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Development of the Activation Analysis Computational Methodology for the  
Spallation Neutron Source (SNS)

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# Development of the Activation Analysis Computational Methodology for the Spallation Neutron Source (SNS)

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## ABSTRACT

For the design of the proposed Spallation Neutron Source (SNS), activation analyses are required to determine the radioactive waste streams, on-line material processing requirements, remote handling/maintenance requirements, potential site contamination and background radiation levels. For the conceptual design of the SNS, the activation analyses were carried out using the high-energy transport code HETC96 coupled with MCNP to generate the required nuclide production rates for the ORIHET95 isotope generation code. ORIHET95 utilizes a matrix-exponential method to study the buildup and decay of activities for any system for which the nuclide production rates are known. In this paper, details of the developed methodology adopted for the activation analyses in the conceptual design of the SNS are presented along with some typical results of the analyses.

## 1. INTRODUCTION

The Department of Energy has initiated a conceptual design study for the Spallation Neutron Source (SNS)<sup>1</sup> and given preliminary approval for the proposed facility to be built at Oak Ridge National Laboratory. The conceptual design of the SNS initially consists of an accelerator system capable of delivering a 1 GeV proton beam with 1 MW of beam power in an approximate 0.5  $\mu$ s pulse at a 60 Hz frequency onto a single target. The SNS will be upgraded in stages to a 4 MW facility with two target stations (a 60 Hz station and a 10 Hz station).

Activation analysis is one of the important components in the radiation transport analysis which will impact conventional facility design and all maintenance operations. Activation analyses are required to determine the radioactive waste streams, on-line material processing requirements (mercury, liquid hydrogen, cooling water, etc.), remote handling/maintenance requirements, and potential site contamination. The analyses are also required to determine background levels within all parts of the facility for normal operation and postulated accident scenarios.

In this paper, details of the activation analysis methodology used for the SNS conceptual design are presented along with some typical results.

## 2. METHODOLOGY

A flow diagram of the activation analysis methodology used in the conceptual design of the SNS is shown in Fig. 1. The analysis flow can be divided into two parts: (1) the radiation transport calculation; and (2) the activation calculation. These two components are described in the following subsections.

### 2.1 RADIATION TRANSPORT CALCULATION

The CALOR96 code system<sup>2</sup> is the main calculational tool used for the numerical radiation transport analysis. The three-dimensional, multimedia, high-energy nucleon-meson transport code HETC96 was used to obtain a detailed description of the nucleon-meson cascade. This Monte Carlo code takes into account the slowing down of charged particles via the continuous slowing-down approximation; the decay of charged pions and muons; and inelastic nucleon-nucleus and charged-pion-nucleus (excluding hydrogen) collisions through the use of a multitude of high energy physics models. In particular, HETC96 utilizes; an intermediate-energy intranuclear-cascade evaporation model ( $E < 3$  GeV); an intermediate-energy intranuclear-cascade-pre-equilibrium evaporation model ( $E < 2$  GeV); a scaling model ( $3 \text{ GeV} < E < 5 \text{ GeV}$ ) and a multi-chain fragmentation model ( $E > 5 \text{ GeV}$ ); and inelastic nucleon-hydrogen and charged-pion-hydrogen collisions via the isobar model ( $E < 3 \text{ GeV}$ ) and a fragmentation model ( $E > 3 \text{ GeV}$ ). Also accounted for are elastic neutron-nucleus ( $E < 100 \text{ MeV}$ ) collisions, and elastic nucleon and charged-pion collisions with hydrogen. The intranuclear-cascade-evaporation model and the intranuclear-cascade-pre-equilibrium evaporation model are the principal physics models in the HETC96 code utilized in the

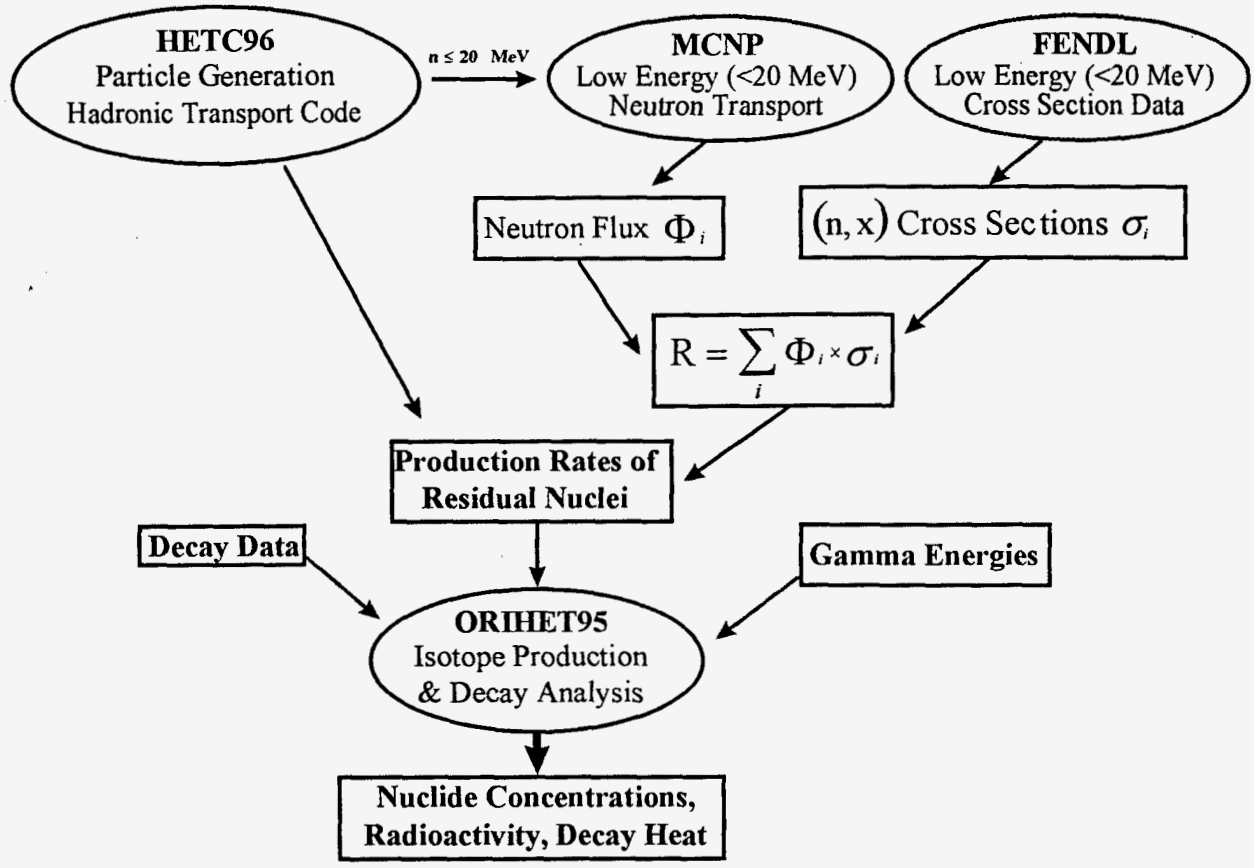


Fig.1 A flow diagram of the SNS activation analyses.

SNS analyses. These models have been used for a variety of calculations and agree quite well with experimental results. For the SNS analyses, the MCNP code<sup>3</sup> was coupled to HETC96 in order to provide the proper source for the low energy ( $E < 20$  MeV) neutron transport. MCNP is a general purpose, continuous-energy, generalized geometry, time-dependent, coupled neutron-photon-electron Monte Carlo transport code system. These transport code calculations provide the necessary information for the activation analyses such as nuclide production rates and neutron flux.

## 2.2 ACTIVATION CALCULATION

### 2.2.1 Nuclide Production Rates

The principal component of the activation analysis is the calculation by ORIHE95<sup>4</sup>, an isotope generation and depletion code. As shown in the Fig.1, HETC96 directly provides nuclide production rates as one of the calculation results. To obtain the nuclide production rates due to neutrons with energies below 20 MeV, reaction rates were calculated using the nuclear data base, the FENDL Activation Library<sup>5</sup>, and neutron fluxes calculated by MCNP. The FENDL Activation Library contains pointwise cross sections for all stable and unstable target nuclides with half-lives longer than 1/2 day. The FENDL Activation Library includes 636 target nuclides with approximately 11,000 reactions with non-zero cross sections below 20 MeV. Group averaged cross section were generated by an ENDF/B utility program, GROUPIE<sup>6</sup>, to match the energy bin structure of the MCNP calculations to calculate the nuclide production rates. Nuclide production rates for certain components were calculated by

$$R_i = \sum_k \phi_j \sigma_k N_i V_j f_1 f_2 / A, \quad k=1, \dots, n \quad (1)$$

where

- $R_i$  = production rate of nuclide  $i$  ( $\text{g}\cdot\text{mol}\cdot\text{s}^{-1}$ ),
- $\phi_j$  = neutron flux in component  $j$  ( $\text{cm}^{-2}$ ),
- $\sigma_k$  = group averaged cross section of  $(n,x)$  reaction which produces nuclide  $i$  ( $\text{cm}^2$ ),
- $n$  = number of reactions which produce nuclide  $i$  in component  $j$ ,
- $N_i$  = number density of precursor of nuclide  $i$  via  $k$ th reaction ( $\text{cm}^{-3}$ ),
- $V_j$  = volume of component  $j$  ( $\text{cm}^3$ ),
- $f_1$  = number of protons per second ( $\text{s}^{-1}$ ),
- $f_2$  = normalization factor to get neutron flux per incident proton
- $A$  = Avogadro's number ( $(\text{g}\cdot\text{mol})^{-1}$ ).

In the activation analyses of the SNS, production rates of gaseous light nuclides ( $^1\text{H}$ ,  $^2\text{H}$ ,  $^3\text{H}$ ,  $^3\text{He}$  and  $^4\text{He}$ ) were also required. These gas production rates were also calculated via Equation 1 using cross sections which result in producing the gaseous light nuclides. The calculated gas production rates were included in the nuclide production rates. Nuclide production rates due to neutrons with energies below 20 MeV were combined with those calculated from HETC96 directly. The combined nuclide production rate data were used as input data to ORIHET95.

### 2.2.2 ORIHET95 Calculation

ORIHET95 was developed from the original Oak Ridge isotope generation and depletion code, ORIGEN<sup>7</sup> which utilizes matrix-exponential methods to study the buildup and decay of nuclide in reactor cores. The ORIHET95 code was design to study the buildup and decay of activity in any system for which the nuclide production rates are known. Nuclides treated in the code are constructed from input production rates of the problem and nuclide decay libraries. The code uses a nuclide data library which contains information on half lives and decay modes of the nuclides, and a gamma data library which contains the number of gamma lines and their energies. These libraries were accompanied with the distribution of the code. The nuclide library was taken from the original ORIGEN library and from the 7th edition of the Table of Isotopes<sup>8</sup>. The gamma library was used to calculate gamma-ray spectra and was formed from an edited version of the Darmstadt gamma-ray atlas<sup>9</sup>. Since the incident proton energy was 1 GeV in the present analyses, it was possible to produce nuclides which were not listed in the libraries. It was found that the production of unlisted nuclides could be ignored because their half lives were always very short and they decayed into short lived nuclides without emitting gamma rays. Also, production rates of these nuclides were smaller than the main contributors to the activities by several orders of magnitude.

The output of the ORIHET95 calculation includes; (1) nuclide concentrations in units of  $\text{g}\cdot\text{mol}/\text{sec}$  and Curies (Ci), (2) gamma-ray spectra, and (3) energy deposition in units of Joules and Watts. These outputs can be obtained for both buildup and decay, and for arbitrary time sequences.

## 3. TYPICAL RESULTS OF ACTIVATION ANALYSES

In this section, some typical results for the SNS target station analyses are presented. The SNS target station has the primary function of generating low energy ( $< 1$  eV) neutron beams for use by neutron scattering instruments. The proton beam target is liquid mercury flowing inside a stainless steel container. The target is positioned within a composite iron and concrete shielding monolith. Two ambient water moderators are positioned below the target and two supercritical hydrogen cryogenic moderators are positioned above the target, with the target and moderators surrounded by a heavy water cooled beryllium reflector region. The SNS core region includes the target, moderators, inner beryllium reflector, and outer nickel reflector contained inside a 2 meter diameter also with a helium atmosphere. Water cooling is used to cool the mercury, shielding, vessels, reflectors, and other assemblies inside the shielding monolith. Results of the activation analysis shown in this paper are given for the initial operating conditions: proton energy 1 GeV, beam power 1 MW, and 1 year continuous operation.

### 3.1 Nuclide Concentration

Figure 2 shows the elemental spallation and transmutation products of the target mercury bombarded by a 1 GeV, 1 MW proton beam as a function of time of operation (1 month, 1 year, and 20 years). The results show that

(1) the spallation and transmutation reactions are distributed across a wide mass number range from Pb to Rh, (2) the decay activities from almost all the nuclides are saturated at 1 month with the exceptions tritium, Rh, Ag, and Sn. Figure 3 shows decay activities of long lived spallation and transmutation isotopes in the target mercury irradiated by a 1 GeV, 1 MW proton beam. The decay activities are plotted as a function of time after shutdown (initial, 1 month, and 1 year). This kind of analysis provides information as to what kinds of isotopes must be considered in the Environmental Impact Statement (EIS) and safety analysis of the facility.

### 3.2 Total Activity

Comparisons of the total activity of different target components is shown in Fig.4 and Fig.5. Figure 4 shows buildup of the activities as a function of time of operation from 1 month to 30 years while decay of the activities is shown in Fig.5 as a function of time after shutdown from shutdown to 5 years. The results indicate that the target mercury would initially be the hottest component among the target components and the Be/D<sub>2</sub>O reflector and the Ni inner plug, which are removed in some target maintenance operations, would also have high activity. The activity of the target components is required to determine target material processing requirements and target component remote handling/maintenance requirements.

### 3.3 Gamma-Ray Spectrum

Figure 6 shows gamma-ray spectra from target components after 1 year continuous operation of the target station with 1 MW proton beam power. The gamma-ray spectra were used to determine shielding requirements of the remote handling cells for maintenance of the target components during normal operation and postulated accident scenarios<sup>10</sup>.

### 3.4 Energy Deposition

OIRIHET95 also has the capability of calculating energy deposition in the SNS target components due to the decay activation. The energy deposition calculations are required to assess shutdown cooling, used component storage, and waste management requirements. Figure 7 shows the decay of thermal power in the target mercury irradiated by a 1 MW proton beam. The analysis was used to determine the decay heat removal requirements of the mercury storage and also the requirements for the venting system of the target mercury that will extract the volatile substances.

## 4. CONCLUSION

A methodology for performing activation analyses of the proposed Spallation Neutron Source (SNS) was developed for the conceptual design of the facility. The methodology utilizes the existing FENDL Activation Library cross-section data base to calculate nuclide production rates due to neutrons with energies below 20 MeV. The main part of the activation analysis was adopted from a scheme used in the HERMES system<sup>4</sup> of KFA Jülich using ORIHET95. The results of ORIHET95 provide necessary information to determine design requirements of the SNS. To demonstrate the methodology, typical calculated results of the spallation and transmutation products, total activities, gamma-ray spectra and energy deposition were presented for the target station components in the conceptual design of the SNS. The developed procedure will be refined and used for the further detailed design of the SNS.

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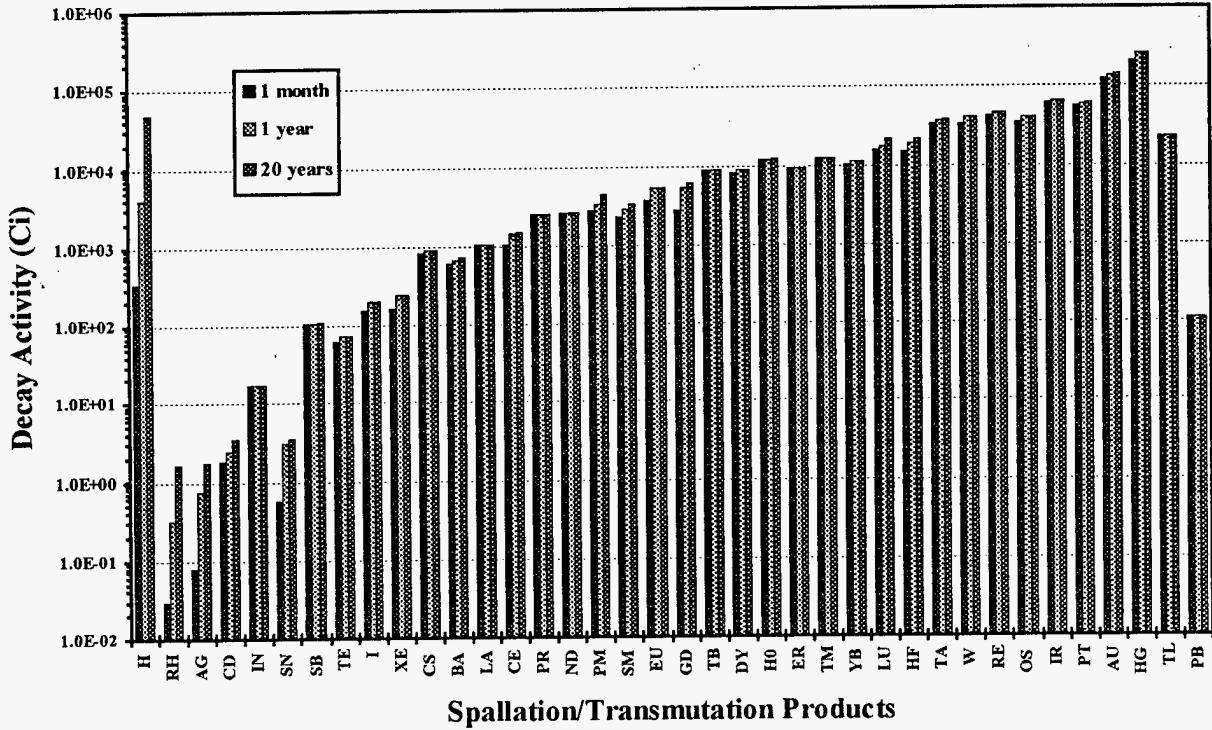


Fig.2. Mercury spallation/transmutation product decay activation as a function of time of operation (1 MW proton beam power, 1 year operation).

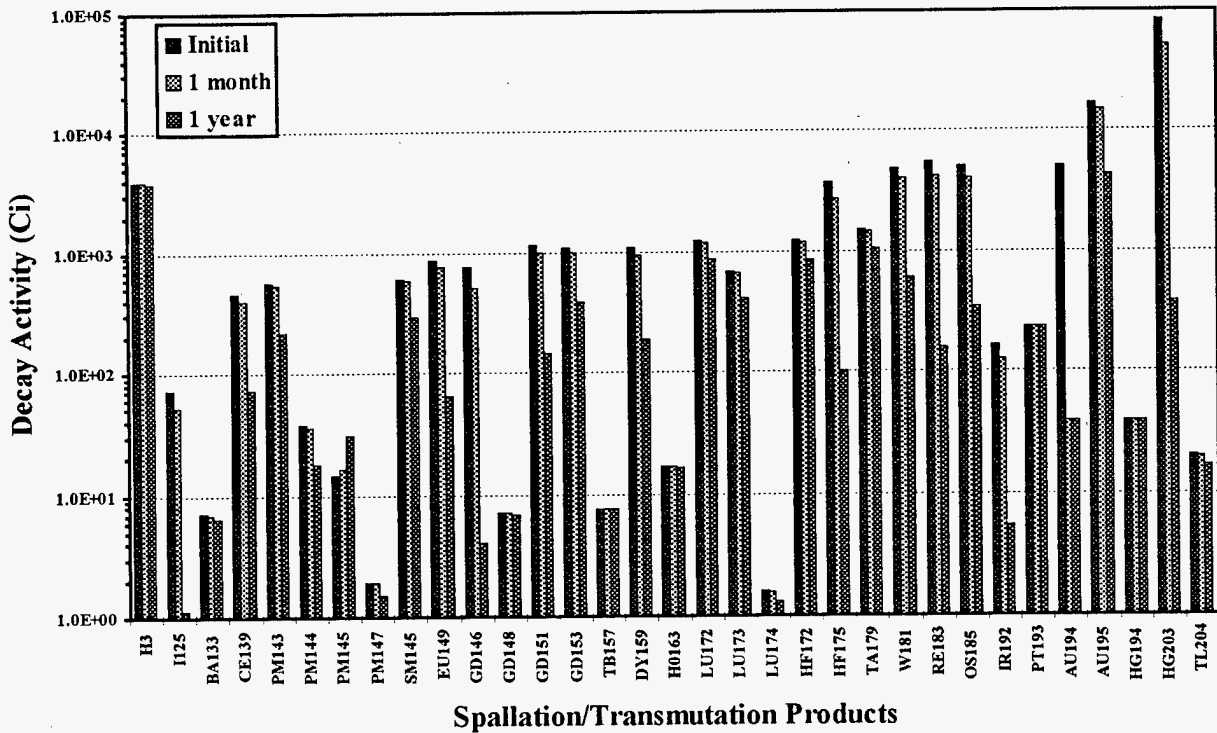


Fig.3. Long-lived Hg spallation/transmutation isotopes decay activation as a function of time after shutdown (1MW proton beam power, 1 year operation).



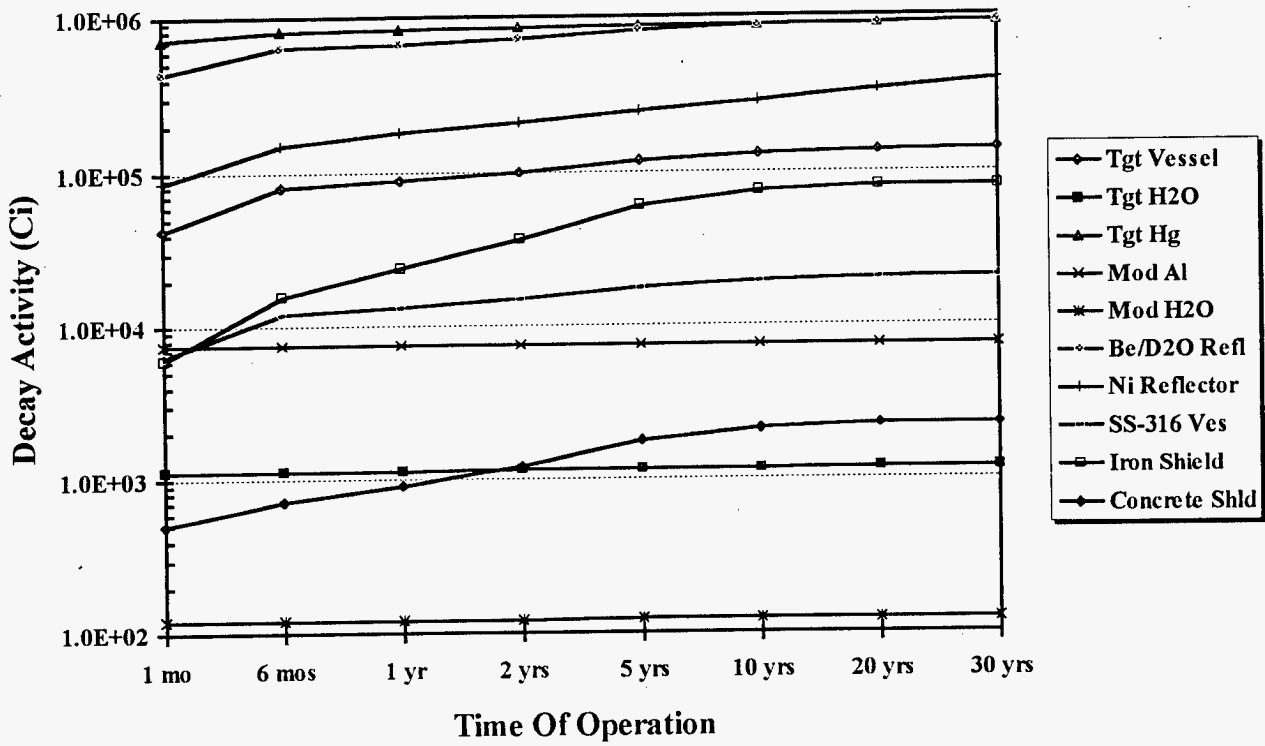


Fig.4. Target station components' decay activation as a function of time of operation (1 MW proton beam power).

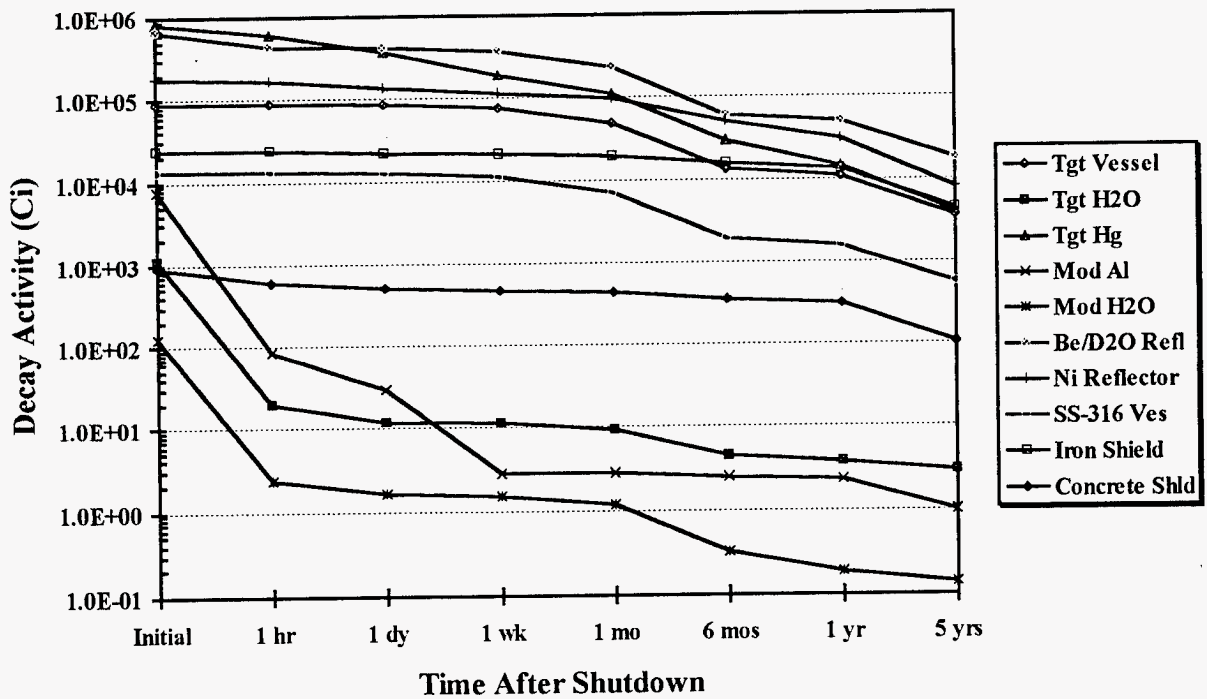


Fig.5. Target station components' decay activation as a function of time after shutdown (1 MW proton beam power).

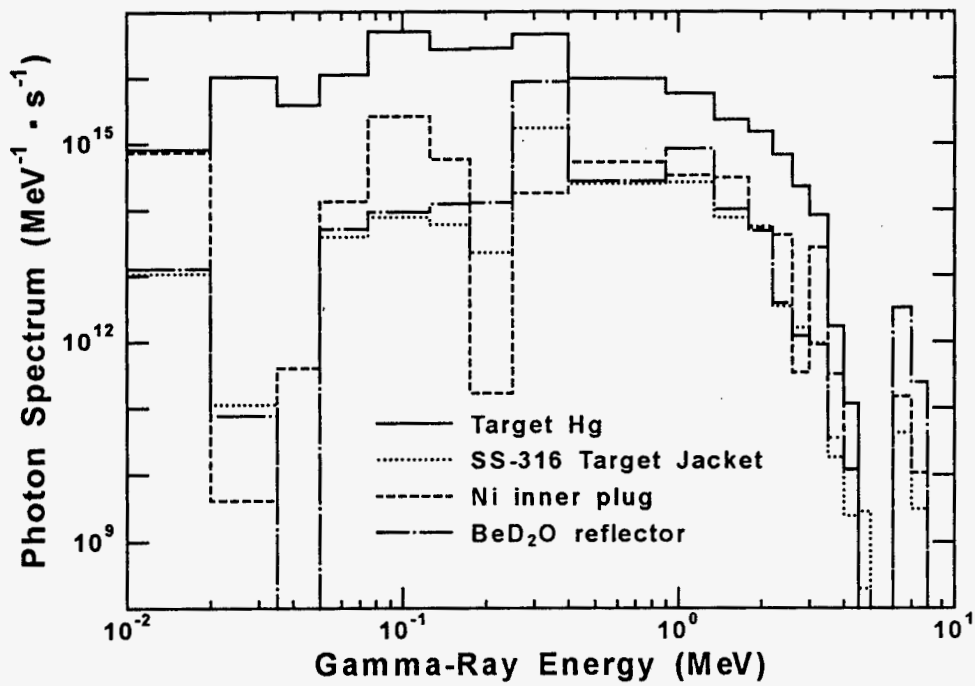


Fig.6. Gamma-ray spectra from different target components due to a 1 GeV, 1MW proton beam after 1 year operation.

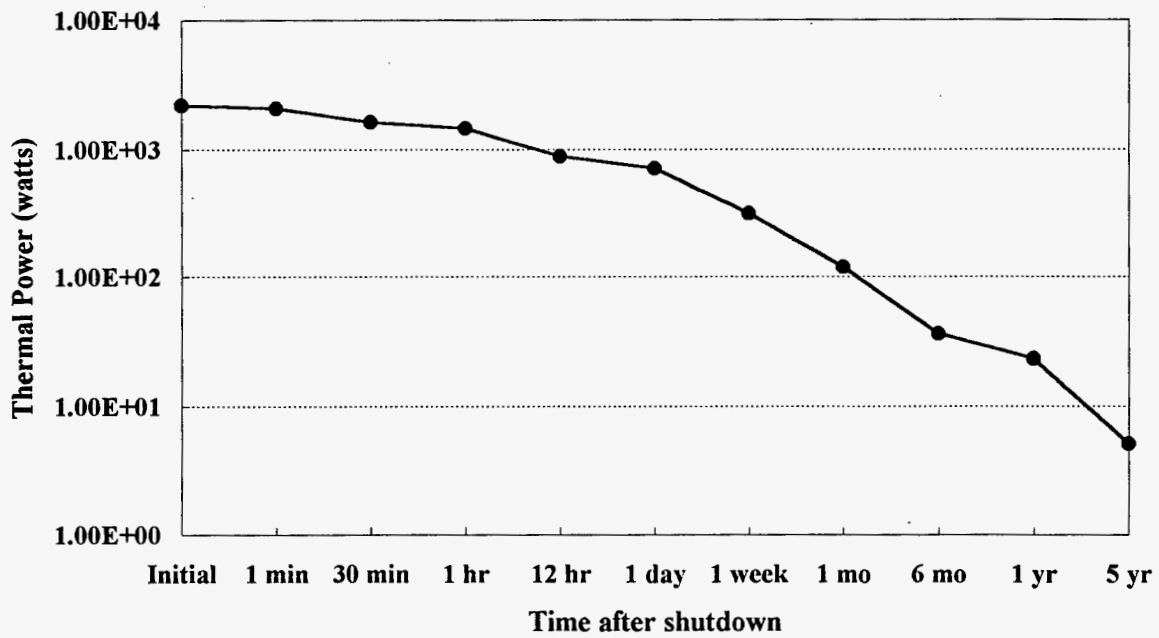


Fig.7. Thermal power of target Hg as a function of time after shutdown (1 MW proton beam power, 1 year operation).

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