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From: Loren Zaremba

Subject: Activity Report, January 5, 1987 - January 25, 1987

In the three week period from January 5 through January 25, 1987 (Weeks 13, 14, and 15 of my contract) I began working on the User's Manual for my computer programs which relate to thermal analysis. I currently have three programs for this purpose:

1) QFIT2 - A program for obtaining a least squares fit to a decay heat curve using a set of exponentially decaying functions. The program contains a limited search routine for determining a best set of decay rates. The user specifies the number of exponential functions to be used in the search, initial values for the decay rates, the search stepsizes for each rate, and the number of steps. The functions determined using QFIT2 are used as input data by the programs TEMP and TEMPH which both assume that the decay heat can be represented by a superposition of exponentially decaying sources.

2) TEMP - This program is a modification of a program developed by the University of Minnesota for ONWI. The modification makes it much easier for the user to simulate a repository by allowing containers to be emplaced as entire rows, rather than one at a time as in the original version. The program TEMP is only able to model a repository in which the waste containers are vertically emplaced.

3) TEMPH - This program is very similar to TEMP, but it is able to simulate horizontally emplaced waste containers. It was developed specifically for the purpose of modeling BWIP's Advanced Conceptual Design which was used in their Environmental Assessment and more recently in the "Waste Package Preliminary Reliability Analysis Report" .

The first task in preparing a data set for QFIT2 is deciding upon the inital values for the exponential decay rates to be used in the search for the best least squares fit to the decay heat curve. During the development and early applications of this program I took the approach of starting with a set of about five decay rates ranging from 1 to 100,000 years at approximately equal logarithmic intervals. However, after I began the User's Manual I decided to examine the question of decay rates more closely. This decision was partially prompted by material which I found in Proposed American National Standard 5.1 - Decay Heat Power in Light Water Reactors, which John Vogelwede brought to my attention several months ago.

Relay #

3875

ANS 5.1 contains procedures for estimating decay heat power based on reactor operating history. This document also contains parameters for exponential fits to the decay heat power from fission products (without neutron absorbtion in the fission products) for the three fissionable nuclides U-235, Pu-239 and U-238. However, these parameters appear to be of limited utility because the standard clearly states that it does not apply, and should not be extrapolated beyond 1.0E+09 sec (about 30 years). Also, the derivation of the exponential fits is neither explained nor referenced. Despite these drawbacks, several useful references are provided. After examining ANS 5.1 in detail I began reviewing some of these references, and I also examined Energy Research Abstracts to obtain some more recent source material.

ANS 5.1 references a paper entitled "Measured and Calculated Rates of Decay Heat in Irradiated U-235, U-233, Pu-239 and Th-232" by S.B. Gunst, D.E. Conway and J.C. Connor (Nucl. Sci. and Eng.,Vol. 56, 241-262,1975) which provides some insight into the sources of decay heat for longer cooling times. At these times actinides are predominant contributors. This paper provides a table showing the nine isotopes which were used in the decay heat calculations, their decay modes, and the energies per decay.

A report on an NRC-sponsored study at Oak Ridge entitled "Fuel Inventory and Afterheat Power Studies of Uranium-Fueled Pressurized Water Reactor Fuel Assemblies Using the SAS2 and ORIGEN2 Modules of SCALE with an ENDF/B-V Updated Cross-Section Library" (NUREG/CR-2397,September 1982) also contains useful information. One of the most important parts of this study is the comparison of the results of the ORIGEN runs with calculations using the ANS 5.1 procedure for times up to 300 years. The two methods are in good agreement, and the differences are smallest at the later times. The authors state that there is really no reason not to use the ANS 5.1 procedure for times greater than 1.0E+09 sec, and that decreased neutron absorbtion by fission products is responsible for the improved agreement at later times.

Two papers by F. Schmittroth at Hanford also contain useful information regarding the nuclear physics aspects of the decay heat curve. The first, "Decay-Heat and Gamma-Dose-Rate Prediction Capability in Spent LWR Fuel" (HEDL-TC-1787, August 1982) provides a table of the important actinides and their uncertainties. A later paper entitled "ORIGEN2 Calculations of PWR Spent Fuel Decay Heat Compared with Calorimeter Data" (HEDL-TME 83-32,January 1984) concludes that uncertainties increase for high-burnup and very long decay time conditions.

In the next two weeks (weeks 16 and 17) I plan to complete my review of the literature relating to decay heat. If sufficient information is available I will include a discussion of the physical basis for choosing the decay rates for QFIT2, and some of the sources of uncertainty in decay heats, as an Appendix to the User's Manual.