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OAK RIDGE NATIONAL LABORATORY
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# CONTENTS

# ABSTRACT

An approach to extend the present ORNL sensitivity program to include functionals of the time-dependent nuclide density field is developed. An adjoint equation for the nuclide field has been derived previously using generalized perturbation theory; our derivation makes use of a variational principle and results in the same equation. The physical significance of this equation is discussed and compared to the time-dependent neutron adjoint equation. Computational requirements for determining sensitivity profiles and uncertainties for functionals of the time-dependent nuclide density vector are developed within the framework of the existing FORSS system, significantly extending the current capability. The development, testing, and use of an adjoint version of the ORIGEN isotope generation and depletion code are documented. Finally, a sample calculation is given which estimates the uncertainty in the plutonium inventory at shutdown of a PWR due to assumed uncertainties in uranium and plutonium cross sections.

# I. INTRODUCTION

Cross section sensitivity programs at Oak Ridge[1,2,3] and elsewhere[4,5,6] have flourished both theoretically and computationally during the last several years, culminating in recent uncertainty estimates[7] for performance parameters of large LMFBR reactors, including both differential and integral information. This work has largely been focused on the time-independent problem for functionals of the neutron flux. Previously, Gandini[8] has described a formulation to enable one to compute sensitivities, and uncertainties if data covariance files are available, for linear functionals of the nuclide density field evaluated at some specified time. It is the purpose of this study to: (1) review the various derivations of equations for this research, extending the application to arbitrary time-dependent linear functionals and functional ratios of the nuclide density field; (2) indicate the code development requirements for the implementation of such a procedure at ORNL; (3) present the results of a typical sample problem; and (4) indicate future directions for the current program with respect to transmutation and decay.

It should not be surprising that an adjoint equation describing the nuclide field can be formulated in a manner analogous to the procedure used by Lewins[9,10] in deriving an adjoint equation for the time-dependent neutron field. The time-dependent neutron and nuclide fields obey the coupled, non-linear equations commonly referred to as the depletion equations. Over "small" time intervals these equations can be approximately decoupled (one assumes the neutron flux is time-independent during a depletion time interval and subsequently recalculates the flux with updated nuclide concentrations) into the linear, time-dependent Boltzmann equation and the linear, time-dependent transmutation equation. These decoupled equations look very similar: each field equation contains a linear operator (which is a function of the other field) operating on the field density and a time derivative of the field variable. Gandini[8] exploited this similitude to derive an adjoint nuclide field equation by simple analogy to the adjoint time-dependent neutron field equation, and has applied this equation to analytical and numerical examples.[11] Our approach differs in that we derive the adjoint nuclide equation from first principles (using a variational method) and then show from physical arguments the analogy to the neutron adjoint. This procedure has the advantage of handling adjoints for generalized nuclide-dependent functionals which may be of future interest (e.g., density ratios), as well as providing a rigorous foundation on which to base our uncertainty analysis program.

The implementation of sensitivity theory at Oak Ridge for the point-depletion equation can most easily be achieved by modification of the ORIGEN[12] isotope generation and depletion code. The matrix exponential solution technique employed in ORIGEN allows for straightforward extension to solution of the time-dependent adjoint equation. Moreover, since virtually the entire nuclide data field is considered, a wide variety of questions related to the transmutation process can be addressed simultaneously. (Situations with significant spatial flux gradients and/or spatial nuclide gradients are best addressed with space-dependent depletion codes.) A modified version of the code designated ORIGEN-A (Appendix B) has already been developed and tested. This program is used to obtain nuclide adjoint solutions for the particular case of "final-time functionals;" its first application to sensitivity analysis is reported in this paper.

## II. DERIVATION OF ADJOINT NUCLIDE FIELD EQUATION

The time-dependent behavior of all nuclides present in a power reactor obeys the nuclide transmutation equation given by:[13]

$$\underline{\underline{M}}(\phi\sigma,\lambda)\ \underline{N}(\overline{r},t) = \frac{\partial}{\partial t}\ \underline{N}(\overline{r},t)\ , \quad t > t_0 \tag{1}$$

$$\underline{N}(\overline{r},t_0) \equiv \underline{N}_0(\overline{r}), \quad \text{at } t = t_0 \tag{2}$$

where

$\underline{\underline{M}}$ = the "burn-up operator," a function of nuclide microscopic reaction rates and decay constants (see Appendix A). Explicit designation of the yield (e.g., from fission) has been suppressed for convenience.

$\underline{N}(\bar{r},t)$ = the space-time dependent nuclide field vector whose components--$N_i(\bar{r},t)$, i = 1, number nuclides--represent the atom density of the $i^{th}$ nuclide at position $\bar{r}$ and time t.

$\underline{N}_0(\bar{r})$ = initial charge of nuclides in the reactor.

In reactor design studies, it is frequently desired to determine some performance parameter that is a function of the time-dependent nuclide field vector. Such an integral parameter will be referred to as a "response" in this paper. The specific types of responses which will be considered are the following:

(a) Functional of flux and atom densities evaluated at a specified instant in time (designated a "final-time functional"),

$$R[\phi,\underline{N},\underline{h}] = < \phi\underline{h}^T\underline{N}\delta(t - t_f) > .$$

(b) Functional of flux and atom densities integrated over time (designated a "time-integrated functional"),

$$R[\phi,\underline{N},\underline{h}] = < \phi\underline{h}^T\underline{N} > .$$

(c) Ratio of functionals of type (a),

$$R = \frac{< \phi\underline{h}_1^T\underline{N}\delta(t - t_f) >}{< \phi\underline{h}_2^T\underline{N}\delta(t - t_f) >} .$$

(d) Ratio of functionals of type (b)

$$R = \frac{< \phi\underline{h}_1^T\underline{N} >}{< \phi h_2^T\underline{N} >} .$$

In these expressions, "T" indicates the transpose operation, and $\underline{h}$ is a "realization vector" which selects the appropriate nuclides for the response of interest. The brackets indicate integration over time, space, energy, and angle for reaction responses; and $t_f$ is the observation time for the response. If the response is purely nuclide densities, then $\phi$ should be set to 1 in (a)-(d), and the brackets denote integration over only space and time. In general, the $i^{th}$ component of $\underline{h}$ may be a function (eq., a reaction cross section for the $i^{th}$ nuclide in a reaction rate response), or a "1" (for the $i^{th}$ nuclide in a nuclide density response), or a "0" (if $i^{th}$ nuclide does not appear in the response).

For the derivations which follow, all required nuclear data such as the various $\sigma$'s and $\lambda$'s for each of the nuclide components of $\underline{N}$ are assembled in a collection that will be called the "reference data vector," $\underline{S}(\alpha)$. For our purposes, the $i^{th}$ component of the data vector, $S_i$, corresponds to the data $\alpha_i$ that appear at some location (possibly at multiple locations) in the burn-up matrix, and thus the number of components of $\underline{S}$ is equal to the number of different data parameters contained in the burn-up operator. It is the objective of our sensitivity development to calculate the rate of change in the calculated response with respect to changes in the nuclear data ($\sigma$ and $\lambda$) that appear in the data vector.

Consider some perturbation in a parameter denoted arbitrarily by $\alpha$ found in the reference nuclear data set $\underline{S}$:

$$\underline{S}' = \underline{S} + \delta\underline{S} \tag{3}$$

due to

$$\alpha' = \alpha + \delta\alpha \tag{4}$$

This change will cause a redistribution of the time-dependent nuclide and neutron fields about their unperturbed values:

$$\phi' = \phi_0 + \delta\phi \ , \tag{5}$$

$$\underline{N}' = \underline{N}_0 + \delta\underline{N} \ . \tag{6}$$

The final result is a change in the response,

$$R' = R_0 + \delta R \ . \tag{7}$$

The perturbed response is naturally a function of the "new" nuclear data set, as well as the perturbed flux and nuclide field vector.

The rate of change of the response can be expressed as a total functional derivative[14] with respect to $\alpha$:

$$\frac{dR}{d\alpha} = \left\langle \left(\frac{\partial R}{\partial \underline{h}}\right)^T \frac{d\underline{h}}{d\alpha} + \left(\frac{\partial R}{\partial \underline{N}}\right)^T \frac{d\underline{N}}{d\alpha} + \frac{\partial R}{\partial \phi}\frac{d\phi}{d\alpha} \right\rangle . \tag{8}$$

In this expression the vector derivatives are defined by

$$\left(\frac{\partial R}{\partial \underline{h}}\right)^T = \left(\frac{\partial R}{\partial h_1}, \frac{\partial R}{\partial h_2}, \frac{\partial R}{\partial h_3}, \text{etc.}\right) .$$

The first term of Eq. (8) represents the direct effect, or change in the response due to a change in a cross section appearing explicitly in the response definition. Hence the evaluation of these derivatives is straightforward. In the current work, the third term in Eq. (8) is neglected by assuming that small perturbations in nuclear data do not severely distort the time-dependent flux behavior. Recently Kallfelz has suggested a method[15] that can partially account for this effect using static, generalized perturbation theory applied over a series of time intervals. However, this procedure has not been incorporated in the present analysis, which is restricted to point-depletion. The major effort, therefore, lies in formulating an expression for the change in response R due to a change in a nuclear data element which affects the transmutation process and, thus, the nuclide field concentrations.

Consider the second term of Eq. (8), with the assumption that the flux field remains unchanged over the time interval of interest $(t_0,t_f)$. The value for $d\underline{N}/d\alpha$ can be found by implicit differentiation of the nuclide field equation:

$$\frac{d}{d\alpha}\left(\underline{\underline{M}}\,\underline{N} - \frac{\partial}{\partial t}\underline{N}\right) = \frac{\partial \underline{\underline{M}}}{\partial \alpha}\underline{N} + \underline{\underline{M}}\frac{d\underline{N}}{d\alpha} - \frac{\partial}{\partial t}\frac{d\underline{N}}{d\alpha} ,$$

assuming that all required derivatives exist. Rearranging gives the following:

$$\underline{\underline{M}}\left(\frac{d\underline{N}}{d\alpha}\right)=\frac{\partial}{\partial t}\left(\frac{d\underline{N}}{d\alpha}\right)-\frac{\partial\underline{\underline{M}}}{\partial\alpha}\underline{N} \tag{9}$$

If we define an auxiliary equation of the form

$$\underline{\underline{M}}^*\underline{N}^* = \frac{-\partial}{\partial t}\underline{N}^* + \frac{\partial R}{\partial\underline{N}}\text{ , where } \underline{\underline{M}}^* = M^T \text{ ,} \tag{10}$$

then Eq. (9) and (10) can be combined to give

$$\left\langle\frac{\partial}{\partial t}\left(\frac{d\underline{N}^T}{d\alpha}\underline{N}^*\right)\right\rangle+\left\langle\frac{\partial R^T}{\partial\underline{N}}\frac{d\underline{N}}{d\alpha}-\underline{N}^{*T}\frac{\partial\underline{\underline{M}}}{\partial\alpha}\underline{N}\right\rangle = 0 \tag{11}$$

Finally, solving for the second term in (8):

$$\left\langle\frac{\partial R^T}{\partial\underline{N}}\frac{d\underline{N}}{d\alpha}\right\rangle=\left[\frac{d\underline{N}^T}{d\alpha}\underline{N}^*\right]_{t=0}-\left[\frac{d\underline{N}^T}{d\alpha}\underline{N}^*\right]_{t=t_f}+\left\langle\underline{N}^{*T}\frac{\partial\underline{\underline{M}}}{\partial\alpha}\underline{N}\right\rangle \text{ ,} \tag{12}$$

with the first two terms on the RHS integrated over space.

We can assume that $(d\underline{N}/d\alpha)_{t=0}$ is zero, since $\underline{N}_0$ is specified independant of $\alpha$. With the additional condition that $\underline{N}^*(t_f) = 0$, the governing equation for $\underline{N}^*$ is specified to be a final value problem. [Note however that if R is a delta-function, the source in Eq. (10) is equivalent to a non-homogeneous final condition.] It will later be shown that $\underline{N}^*$ is the "nuclide adjoint function." From (12), the second term of Eq. (8) reduces simply to

$$\left\langle\underline{N}^{*T}\frac{\partial\underline{\underline{M}}}{\partial\alpha}\underline{N}\right\rangle \tag{13}$$

The preceding brief dirivation, which was based on determining the "slope" of the response in $\alpha$-space, is useful in illustrating the physical procedure involved in sensitivity theory. However, this differential development will not be pursued further in this paper. Instead we will employ an alternate technique (that produces equations similar to those previously derived) for which the error approximations inherent in sensitivity analysis are more apparent.

In the evaluation of the second term of Eq. (8) a formulation is sought which is insensitive to first order errors in the change in nuclide density, i.e.,

$$\delta R = [a\delta\alpha + b\delta \underline{N}^2] \ . \tag{14}$$

The increment $\delta R$ is first order in $\delta\alpha$ but second order in $\delta\underline{N}$. It is then only necessary to evaluate the coefficient "a" of $\delta\alpha$ to obtain estimates of $\delta R$ accurate through first order in $\delta\underline{N}$.

A systematic procedure based on a variational principle has been suggested by Pomraning[16] and Stacey[17] to achieve this stationary condition. With this method, the transmutation equation is treated as a constraint condition on the response; and as such, is appended to the functional with an unspecified Lagrange multiplier $\underline{N}^*$:

$$K[\phi,\underline{h},\underline{N},\alpha,N^*] = R[\phi,\underline{h},\underline{N}] + < \underline{N}^{*T} \left[ \underline{\underline{M}}(\alpha)\underline{N} - \frac{\partial N}{\partial t} \right] > \tag{15}$$

The explicit dependence on $\overline{r}$ and t has been suppressed where convenient. The K functional is an explicit function of all the data parameters found in the "data vector" $\underline{S}$, since these values are contained in the $\underline{\underline{M}}$ operator.

From Eq. (15) we see that if the unperturbed value for $\underline{N}$ $\left[\text{i.e., the solution to } \underline{\underline{M}}\ \underline{N} = \frac{\partial}{\partial t}\underline{N},\ \underline{N}(o) = \underline{N}_0\right]$ is used to evaluate K, then

$$K[\phi,\underline{h},\underline{N},\alpha,\underline{N}^*] = R \ . \tag{16}$$

Furthermore, if $\alpha'$ and $\underline{N}'$ are perturbed values that obey the relation

$$\underline{\underline{M}}'(\alpha')\underline{N}' = \frac{\partial}{\partial t}\underline{N}',\ \underline{N}'(o) = \underline{N}_0' \ , \tag{17}$$

then

$$K'[\phi,\underline{h},\underline{N}',\alpha',\underline{N}^{*\prime}] = R' \ . \tag{18}$$

where $\underline{N}^*$ is as yet an unspecified Lagrange function evaluated using data set $\alpha$. For purposes of evaluating the second term of Eq. (8), $\phi$ and $\underline{h}$ are unaffected by data set alteration ($\alpha'$).

Expanding the left-hand side of Eq. (18) in a function Taylor series about the unperturbed variables and suppressing the $\phi$ and $\underline{h}$ dependence gives

$$K' = K[\phi,\underline{h},\underline{N},\alpha,N^*] + \left\langle \left(\frac{\partial K}{\partial \underline{N}}\right)^T (\underline{N}' - \underline{N}) + \left(\frac{\partial K}{\partial \underline{N}^*}\right)^T (\underline{N}^{*\prime} - \underline{N}^*) + \frac{\partial K}{\partial \alpha}(\alpha' - \alpha) \right\rangle + \ldots \text{ higher terms} \ . \tag{19}$$

If the partial derivatives $\frac{\partial K}{\partial \underline{N}}$ and $\frac{\partial K}{\partial \underline{N}^*}$ can be made to vanish, then using Eqs. (16), (18), and (19)

$$R' - R = \left\langle \left(\frac{\partial K}{\partial \alpha}\right)_{\underline{N},\underline{N}^*} (\alpha' - \alpha) \right\rangle + \text{second-order terms in } (\delta\underline{N}),\ (\delta\underline{N}^*) \tag{20}$$

which is the desired result.

To determine the appropriate stationary conditions, consider first the variation of K with respect to $\underline{N}^*$ (i.e., the 3rd term on the right-hand side of Eq. 19):

$$(\delta K)_{\delta\underline{N}^*} = \left(\frac{\partial K}{\partial \underline{N}^*}\right)^T \cdot \delta\underline{N}^* = < \delta\underline{N}^{*T} \left[ \underline{\underline{M}}\ \underline{N} - \frac{\partial}{\partial t}\underline{N} \right] > \ , \tag{21}$$

which gives the expected Euler condition

$$\underline{\underline{M}}\ \underline{N} = \frac{\partial}{\partial t}\underline{N} \ . \tag{22}$$

The solution to the unperturbed burn-up equation (Eq. 22) makes K stationary with respect to arbitrary variations in the function $\underline{N}^*$.

Taking the variation with respect to $\underline{N}$ (i.e., the second term on the right-hand side of Eq. 19) gives

$$(\delta K)_{\delta \underline{N}} = \frac{\partial K}{\partial \underline{N}}^{T} \delta \underline{N} = < \left[ \delta \underline{N}^{T} \left( \frac{\partial R}{\partial \underline{N}} + \underline{\underline{M}}^* \underline{N}^* + \frac{\partial}{\partial t} \underline{N}^* \right) \right] > +$$

$$\int - \delta \underline{N}^{T}(t_f) \underline{N}^*(t_f) + \delta \underline{N}^{T}(t_0) \underline{N}^*(t_0) dV \qquad (23)$$

In obtaining the above equation, the following adjoint properties were employed:

$$< \underline{N}^{*T} \underline{\underline{M}}\ \underline{N} > = < \underline{N}^{T}\ \underline{\underline{M}}^* \underline{N}^* > , \qquad (24)$$

where $\underline{\underline{M}}^*$ = transpose $\underline{\underline{M}}$, and

$$\int_t \underline{N}^{*T} \frac{\partial}{\partial t} \underline{N}\, dt = \underline{N}^{T}(t_f) \underline{N}^*(t_f)$$

$$- \underline{N}^{T}(t_0) \underline{N}^*(t_0) - \int_t \underline{N}^{*T} \frac{\partial}{\partial t} \underline{N}^*\, dt , \qquad (25)$$

where $t_f$ is the final time in the time domain for $\underline{N}$.

At this point, there are several ways of reducing the expression in Eq. (23), the appropriate method depending on the specific response of interest. For example, consider the case of the response being a final-time, linear functional at $t_f$ (i.e., response type "a"). Then

$$\frac{\partial R}{\partial \underline{N}} = \int_E \int_\Omega \underline{h} \phi(t) d\Omega dE\ \delta(t - t_f) = \text{space-dependent delta function} ; \qquad (26)$$

$$\int \delta \underline{N}^{T} \frac{\delta R}{\delta \underline{N}} dV = \delta \underline{N}^{T}(t_f) \int_E \int_\Omega \underline{h} \phi(t_f) d\Omega dE\ dV \qquad (27)$$

If we set $\underline{N}^*(t_f) \equiv \underline{N}^*_{\underline{F}(r)} = \int_E \int_\Omega \underline{h}\phi(t_f)d\Omega dE$, then the $\delta\underline{N}(t_f)$ boundary term vanishes in equation (23). Excluding the initial condition perturbation $\delta\underline{N}_0$, the remainder of the expression for $\delta K$ will vanish if $\underline{N}^*$ obeys the final value equation,

$$\underline{\underline{M}}^*\underline{N}^* = \frac{-\partial}{\partial t}\underline{N}^* \ , \quad \underline{N}^*(t_f) = \underline{N}^*_{\underline{F}} \tag{28}$$

If the response R is a ratio specified at $t = t_f$ (response type "c"), then Eq. (28) still holds, but the final condition is now

$$\underline{N}^*_{\underline{F}(r)} = \frac{< \underline{N}^T\underline{h}_1\phi\delta(t - t_f) >}{< \underline{N}^T\underline{h}_2\phi\delta(t - t_f) >}\left\{\frac{\int_E \int_\Omega \phi(t_f)\underline{h}_1 d\Omega dE}{< \underline{N}^T\underline{h}_1\phi\delta(t - t_f) >} - \frac{\int_E \int_\Omega \phi(t_f)\underline{h}_2 d\Omega dE}{< \underline{N}^T\underline{h}_2\phi\delta(t - t_f) >}\right\} . \tag{29}$$

For the case of a time-integrated, linear functional (response type "b"), the $\delta\underline{N}(t_f)$ term is made to vanish by choosing $\underline{N}^*_{\underline{F}(r)} = 0$. The appropriate condition for $\underline{N}^*$ is now an inhomogeneous equation with a homogeneous final condition,

$$M^*\underline{N}^* = -\frac{\delta}{\delta t}\underline{N}^* - \underline{Q}^*$$

$$\underline{N}^*_{\underline{F}(r)} = 0 \ , \tag{30}$$

where the time-dependant fixed source is defined by

$$\underline{Q}^*(r,t) \equiv \frac{\partial R}{\partial \underline{N}} = \int_E \int_\Omega \phi(t)\underline{h} d\Omega dE \ . \tag{31}$$

For the integrated functional ratio (response type "d"), Eq. (30) still holds, but now

$$\underline{Q}^* = \frac{< \underline{N}^T \underline{h}_1 \phi >}{< \underline{N}^T \underline{h}_2 \phi >} \left\{ \frac{\int_E \int_\Omega \phi(t) \underline{h}_1 d\Omega dE}{< \underline{N}^T \underline{h}_1 \phi >} - \frac{\int_E \int_\Omega \phi(t) \underline{h}_2 d\Omega dE}{< \underline{N}^T \underline{h}_2 \phi >} \right\} . \qquad (32)$$

With the equations for the adjoint nuclide field defined by the methods discussed, it is now possible to write (for an unperturbed flux field)

$$\Delta R = \left\langle \frac{\partial R}{\partial \alpha} \delta\alpha \right\rangle + < \left( \underline{N}^{*T} \frac{\partial}{\partial \alpha} \underline{\underline{M}}\, \underline{N} \right) \delta\alpha > + \int \delta \underline{N}_0{}^T \underline{N}^* \, dV \ . \qquad (33)$$

Note that R can be evaluated for any $\delta\alpha$ ($\alpha$ in $\underline{S}$) and for any $\delta\underline{N}_0$, without requiring a new calculation for $\underline{N}$ and $\underline{N}^*$, and in this property lies the power of the perturbation approach to sensitivity analysis. For no change in the initial condition, Eq. (33) reduces to the response change arising from data changes only, previously derived in Eq. 13.

## III. MAGNITUDE OF ERRORS

The burn-up operator $\underline{\underline{M}}(\sigma\phi,\lambda)$ can be written as the sum of two operators, one representing nuclide transmutation by radioactive decay, the other transmutation by reactions with the neutron field:

$$\underline{\underline{M}}(\sigma\phi,\lambda) = \underline{\underline{R}}(\sigma\phi) + \underline{\underline{D}}(\lambda) \ . \qquad (34)$$

A change in some nuclear data value will result in

$$\delta\underline{\underline{M}} = \underline{\underline{R}}(\delta(\sigma\phi)) + \underline{\underline{D}}(\delta\lambda) = \frac{\partial \underline{\underline{R}}}{\partial \sigma} \delta\sigma + \frac{\partial \underline{\underline{R}}}{\partial \phi} \delta\phi + \frac{\partial \underline{\underline{R}}}{\partial \lambda} \delta\lambda$$

$$+ \text{ 2nd order term in } \delta\phi \text{ and } \delta\sigma \qquad (35)$$

In particular, note that there is a perturbation in the reaction rate operator due to the flux change $\delta\phi$. Since the flux field is a function both of the data appearing explicitly in the Boltzmann equation, and of the nuclide field vector, a change in either or both of these variables will affect the flux; e.g., a change in data contained in the burn-up operator (and possibly also contained in the Boltzmann operator) will perturb the nuclide field, which then alters the flux field. This flux change is fed back as additional perturbation to the burn-up operator, and so on. For the present study, we will neglect this nonlinearity and assume that any changes to the nuclear data parameters contained in the burn-up operator do not significantly affect the neutron field, so that over some time period

$$\delta\underline{\underline{M}} \cong \phi\underline{\underline{R}}(\delta\sigma) + \underline{\underline{D}}(\delta\lambda) \ . \qquad (36)$$

It should be pointed out that the $\delta\phi$ term is a first-order error and therefore an estimate of the response change based on equation (33) may be inaccurate for data uncertainties which severely distort the time-dependent flux over the time interval of interest. If one requires first-order accuracy to variations in both fields simultaneously, coupled neutron-nuclide perturbation theory must be employed.

To illustrate the role of the nuclide adjoint function in 1st-order perturbation theory, an alternate derivation of Eqs. (26) and (33) will now be presented.(a) For this approach, we chose to write a specified final-value response functional $R[\underline{N}] = < \phi\underline{h}^T\underline{N}(t_f)\ \delta(t-t_f) >$ as follows

$$R[\underline{N}] = \int_{t_0}^{t_f} \frac{d}{dt}\,(\underline{N}^T\underline{N}^*)dt + \underline{N}^{*T}(t_0)\underline{N}(t_0) \ , \qquad (37)$$

---

(a) See reference 10 for the neutron analog.

where $\underline{N}^*$ is an unspecified function in the domain of continuous functions on $[t_0, t_f]$, the only requirement being a fixed end point of $\underline{N}^*(t_f) = \underline{h}\phi$. Phase space variables other than "time" are not explicitly treated in this development; integration over these variables is assumed. Expanding Eq. (37),

$$R[\underline{N}] = \int_{t_0}^{t_f} \left( \underline{N}^{T*} \frac{d\underline{N}}{dt} + \underline{N}^{T} \frac{d\underline{N}^*}{dt} \right) dt + \underline{N}^{T*}(t_0)\underline{N}(t_0) \tag{38}$$

$$= \int_{t_0}^{t_f} \left[ (\underline{N}^{T*} \underline{\underline{M}}\, \underline{N}) + \underline{N}^{T} \frac{d\underline{N}^*}{dt} \right] dt + \underline{N}^{T*}(t_0)\underline{N}(t_0) \ . \tag{39}$$

We will now consider a perturbation in the nuclide field equation (e.g., due to data change):

$$\underline{\underline{M}}' \, \underline{N}' = \frac{\partial}{\partial t} \underline{N}' \ , \tag{40}$$

and Eq. (39) becomes

$$R'(\underline{N}') = \int_{t_0}^{t_f} \left( \underline{N}^{*T} \underline{\underline{M}}' \underline{N}' + \underline{N}'^{T} \frac{d}{dt} \underline{N}^* \right) dt + \underline{N}^{*T}(t_0)\underline{N}(t_0) \tag{41}$$

(assuming no change in the initial concentrations $\underline{N}_0$ or the realization vector $\underline{h}$). Therefore, we see that

$$R'(\underline{N}') = \int_{t_0}^{t_f} \left( \underline{N}^{*T} \underline{\underline{M}}\, N' + \underline{N}^{*T} \delta \underline{\underline{M}}\, \underline{N} + \underline{N}^{*T} \delta \underline{\underline{M}} \delta \underline{N} + \underline{N}'^{T} \frac{d\underline{N}^*}{dt} \right) dt$$

$$+ \underline{N}^{*T}(t_0)\underline{N}(t_0) \ . \tag{42}$$

Applying the adjoint property to the $\underline{\underline{M}}$ and $\frac{d}{dt}$ operators,

$$R'[\underline{N}'] = \int_{t_0}^{t_f} (\underline{N}^{T*}\delta\underline{\underline{M}}\ \underline{N})dt + \int_{t_0}^{t_f} \underline{N}'^{T}\left(\underline{\underline{M}}^*\underline{N}^* + \frac{d\underline{N}^*}{dt}\right)dt$$

$$+ \int_{t_0}^{t_f} \underline{N}^{*T}\delta\underline{\underline{M}}\delta\underline{N}dt + \underline{N}^{*T}(t_f)\underline{N}(t_f)\ . \qquad (43)$$

Recall that up until this point, $\underline{N}^*$ has been an arbitrary function. *We will now define it as the function which causes the second integral to vanish*, i.e.,

$$\underline{\underline{M}}^*\underline{N}^* = -\frac{d}{dt}\underline{N}^*$$

$$\underline{N}^* = \phi\underline{h}, \quad \text{at } t = t_f\ .$$

Of course this is merely a restatement of Eq. (28). By definition,

$$\underline{N}^{*T}(t_f)\underline{N}(t_f) = \underline{N}^T(t_f)\ \phi\underline{h} = R[\underline{N}]\ . \qquad (44)$$

Substituting the above relation into Eq. (43) gives the following

$$\delta R = \int_{t_0}^{t_f} \underline{N}^{*T}\delta\underline{\underline{M}}\ \underline{N}dt + \int_{t_0}^{t_f} N^{*T}\delta\underline{\underline{M}}\delta\underline{N}dt\ . \qquad (45)$$

Since the last integral in Eq. (45) is second order, we see that $\underline{N}^*$ is that particular function which makes the response in Eq. (37) insensitive (to first order) to variations in $\underline{N}(t)$. Finally, we can say

$$\delta R = \int_{t_0}^{t_f} \underline{N}^{*T}\delta\underline{\underline{M}}\ \underline{N}dt \quad \text{plus 2nd order terms.} \qquad (46)$$

## IV. PHYSICAL SIGNIFICANCE OF THE TIME-DEPENDENT NUCLIDE ADJOINT

It is well known that the solution to the adjoint time-dependent Boltzmann transport equation can be interpreted as follows:

$\phi^*(t)$ = "importance of a neutron at time t to the response at time, $t_F$."[9] (Note – again, all phase space variables except "time" are implicitly treated.)

Therefore, it is not surprising that a time-dependent nuclide adjoint plays a similar role for final-time functionals in burn-up calculations. We assert the following axiom:

$N_i^*(t)$ = importance of nuclide i at time t to the response at time $t_F$.

For the particular case of the response being some final-time nuclide density, this definition can be stated more quantitatively by

$N_i^*$ = fraction of atoms of nuclide i present at time t, which will be transmuted into components of the response nuclides at time $t_F$.

For the burn-up equation with a fixed neutron flux field, the above definitions show that the adjoint nuclide field is independent of the forward field, and, therefore, a particular adjoint calculation is applicable to all reactor configurations which have the same flux field as used in the original calculation. This fact is analogous to the situation for the neutron adjoint, which is applicable to all neutron flux fields that have a common nuclide field. In both instances the forward field is fixed by the initial conditions, and the adjoint field is fixed by the final response.

The importance property of the nuclide adjoint can be used to directly derive the adjoint transmutation equation from first principles, in a manner similar to the method used by Lewins to derive the neutron adjoint equation.[9] The derivation is based on the principle for "conservation of nuclide importance," which states that a nuclide in an specified neutron environment is as important as its daughters (from both reactions and decays). From this axiom, it is easily seen that the importance of nuclide i at time t is equal to its importance at t + Δt plus the importance of all daughters it produces during Δt. Let $\alpha_i$ be the total transmutation probability per unit time for nuclide i; then $(1 - \alpha_i \Delta t)$ = probability that nuclide i does not transmute during Δt. Let $\alpha_{i \to j}$ be the probability per unit time that nuclide i will transmute into nuclide j. Then applying the conservation of nuclide importance:

$$N_i^*(t) = N_i^*(t + \Delta t)(1 - \alpha_i \Delta t) + \sum_{j \neq i} \alpha_{i \to j} N_j^* \Delta t \ , \tag{47}$$

rearranging terms,

$$\frac{N_i^*(t) - N_i^*(t + \Delta t)}{\Delta t} = -\alpha_i N_i^*(t + \Delta t) + \sum_{j \neq i} \alpha_{i \to j} N_j^* \ . \tag{48}$$

Finally, taking the limit Δt → 0,

$$\sum_j \alpha_{i \to j} N_j^* = - \frac{d}{dt} N_i^* \ , \tag{49}$$

where $\alpha_{ii}$ is defined to $-\alpha_i$. This equation can be written in vector notation as

$$- \frac{d}{dt} \underline{N^*} = \underline{\underline{A}}\ \underline{N^*} \ . \tag{50}$$

Comparing the elements of $\underline{\underline{A}}$ to the elements of the burn-up matrix $\underline{\underline{M}}$ (see Appendix A), we see that $\underline{\underline{A}}$ = transpose $\underline{\underline{M}} = \underline{\underline{M}}^*$. Therefore $\underline{\underline{M}}^* \underline{N^*} = - \frac{d}{dt} \underline{N^*}$.

The importance conservation property of the adjoint-nuclide field also makes possible the creation of a "nuclide channel theory." The concept of neutron channel theory has been introduced in an earlier paper as a method to determine the mechanism by which neutrons flow from the forward source to the response detector, so as to locate spatial streaming paths.[18,19] A similar idea can be applied to the nuclide field to find the major "nuclide paths" by which atoms are transformed from the initial isotopic concentrations into the final response concentrations.

To this end, a quantity known as the "nuclide contributon density" can be defined to be:

$c_i(t)$ = number of atoms of nuclide i, per $\text{cm}^3$, present at time t which become response atoms at time $t_F$.

It is easy to see from the definition of the adjoint,

$$c_i(t) = N_i(t)N_i^*(t) \ . \tag{51}$$

Because the final response must originate from some nuclide present in the system,

$$\sum_i c_i(t) = \text{final response} \ , \tag{52}$$

for all t in the interval $[t_0,t_f]$, which can be written as

$$\underline{N}^T(t)\underline{N}^*(t) = \text{constant} = \underline{h}^T \ \underline{N}(t_f) = \text{response} \ . \tag{53}$$

A knowledge of $c_i(t)$ for all nuclides allows one to determine which isotopes at time t contribute most heavily to the response of interest. This property could possibly be beneficial to optimization studies in reactor design.

## V. TIME-DEPENDENT UNCERTAINTY ANALYSIS

Time-dependent uncertainty analysis is similar to the static uncertainty theory previously developed, and some of the following derivations are based on earlier works. The established approach is to use the results of Section II to define "sensitivity coefficients" which can be used in conjunction with covariance files for basic nuclear data to develop uncertainties in responses of interest. For the present study, the sensitivity coefficients are defined with time-dependent vectors, compared with energy functions for the static case.

The existing evaluations of nuclear data can be thought of as representing the mean value (albeit weighted) derived from a distribution of microscopic measurements. With the issue of ENDF/B-IV — and greatly extending into ENDF-V — the second moments of the distribution of measurements (i.e., the variances and covariances) representing correlated uncertainties are specified to provide the analyst with a measure of the quality of the data.[20,21]

To briefly demonstrate how sensitivity theory is combined with data uncertainty files, let us consider a reference data collection (assumed to be the mean value of several measurements) that will again be designated as the "data vector" $\underline{S}(\alpha_i)$. As before, the elements $\alpha_i$ of $\underline{S}$ represent the decay data, microscopic reaction rates ($\sigma\phi$), etc., that are to be used in some depletion calculations. With this collection of data, the expectation value of the response is calculated to be $R(\underline{S})$.

If some other data vector $\underline{S}_n$ were used in the calculation, then another value for the response would be obtained, $R_n(\underline{S}_n)$. The distribution of all such possible calculated responses, due to the distribution of nuclear data, is described by the response variance, given by

$$V = \frac{1}{N} \sum_{n=1}^{N} (R_n - R)^2 , \tag{54}$$

with N = number of data vectors used in computing the mean set $\underline{S}$; i.e., N is related to the number of measurements for the $\alpha$'s in $\underline{S}$.

Expanding $R_n$ in a first-order Taylor series about the expectation value gives

$$R_n = R + \frac{\partial R(S)^T}{\partial \underline{S}} (\underline{S}_n - \underline{S}) \ , \tag{55}$$

where the vector derivative $\frac{\partial}{\partial \underline{S}}$ is defined to be the column vector operator with components $\frac{\partial}{\partial \alpha_i}$ .

Substituting Eq. (55) into Eq. (54) results in

$$V = \frac{1}{N} \sum_n \left( \frac{\partial R^T}{\partial \underline{S}} \Delta \underline{S}_n \right)^2 \tag{56}$$

Now defining a diagonal matrix of the form

$$D = \begin{pmatrix} \alpha_1 & 0 & 0 \ldots \\ 0 & \alpha_2 & 0 \ldots \\ \vdots & & \\ 0 & 0 \ldots & \alpha_m \end{pmatrix} \quad \begin{array}{l} \text{where } \alpha_1 = \text{first component of } \underline{S} \ , \\ \phantom{\text{where }} \alpha_2 = \text{second component of } \underline{S} \ , \\ \phantom{\text{where }} \vdots \\ \phantom{\text{where }} \alpha_i = i\text{th component of } \underline{S} \end{array}$$

Equation (56) can be written

$$V = \frac{1}{N} \sum_n \left\{ \frac{\partial R^T}{\partial \underline{S}} \left( \underline{\underline{D}} \frac{1}{\underline{\underline{D}}} \right) \Delta \underline{S}_n \right\}^2$$

$$= R^2 \frac{1}{N} \sum_n \left( \frac{\underline{\underline{D}}}{R} \frac{\partial R}{\partial \underline{S}} \right)^T \left( \frac{1}{\underline{\underline{D}}} \Delta \underline{S}_n \Delta \underline{S}_n^T \frac{1}{\underline{\underline{D}}} \right) \left( \frac{\underline{\underline{D}}}{R} \frac{\partial R}{\partial \underline{S}} \right) \ . \tag{57}$$

Noting that $\frac{\partial R}{\partial \underline{S}}$ is independent of the summation index, Eq. (57) is finally expressed as

$$\frac{V}{R^2} = \underline{P}^T \underline{\underline{C}} \, \underline{P} = \text{relative response variance} \ , \tag{58}$$

where

$$\underline{P} = \frac{\underline{\underline{D}}}{R} \frac{\partial R}{\partial \underline{S}} \tag{59}$$

$$\underline{\underline{C}} = \frac{1}{N} \sum_{n} \left( \frac{1}{\underline{\underline{D}}} \Delta \underline{S}_n \Delta \underline{S}_n^T \frac{1}{\underline{\underline{D}}} \right) \tag{60}$$

The matrix $\underline{\underline{C}}$ formed by the dyadic square of $\Delta \underline{S}_n$ is called the "relative covariance matrix," and the vector $\underline{P}$ is called the "sensitivity vector." Let us consider one component of $\underline{P}$:

$$P_i = \frac{\alpha_i}{R} \frac{\partial R}{\partial \alpha_i} = \frac{\partial R / R}{\partial \alpha_i / \alpha_i} \; . \tag{61}$$

Equation (8) can be used to evaluate the partial derivative accurate through first order:

$$\frac{\partial R}{\partial \alpha_i} = \left\langle \; \underline{N}^{*T} \frac{\partial}{\partial \alpha_i} \underline{\underline{M}} \; \underline{N} \right\rangle \; . \tag{62}$$

If we assume as an example that the data $\alpha_i$ appears only in position $(k,\ell)$ of the burn-up matrix, then $\frac{\partial}{\partial \alpha_i} \underline{\underline{M}}$ is a matrix with zeros in all positions except $(k,\ell)$, where its value is $\frac{\partial}{\partial \alpha_i} (m_{k\ell})$. Therefore in general

$$P_i = \frac{\alpha_i}{R} \sum_{k,\ell} \left\langle \left[ N_k^*(t) \, \frac{\partial m_{k\ell}}{\partial \alpha_i} \, N_\ell(t) \right] \right\rangle \; . \tag{63}$$

Thus we see that uncertainty analysis involves both a knowledge of the data covariances and the sensitivity vector. We will now consider a sample problem to illustrate the procedure for determining the sensitivity vector; questions concerning the covariance matrix will not be addressed.

## VI. PROBLEM SPECIFICATION

Time-dependent sensitivity theory was applied to the analysis of a thermal reactor depletion calculation that was specified by the Electric Power Research Insitute (EPRI).[22] A point-model of the homogenized fuel zone was used in the sensitivity calculation, with the initial concentrations listed in Table 1. The time dependent thermal flux (Table 2) was obtained from an earlier non-linear burn-up calculation supplied by EPRI.

Point depletion calculations for the forward and adjoint nuclide fields were performed with the computer code ORIGEN-A, a modified version of ORIGEN (described in detail in Appendix A). ORIGEN solves a zero dimensional version of the burn-up equations using the matrix exponential technique, a method which allows a wide variety of nuclides to be included in the depletion calculation. Nuclear data was obtained directly from the ORIGEN PWR library[12] (three cross section groups) for computational convenience.

The calculated response was the total plutonium inventory ($^{239,240,241,242}$Pu) at end of cycle ($t_f$ = 25614 hours). The standard deviation in this response was estimated using approximate standard deviations for the $^{238}$U capture and $^{239}$Pu fission cross sections.

Uncertainties in these cross sections are the two major causes for uncertainty in the Pu production. Most other pertinent data have either low sensitivity coefficients or small uncertainties (as for decay constants); therefore consideration only of the $^{238}$U and $^{239}$Pu cross sections can provide a reasonable lower bound for the total standard deviation of the plutonium inventory at end of cycle.

## VII. RESULTS

The values for the most important time-dependent actinide densities found in the forward ORIGEN-A calculation are shown in Figs. 1 and 2. As expected, the concentrations of uranium and plutonium isotopes dominate the results of the forward case, with $^{238}$U being the most predominate by far, due to its large initial concentration. Figure 3 shows the major chains for plutonium build-up.

Table 1. Initial concentrations for homogenized fuel

| Nuclide | Number density |
|---|---|
| $^{16}$O | 4.37-02 |
| $^{135}$X | 0.0 |
| $^{149}$Sm | 0.0 |
| $^{234}$U | 4.45-06 |
| $^{235}$U | 5.67-04 |
| $^{236}$U | 3.53-06 |
| $^{238}$U | 2.13-02 |
| $^{239}$Pu | 0.0 |
| $^{240}$Pu | 0.0 |
| $^{241}$Pu | 0.0 |
| $^{242}$Pu | 0.0 |
| $^{241}$Am | 0.0 |

Table 2. Time-dependent thermal flux

| Time interval | $t_i$ (hr) | $\phi$ (x $10^{13}$) neutrons/cm$^2$·sec |
|---|---|---|
| 1 | 75.34 | 4.52 |
| 2 | 376.68 | 4.54 |
| 3 | 1506.68 | 4.51 |
| 4 | 3013.42 | 4.43 |
| 5 | 4520.13 | 4.38 |
| 6 | 6026.84 | 4.37 |
| 7 | 7533.55 | 4.38 |
| 8 | 9040.26 | 4.41 |
| 9 | 10546.97 | 4.46 |
| 10 | 12053.68 | 4.51 |
| 11 | 13560.39 | 4.58 |
| 12 | 15067.10 | 4.65 |
| 13 | 16573.81 | 4.72 |
| 14 | 18080.52 | 4.81 |
| 15 | 19587.13 | 4.89 |
| 16 | 21093.94 | 4.98 |
| 17 | 22600.65 | 5.07 |
| 18 | 24107.36 | 5.17 |
| 19 | 25614.07 | 5.26 |

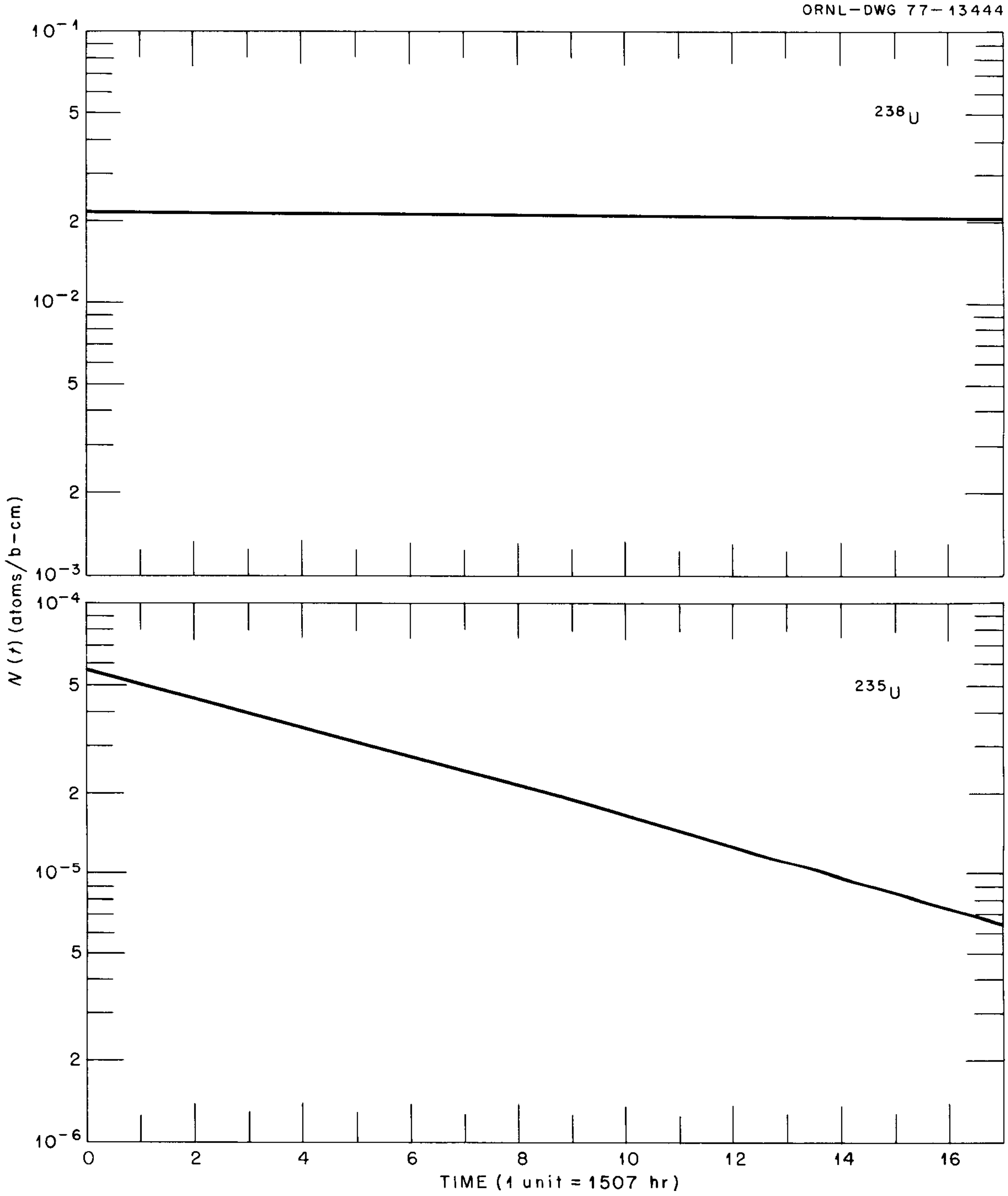

Fig. 1. Uranium atom densities.

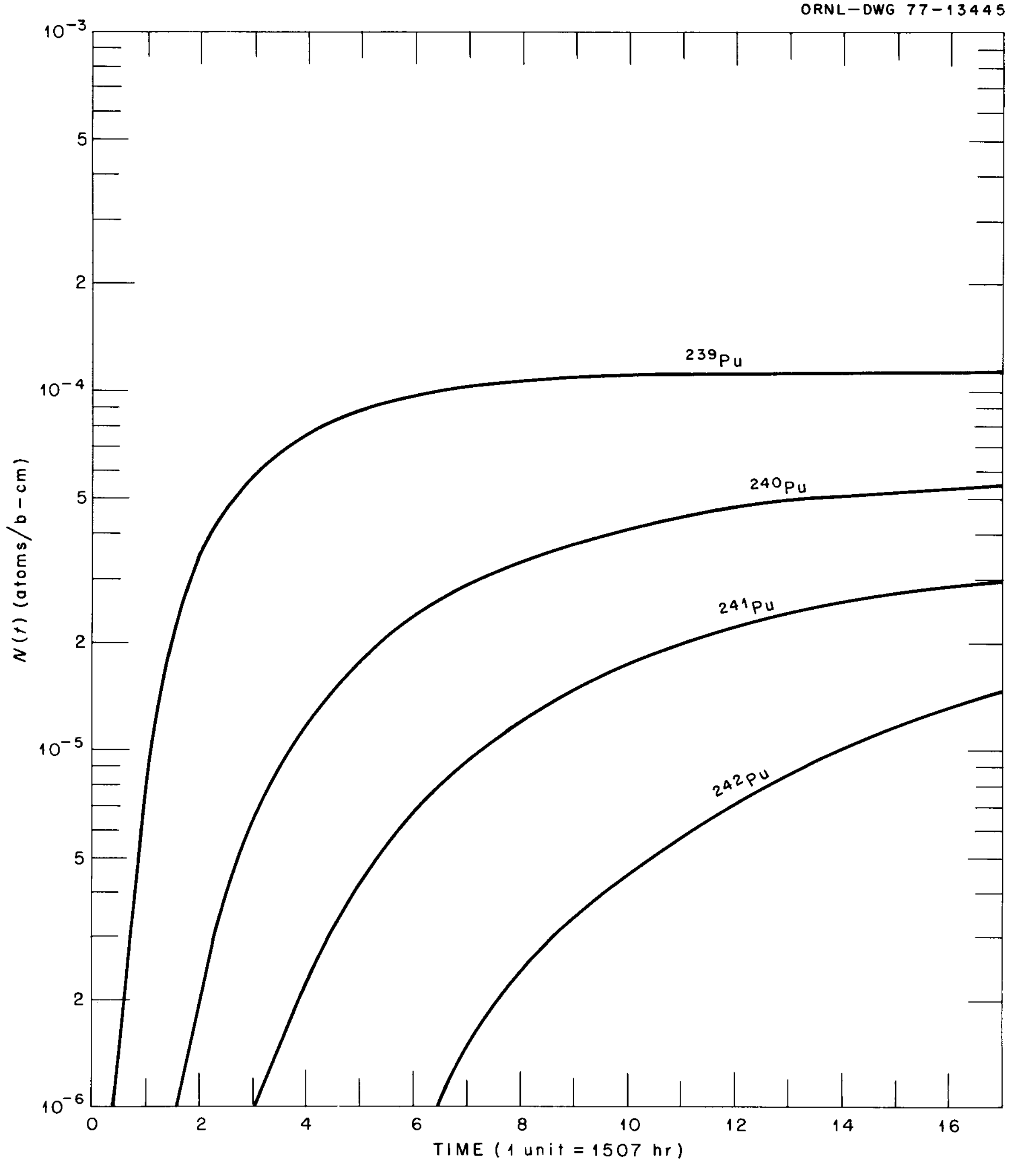

Fig. 2. Plutonium atom densities.

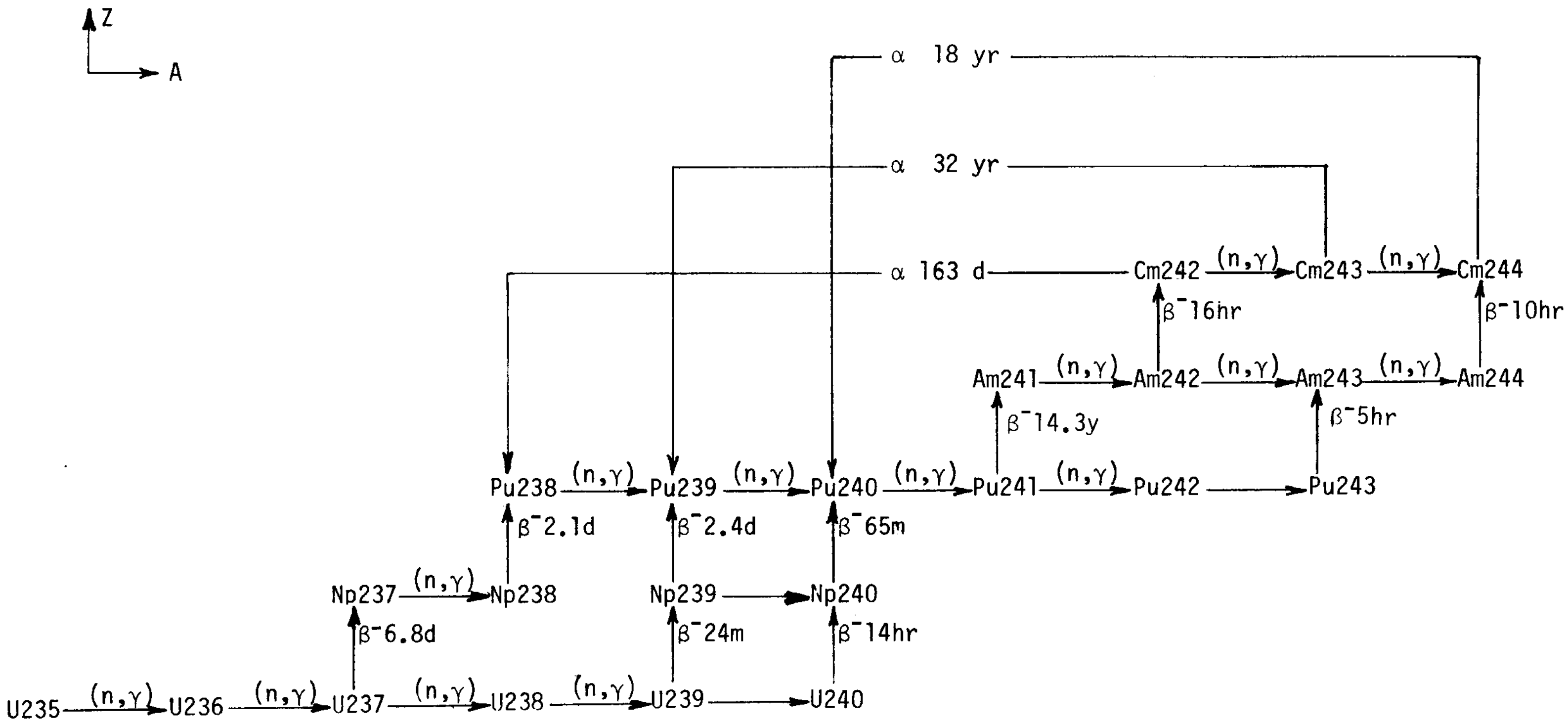

Fig. 3. Major chains for plutonium production

Figures 4-8 summarize the results of the adjoint ORIGEN-A calculation. For this run the "initial" (actually, final)(a) values were zero for all nuclides except $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, and $^{242}$Pu, which had concentrations of 1.0, since this is the realization vector corresponding to a response of "plutonium inventory at shutdown." The flux in Eq. (27) was omitted because reaction rates are not being considered.

At first sight it may be surprising to see some of the more uncommon isotopes (such as $^{237}$U, $^{242}$Cm, etc.) appearing among the important isotopes for producing plutonium. It may be equally surprising that the dominant nuclide in the forward calculation — $^{238}$U — is not among the most dominant adjoint values! The results appear more reasonable when one realizes that the "importance" of a nuclide is <u>independent</u> of its concentration. Even though nuclides such as $^{240}$Np have only a small number of atoms present at any given time, any atom which is present has a high probability of being transformed into a plutonium atom by shutdown. The importance of $^{238}$U atoms ($\sim 10^{-3}$) is comparatively low due to its having a smaller capture cross section(b) (∿3 b) than more important isotopes, such as $^{237}$Np (∿170 b). Therefore a $^{238}$U atom has less probability of being transformed into Pu than does a $^{237}$Np atom; i.e., a smaller <u>fraction</u> of $^{238}$U will transmute into Pu, although the absolute number of $^{238}$U atoms which contribute to the response is much greater than for $^{237}$Np, since there are far more $^{238}$U atoms than Np atoms present in the reactor.

An examination of several nuclide adjoints will perhaps give the reader a better physical insight. The Pu response isotopes themselves are obviously important, especially at times near $t_f$. At earlier times, the high fission cross section makes an atom of a fissile Pu isotope quite likely to disappear before it lives to $t_f$. The adjoint for $^{238}$Pu decreases near $t_f$ because it was not directly contained in the response.

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(a) See Appendix A, for inverted solution to the adjoint equation.

(b) Cross sections quoted are 2200 m/s values.

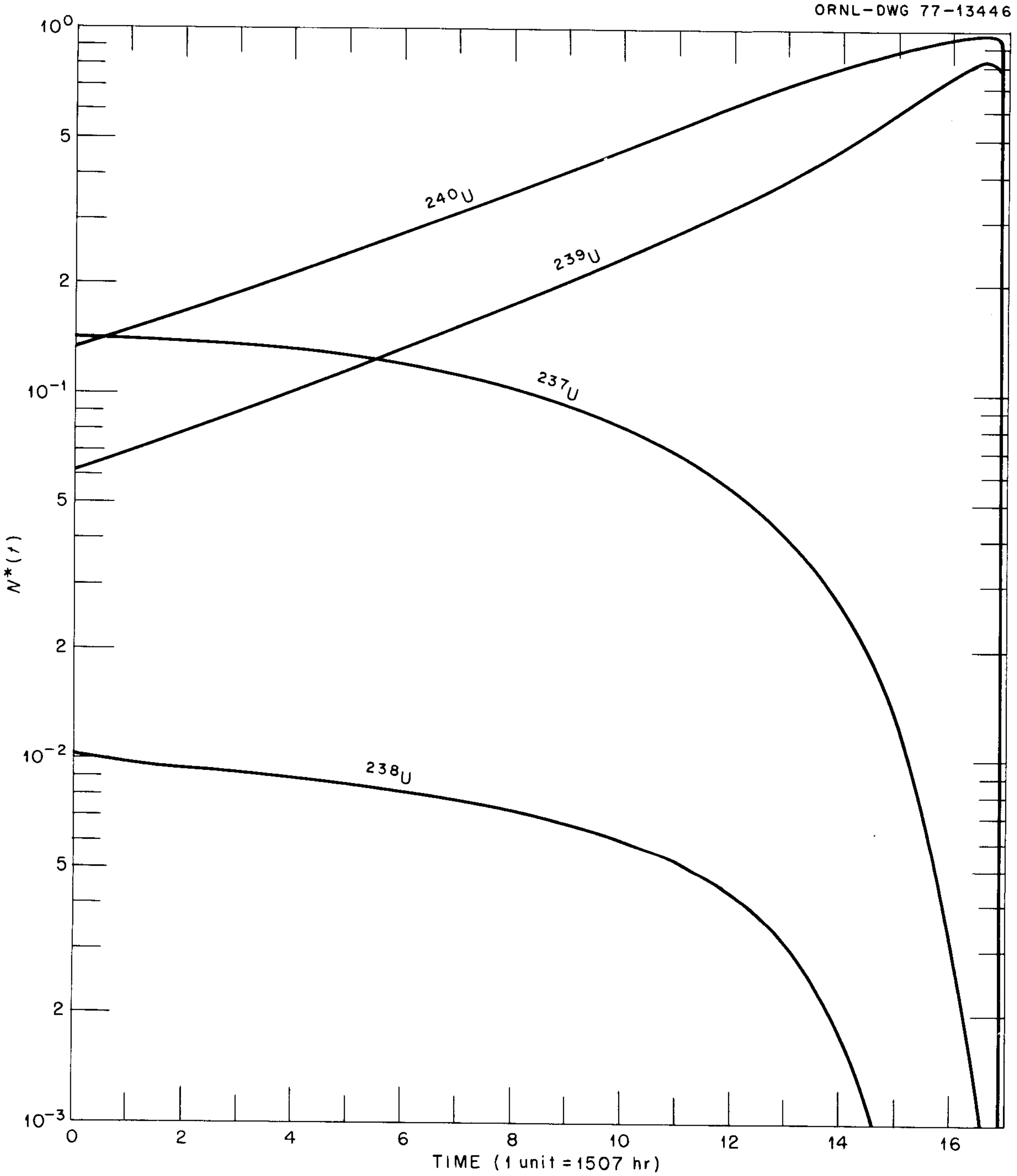

Fig. 4. Uranium adjoint functions.

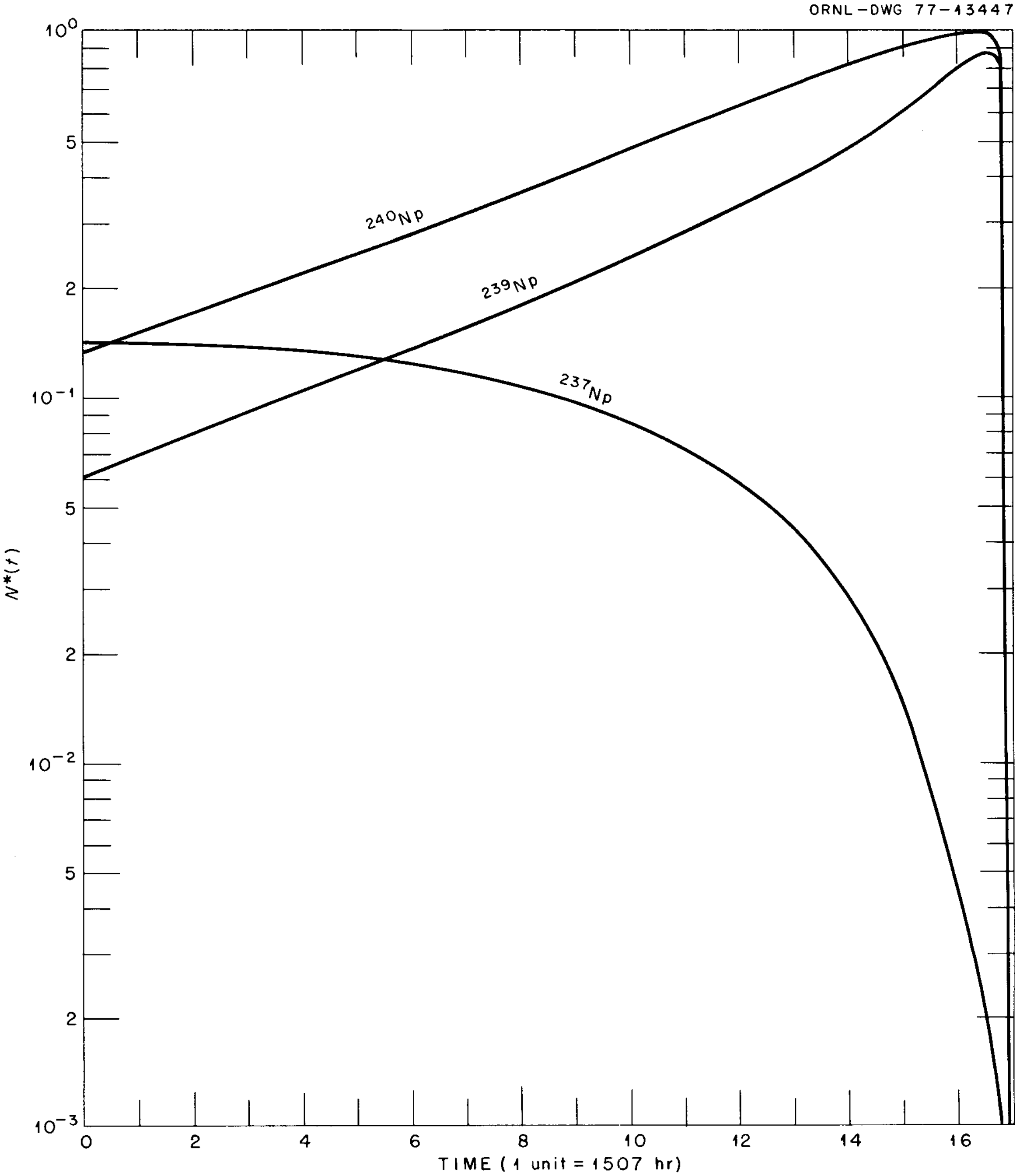

Fig. 5. Neptunium adjoint functions.

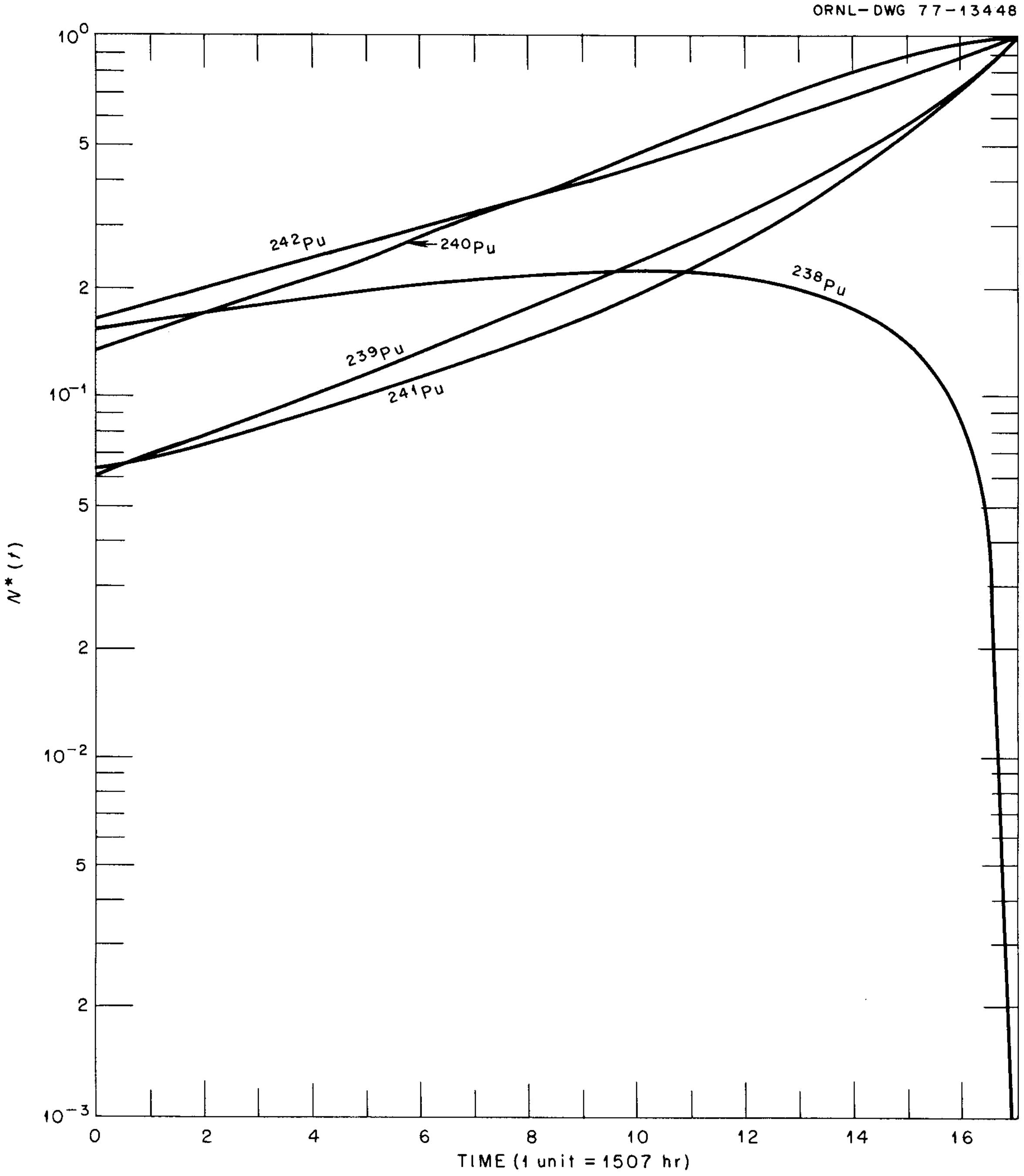

Fig. 6. Plutonium adjoint functions.

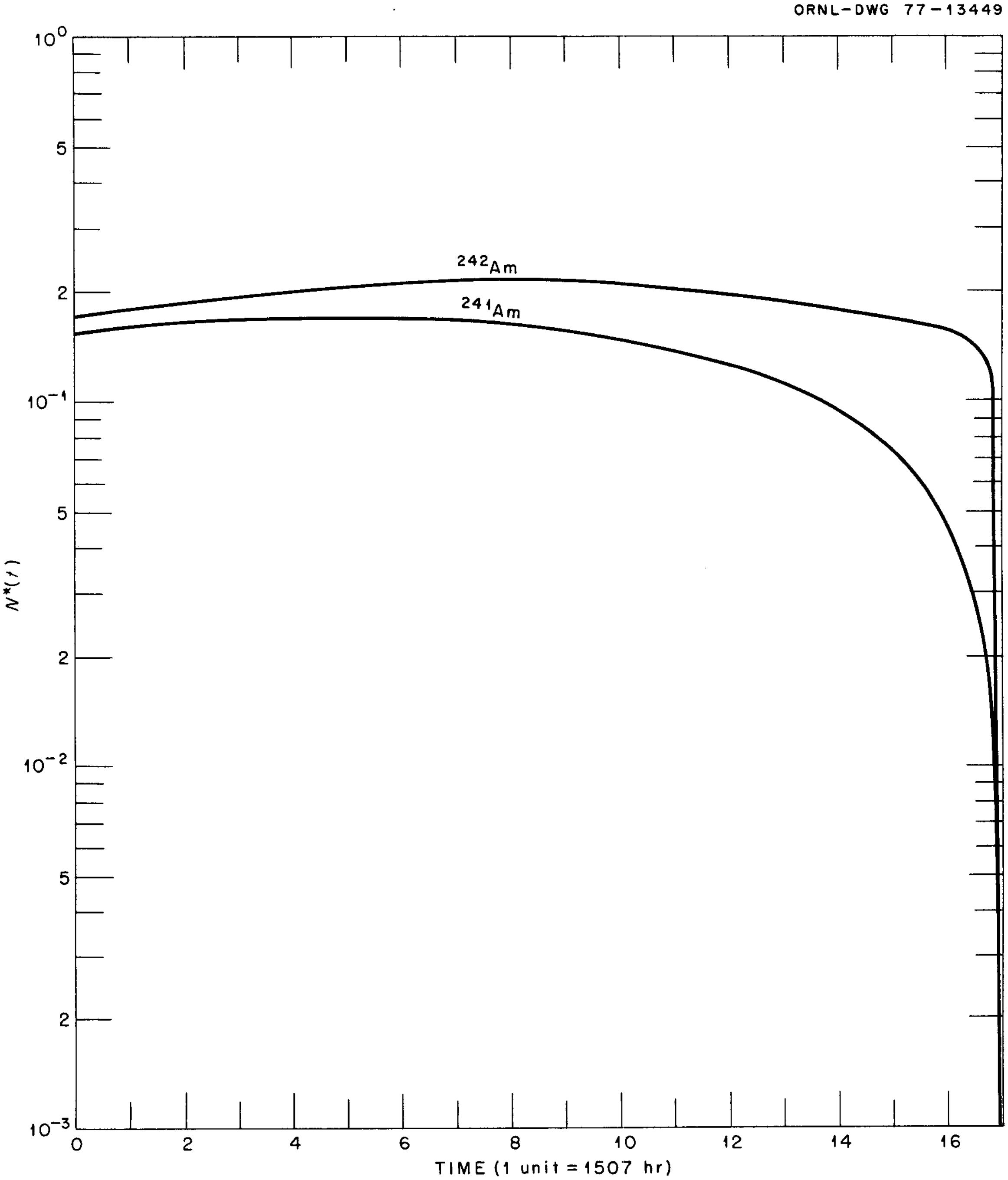

Fig. 7. Americium adjoint functions.

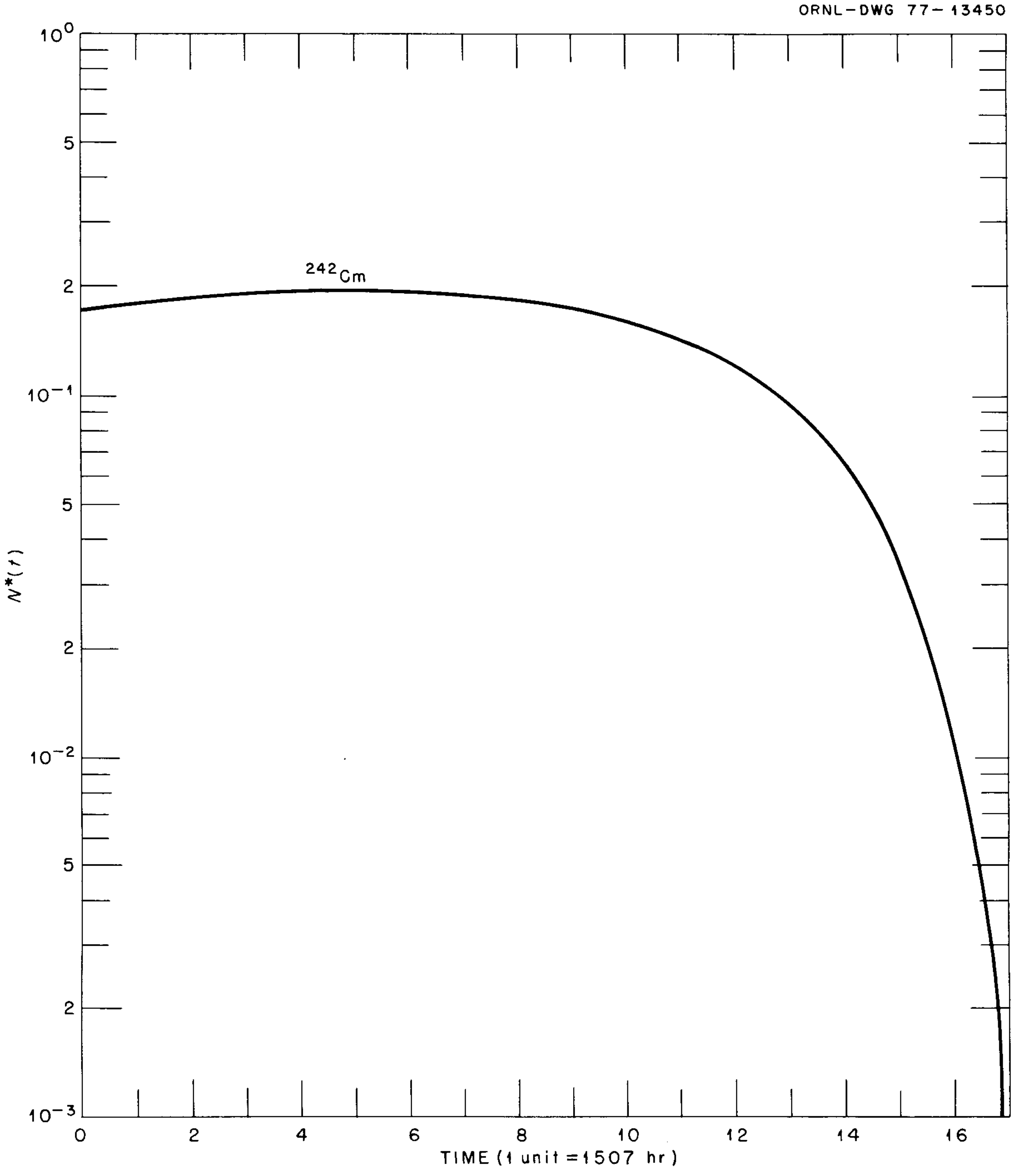

Fig. 8. Curium adjoint function.

Actinides with a higher atomic number than 94 are usually important through their decay modes. For example, $^{242}$Cm has a moderate absorption cross section (∿30 b) and a relatively short half-life (163 d); therefore it has about thirty times greater probability of decaying to $^{238}$Pu before it captures a neutron to become $^{243}$Cm — note the similarity in the $^{238}$Pu adjoint curve and the $^{242}$Cm, adjoint curve. Furthermore, even if the $^{242}$Cm atom does transmute to $^{243}$Cm, there is still a possibility that the $^{243}$Cm isotope will decay to $^{239}$Pu.

Americium-242 is important because it decays by beta emission to $^{242}$Cm and by electron capture directly to $^{242}$Pu, and its short half-life ($t_{1/2}$ = 16 hours) makes the transition likely over a long time period. In fact, even at one time interval before shutdown its adjoint is still quite high. At early times the isotope $^{237}$U is an important nuclide whose mode of contribution is fairly complicated to assess. Its short half-life (7 days) and large capture cross section (480 b) provide two possible methods for the nuclide to transmute into Pu. If $^{237}$U captures a neutron, it becomes $^{238}$U and follows the familiar procedure for creating $^{239}$Pu. The alternate method is for $^{237}$U to decay by beta emission to $^{237}$Np. Since this nuclide has a long half-life (2 x $10^6$ y), it is probable that an atom will capture a neutron ($\sigma_c$ = 169) and become $^{238}$Np, which then decays ($t_{1/2}$ = 2.12 days) into $^{238}$Pu. An examination of Figs. 3 and 4 reveals that over most of the cycle, $^{237}$U is more important than $^{238}$U, but slightly less important than $^{237}$Np, a fact which leads one to believe that the second contribution mode is more important.

Table 3 (see Eq. 51) contains the values of the contributon densities for the major nuclides. It is seen that until near the end of cycle the response stored in the $^{238}$U atoms overwhelms all others, due to its large initial charge. At time step 17, Pu begins to dominate, as the $^{238}$U atoms are "running out of time" in which they can transmute into Pu. Notice the initial contributon density for $^{238}$U is 2.15 x $10^{-4}$, which was found to be exactly the value of the plutonium inventory at shutdown (see last row in Table 3). This indicates — as expected — that initially the entire response is contained in the $^{238}$U atoms:

$$R(t_f) = (N_0 N_0^*)_{^{238}U} .$$

Table 3. Major contributon densities (atoms/cm$^3$ x 10$^{-24}$)

| Time interval | $^{238}$U | $^{239}$Pu | $^{240}$Pu | $^{241}$Pu | $^{242}$Pu |
|---|---|---|---|---|---|
| 1 | 2.15-4 | 0 | 0 | 0 | 0 |
| 2 | 2.15-4 | 0 | 0 | 0 | 0 |
| 3 | 2.15-4 | 0 | 0 | 0 | 0 |
| 4 | 2.13-4 | 2.36-6 | 0 | 0 | 0 |
| 5 | 2.09-4 | 4.63-6 | 1.08-6 | 0 | 0 |
| 6 | 2.06-4 | 6.80-6 | 2.27-6 | 0 | 0 |
| 7 | 2.01-4 | 8.94-6 | 3.82-6 | 0 | 0 |
| 8 | 1.97-4 | 1.12-5 | 5.71-6 | 0 | 0 |
| 9 | 1.91-4 | 1.36-5 | 7.92-6 | 1.04-6 | 0 |
| 10 | 1.86-4 | 1.63-5 | 1.05-5 | 1.54-6 | 0 |
| 11 | 1.78-4 | 1.91-5 | 1.35-5 | 2.13-6 | 1.18-6 |
| 12 | 1.70-4 | 2.24-5 | 1.70-5 | 2.89-6 | 1.76-6 |
| 13 | 1.60-4 | 2.63-5 | 2.09-5 | 3.82-6 | 2.53-6 |
| 14 | 1.49-4 | 3.11-5 | 2.53-5 | 5.02-6 | 3.50-6 |
| 15 | 1.35-4 | 3.71-5 | 3.03-5 | 6.57-6 | 4.73-6 |
| 16 | 1.19-4 | 4.43-5 | 3.58-5 | 8.65-6 | 6.22-6 |
| 17 | 9.81-5 | 5.39-5 | 4.15-5 | 1.15-5 | 8.10-6 |
| 18 | 7.29-5 | 6.70-5 | 4.73-5 | 1.55-5 | 1.03-5 |
| 19 | 4.04-5 | 8.58-5 | 5.22-5 | 2.15-5 | 1.30-5 |
| 20 | 0 | 1.14-4 | 5.48-5 | 3.02-5 | 1.62-5 |

Table 4. Time-dependent sensitivity profile for Pu inventory at shutdown

| Time interval | $^{238}$U (n,$\gamma$) | $^{239}$Pu (n,f) |
|---|---|---|
| 1 | 5.24-4 | 0 |
| 2 | 2.13-3 | 0 |
| 3 | 8.58-3 | -1.06-3 |
| 4 | 1.29-2 | -4.16-3 |
| 5 | 1.48-2 | -6.71-3 |
| 6 | 1.70-2 | -9.23-3 |
| 7 | 1.97-2 | -1.19-2 |
| 8 | 2.31-2 | -1.47-2 |
| 9 | 2.69-2 | -1.79-2 |
| 10 | 3.15-2 | -2.14-2 |
| 11 | 3.72-2 | -2.55-2 |
| 12 | 4.39-2 | -3.04-2 |
| 13 | 5.24-2 | -3.64-2 |
| 14 | 6.29-2 | -4.39-2 |
| 15 | 7.65-2 | -5.34-2 |
| 16 | 4.35-2 | -6.56-2 |
| 17 | 1.20-1 | -8.23-2 |
| 18 | 1.53-1 | -1.06-1 |
| 19 | 8.70-2 | -1.41-1 |
| Total | 0.835 | -0.671 |

The differential time-dependent sensitivity profiles for $^{238}$U capture and $^{239}$Pu fission are given in Table 4. Because the capture cross section appears as both a loss and a gain (a negative effect due to burn-up of a fertile isotope; a positive effect due to production of $^{239}$Pu), errors in this value tend to cancel somewhat in the determination of the response uncertainty. The uncertainty for $^{239}$Pu fission cross section impacts the response directly since it is a loss mechanism for the response nuclide of interest.

Detailed covariance files for the thermal energy range are only now being developed, and were not available for the present work. Estimated standard deviations of 3% for both the $^{238}$U capture and the $^{239}$Pu fission cross sections were used in this study. These values were obtained by assuming cross section uncertainties of 1% in the thermal range and 5% in the epithermal range, with 3:1 weighting function over these ranges, respectively.[23,24] Based on these approximate uncertainty estimates, the associated relative standard deviation in plutonium production is found to be ∿3%, arising from $^{238}$U capture uncertainty; and ∿2% arising from $^{239}$Pu fission uncertainty. This results in a relative standard deviation of approximately 3% in plutonium inventory at shutdown.

It is important to note that the value for the standard deviation does not reflect uncertainties in half-lives, branching ratios, or reaction cross sections in nuclides other than $^{238}$U and $^{239}$Pu; nor does it contain any cross correlation between $^{238}$U and $^{239}$Pu data. The calculated value is only intended as a lower bound for the response uncertainty. More accurate results will be obtained after more complete error files are made available on the ENDF-5 data evaluation, soon to be released.

## VIII. SUMMARY AND CONCLUSIONS

Sensitivity and uncertainty analysis for functionals of the time-dependent nuclide density field has been implemented into the present ORNL sensitivity program using methods that are similar to those developed for the static case. The computer code ORIGEN-A (see Appendix B) has extended the capability of the ORIGEN burn-up code to allow calculation of nuclide adjoint functions for final-time, linear functionals and functional ratios, as well as the normal forward calculation. When the forward and adjoint values are coupled, sensitivity coefficients can be computed for all nuclear data contained in the burn-up matrix (e.g., microscopic cross sections, decay constants, yields, branching ratios, etc.). The sensitivity coefficients relate changes in response to changes in nuclear data.

The concept of "nuclide importance" has been quantified and compared to its predecessor "neutron importance." This allowed for the development of a "nuclide channel theory," which indicates the isotope "channels" through which a nuclide field is transformed from its initial configuration to some final response.

Uncertainty analysis for nuclide density functionals was shown to be based on methods similar to those already in use in the FØRSS system. Extensions of existing programs are required with respect to achieving compatability with the ORIGEN-A output and accessing uncertainties in decay constants, yields, etc.

A sample calculation illustrated the generation of nuclide adjoints and their use in channel theory and in time-dependant sensitivity/uncertainty analysis. For assumed standard deviations of 3% in $^{238}$U capture and $^{239}$Pu absorption cross sections, the minimum uncertainty in the plutonium inventory after approximately three years of a PWR reactor operation was found to be near 3%.

## ACKNOWLEDGMENTS

The authors wish to thank O. W. Hermann and C. W. Kee for their assistance in fathoming the logic of the ORIGEN code to implement the programming for adjoint calculations. Appreciation is also extended to O. Ozer of the Electric Power Research Institute, who suggested the sample problem and provided necessary depletion parameters.

# APPENDIX A: NUMERICAL SOLUTION TO THE LINEARIZED ADJOINT BURN-UP EQUATION

The burn-up equation is a statement of mass balance for a radioactive nuclide field subjected to a neutron flux. The equation for nuclide species i can be written:

$$\frac{dN_i}{dt} = -(\sigma_{ai}\phi + \lambda_i)N_i + \sum_{j\neq i} (\sigma_{j\to i}\phi + \lambda_{j\to i})N_j \ . \tag{A1}$$

In matrix notation, the above equation is merely:

$$\underline{\underline{M}}(\alpha_{j\to i})\underline{N} = \frac{\partial}{\partial t}\underline{N} \ ,$$

$\alpha_{j\to i}$ = probability per unit time that isotope i will be produced from isotope j, and $\alpha_{ii} = -\sum_j \alpha_{i\to j}$.

In Eq. (A1), the value for $\underline{N}$ can be found with the matrix exponential technique as

$$\underline{N}(t) = \exp(\underline{\underline{M}}t)\ \underline{N}_o \ , \tag{A2}$$

where exp ($\underline{\underline{M}}$t) is the time dependent matrix given by the infinite series

$$\underline{I} + \underline{\underline{M}}t + \frac{\underline{\underline{M}}^2 t^2}{2!} \ldots \equiv \underline{\underline{B}}(t) \ . \tag{A3}$$

Of course in reality the series is truncated at some finite number of terms dictated by the tolerance placed on $\underline{N}(t)$. The computer code ORIGEN solves the burn-up equations using this method, and a discussion of the numerical procedures involved in its implementation can be found in reference 12.

Note that the matrix $\underline{\underline{B}}(t)$ is independent of the initial conditions $\underline{N}_0$; therefore, in theory it is possible to obtain a solution for a given $\underline{\underline{M}}(\phi)$ that does not depend on the initial reactor configuration. Then the time-dependent nuclide field is

$$\underline{N}(t) = \underline{\underline{B}}(t)\underline{N}_o \qquad \text{for any } \underline{N}_0 \ , \tag{A4}$$

Unfortunately the nuclear data matrix $\underline{\underline{B}}$ is problem dependant (through the flux) and is too large ($\sim$800 by 800 words for each time step in ORIGEN) to be used efficiently. It is more advantageous to recalculate $\underline{N}(t)$ for each $\underline{N}_0$.

As previously discussed the adjoint burn-up equation is

$$-\frac{d}{dt}\underline{N}^* = \underline{\underline{M}}^T\underline{N}^* \ . \tag{A5}$$

Equation (A5) can be expressed in a form compatible with the present ORIGEN computational technique (i.e., a <u>positive</u> time derivative) by making a change of variable:

$$t' = t_f - t$$

$$-\frac{d}{dt} = \frac{d}{dt'} \tag{A6}$$

$$\underline{N}^*(t_f) = \underline{N}^*(t'=0)$$

Then the adjoint solution is merely

$$\underline{N}^*(t') = e^{\underline{\underline{M}}^T t'}\ \underline{N}^*(t'=0), \qquad 0 < t < t_f \tag{A7}$$

$$\underline{N}^*(t) = \underline{N}^*(t_f - t') \ ,$$

$$\underline{N}^*(t_f) = \underline{N}^*(t'=0) \equiv \underline{N}^*_f \tag{A8}$$

which is the same equation solved by the forward ORIGEN code, except the data matrix is transposed.

Equation (A7) can be written as

$$\underline{N}^*(t) = \exp\,[\underline{\underline{M}}^T(t_f - t)]\;\underline{N}^*_f\;. \qquad \text{(A9)}$$

It is easy to show that

$$\exp\,(\underline{\underline{A}}^T) = (\exp\,\underline{\underline{A}})^T\;, \qquad \text{(A10)}$$

and therefore

$$\underline{N}^*(t) = \underline{\underline{B}}^T(t_f - t)\underline{N}^*_f \qquad \text{(A11)}$$

It is interesting to note that

$$\begin{aligned} \underline{N}^T(t)\underline{N}^*(t) &= [e^{\underline{\underline{M}}t}\underline{N}_o]^T[e^{\underline{\underline{M}}^T(t_f - t)}\underline{N}^*_f] \\ &= \underline{N}_o^T\;[e^{\underline{\underline{M}}^T(t - t + t_f)}]\;\underline{N}^*_f \\ &= \underline{N}^{*T}_f\;e^{\underline{\underline{M}}t_f}\;\underline{N}_o = \underline{N}^{*T}_f\;\underline{N}_f = R \end{aligned} \qquad \text{(A12)}$$

This result was derived earlier, as a conservation law for the total "value" of the nuclide field.

One of the more puzzling difficulties encountered in providing adjoint capability for the ORIGEN code arose in the treatment of nearly stable (both in decay and in reaction) product nuclides such as $He^4$, $H^2$, etc. When the parent-daughter relation among nuclides is reversed by transposing $\underline{\underline{M}}$, it is possible for nuclides which previously had no daughters to have transmutation products, since their parents are then identified as daughters. The presence of a zero (or very small) transition probability for a nuclide with daughter products causes a series of numerical problems in ORIGEN, the final result being a "divide check."

The solution to this problem is discussed below, for a hypothetical decay chain of three nuclides — A, B, C — the last of which is stable. We assume the appropriate burn-up equations are the following:

$$\begin{bmatrix} -\lambda_A & 0 & 0 \\ \lambda_{AB} & -\lambda_B & 0 \\ 0 & \lambda_{BC} & 0 \end{bmatrix} \begin{bmatrix} N_A \\ N_B \\ N_C \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} N_A \\ N_B \\ N_C \end{bmatrix} \qquad \text{(A13)}$$

The adjoint system is

$$\begin{bmatrix} -\lambda_A & \lambda_{AB} & 0 \\ 0 & -\lambda_B & \lambda_{BC} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} N_A^* \\ N_B^* \\ N_C^* \end{bmatrix} = \frac{-d}{dt} \begin{bmatrix} N_A^* \\ N_B^* \\ N_C^* \end{bmatrix} \qquad \text{(A14)}$$

The equation for $N_C^*$ is

$$\frac{d}{dt} N_C^* = 0 \qquad N_C^* = \text{constant} \qquad \text{(A15)}$$

Therefore $N_C^* = (\underline{h})_C$, where $\underline{h}$ is the input realization vector. Since this value is fixed by the specified final condition, the calculation of stable-nuclide adjoints is omitted from ORIGEN.

Considering Eq. (A14) again, and omitting the equation for $N_C^*$,

$$\begin{bmatrix} -\lambda_A & \lambda_{AB} \\ 0 & -\lambda_B \end{bmatrix} \begin{bmatrix} N_A \\ N_B \end{bmatrix} = \frac{-d}{dt} \begin{bmatrix} N_A \\ N_B \end{bmatrix} - \begin{bmatrix} 0 \\ (\underline{h})_C \lambda_{BC} \end{bmatrix} \qquad \text{(A16)}$$

Thus we see that a stable nuclide can give rise to a fixed source term in the adjoint burn-up equation, depending on the value of $\underline{h}$.

In summary, Eqs. (A7) and (A8) can be incorporated into the ORIGEN to allow adjoint solutions, with four modifications:

a) enter "initial" charge as $\underline{N}_f^*$, the response realization vector,
b) reverse the parent-daughter relationship among nuclides,
c) reverse flux and time arrays,
d) interpret all results backwards in the time variable.

With these modifications, as well as several changes in the numerical methods, the ORIGEN code is called ORIGEN-A, which is presently in use at ORNL.

## APPENDIX B. Origen-A Description

The ancestry of the ORIGEN-A Code goes back several generations. ORIGEN-A is the result of modifications made by M. L. Williams to the ORIGEN-S program soon to be released as part of the SCALE computer code system.[25] O. W. Hermann was the main author of ORIGEN-S, which represented an updated version of the original ORIGEN Code written by M. J. Bell. The most important new features in ORIGEN-S over ORIGEN was the addition of variable dimensioning and of FIDO input[26] capability.

The input to the ORIGEN-A Code is nearly identical to that for ORIGEN-S, except for a few adjoint input parameters. The input description in APPENDIX C was originally written by Hermann for ORIGEN-S, with a description of the required adjoint parameters added for this publication. The new input required for adjoint calculations is marked with an asterisk in the margin.

The modifications made to the ORIGEN-S computer program are listed below:

### B.1. ORIGEN-A: New and Modified Subroutines Added to ORIGEN

| | |
|---|---|
| XNUDATA | - Transposes light element, fission product, and actinide libraries. |
| XORIGEN | - Prints forward or adjoint field by nuclide and time interval<br>- Initializes adjoint arrays<br>- Reverses time and flux print for adjoint calculation<br>- Calls adjoint source routines |
| FLIP | - Reverses the order of 1-D arrays |
| BLADJ | - Sets up base locations for stable-nuclide adjoint source |
| MSBF | - Multiplies portion of adjoint source by flux at each time step |
| ADJSRC | - Constructs stable nuclide source<br>- Deletes stable nuclide data from nuclear data matrix |

## APPENDIX C. ORIGEN-A Code Input (Using FIDO)

The ORIGEN-A Code determines the forward concentrations or the adjoint for elements or isotopes that are present after various time durations. These calculations may consider only the effect of radioactive decay or the effect of irradiation and decay within a given reactor flux.

An interpretation of certain words and phrases used in the input instructions is presented first. Reference to these somewhat arbitrary definitions may enhance some of the explanations in the input description. This description was modified from the original ORIGEN-S input description written by O. W. Hermann for the ORIGEN module of the SCALE code system.

### C.1. Cases and Subcases

The input data for a job may contain stacked "cases" and "subcases" as described here.

A "case" is defined as that part of a job which includes all of the problems solved after starting with both a different nuclear library and new material concentrations, unless the "blending feature" is used. The flag, NG0, is used to specify the type of the next problem. If NG0 = 0, the following problem uses both new concentrations and a different library. If NG0 = 0 and N0BLND = 1 (the flag set for no "blending"), the next problem is the start of a new case.

If a "blending case" is requested (specified by N0BLND > 1), even a problem starting with both new concentrations and a different library can be a subcase of the blended case. A new case starts after NG0 = 0, only if the number of subcases where KBLEND was set positive equals the value of N0BLND.

### C.2. Nuclide or Isotope Identification Number

A six-digit "nuclide" integer is used to identify each isotope, including its isomeric state. This is called a "Nuclide ID No." in the input instructions. The following equation is used:

Nuclide ID No. = IZ * 10000 + IW * 10 + IS where,

IX = the atomic number,
IW = the atomic weight,
IS = 0, for ground state,
IS = 1, for metastable state.
IS > 1, for additional metastable state levels.

## C.3. Main Features of the Code

The code solves problems having the following characteristics or features:

1. An "irradiation" problem is solved using a set of initial nuclide of element concentrations and the "nuclear data library" for a given reactor flux.
2. A "post-irradiation" problem is solved. It may be part of irradiation subcase or a new subcase.
3. A "decay-only" problem is solved, involving no irradiation.
4. A problem is solved using "continuous feed" feature, where the concentrations are enhanced with a continuous rate of feed for given isotopes. This applies to fluid fuel reactors.
5. A problem is solved using "continuous chemical processing" feature, where the concentrations of given elements are depleted by a continuous removal rate through chemical processing.
6. A "continuation" problem may be requested, where an irradiation or decay subcase begins with the concentrations prevailing at any time specified during the last subcase.
7. Either the same or a different "nuclear data library" may be requested in a continuation subcase. This allows for different flux spectra or an "experiment position change" within a reactor.
8. A continuation problem is solved using "batch removal" feature, where given fractions of specified elements are removed through chemical batch processing before calculation continues.
9. A "blending case" is executed, which always will contain several subcases. Different concentrations are used in two or more of the subcases. A given fraction of the material from each of the streams,

or subcases, at specified times are added together to form the initial concentrations for subsequent "blended stream" subcases. While different libraries are permitted, there may not be any variation in the list of nuclides in the libraries. Any number of problems not related to blending may be solved in subcases within the case, if requested.

10. The output tables of results and libraries are completely optional. The answers may be printed in three types of tables pertaining to the "nuclides" of the three different libraries. Tables may be given for results listed only by "elements" of the libraries. Also. summary tables, including both nuclide and element type tables, may be requested. Lines are deleted from the latter tables, if values are below specified cutoffs. Also, the results at alternate time periods are deleted from summary tables. All of the tables may be "optionally printed" for the nonirradiation period in a variety of units pertaining to quantity, activity, heat, or radiation hazard standards. Irradiation period quantity results may be printed in tables listed by either nuclides or elements. Lines for element results below a requested cutoff are suppressed. The output of any of the tables described above may be separately suppressed. Also, a set of several tables of time dependent photon sources and neutron sources may be printed or suppressed.
11. Each of the printed tables for the six library files may be separately suppressed. Also, the library prologue and the list of air and water hazard factors may be omitted. If not required for the case, any of the three libraries may be skipped without changing Job Control Language cards.
12. Various punched-output options are available. Concentrations of all nuclides or totals of a printed output table, in various units, may be punched. Sources which may be punched include: final gamma sources of light elements or fission products, the gamma source at any time period for the three libraries combined, and the alpha-neutron and spontaneous fission neutron sources of the actinides.

13. The total neutron production and absorption and the k-infinity of the heavy elements for each time period may be printed for forward cases.
14. The "line gamma source option" may be requested. This feature produces a data set containing the gamma source for each fission product nuclide at the end of requested time periods. Each source includes the photons per second for every line (energy level) of the nuclide corresponding to data obtained from the ENDF/B-IV Library, Section 457 (or, any later ENDF/B Library). Also, the integrated fission product gamma source intensity is printed for the time periods requested. Not applicable to adjoint calculations.

*15. An adjoint calculation may be requested by setting JOPT (10) = 1. In this case, the printed values correspond to the "importance" of the specified nuclides at the specified times. In most cases, the units for initial charge should be gram-atoms (see $3). Flux (59*) and times (60*) are entered in the same order as in forward case, but the order of "continuation problems" must be reversed. See "Special Instructions for Adjoint Calculation."

### C.4. Estimate of Storage Array Size and Job Region Size

The ORIGEN Code utilizes a technique permitting object-time dimensions, or "flexible dimensions." The user may allocate only the quantity of computer core needed for any specific problem. In order to efficiently use flexible dimensions, an adequate value for the Storage Array Size should be determined. The value used for the Storage Array Size must be supplied as the dimension of the array named "L" and the value of LMAX, which are given in the short FORTRAN MAIN routine in ORIGEN. Then, MAIN is compiled as part of the entire job execution. If a Region Size is required by the computer system being used, it may be found from LMAX and the remaining core and buffer sizes needed by the code.

The following characteristics in the formula for LMAX may be useful:

1. Some of the input parameters used in the formula (e.g., IZMAX) may exceed the necessary dimension size, which is not known exactly the

first time a particular library is requested. This may cause an unavoidable "over-estimate" of LMAX.

2. A few small parameters are deleted from the formula and replaced with additions to the constants. Although this change causes the calculation to be slightly inaccurate, it reduces the length of the formula and assures a safe "over-estimate" of LMAX.
3. The actual sizes needed, during execution, for LMAX and the terms A through H in the formula are printed for each subcase. Proper use of these printed values in later jobs using the same parameters may substantially reduce the length of the formula.
4. The calculation requires use of a maximum value of some of the terms in the formula. This is denoted by MAX(....), similar to FORTRAN. If the short comparison test applying to a term is true, the longer computation for the term is not required. (See A, B, and C)
5. A default value is shown in each equation. It is the result obtained if all parameters used in the equation equal the corresponding default values in the input instructions.
6. Always use the largest value of LMAX calculated for all subcases within the job. Note that the terms A, B, and C are constant for all subcases using the same data library.

LMAX = A + MAX(B,C,H,I) + 100 = 43,860 (default)

A = (ITMAX+LPU)*(9 - 2*MPCTAB) + 3*(IAMAX+LPU) + 2*IZMAX
+ ILMAX + LPU +650 = 15,160 (default)

B = 2*(ITMAX+LPU)*(NREACT+MPCTAB+1) +IFMAX*NFIS0 + 2*IZMAX
+ 8*LPU + 9*NGRP + 100 = 22,200 (default)

or,

B = 0, if 2*(NREACT+MPCTAB) + NFIS0 < 15 + M0UT

C = NENLE*(ILMAX+1) + NENAC+(LAMAX+LPU+2) + NENFP*(IFMAX+1)
+ ITMAX + 200 = 15,270 (default)

or,

C = 0, if MAX(NENLE,NENAC,NENFP) < 20 + M0UT

D = (ITMAX+LPU+3)*(M0UT+8) + MPR0S*(NPR0S+2) + 2*NSHRT
+ 3*NTERM + 100 = 15,750 (default)

E = 2*(ITMAX+LPU), if N0BLND > 1

or,

E = 0, if NOBLND = 1 (default)

F = 2*(IZMAX + 4*LPU) + 8*(ITMAX+LPU) + NTERM = 12,850 (default)

G = (MAX(NENLE,NENAC,NENFP)+8)*(MOUT+2) + MAX(NENLE*ILMAX, NENAC*(IAMAX+LPU),NENFP*IFMAX) = 6,312 (default)

H = D + E +MAX(F,G) = 28,600 (default)

I = ITMAX + NELEM + N1MAX + 2*N2MAX + MOUT

If a Job Region Size is required, it is derived from LMAX. When using the current computer system at ORNL (10-1-74), the following formula may be used:

Region Size = (84 + 4*LMAX/1024)K Bytes

*7. Adjoint calculations require 2,000 additional words for data storage.

## C.5. Data Sets Required and Unit Assignments

The following table gives information concerning data sets needed for Job Control Language. The data sets are referred to by their variable name in the code. If the unit number is defined in the input, the name of the array in which it may be entered is indicated. If the unit number is always set by the code, its value is shown. Also, any other necessary information is given.

Data Set Unit Assignments

| Name | Unit | Function and Comments |
|---|---|---|
| N5 | 5 | All input data cards. |
| N6 | 6 | Printed output giving "FIDO data edit" of array entry lengths for data read prior to processing library. |
| NDUM | 9 | Same as function of N6 for all cards read after processing library. If KOUT = t, the pages printed from unit 9 follow those from unit 6. |
| KOUT | 3$ | Printed output of ORIGEN Code, excluding FIDO data edit. |

Data Set Unit Assignments (Continued)

| Name | Unit | Function and Comments |
|---|---|---|
| NDSET | 3$ | Nuclear Data Library which contains one to six files or data sets, depending on method produced. (See ORNL-4628, Section 3) |
| NDISK | 11 | Unformatted (binary) scratch data set, usually on a disk. Space allocation should accommodate (in bytes) four times the value of "C" in Storage Array Size Formula. BLKSIZE = 1000, usually, is reasonable. Larger values may require an increase in Region Size. |
| NPUN | 56$ | Punched output of ORIGEN Code. If punched cards are not requested (NPUN=0), the data definition card is not needed. |
| NDF | 81$ | ENDF/B Library, needed if using gamma source option (LNGAM = 1 in 81$ Array). |
| *J0PT(11) | 54$ | If J0PT(11) = N, nuclide adjoint or forward concentrations will be written on Logical Unit N. A separate record is written for each time step; each record is "number of nuclides" long. |
| LDSET | 81$ | Unformatted (binary) data set for the gamma sources produced. Need if LNGAM = 1 in 81$ Array. See below for the data set format. |

## C.6. Format of LDSET - The Gamma Source Data Set

A Gamma Source Data Set, written in the binary mode, can be produced in forward calculations. If LNGAM - 1 (see 81$ Array), this data set is requested. The records are described as follows (word length is 4 bytes -- single precision):

Record No. 1 - 20 words.

Copy of the title card (read after Data Block 6) for the first time period in which gamma source is requested.

Record No. 2 - 4 words, all integers except no. (2).

1. Nuclide ID No. of first fission product
2. Sum of the photons/second for the nuclide
3. Number of lines in the nuclide gamma spectrum
4. Number of words is next record, or, twice (3)

Record No. 3 - no. of words = value of word 4, all are floating point.

1. Line energy (MeV) in gamma spectrum
2. Photons/second for line (1) after time period

.

.

.

continued pairs of line energy and gamma decay rate for all lines in gamma spectrum of nuclide.

Record No. 4 - 4 words

Same as Record No. 2 for next fission product nuclide in the ENDF/B file.

Record No. 5

Same as Record No. 3 for Record No. 4 nuclide.

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(Continued for all fission product nuclides in ENDF/B file.)

Last Record (for this time period) - 4 words

Read same as Record No. 2 with all integers except (2).

1. A zero
2. Total photons/second for all the above nuclides
3. A zero
4. A zero

All of the above records are repeated in the same file for all other requested time periods.

## C.7. ORIGEN-A Input Instructions

NOTE: Default values are given in parentheses. (Assume data required unless a condition is specified.)

Data Block 1 - New Case Trigger

0$ - Make 5th entry equal to "NDSET" in 3$
1$ - (1 entry)
NØBLND = 0/1/N job terminator/no blending/N streams blended. (1)
T - terminator

Data Block 2 - New Library

TITLE - Title. Format (20A4)
2* - Required if NØBLND > 1. (NOBLND entries)
  FACT = fraction of each blended stream.
3$ - Library Constants. (33 entries)
  1. NDSET = library unit no. (27)
  2. NØLIB = no. of libraries in NDSET. (4)
  3. NTYPE = 0/1/>1 card image/binary/future type library. (0)
  4. NGRP = 0, if NTYPE = 0 or 1.
     = no. of energy groups in cross sections. (0)
  5. KØUT = printed output unit no. (6)
  6. MPCTAB = 0/1 air, water hazards requested/not requested. (0)
  7. INPT = 0/1 read photon library from NDSET/cards. (0)
  8. IR = 1/0 print transition matrix/do not print. (0)
  9. LPU = 0/1 read all actinide data from NDSET/part from cards. (0)
  10-15. NN1, NN2, NN3, NN4, NN5, NN6:
     NN1 = 1/0 print Ith library table/do not print. (0)
  *16. NN7 = Triger for concentration units in 74* Array (0):
     = 0/1/2/3 units in gram-atoms/wt. ppm/grams/atom ppm. (Make 0 for adjoint calculation)
  17. NN8 = -1, suppress print of library prologue;
     = 0, print wanted. (-1)
  18. ITMAX = total no. of library nuclides. (850)
  19. ILMAX = no. of kind 1 nuclides. (500)
  20. IAMAX = no. of kind 2 nuclides. (120)

21. IFMAX = no. of kind 3 nuclides. (500)
22. IZMAX = no. of off-diagonal matrix elements. (3000)
23. NREACT = max. no. of reactions for any nuclide. (7)
24. NFIS0 = no. of fission isotopes. (5)
25. NELEM = max. atomic no. in calculation. (99)
26. NM0 = month in date of library.
27. NDAY = day in date.
28. NYR = year in date.
29. NENAC = no. of actinide photon energy groups. (18)
30. NENLE = no. of light element photon groups. (12)
31. NENFP = no. of fission product photon groups. (12)
32. NREAD = not used. (0)
33. MREAD = not used. (0)

4* - Library Constants. (4 entries)

1. THERM = ratio of neutron reaction rate of 1/v absorber to thermal neutron flux. (1.0)
2. RES = resonance flux per unit lethargy/thermal flux. (1.0)
3. FAST = ratio of flux > 1 MeV/thermal flux. (1.0)
4. ERR = truncation limit. ($10^{-25}$)

5$ - Library Position Number. (1 entry)

NLIBE = Reactor Library position in NDSET (3):
= 1/2/3/4 for HTGR/LWR/LMFBR/MSBR Reactor (ORNL Library, 10-1-74).

*54$ - Special Options - not required. (12 entries)

(May include 54$ in Data Block 5)

J0PT = triggers to obtain special option

JOPT(I)= N/O request option/not requested. Entry positions (I) trigger the following: (1) compute K-infinity, (2) punch concentrations, (3) punch total gamma sources of Kind 1 and 3, (4) punch alpha-n and spontaneous fission sources, (5) punch combined g gamma source, (6) punch totals of nuclide tables N of each "Kind", (7) punch for element tables N, (10) perform adjoint calculation (11) write results on N.

T - terminator

Data Block 3 - Actinide Nuclide cards required only if LPU  0.

6$ - (LPU entries)

NEWCX = Nuclide ID Nos. of actinides read in by cards.

T - terminator

Extra Card Input: If LPU  0, read LPU cards for cross section data of the NEWCX nuclides.

Data Block 4 - Photon Energy Group Structures. First data array is required, always

35$ - Required. (1 entry).

LFLAG = 0, if default photon energy group structure and U-235 fission photon distribution to be used as given in original ORNL Libraries (10-1-74).
= 1, if any group structures read in this data block.

36* - Optional. (NENAC entries)

EACTGP = Actinide photon energy group structure.

37* - Optional. (NENLE entries)

EGRØUP = Light element photon energy groups.

38* - Optional. (NENAC entries)

SFGAMA = Photons/fission for U-235 in structure of EACTGP.

39* - Optional. (NENFP entries)

EFPGRP = Fission products photon energy groups.

T - terminator

Extra Card input: If INPT - 1, read in entire photon libraries. (fixed format)

Data Block 5 - New subcase with same library

56$ - Subcase Integer Control Constants. (20 entries)

1. MMN = no. of irradiation intervals. (0)
2. MØUT = no. of time intervals in subcase;
= 0, job terminator. (10)
*3. INDEX = 0/1 power read in 58*/read flux in 59*. (0)
(Make 1 for adjoint calculation)
4. NTABLE = 0, any output printed if not suppressed in 65$;
= 1, print summaries of "Class 3", per 65$. (0)

5. MSTAR = time period for CUTOFF, photon sources. (0)
= 0, cut off feature not used, and JT0 - 1 or 4.
6. NG0 = Next problem indicator (0):
= -1, new concentrations and same library;
= 0, new concentrations and library;
= 1, old concentrations and same library;
= 3, old concentrations and new library.
7. MPR0S = 0, for no continuous chemical processing;
= N, for N groups of elements continuously processed. (0)
8. NPR0S = 0, if MPROS = 0;
= N, the max. no. of elements in a process group. (0)
9. MFEED = 0, for no continuous feed;
= N, if N elements are continuously feed. (0)
10. MSUB = 0, for new concentrations (Last NG0 = -1 or 0);
= N, if old concentrations are from time interval N;
= -N, where N means the same, but with batch processing. (0)
11. NTERM = max. no. of exponential expansion terms. (50)
12. NSHRT = max. no. of short-lived precursors in chain. (100)
13. NXCMP = no. of new nuclide or element concentrations. (0)
14. NUNIT = 1/2/3/4/5/6 time (in 60*) in sec./min./hrs./days/yrs./other. (4)
15. NTI = 0, no title cards read at Data Block 6;
= 1, TITLE read;
= 2, BASIS read;
= 3, both are read. (0)
16. NPUN = 0/N no punch/punches concentrations on unit N. (0)
17. JTO = 0, all non-irradiation tables output;
= 1, all output results suppressed;
= 2, may suppress only by 65$ or 66$;
= 3, suppresses all except photon tables;
= 4, suppresses photon tables and by 65$ or 66$. (0)

18. NUC = 0, suppresses "irradiation" nuclide tables;
= 1, suppressed only by 66$. (0)

19. NEL = same as NUC for element tables. (0)

20. KBLEND = -1, if subcase uses total of previous blended streams;
= 0, no blended stream saved or used;
= N, concentrations at time period, N, multiplied times next value of FACT are added as part of blend. (0)

57* - Subcase Floating Point Constants. (5 entries)

1. TM0 = code uses T(1)-TM0 as first interval in calculation. Code sets to 0.0 at start or after NG0 = 0. (0.0)
2. RH0 = total material density (gm./cc.). Needed for tables in units of atoms/barn-cm., if NN7 = 1 or 3. (0.0)
3. CUT = an option for deleting elements in tables under 66$ control. If the concentration in units of 74* is less than CUT for any element, it is deleted. (0.0)
4. FRACPW = (T(MMN) - TM0)/(sum of time of all irradiation subcases). (1.0)
5. TC0NST = If NUNIT = 6, no. of sec. in the special time unit.

T - terminator

Data Block 6 - Subcase Arrays and Titles

TITLE - Subcase Title, if NTI = 1 or 3. Format (20A4)

BASIS - Basis of Calculation, if NTI = 2 or 3. Format (10A4)

58* - Power required if INDEX = 0 and MMN > 0. (MMN entries)

POWER = thermal power in time intervals of 60* (consecutive values or MMNth value cannot be zero.)

59* - Flux required if INDEX = 1 and MMN 0. (MMN entries)

FLUX = thermal flux in neutrons/cm.$^2$-sec., (consecutive values or MMNth value cannot be zero).

60* Printout Times. (M0UT entries)

T = elapsed times since start of case. These are printed. See TM0.

61* - Output Cutoffs - required if MSTAR  0 and summaries in 65$. (7 entries)

CUTOFF = cutoff values for deleting lines from 7 types of summary tables. This is compared with result at time period MSTAR.

62* - Removal Constants - required if MPR0S > 0. (MPR0S entries)

PRATE = group removal constants in continuous chemical processing.

63$ - No. of Elements - required if MPR0S > 0. (MPR0S entries)

N0PR0S = no. of elements being processed in each group.

64$ - Atomic Numbers - required if MPR0S > 0. (entries - MPR0S* NPR0S)

NZPR0S = atomic nos. of all processed elements in sets of entries equal to NPR0S. After the corresponding N0PR0S elements, remaining entries are "0".

65$ Array - Required if [17th] JT0 = 2 or 4. (63 entries)

NT0 = an output suppression array for all "non-irradiation" tables except the photon tables or those already suppressed with [4th] NTABLE = 1 and MPCTAB = 1 (6th entry in 3$ Array):

= 0, suppresses the table (or the two summary tables) denoted by the entry position;

= 1, prints the output for the entry position. (If NN7 = 1 or 3, only the first three entries in the set for of each "Kind" have any effect. Tables controlled by other entries are not printed. If NN7 = 1 or 3, further control of output is specified in 66$ Array.)

There are 84 tables controlled with the 63 entries here. Separate tables are printed for each of the three libraries. They may be listed according to nuclides or elements. The computed quantities may be given in seven different types of units for all time periods or alternate time periods. A convention is used to explicitly explain this method. First the definitions of "Class", "Type", and "Kind" are given. These words are used to show which table corresponds to an entry position.

Class 1 is a table where the list is given by nuclides.

Class 2 is a table where the list is given by elements.

Class 3 are two table summaries of alternate time periods of nuclides and elements. (See [5th] MSTAR and 61* Array.)

Type 1 table values have units of gram-atoms, if NN7 = 0 or 2. (If NN7 = 1 or 3, Type 1 refers to the three units controlled by KW or 66$ Array.)

Type 2 table values have units of grams.

Type 3 table values have units of curies.

Type 4 table values have units of alpha plus beta plus gamma watts of thermal power.

Type 5 table values have units of gamma watts.

Type 6 table values have units of meters of air which dilute to $RCG_a$.

Type 7 table values have units of meters of water which dilute to $RCG_w$.

Kind 1 table nuclides are from Light Element Library.

Kind 2 table nuclides are from Actinide Library.

Kind 3 table nuclides are from Fission Products Library.

The table output is controlled by the position of the entry in 65$ Array as follows:

Entry 1 refers to Class 1, Type 1, Kind 1.
Entry 2 refers to Class 2, Type 1, Kind 1.
Entry 3 refers to Class 3, Type 1, Kind 1.
Entry 4 refers to Class 1, Type 2, Kind 1.
. . . .
. . . .
Entry 21 refers to Class 3, Type 7, Kind 1.
Entry 22 refers to Class 1, Type 1, Kind 2.
. . . .
. . . .

Entry N refers to Class I, Type J, Kind K according to the following:

N = I + (J-1)*3 + (K-1)*21

. . .

Entry 63 refers to Class 3, Type 7, Kind 3.
Or, this follows the Fortran form for NTØ(3, 7, 3):
(((NTØ(CLASS, TYPE, KIND), CLASS=1,3),TYPE=1,7),KIND=1,3).

66$ Array - Required if [1st] MMN   0 and [17th] JTØ = 0, 2, 4.
(12 entries)

KW = "irradiation period" output table control options. If NN7 = 1 or 3 (3$ Array), KW also applies to "non-irradiation" output tables.
= 0, suppresses the table denoted by the entry position;
= 1, prints the tables controlled by the entry position, except that all tables in a "Class" can be suppressed with [18th] NUC = 0, [19th] NEL = 0, or suppression in 65$ data. Also, elements are deleted from tables as specified by CUT in 57* Array. "Type" units must correspond to those denoted by NN7. If NN7 = 0 or 2, tables may be printed in Type 1 units, only. An entry for any other table has no effect. If NN7 = 1 or 3 and using ppm in 74* Array, tables may be printed in units of Types 2, 3 or 4 (defined below) and obtained during both the irradiation or non-irradiation periods. (Note, if NN7 = 0 or 2, the entries control tables during the irradiation period only.) Using terms from above (in 65$ Array), define Class 1 and 2 and Kind 1, 2 and 3 the same. Use new meaning as follows:

Type 1 table values have units of gram-atoms.
Type 2 table values have units of weight ppm.
Type 3 table values have units of atom ppm.
Type 4 table values have units of atoms/(barn-cm).

The tables referred to by the 12 entries positions in 66$ Array are as follows:

Entry 1 refers to Type 1, Kind 1, Class 1 and 2.
Entry 2 refers to Type 2, Kind 1, Class 1 and 2.
Entry 3 refers to Type 3, Kind 1, Class 1 and 2.
Entry 4 refers to Type 4, Kind 1, Class 1 and 2.
Entry 5 refers to Type 1, Kind 2, Class 1 and 2.
Entry 6 refers to Type 2, Kind 2, Class 1 and 2.

. . . .

Entry 12 refers to Type 4, Kind 3, Class 1 and 2.

Note that no Class 1 nor Class 2 tables are printed unless [18th] NUC = 1 or [19th] NEL = 1, respectively.

73$ - ID of Nuclides - required for new case or if last NG0 = -1 or 0. (NXCMP entries)

INUC1 = Nuclide ID No. (if NEX1 - 1, 2, or 3) or Element ID No. (if NEX1 - 4, and IW - 0 in ID no.) for the concentrations in 74*.

74* - Concentrations required with 73$. (NXCMP entries)

XC0M1 = concentrations for nuclides and elements in 73$ in gram-atoms (NN7 = 0), wt. ppm (NN7 = 3).

75$ - Library Kinds - required with 73$. (NXCMP entries)

NEX1 = 1/2/3 where Nuclide ID No. applies to Library "Kind" 1/2/3.
= 4 for element in "Kind" 1 Library.

76$ - ID of Nuclides - required if MFEED > 0. (MFEED entries)

INUC2 = same as INUC1, applied to continuous feed option.

77* - Feed Rates - required if MFEED > 0. (MFEED entries)

XC0M2 continuous feed rates (gram-atoms/sec./fuel unit).

78$ - Library Kind - required if MFEED > 0. (MFEED entries)

NEX2 = same convention as NEX1, applies to 76$

79* = Element Fractions - required if MSUB < 0. (NELEM entries)

FREPR0 = fractions of elements retained in batch chemical processing, where entry position no. - element atomic no.

81$ - Gamma Source Constants - required if LNGAM - 1. ( 6 entries)
1. LNGAM = 1/0 gamma source requested/not requested. (0)
2. LDSET = output gamma source unit no. (15)
3. NDF = ENDF/B unit no. (18)
4. MNDF = 2/1 - ENDF/B mode: card image/binary. (2)
5. N1MAX = max. no. of fl. pt. words in ENDF record. (3000)
6. N2MAX = max. no. of ENDF photon lines. (1000)

82$ - Source Triggers - required if LNGAM - 1. (MOUT entries)
M = 1/0 - in Nth entry, request/no request for gamma source at Nth time period.

T - terminator

IA - Source Title Card for each 84$ Array request.
Format (20A4).

FORMT = Variable Format - required if JOPT(2)   0. Format (20A4).
Requires 3 cards.
= the format used for concentrations punched on cards.

Terminate job with card containing "END" starting in Column 1.

*END OF INPUT INSTRUCTIONS*

## C.8. *SPECIAL INSTRUCTIONS FOR ADJOINT CALCULATIONS

If an adjoint calculation is performed, certain options in the forward sense are not applicable--such as blending streams, batch chemical processing, gamma-source, etc. These options obviously should not be used for adjoint calculations.

Flux should always be specified rather than power (INDEX in 56$) for adjoint calculations. Otherwise ORIGEN will try to calculate the flux from the input power using nuclide adjoints rather than nuclide density, with nonsense results. The order in which the time and flux arrays (59*, 60*) are entered is the same as in the forward case--the code reverses these arrays internally.

The "initial" charge entered in the 73$ and 74* actually corresponds to the response realization vector at the final time of detection (see text).

Consider the following examples:

i) For a response corresponding to "Pu-242 atom density at shutdown", $R = \underline{h}_{Pu^{242}}\,\underline{N}$, and we have

73$$ 942420     74** 1.0

ii) For a response corresponding to "U-238 capture rate at shutdown", $R = (\sigma_c\underline{h})_{U^{238}}\,\phi\,\underline{N}$ ,

we have

73$$ 922380     74** $(\sigma_c)_{U^{238}}\phi(t_f)$

iii) For a response corresponding to "Pu-239/U-238 ratio at shutdown",

$$R = \frac{\underline{h}_{Pu^{239}}\,\underline{N}}{\underline{h}_{U^{238}}\,\underline{N}}$$

we have

73$$ 922380 $^{c}$A2390  74* $\left(\frac{-N_{239}(t_f)}{N_{238}(t_f)} \cdot \frac{1}{N_{238}(t_f)}\right) \left(\frac{N_{239}(t_f)}{N_{238}(t_f)} \cdot \frac{1}{N_{239}(t_f)}\right)$

The order of continuation problems should be reversed in adjoint calculations. For example, suppose that a computation consisted of an initial calculation from t=0 to t=100, and a continuation case from t=100 to t=200. This would be accomplished in the forward case by two calculational steps: in the first, TMO in 57** array is 0.0, and the last entry in the 60** array is 100.0; in the second step, TMO=100.0 and the last 60** entry is 200.0. For the adjoint calculation, the first step has TMO=100.0 and the last 60** entry is 200.0, the second step has TMO=0.0, and the 60** array ends at 100.0.

## C.9. Example Input Description

The following pages present sample input for a forward and adjoint ORIGEN-A calculation. The problem considered is for a fast reactor, operated for 1374 days. The initial change for the forward case is the concentration for a Pu-239 sample with Pu-240, Pu-241, Pu-242, and AM-241 impurities. The charge for the adjoint calculation corresponds to a response of "Am-241 concentration at shutdown."

Note in particular the reversal in the order of the sub-cases for the adjoint calculation. The 59** (flux) and 60** (time) arrays are in the same order for the two calculations.

## Sample Input for Forward Calculation

```
      PRIMARY MODULE ACCESS AND INPUT RECORD ( SCALE DRIVER - MARCH 25,1977 )
MODULE ORIGENS  WILL BE CALLED  TIME OF DAY 21.16.47  DATE 78.031

   0$$  A5  27  E
   1$$  1  T
   NEW VERSION ENDFB-5,ZPPF/EXF FLUX WT'ED
   3$$  A11 1  A16 2  A18 110  -1  107  -1  2000    E
   5$$  3   T
  35$$  0  T
  56$$  10  10  1  0  1  1  A13 5  4  3  A17  2  1   E
  57**  A3 1.0-13    E   T
  P.SAMPLE--IRRAD IN EBR DAYS 0-193
   CHFG FRM J HINES(ANL)-GW PL SAMPLE
  59**  5R1.24+15  5R1.0-25
  60**  315.0  4I25.0  193.0
   73$$  942390 942400 942410 942420 952410
  74**  130.36  6.292  .4485  .026  .111       75$$   F2
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  193.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 193-309
  59**  5R1.15+15  3R1.0-25  .611+15  1.0-25
  60**  3I206.4  2I260.0  290.0  297.0  309.0
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  309.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 309-455
  60**  329.0  349.0  1I351.0  1I372.0  1I424.0  451.0  455.0
  59**  2R1.27+15  1.0-25  2R1.45+15  2R1.0-25  2R.515+15  2.18+15
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  455.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 455-500
  60**  457.0 461.0 480.0 487.0 488.0 492.0 494.0 497.0 498.0 500.0
  59** 1.0-25 .762+15 1.0-25 2.01+15 1.0-25 1.11+15 1.0-25 1.15+15
   1.0-25  1.20+15
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  500.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 500-557
  60**  506.0 513.0 514.0 517.0 520.0 524.0 526.0 538.0 540.0 557.0
  59**  1.0-25 1.45+15 1.0-25 1.57+15 1.0-25 1.89+15 1.0-25 1.24+15
   1.0-25  1.93+15
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  557.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 557-639
  60**  568.0 577.0 581.0 583.0 587.0 594.0 597.0 619.0 624.0 639.0
  59**  1.0-25 1.03+15 1.0-25 .59+15 1.0-25 1.44+15 1.0-25 1.59+15 1.0-25
   2.14+15
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  639.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 639-675
  60**  641.0 645.0 649.0 651.0 655.0 656.0 659.0 664.0 668.0 675.0
  59**  1.0-25 2.04+15 .639+15 1.0-25 .971+15 1.0-25 1.29+15 1.0-25
   1.09+15  1.0-25
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  675.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 675-722
  60**  682.0 683.0 688.0 690.0 698.0 700.0 709.0 710.0 712.0 722.0
  59**  1.12+15 1.0-25 1.38+15 1.0-25 2.29+15 1.0-25 2.26+15 1.0-25
   2.73+15  1.0-25
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  722.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 722-828
  60**  742.0 743.0 749.0 750.0 752.0 753.0 1I758.0  812.0 828.0
  59**  1.82+15 1.0-25 1.77+15 1.0-25 1.53+15 1.0-25 1.91+15 2R1.0-25
   .799+15
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  828.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 828-937
  60**  844.0 853.0 868.0 871.0 889.0 890.0 897.0 905.0 933.0 937.0
  59**  .799+15 1.0-25 1.64+15 1.0-25 1.95+15 1.0-25 1.89+15 1.0-25
   1.83+15  1.0-25
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  937.0        A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 937-1106
  60**  957.0 959.0 968.0 970.0 998.0 1009.0 1027.0 1032.0 1045.0 1106.0
  59**  1.71+15 1.0-25 1.69+15 1.0-25 1.82+15 1.0-25 1.82+15 1.0-25
   1.97+15  1.0-25
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  1106.0       A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 1106-1207
  60**  1131.0 1135.0 1140.0 1149.0 1152.0 1162.0 1181.0 1185.0 1205.0
   1207.0
  59**  1.31+15 1.0-25 1.58+15 1.97+15 1.0-25 1.69+15 2.07+15 1.0-25
   2.05+15  1.0-25
  66$$   4Z  1  22  1    E   T
  56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  1207.0       A3 1.0-13  E   T
  F.SAMPLE--IRRAD IN EBR DAYS 1207-1342
  60**  1212.0 1229.0 1259.0 1267.0 1295.0 1298.0 1317.0 1327.0 1337.0
    1342.0
  59**  1.34+15 1.0-25 1.91+15 1.0-25 2.06+15 1.0-25 2.02+15 1.0-25
   1.92+15  1.0-25
  66$$   4Z  1  22  1    E   T
  56$$   3   3  1  0  1  1  A10 10  A15 1  A17 2  1  E
  57**  1342.0       A3 1.0-13  E   T
  P.SAMPLE--IRRAD IN EBR DAYS 1342-1374
  60**  1356.0 1359.0 1374.0
  59**  1.96+15 1.0-25 2.0+15
  66$$   4Z  1  22  1    E   T
  END

MODULE ORIGENS  IS FINISHED.  USER COMPLETION CODE  0016. CPU TIME USED    22.69 (SECONDS). I/O'S USED    1026
```

## Sample Input for Adjoint Calculation

```
      PRIMARY MODULE ACCESS AND INPUT RECORD ( SCALE DRIVER - MARCH 25,1977 )
MODULE ORIGENS  WILL BE CALLED  TIME OF DAY 11.41.01  DATE 78.025

    0$$  A5  27  E
    1$$  1  T
    ORIGINAL ORIGEN 'FAST' REACT LIB
    3$$  A11 1  A16 0  A18 110  -1  107  -1  2000     E
   54$$   A10 1
    5$$  3   T
   35$$  0  T
   56$$  3  3  1  0  1  1  A13 1  4  3  A17 2  1     E
   57**  1342.0     A3 1.0-13  E   T
     AM 241 ADJOINT FOR EBR EXP,DAYS 1374-1342
    CHRG=1.0 AM241
   60**  1356.0 1359.0 1374.0
   59**  1.96+15 1.0-25 2.0+15
   73$$   952410  74**  1.0   75$$  F2
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10  3  A15 1  A17 2  1  E
   57**  1207.0     A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 1207-1342
   60**  1212.0 1229.0 1259.0 1267.0 1295.0 1298.0 1317.0 1327.0 1337.0
     1342.0
   59**  1.34+15 1.0-25 1.91+15 1.0-25 2.06+15 1.0-25 2.02+15 1.0-25
     1.92+15  1.0-25
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  1106.0     A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 1106-1207
   60**  1131.0 1135.0 1140.0 1149.0 1152.0 1162.0 1181.0 1185.0 1205.0
     1207.0
   59**  1.31+15 1.0-25 1.58+15 1.97+15 1.0-25 1.89+15 2.07+15 1.0-25
     2.05+15  1.0-25
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  937.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 937-1106
   60**  957.0 959.0 968.0 970.0 998.0 1009.0 1027.0 1032.0 1045.0 1106.0
   59**  1.71+15 1.0-25 1.89+15 1.0-25 1.82+15 1.0-25 1.82+15 1.0-25
     1.97+15  1.0-25
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  828.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 828-937
   60**  844.0 853.0 868.0 871.0 889.0 890.0 897.0 905.0 933.0 937.0
   59**  .799+15 1.0-25 1.64+15 1.0-25 1.95+15 1.0-25 1.89+15 1.0-25
     1.83+15  1.0-25
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  722.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 722-828
   60**  742.0 743.0 749.0 750.0 752.0 753.0 11758.0  812.0 828.0
   59**  1.82+15 1.0-25 1.77+15 1.0-25 1.53+15 1.0-25 1.91+15 2R1.0-25
     .799+15
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  675.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 675-722
   60**  682.0 683.0 686.0 690.0 698.0 700.0 709.0 710.0 712.0 722.0
   59**  1.12+15 1.0-25 1.38+15 1.0-25 2.29+15 1.0-25 2.26+15 1.0-25
     2.73+15  1.0-25
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  639.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 639-675
   60**  641.0 645.0 649.0 651.0 655.0 656.0 659.0 664.0 668.0 675.0
   59**  1.0-25 2.04+15 .639+15 1.0-25 .971+15 1.0-25 1.29+15 1.0-25
     1.09+15  1.0-25
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  557.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 557-639
   60**  568.0 577.0 581.0 583.0 587.0 594.0 597.0 619.0 624.0 639.0
   59**  1.0-25 1.03+15 1.0-25 .59+15 1.0-25 1.44+15 1.0-25 1.59+15 1.0-25
     2.14+15
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  500.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 500-557
   60**  506.0 513.0 514.0 517.0 520.0 524.0 526.0 538.0 540.0 557.0
   59**  1.0-25 1.45+15 1.0-25 1.57+15 1.0-25 1.89+15 1.0-25 1.24+15
     1.0-25  1.93+15
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  455.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 455-500
   60**  457.0 461.0 480.0 487.0 488.0 492.0 494.0 497.0 498.0 500.0
   59** 1.0-25 .762+15 1.0-25 2.01+15 1.0-25 1.11+15 1.0-25 1.15+15
     1.0-25  1.20+15
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  309.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 309-455
   60**  329.0  349.0  11351.0  11372.0  11424.0  451.0  455.0
   59**  2R1.27+15  1.0-25  2R1.45+15  2R1.0-25  2R.515+15  2.18+15
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  193.0      A3 1.0-13  E   T
   P.SAMPLE--IRRAD IN EBR DAYS 193-309
   59**  5R1.15+15  3R1.0-25  .611+15  1.0-25
   60**  31206.4  21260.0  290.0  297.0  309.0
   66$$   4Z  1  2Z  1    E   T
   56$$  10  10  1  0  1  1  A10 10  A15 1  A17 2  1  E
   57**  0.0  A3 1.0-13    E   T
   P.SAMPLE--IRRAD IN EBR DAYS 0-193
   59**  5R1.24+15  5R1.0-25
   60**  315.0  4125.0  193.0
   66$$   4Z  1  2Z  1    E   T
   END
MODULE ORIGENS  IS FINISHED.  USER COMPLETION CODE  0016. CPU TIME USED    20.47 (SECONDS). I/O'S USED    1048
```

## C. 10. Job Control Cards for Local Use of ORIGEN-A

```
// EXEC SCALE,PARM.LKED='MAP,LIST,OVLY',REGION=270K
//LKED.SYSPRINT DD DUMMY
//LKED.ORIGEN    DD   DISP=SHR,DSN=CAD10.OWH13884.ORIGENSC
//LKED.OOVLY     DD   DISP=SHR,DSN=CAD10.OWH13884.ORIGOVLY
//LKED.ADJNT DD DISP=SHR,DSN=CAD10.OWH13884.ADJNTX
//LKED.SYSIN DD *
 ENTRY ORIGNS
  INCLUDE ADJNT
 INCLUDE ORIGEN
 ALIAS Q#$004
 INCLUDE OOVLY
 NAME ORIGENS(R)
//GO.FT10F001 DD UNIT=SYSDA,DSN=&&NTGRL,DISP=(NEW,DELETE),
// SPACE=(1000,(40,6),RLSE),
//  DCB=(RECFM=VBS,LRECL=X,BLKSIZE=1000,BUFL=1000)
//GO.FT11F001 DD UNIT=SYSDA,DSN=&&GAMMA,DISP=(NEW,DELETE),
// SPACE=(1000,(40,6),RLSE),                                                   *//
//  DCB=(RECFM=VBS,LRECL=X,BLKSIZE=1000,BUFL=1000)
//GO.FT13F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133,BUFL=150)                  *//
//GO.FT96F001 DD DUMMY,DCB=(RECFM=VBS,BLKSIZE=100,BUFL=100)                    *//
//GO.FT07F001 DD DUMMY,DCB=(RECFM=FB,LRECL=80,BLKSIZE=80)
//GO.FT21F001 DD DISP=SHR,DSN=CAD10.OWH13884.BINRYLWR
//GO.FT22F001 DD DISP=SHR,DSN=CAD10.OWH13884.BINLMFBR
//GO.FT23F001 DD DISP=SHR,DSN=CAD10.OWH13884.BNBIGLWR
//GO.FT24F001 DD DISP=SHR,DSN=CAD10.OWH13884.NEWBNLB1
//GO.FT25F001 DD DISP=SHR,DSN=CAD10.OWH13884.NEWBNLB2
//GO.FT26F001 DD DISP=SHR,DSN=CAD10.OWH13884.NEWBNLB3
//GO.FT27F001 DD DISP=SHR,DSN=CHEMTECH.CWK13992.OLDLITE
//GO.FT27F002 DD DISP=SHR,DSN=CHEMTECH.CWK13992.OLDACT
//GO.FT27F003 DD DISP=SHR,DSN=CHEMTECH.CWK13992.OLDFISS
//GO.FT27F004 DD DISP=SHR,DSN=CHEMTECH.CWK13992.GLITE                          *//
//GO.FT27F005 DD DISP=SHR,DSN=CHEMTECH.CWK13992.GACT                           *//
//GO.FT27F006 DD DISP=SHR,DSN=CHEMTECH.CWK13992.GFISS                          *//
//GO.FT28F001 DD DISP=SHR,DSN=CHEMTECH.CWK13992.LITELIB                        *//
//GO.FT28F002 DD DISP=SHR,DSN=CHEMTECH.CWK13992.ACTINIDE                       *//
//GO.FT28F003 DD UNIT=2314,VOL=SER=CADPK1,DSN=GWM.LMP15316.FISPNEW,            *//
//      DISP=SHR                                                               *//
//*                       NOISSIF.29931KWC.HCETMEHC=NSD,RHS=PSID DD 300F82TF.OG//
//GO.FT28F004 DD DISP=SHR,DSN=CAD10.OWH13884.GLITEDUM
//GO.FT28F005 DD DISP=SHR,DSN=CHEMTECH.CWK13992.GACT                           *//
//GO.FT28F006 DD DISP=SHR,DSN=CAD10.OWH13884.GFISNOBR                          *//
//*                      NOISSIFG.29931KWC.HCETMEHC=NSD,RHS=PSID DD 600F82TF.OG//
//GO.SYSIN DD *
=ORIGENS
```

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