To: Kien Chang

From: Loren Zaremba

Subject: Comments on NNWSI Waste Package Performance Model

Date: August 27, 1987

An interesting report recently appeared among the new acquisitions in the Phillips building library. It is entitled " Waste Package Performance Assessment: Deterministic System Model Program Scope and Specification", by W.J. O'Connel and R.S. Drach of Lawrence Livermore National Laboratory, UCRL-53761, October 1986. It is important because it is the first document I have seen which provides a reasonably detailed discussion of the tuff program's approach to waste package performance assessment. Lawrence Livermore has been given the responsibility for developing this approach and the associated computer models. As the title states, this report discusses the scope and specifications for the waste package performance assessment modeling. It does not provide details on the operation of the codes, which have not yet been developed.

The performance assessment methodology outlined in this report is to be implemented in a code called PANDORA (Performance Assessment of NNWSI Design Omitting Random Aspects). LLNL is adopting an iteritive approach to development of their models. As the acronym for this first effort implies, their first model will be deterministic. Probabilistic aspects, such as the uncertainty in the model parameters will be incorporated in future models.

The LLNL approach appears to be rather heavily influenced by WAPPA. Although the authors state several instances where WAPPA is inappropriate for application to the tuff problem (e.g. unsaturated vs. saturated flow) and point out several technical errors in WAPPA (e.g. in the radiation model), there are numerous similarities and some of WAPPA's process models will be utilized with minor modifications.

PANDORA will consist of a driver and seven physical process models. In addition the code will incorporate a waste package model to keep track of current conditions. The approach used in the waste package model is almost identical to that used in WAPPA. It will be a one dimensional radial model in which the inner and outer radii of annulli will be keyed to a data base of material properties. The program will add corrosion layers for metals and insert gas gaps in any voids. The seven physical process models and the approach to be used in each are as follows:

1) Radiation Model - The purpose of this model is to calculate the heat

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and radiation output of the wasteform vs. time and the dose rates throughout the waste package. It will consist of four submodels; source, gamma ray dose, alpha particle dose, and spontaneous fission/ neutron dose. Some of the important features of the submodels are:

a) Source Submodel - This submodel will interpolate ORIGEN2 generated tables to adjust for burnup and quantity of waste. This is the same approach as that used in WAPPA.

b) Gamma Ray Dose Submodel - This submodel will compute the gamma doses at the wasteform surface and the outside surfaces of metal barriers. These are of interest because they may be related to wasteform alteration and corrosion enhancement by radiolysis, respectively. The approach to be used is to scale results from a reference calculation using the Monte Carlo radiation transport code MORSE-L. Gamma absorbed dose at the wasteform surface would be scaled linearly with gamma energy per unit volume of wasteform and inversely with wasteform mass density. Gamma ray attenuation by the barriers would obtained by adjusting the MORSE-L calculation for differences in mass thickness.

c) Alpha Particle Dose Submodel - This submodel is only of academic at present because an approach for computing wasteform alteration due to alpha damage has not been developed. The dose submodel will use the average alpha energy and the dose will be given as the product of the alpha generation rate, average energy, average range and a geometric factor.

d) Spontaneous Fission/Neutron Dose Submodel - This submodel will operate like the alpha dose submodel. Again, the output will not be used until a wasteform alteration model is developed.

2) Thermal Model - PANDORA's thermal model will be almost identical to WAPPA's. It will compute the temperature as a function of radial position and time using the same closed form solutions to the heat equation that are use in WAPPA. As in WAPPA, the temperature history at the borehole wall will have to be supplied in the input data.

3) Mechanical Model - The mechanical model will also be almost identical to that used in WAPPA. It will use the same basic set of plain strain stress equations and obtain an overall solution by solving the matrix equations by equalizing pressure contact between solids. However, since no hydrostatic or lithostatic pressure on the container are expected, the residual stress at the closure weld may be the most important for container failure. The peak value expected for this stress will be added to the stress calculated at the container surface.

4) Waste Package Environment Model - The purpose of this model is to evaluate the flow of water, steam and air. An unsaturated nonisothermal

flow code called TOUGH will be used to calculate the rewetting of the rock and water flow during the transient period. In steady state, a simplified model will be used. This is a conservative model in which the water flow through the package will be assumed to be the product of the steady state flux (about 1mm/yr) and an effective area equal to the spacing between the packages. Two scenarios will be considered. The first, which is called the bathtub, is applicable to vertically emplaced containers. In this model the closure weld will be penetrated first and the container will gradually fill with standing water. After it is full, the inflow of new water will be balanced by the outflow. For horizontally emplaced containers, a trickle model will be used. In this model the closure weld will be assumed to be penetrated in several places and allow water to flow through. Very little discussion is provided regarding the details of this model.

5) Corrosion Model - Only generalized, or uniform corrosion will be considered in the initial modeling. The first model will use a look-up table of corrosion rates in air/steam, air/water vapor and water, and the rates of removal of corrosion layers by water. The tables will provide these rates as functions of temperature and water gamma dose.

6) Waste Form Alteration - The name of this model is slightly misleading because it does not include alpha dose effects on wasteform integrity. Initially, the model will only compute wasteform dissolution and thus should probably be called a wasteform dissolution model. For spent fuel, five release mechanisms are included. The first is release of radionuclides in the oxidized layer in the outer surface of the zircoloy, which is expected to occur rapidly. The second mechanism will be release of radionuclides in the cladding itself. The third is release of radionuclides in the stainless steal and Inconel assembly components, and the fourth will gasses from the fuel/cladding gap. The fifth mechanism is the one most models consider, i.e. from the spent fuel pellet matrix. The rapid releases such as from oxide coatings and gases will be obtained from tables of experimental data. Matrix release will be assumed to be by means of congruent dissolution with limits imposed by the solubility of individual radionuclides. In the bathtub scenario for vertically emplaced containers, the departing water will carry the solubility limit of uranium and a congruent amount of other materials. No details are provided for the trickle scenario which will be applied to horizontally emplaced containers. For glass wasteforms release will be by the matrix alone.

7) Waste Transport Model - This model will provide the flux of radionuclides at the borehole wall. For soluble nuclides, transport will be by advection, and will be delay by container fill time in the bathtub scenario. Transport of gaseous nuclides will be by diffusion, and they will be mobilized immediately after penetration of the container.

Although PANDORA contains a number of interesting features, it appears to suffer from a number of the problems that have made WAPPA of limited utility. Like WAPPA, it is extremely data intensive. Until this data is available, the model will be useless. The approach advocated by Pigford, and exemplified to some extent by the BWIP approach, is to use reliable models of physical processes, such as diffusion. This approach is capable of providing near term results and is not subject to problems such as extrapolating short term experimental data to extremely long times. Also, like WAPPA, PANDORA appears to be overly ambitious. The waste package model which keeps track of conditions is really not necessary for the simple package designs which have been considered thusfar. Also, the radiation model is unnecessary because the effects of radiation are very poorly known at present. The mechanical model will also be of very limited utility because no hydrostatic or lithostatic stresses are expected. The thermal model suffers from the same problem as WAPPA's, i.e. it requires another model to calculate the temperature history at the borehole wall. In our modeling we provide the thermal history at locations of interest in terms of response functions, which simplifies the temperature calculations considerably.

Despite the modeling problems, the report provides valuable insight into the methodology being considered for evaluating tuff waste packages and it should be very helpful in our review of the Tuff Site Characterization Plans.

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