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20 November 1987
88.rbm.11

Mr. K. C. Chang
Mail Stop 623-SS
U. S. Nuclear Regulatory Commission
Washington, DC 20555

Dear Kien:

Services Rendered on High Level Waste Repository
Performance Assessment Development 11/1/87-11/14/87

During this reporting period the Methodology Demonstration report was completely assembled in a final copy for publication. The original and a copy were submitted for publication.

I have continued the work on corrosion processes expected to occur in low carbon stainless steels and copper in the tuff environment. The data required to use the models has proven to be more difficult to obtain than expected. Dr. Boyars has been attempting to obtain the various values that are available. They are scattered through out the literature in a number of obscure journals. In some cases the data are in forms that require some effort to convert to a usable format.

The development of a consistent temperature dependent model of copper corrosion has proceeded slowly. The difficulty is that the available data measured at different temperatures results in some serious discrepancies. These discrepancies are exhibited when a temperature dependent rate model is integrated to calculate the total corrosion as a function of time. The data available, which are in terms of weight loss as a function of time for a constant temperature, do not appear to be internally consistent. That is, the initial rates extrapolated from the earliest time weight loss data, do not fit the temperature dependent rate equations that have been proposed. Also the rates at some temperatures appear to be a function of the thickness of the corrosion layer, in contradiction to the proposed theory. It is difficult to determine whether these results are a consequence of experimental variations or a weakness in the proposed mechanism that controls the corrosion process. I am having discussions with Lawrence Livermore Laboratory personnel in an effort to resolve these questions.

I have briefly explored the area of chaos theory applied to pitting corrosion. Chaos theory is a relatively recent advance in mathematical physics applicable to non-linear systems. Pitting corrosion is unquestionably a non-linear system of the type that has been analyzed with chaos theory with considerable success. The fact that pitting corrosion appears to be stochastic in nature is highly suggestive that it may be fruitfully analyzed using the tools of chaos theory. My knowledge of the mathematics is very limited at present and consequently its application is speculative. I am studying the area on my own time and hope to gain sufficient understanding in the next several months to make a better estimation of its applicability. If it appears that it has promise I would propose to pursue it then.

The analysis of the tuff repository as an engineered barrier system will be quite difficult unless some very unrealistic simplifications are applied to the problem. This is most evident in the area of transport phenomena. Although it seems reasonable to be able to model the corrosion processes with a reasonable degree of success, the transport of radionuclides from individual containers to the boundary of an individual horizontal drift and the combination of all parts of the EBS into a single source term presents some formidable difficulties. Because the medium is unsaturated, the relatively tractable solution of diffusive and advective transport do not apply. When a thermal gradient is imposed the resulting equations must involve extremely complex two-phase unsaturated flow that includes numerous coupled processes. There are no closed form solutions to the problems, and often the only approach is a complex computer simulation. Even in this case there is no guarantee that a stable equilibrium result will be present.

In other words, the physical reality is that the system can exhibit a large range of behavior within certain limits. Within these limits, the behavior cannot be predicted because very small changes in the input conditions can have large effects on the observed behavior. Futhermore, the behavior will not be stable; that is, it will vary continuously within the limits established by the initial and boundary conditions. This is a characteristic feature of any set of coupled second order partial differential equations. It is only in special cases that stable equilibrium solutions will exist.

Predictability in such systems is possible only in a very general sense. Given adequate exploration of the system by computer simulation, it may be possible to establish an envelope of behavior that will be useful for prediction in the probabilistic sense; however, even this may not be possible if the system "constants" such as permeability, diffusivity, conductivity, etc. have large variations that must be accounted for in the simulations. Variations in initial conditions have yet another range of effects. Thus the temperature, and quantity of groundwater will change the limits of the range of behavior of the system.

Whether useful simplifications of this type of complex behavior can be developed is an open question. It is know that even the analysis of coupled heat/mass-transport problems that have established closed form solutions can involve large amounts of computer time. Consequently the necessity of having useful simplifications in order to explore the behavior of a real system is crucial. Without such simplifications, only a few cases could be studied and the results would almost certainly not be representative of the actual behavior of the system.

I will continue to explore the implications of these questions with Gary Fuller in an attempt to develop a useful model of mass transport in the tuff environment.

I am enclosing three (3) copies of the voucher for professional services for your approval. As of 14 Nov. 1987 I have charged 48.5 days against the total of 130 days authorized in my contract.

If you have any questions please feel free to call me.

Sincerely,

Robert B Moler

Robert B. Moler

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