, the simpler approach was chosen.

Section A.5 - The comment states that our conclusion regarding the model dependence of the importance of pitting is not correct. The conclusion was intended to point out the limitations of corrosion modeling approaches which ignore pitting. However, we agree that further fundamental investigation is necessary.

Section D.1 - The first comment states that our discussion regarding the nonconservative nature of transport models which do not include decay is incorrect. It also includes a mathematical argument that radioactive decay has the opposite effect. In their paper entitled "Prediction of Waste Performance in a Geologic Repository", published in the 1984 Material Research Society Symposium Proceedings, Pigford and Chambre' state that:

"For C-14, with a half life of 5730 years, decay not only increases the rate of mass transfer into the backfill, because it steepens the concentration profile, but it also increases the transient and steady-state rate of mass transfer into the rock. For a radionuclide with a half life as short as 15.3 years decay considerably increases the mass transfer rate into the backfill, but the half life is short enough that it all decays while diffusing in the backfill. Thus, there is a range of half lives for which the rate of mass transfer into the rock is greater than the steady state value for no decay."

The mathematical argument presented in the comment is not correct. Substitution of a decay dependent concentration in the diffusion equation results in a new equation and hence a new concentration profile. The concentrations with and without decay cannot be simply related by an exponential decay factor.

The second comment states that although the rationale for ruling out advection is understood, NRC must be prepared to include this mode in the analysis. This is probably true, however, the need to include advection in waste package analyses, which may include a packing material, may not be as great as in far field analyses.

Section D.2.3 - The comment states a hope that our conclusion that early times are of little interest was not based on analyses with Oliver's model alone. Our conclusion was not that early times are of little interest in general, but that in some cases the fact that it may be difficult to obtain a solution at early times with this model may not be important because significant release does not occur until much later.

Section D.2 - The first comment states that the use of an intermediate porosity value to simulate a multiple porosity zone is dangerous, and can lead to an underestimate of the maximum release rate. In general, several values of porosity were tried and compared with the predictions of a multi-media model. The purpose of this comparison was to avoid underestimating release rates. The same comment also states that comparing analytical models with numerical models to ascertain the validity of the numerical models is dangerous. This depends on the situation. If for some reason, such as computational speed, it is necessary to use an analytical model which cannot simulate an important feature of the waste package, such as packing, it may be useful to compare the analytical model with numerical model results to determine the effect of the omission and/or obtain a correction factor.

The second comment states that comparison of the cylindrical and spherical models is invalid because their volumes were different. There seems to be some confusion here. We did not compare the cylindrical and spherical models on the basis of equal surface areas. In fact, the cylindrical model simulates the waste package as an infinitely long cylinder, and consequently it is impossible to calculate its surface area or volume. The text states that Chambre' chose the radius of his sphere to provide the same surface area as the waste package he was attempting to simulate. Since a sphere has one dimensional parameter, and a fixed surface to volume ratio, he could not obtain the same surface area and volume as the waste package simultaneously.

Section D.3 - The comment states that the difficulty of the linear transport model in predicting release rates at large times is identical to that for the Oliver model at short times. The difficulties are not at all related. We had no problem achieving convergence with the linear model. The difficulty with the linear model was related to its dimensionality and the fact that it predicts a steady state release rate equal to zero.

Section D.4 - The comment states concern that the prolate spheroid model was considered the most satisfactory because it provided the highest estimated release rates. This was not the case. The prolate spheroid model was considered desireable because it is three dimensionsal and approximates a cylinder. However, it does have the disadvantage of being a single medium model, and thus cannot model both packing and rock. Simulating a finite cylinder by using several line sources or point sources arranged along several lines has been considered. In fact, the solution to the latter problem is used in the thermal code which we used to determine the temperature history of the repository. However, the analytic solution used in that code is again applicable only to a homogeneous medium.