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(Return to WM, 623-SS)

To: Kien Chang

From: Loren Zaremba

87 JUN -5 A11:43

Subject: Activity Report, May 18 - May 31, 1987

PART II OF USER'S MANUAL

During the period from May 18 - May 31 (weeks 31 and 32 of my current contract) I continued to test the operation of the computer code called CONVO on the NIH computer. Also, upon the advice of John Vogelwede, I began to examine NRC's formal requirements for the documentation of software to ensure that the User's Manuals conform with these requirements.

CONVO Tests -

The CONVO tests were made using the new data in BWIP's "Waste Package Preliminary Reliability Analysis Report" (SD-BWI-TI-287). Some of the changes in the data and methods from those employed in BWIP's Draft Environmental Assessment were summarized in my last Activity Report. The CONVO tests were made to compare the predictions of our model with BWIP's latest results.

In the first test, the container lifetime predictions were compared. The median container lifetime predicted by CONVO (10,020 yrs) was in excellent agreement with BWIP's result (9,932 yrs). BWIP's corrosion model was used in this test, but the thermal history of the container surface used by CONVO in this run was obtained using a response surface developed with the TEMP code. BWIP used a thermal history calculated using the finite element code HEATING5. Also, CONVO used a standard Monte Carlo sampling method and BWIP used stratified sampling. Despite these differences, there was very little difference in predicted median container lifetimes.

In the remaining tests, the expected maximum release rates and cumulative releases at 10,000 yrs were examined. CONVO contains three optional radionuclide transport models for computing these releases. In the tests, two of these -- the linear two-medium model and one-medium prolate spheroid model were compared with BWIP's calculations. CONVO's third transport model, a cylindrical transport model, requires long run times and was not well-suited to these tests. For both the linear and prolate spheroid model, the expected releases were calculated by convolving the container failure pdf obtained with the BWIP corrosion model and the average release rate predicted by the transport model.

The attached table shows a comparison of the CONVO results using the two different transport models with the values reported by BWIP. BWIP used the finite element code CHAINT-MC for its transport calculations, which simulated the packing as well as 3 different rock layers (damaged, disturbed and intact). CHAINT-MC is a radial two-dimensional model. In the CONVO runs, the properties of intact rock were used in the one-medium prolated spheroid model, and the properties of packing and intact rock were used in the two-medium linear model.

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For the two long-lived nuclides, Cs-135 (2.30x10**6 yrs) and Se-79 (6.50x10**4 yrs), the maximum release rate and cumulative release predict by CONVO using the prolate spheroid model are about twice those reported by BWIP. For the two intermediate-lived nuclei, Am-241 (432 yrs) and Am-243 (7380 yrs), the releases predicted by these methods are comparable. The releases predicted by CONVO using the linear model are much less than those predicted by BWIP in all cases, but the discrepancy is less for the long-lived nuclides.

In these limited tests there appears to be a tendency towards an increase in predicted release with the dimensionality of the model. This is expected because increased dimensionality tends to increase the volume of available solution, and this increases the concentration gradient. However, the fact that CHAINT accounts for radioactive decay, which tends to increase release rates for intermediate-lived nuclides, appears to compensate for this to a large extent.

Documentation Requirements --

John Vogelwede provided me with references to two NRC publications which provide the Agency's requirements with regard to software documentation; Bulletin 0904-3 and NUREG-856. I have begun to examine these publications and will revise the User's Manuals accordingly. However, John said that after glancing at Part I, it appeared to him that the draft generally fulfilled NRC's requirements. Consequently, only minor revisions may be necessary.

PROPOSED FUTURE TASKS

As requested, I have developed a list of proposed projects for the next consulting contract period, which will begin July 1, 1987. I have provided this list on an attached sheet for your convenience. Please call me if you would like to discuss these projects and/or their justifications in greater detail.

Comparison of Radionuclide Release Rates Predicted by CONVO with BWIP Results.

Max. Fractional Release Rate (1/yr)

Nuclide	CONVO-Linear	BWIP-CHAINT	CONVO-Prolate
Cs-135	0.81x10**-7	4.94x10**-7	8.49x10**-7
Se-79	1.86x10**-7	8.10x10**-7	21.0x10**-7
Am-241	0.11x10**-12	1.90x10**-12	1.13x10**-12
Am-243	0.63x10**-13	6.78x10**-13	6.59x10**-13

Cumulative Release at 10,000 yrs (CI/MTHM)

Nuclide	CONVO-Linear	BWIP-CHAINT	CONVO-Prolate
Cs-135	0.33x10**-4	1.47x10**-4	2.69x10**-4
Se-79	0.99x10**-4	4.11x10**-4	8.09x10**-4
Am-241	0.14x10**-6	1.00x10**-6	1.07x10**-6
Am-243	0.15x10**-8	1.08x10**-8	1.16x10**-8

Proposed Consulting Tasks for Next Contract Period

Loren A. Zaremba

Proposed tasks for the next contract period (7-1-87 to 6-30-88) are listed below. Since it is unlikely that I will be able to complete all of these tasks in the time available, I suggest that priorities be assigned and the tasks be performed in order of priority.

Task I - Support for CONVO Computer Program

There is a continuing need to provide support for the CONVO code, which is currently our principal code for waste package performance assessment. Support would include user assistance and instruction, additional validation and verification, and the installation of modifications and improvements.

Task II - Thermal Code Verification

At the Waste Management '86 meeting in Tucson last year, SANDIA reported the results of tests in which electric heaters simulating decay heat were emplaced in salt at the WIPP facility and temperature vs. time curves were recorded at various locations. In this task, the test results would be compared with the temperatures predicted by the TEMP code, which was used in our waste package performance assessment methodology demonstration last year.

Task III - Transport Code Evaluation

As stated in the conclusions to our waste package performance assessment demonstration report, we have not yet implemented a radionuclide transport code into our methodology which is entirely satisfactory. In this task a survey of recent literature would be made to identify an analytical code which is sufficiently rapid to be used in Monte Carlo calculations, includes radioactive decay, and can simulate at least two media. Recent work at Lawrence Berkeley Labs and Battelle appears promising in this regard. This task would also include installing and testing or or more models to the extent time allows.

Task IV - Engineered Barriers

Other NRC consultants have discussed conceptual approaches to problems associated with the performance assessment of engineered barriers. One of these problems involves the determination of total release rate from all of the packages in the repository at the repository boundary. In this task, the release from a single package would be estimated using the analytical solution for a point or line source and aggregate release would be obtained by superposition. This would also establish a source term for far field analysis.