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Informal Report

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SUVIUS:

**A Circulating and Plateout Activity Program for
Gas-Cooled Reactors with
Arbitrary Radioactive Chains**

**los alamos
scientific laboratory**

of the University of California

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Courtney E. Apperson, Jr.

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SUVIUS: A CIRCULATING AND PLATEOUT ACTIVITY PROGRAM
FOR GAS-COOLED REACTORS WITH ARBITRARY RADIOACTIVE CHAINS

by

Courtney E. Apperson, Jr.

ABSTRACT

A time-dependent method for estimating the fuel body, circulating, plateout, and filter inventory of a high temperature gas-cooled reactor (HTGR) during normal operation is discussed. The primary coolant model accounts for the source, buildup, decay, and cleanup of isotopes that are gas borne inside the prestressed concrete reactor vessel (PCRVR). This method has been implemented in the SUVIUS computer program that is described in detail.

1. INTRODUCTION

The primary coolant of an operating High Temperature Gas-Cooled Reactor (HTGR) carries with it a measurable quantity of gaseous and volatile fission products. This results from the diffusion of fission production from the HTGR fuel, which is made up of fissile and fertile fuel particles contained in a graphite matrix.¹ Although intact fuel particles are assumed to be impervious to volatiles and gases, failed fuel particles and small quantities of manufacturing contamination on fuel particles are sources of fission products to the primary coolant. Experimentally, this source of gaseous fission products can be defined in terms of the ratio of the release rate of an isotope to its birth rate in a specific fuel volume.²

The small fraction of nuclides that migrate from the fuel enter the primary coolant stream. The helium coolant is assumed to be a well-mixed gas and therefore the fission gases are homogeneously distributed in the gas volume. Once in the primary coolant, the gaseous fission products behave according to their nuclear and chemical properties.

Several processes compete for the fission gases as they are borne by the primary coolant around the coolant loop. A filter system is present, which removes all fission gases from the withdrawn fraction before returning the helium coolant to the circuit. As the coolant contacts exposed surfaces inside the primary coolant boundary, some fission gases adsorb onto these surfaces at rates which depend on their chemical properties. Radioactive fission gases are also removed from the primary coolant by decay.

Since fission products are present in the coolant of a gas reactor, it is necessary to quantify them for both safety and operational considerations. A reasonable estimate of the steady-state activity and nuclide distribution is essential to properly predict the consequences of a hypothetical release accident. For routine maintenance of contaminated equipment, a reliable estimate of surface activity is needed before maintenance procedures can be prepared. Bench scale experiments are valuable in establishing a basis for predicting these activities. To extend these experimental data to a level at which they are useful in nuclear reactor design, a substantial amount of calculation is required. An analytic algorithm has been developed, described in the body of the report, to do these calculations efficiently.

The SUVIUS computer program utilizes this algorithm to analytically solve the primary coolant model, which will be discussed in detail. Using experimentally defined fuel data, the SUVIUS code can calculate the inventory of an arbitrary radioactive decay chain in the fuel, coolant, filter system, and on plateout surfaces of an HTGR. These calculations can be done in time-dependent mode and for multiple fuel regions.

II. ANALYTIC MODEL

An analytic model of the HTGR primary coolant loop has been developed to evaluate the release of radioactive materials from the core of gas-cooled reactors. Estimates of the partitioning of fission gases between the cleanup system, plateout surfaces, and the helium coolant are obtained from a mathematical model, which accounts for the source, the decay, the cleanup, and the plateout of each nuclide in an arbitrary radioactive decay chain.

A schematic of the HTGR primary containment model on which the SUVIUS code is based is shown in Fig. 1. The system consists of a reactor core as a source of materials produced by fission ($\bar{S}$), a cleanup system that filters the primary

Fig. 1. Schematic SUIVUS model.

coolant with a removal rate of V , and a primary containment. The surfaces inside the primary containment contacted by the primary coolant act as a sink and remove fission products with a plateout removal rate of π . The filter efficiency is assumed at 100% for all nuclides so that clean helium is returned to the coolant loop from the cleanup system. Plateout depends on the chemical properties of the adsorbent surface and the coolant-borne material such that the deposited fraction can vary from 0 to 1.0.

The elements of the vectors $\vec{B}$, $\vec{N}$, $\vec{F}$, and $\vec{P}$ are the inventories of individual species in an arbitrary decay chain in the fuel, primary coolant, cleanup system, and on plateout surfaces.

The source rate, $\vec{S}$, is assumed to be linear in time and is described by Eq. (1). In this model, it is assumed that the removal and plateout rates of the species considered are constant in time.

$$\vec{S} = \vec{S}_0 + t\vec{S}_1. \quad (1)$$

The linear system of equations, based on these definitions, can be solved analytically. This system can readily be displayed in matrix form.

$$\frac{d\vec{X}}{dt} = A\vec{X} + \vec{S}, \quad (2)$$

where

$$\vec{X} = \begin{bmatrix} \vec{B} \\ \vec{N} \\ \vec{F} \\ \vec{P} \end{bmatrix}, \quad (3a)$$

$$\vec{S} = \vec{S}_0 + t \vec{S}_1 = \begin{bmatrix} \vec{s}_0^B + t \vec{s}_1^B \\ \vec{s}_0^N + t \vec{s}_1^N \\ 0 \\ 0 \end{bmatrix}, \text{ and} \quad (3b)$$

$$A = \begin{bmatrix} -\Sigma & 0 & 0 & 0 \\ \Sigma^* & -\Lambda & 0 & -\lambda^* \\ 0 & V & -\bar{\lambda} & 0 \\ 0 & \pi & 0 & -\lambda \end{bmatrix}. \quad (3c)$$

The components of Eqs. (3a) and (3b) have been defined earlier so the transformation to the supervector $\vec{X}$ and $\vec{S}$ is straightforward. The vector $\vec{X}$ is a vector created by combining all four inventory vectors. A similar procedure is followed to define the vector $\vec{S}$. The source to the fuel body, $\vec{s}^B$, and coolant, $\vec{s}^N$, inventories derives from fission product production, as will be discussed in a later section. Each vector element in $\vec{X}$ and $\vec{S}$ has as many elements as there are nuclides in a given chain, n . This implies that these two supervectors each has $4n$ elements.

All of the elements of matrix A , Eq. (3c), are matrices. The coupling of the system of equations is illustrated by this matrix. It should be noted that

A contains an above-diagonal term. This condition, as well as singularities in A, can be treated analytically with the solution technique employed. All of the component matrices of A are $n \times n$ dimensional; therefore, A is a $4n \times 4n$ matrix.

The submatrix $\bar{\lambda}$ of the supermatrix A denotes the decay chain matrix. The negative off-diagonal elements of $\bar{\lambda}$ include the branching effects. This matrix appears as a term in the definition of several of the submatrices. It stands alone as the only removal term in the cleanup equation.

The submatrices V and π are the diagonal cleanup and plateout rate matrices. These matrices define the source from the primary coolant to the cleanup system and the plateout surface equations.

The diagonal elements of the cleanup rate matrix, V, are identical since all nuclides are assumed filtered at 100% efficiency. Based on the assumption that the coolant is a well-mixed gas, the cleanup removal rate elements, V_{ii} , are the ratio of the purification system flow rate to the circulating helium inventory, $\dot{m}_p/M$. The off-diagonal elements are zero.

The diagonal elements of the plateout removal rate matrix, π , are species dependent. The plateout rate depends on the nuclide and on the base material since some nuclides adsorb on a given base material more readily than others. The rate of removal by plateout is concentration dependent and, therefore, the well-mixed gas assumption does not apply. As the gas advances past a surface that is removing a nuclide, the nuclide concentration is dropping and, therefore, the concentration next to the plateout surface is decreasing. This concentration change is only weakly related to the total concentration of a given nuclide. One way around this problem is to define a constant, τ ,³ the average plateout per pass. This constant is defined as the average fraction of material removed from the coolant by plateout during the time required for the coolant to move around the loop once. Experimental data collected during a time period sufficient for numerous traverses of the coolant circuit are used to evaluate this constant.

If it is assumed that the concentration is reduced linearly during the time required for one traverse of the loop, $M/\dot{m}_s$ (M = total circulating helium inventory, $\dot{m}_s$ = primary coolant flow rate), the relationship between concentration and time can be approximated by an exponential (Fig. 2). Assuming, therefore, that plateout is exponential, a plateout removal rate constant can be defined. Based on this assumption, the relationship between the quantity plated out and the plateout rate is defined by the following equations.

$$dN_i = \pi_{ii} N_i(t) dt, \quad (4a)$$

$$\ln \frac{N_i(t + \Delta t)}{N_i(t)} = -\pi_{ii} \Delta t, \text{ and} \quad (4b)$$

$$N_i(t + \Delta t) = N_i(t) e^{-\pi_{ii} \Delta t}. \quad (4c)$$

The elements of the diagonal matrix, π , are determined by fitting the appropriate data, similar to that of Fig. 2, for a given nuclide to an exponential. The matrix element for any nuclide i is therefore given by Eq. (5), where $t = \frac{M}{\dot{m}_s}$ and $N(t + \Delta t) = (1 - \tau)N(t)$.

$$\pi_{ii} = -\frac{\dot{m}_s}{M} \ln(1 - \tau_i). \quad (5)$$

The removal term in the primary coolant equation is the submatrix Λ as given by Eq. (6).

$$\Lambda = \bar{\lambda} + V + \pi + qR. \quad (6)$$

The R matrix in Λ accounts for transmutation reaction, capture, $n-2n$, $n-\alpha$, and $n-p$, which occur when the coolant is exposed to a neutron flux. The scalar quantity, q , in the equation is the ratio of the time the coolant is in a given neutron flux to the total transit time of the circuit.

The remaining right-hand terms, V , $\bar{\lambda}$, and π in Eq. (6) are the cleanup removal rate, the decay chain, and the plateout removal rate matrices and have been discussed earlier in this section. The fission source to the fuel body equation, $\vec{s}^B$, is treated as a source term, so only the removal term for the fuel body equation, Σ , appears in the A matrix. The submatrix Σ is defined by

$$\begin{aligned} \Sigma_{ii} &= \bar{\lambda}_{ii} + R_{ii} \quad \text{and} \\ \Sigma_{ij} &= (\bar{\lambda}_{ij} + R_{ij})(1 - \bar{G}_i), \quad (7) \\ i &\neq j \end{aligned}$$

Where $\bar{G}_i$ is the time-dependent release rate to birth rate ratio averaged over the time interval and the fuel volume for failed and intact fuel particles for nuclide i , λ is the decay chain matrix, and R is the transmutation reaction matrix.

The source to the coolant is the release of fission products from the fuel body. In the supermatrix A , the submatrix Σ^* is the source from the fuel body to the coolant or

$$\Sigma_{ii}^* = 0 \quad \text{and}$$

$$\Sigma_{ij}^* = -(\bar{\lambda}_{ij} + R_{ij})\bar{G}_i. \quad (8)$$

The plateout decay term, λ , expresses the fact that gases do not plate out but return to the coolant stream. This means that there is a feedback term in the primary coolant equation, λ^* . These terms are defined by

$$\lambda = \bar{\lambda} - \lambda^* \quad (9)$$

and

$$\lambda^* = \bar{\delta} \otimes \bar{\lambda}. \quad (10)$$

The operator $\otimes$ is defined to be the Cartesian product. The elements of the matrix $\bar{\delta}$ are defined by

$$\bar{\delta}_{ij} = \mu_i (1 - \delta_{ij}), \quad (11)$$

where μ_i is 1 if nuclide i is a gas and 0 otherwise, and δ_{ij} is the Kronecker delta. At this point, the analytic model has been defined. Only limited definition has been given of the source vector, $\vec{S}$, and of the release fraction, $\vec{G}_{AVG}$. These two vectors will be discussed further in the following sections.

To provide for an internal independent check on the inventories calculated by the above model, the total fission product inventory is also calculated. The equation required corresponds to the system of linear equations given by

$$\frac{d\vec{X}_{TOTAL}}{dt} = -(\bar{\lambda} + R) \vec{X}_{TOTAL} + \vec{S}_{TOTAL}. \quad (12)$$

The vector $\vec{\lambda}_{\text{TOTAL}}$ contains an element for each nuclide in the chain being considered. The source vector $\vec{S}_{\text{TOTAL}}$ contains fission yield information. The matrices $\vec{\lambda}$ and R are the decay and transmutation matrices. The matrix R should be multiplied by a scalar as in Eq. (6) to account for the fact that the total inventory is not always in the neutron flux. However, a large fraction of the total inventory is always in the fuel body, since very little is released to the coolant; therefore, the scalar multiplying factor is very close to 1. This factor has been set equal to 1 for these calculations.

III. FISSION SOURCE

The vector $\vec{S}_{\text{TOTAL}}$ as used in Eq. (12) is the total fission source. The vector $\vec{S}$ [Eqs. (2) and (3b)], is the total fission source partitioned between the fuel body and primary coolant by the release fraction, $\vec{G}(t)$, which is averaged over the core at a given instant in time.

The birth rate of various elements in TRISO and BISO coated fuel particles is given by Eqs. (13) and (14). Variations in fuel loading and the fraction of the total fissions occurring in TRISO and BISO fuel are included.

$$B_{\lambda}^{\text{TRISO}}(t) = \sum_{n=1}^{\text{NR}} \bar{P} \cdot p_n \cdot \epsilon_{\text{TRISO}} \cdot y_{\lambda}^{\text{TRISO}} \cdot f_n(t) \quad (13)$$

and

$$B_{\lambda}^{\text{BISO}}(t) = \sum_{n=1}^{\text{NR}} \bar{P} \cdot p_n \cdot \epsilon_{\text{BISO}} \cdot y_{\lambda}^{\text{BISO}} \cdot (1 - f_n(t)), \quad (14)$$

where

- $\bar{P}$ = average reactor power (watts),
- p_n = power fraction in region n ,
- ϵ_k = fission/(W·s) in fuel type k ,
- y_{λ}^k = fission yield of nuclide λ in fuel type k , and
- $f_n(t)$ = fraction of fissions occurring in TRISO fuel in region n as a function of time.

All of the variables except ϵ_k and $f_n(t)$ are input parameters. The ϵ_k values are set in the subroutine RELEAS and are based on 193-MeV/fis for ^{235}U . The fraction of fissions in TRISO fuel, $f_n(t)$, is defined in the routine INPB by DATA statements. A typical TRISO fission fraction as a function of time, based on a report by Haire and McEachern,⁴ is used in SUVIUS, Fig. 3.

Fig. 2. Determination of plateout removal rate.

Fig. 3. TRISO fission fraction.

The sum of Eqs. (13) and (14) is the total fission source at a given time,

$$\vec{S}_{\text{TOTAL}}(t) = \vec{B}^{\text{TRISO}}(t) + \vec{B}^{\text{BISO}}(t). \quad (15)$$

The vector $\vec{S}$ can be defined in terms of $\vec{S}_{\text{TOTAL}}$,

$$\vec{S}(t) = \begin{bmatrix} \vec{S}^{\text{B}}(t) \\ \vec{S}^{\text{N}}(t) \\ 0 \\ 0 \end{bmatrix}, \quad (16a)$$

where

$$\vec{S}^{\text{B}}(t) = \vec{S}_{\text{TOTAL}}(t) [\vec{1} - \vec{G}(t)], \quad (16b)$$

$$\vec{S}^{\text{N}}(t) = \vec{S}_{\text{TOTAL}}(t) \vec{G}(t),$$

and $\vec{1}$ represents a vector, all of whose elements are unity.

For small time steps τ on an interval $(0, \tau)$, it is assumed that $\vec{S}_{\text{TOTAL}}(t)$ and $\vec{S}(t)$ can be approximated as a linear function of time,

$$\vec{s}(t) = \vec{s}_0 + t\vec{s}_1, \quad (17)$$

where $\vec{s}_0$ is defined to be $\vec{s}(0)$ and $\vec{s}_1$ is defined by Eq. (18),

$$\vec{s}_1 = \frac{\vec{s}(\tau) - \vec{s}(0)}{\tau}. \quad (18)$$

IV. CORE AVERAGE RELEASE FRACTION

The core average release fraction, $\vec{G}(t)$, appears in Eqs. (7) and (8) and in the partitioned source, Eq. (16). The elements of $\vec{G}(t)$ are the weighted average of experimentally measured release fractions for individual fuel rods containing

100% failed or 100% intact fuel particles over the volume of an HTGR core.⁴ The weighting procedure attempts to reflect the space distribution of temperature, fuel failure, and integrated power at a given point in time.

The vector $\vec{G}(t)$ is evaluated by independently summing the release rates and birth rates from the local regions to form the ratio,

$$\vec{G}(t) = \frac{\sum_{n=1}^{NR} \vec{R}_n(t)}{\vec{S}_{TOTAL}(t)}, \quad (19)$$

where

$\vec{S}_{TOTAL}(t)$ = total birth rate defined by Eq. (15) and

$\vec{R}_n(t)$ = local release rate in region n.

The numerator of Eq. (19) is expanded in Eq. (20) for an individual element of $\vec{R}_n(t)$.

$$\begin{aligned} \sum_{n=1}^{NR} R_{in}(t) = \sum_{n=1}^{NR} \left\{ \left[g_{in}^{TF}(T) \cdot B_{in}^T(t) \cdot f_n^T(t) + g_{in}^{BF}(T) \cdot B_{in}^B(t) \cdot f_n^B(t) \right] \right. \\ + \left[g_{in}^{TC}(T) \cdot B_{in}^T(t) + g_{in}^{BC}(T) \cdot B_{in}^B(t) \right] \\ \left. + \left[N_{in}^T(t) \cdot f_n^T(t) + N_{in}^B(t) \cdot f_n^B(t) \right] \right\}, \quad (20) \end{aligned}$$

where

$B_{in}^\alpha(t)$ = birth rate of nuclide i , in region n for fuel type α , $\alpha = T$ (TRISO) or B (BISO), [see Eqs. (13) and (14)].

$g_{in}^\beta(T)$ = temperature-dependent local release fraction, $\beta = T$ (TRISO failed (TF), BISO failed (BF), TRISO intact (TC), and BISO intact (BC) for nuclide i .

$f_n^\alpha(t)$ = time-dependent failure fraction in region n for fuel type α , $\alpha =$ T(TRISO) or B(BISO).

$f_n^{\sim\alpha}$ = time-dependent failure fraction rate in region n for fuel type α , $\alpha =$ T(TRISO) or B(BISO).

$N_{\lambda n}^\alpha$ = time-dependent inventory of nuclide λ in region n in intact particle type α , $\alpha =$ T(TRISO) or B(BISO).

The first term on the right-hand side of Eq. (20) accounts for the release from failed TRISO and BISO particles. Birth rate factors were developed in detail earlier [see Eqs. (13) and (14)]. The failure fraction is based on one of three fuel failure models, which will be discussed in Section V. Evaluation of the local release factor is derived from experimental data for a fuel compact with 100% failed fuel and is referenced to the total BISO or TRISO birth rate.

Intact particle release is handled by the second term on the right-hand side of Eq. (20). The birth rate terms are the same as before. Experimental data for a fuel compact with 100% intact fuel is used to establish the local release fraction, which is referenced to the total BISO or TRISO birth rate. Since it is assumed that volatiles and gases do not escape an intact particle, the only release in this situation comes from contamination outside of the particles which was accumulated during manufacture.

The final term in Eq. (20) estimates the instantaneous release from an intact particle when it fails. Long-lived fission products build up in a fuel kernel. The radioactive fission gases accumulate in the particle until they reach an equilibrium with their production rate, and the stable fission gases accumulate proportionally with their birth rate. For the short-lived fission gases, the particle inventory is essentially constant for intact and failed kernels since their diffusion rate out of the kernel is much less than their decay rate. The burst of fission gas released upon particle failure can account for a large fraction of the net release to the primary coolant for long-lived and stable nuclides, when integrated over the time required to release the held-up fission product gases.

For a collection of particles assumed to be intact, the inventory available for release at failure is given by

$$\frac{d\vec{N}^\alpha}{dt} = -(\vec{\lambda} + R) \vec{N}^\alpha + \vec{P}^\alpha, \quad (21)$$

where

$\vec{N}^\alpha$ = inventory vector for intact particles of type α , $\alpha = T(\text{TRISO})$ or $B(\text{BISO})$,

$\vec{\lambda}$ = decay chain matrix,

R = transmutation matrix, and

$\vec{P}^\alpha$ = constant source from the kernel to the buffer coating for particles of type α , $\alpha = T(\text{TRISO})$ or $B(\text{BISO})$.

The source is given by

$$\vec{P}^\alpha = g^\alpha(T) \cdot \vec{B}^\alpha(t_f), \quad (22)$$

where

$g^\alpha(T)$ = temperature-dependent release fraction in particle type α ,

$\alpha = T(\text{TRISO})$ or $B(\text{BISO})$ and

$\vec{B}^\alpha(t_f)$ = birth rate in particle type α with an age of t_f .

It is assumed that the release fraction from the kernel to the coating is approximately equal to the release fraction of a failed particle. This assumption is valid since the kernel offers the greatest resistance to the release of fission gases in particles with failed coatings.

The solution to Eq. (21) for an initial inventory, $\vec{N}^\alpha(0)$, in a fresh particle of zero is

$$\vec{N}^\alpha(t) = -(A^{-1}) \left[I - e^{A(t)} \right] \vec{P}^\alpha, \quad (23)$$

where

$$A = -(\vec{\lambda} + R). \quad (24)$$

There is essentially a continuous release due to the burst effect since a small fraction of particles fail in any given time interval. If we consider some of the particles used in Eq. (21) to be failed, the inventory held up in the intact TRISO or BISO particles is

$$N_{in}^{\alpha}(t) = \left[1 - f_n^{\alpha}(t) \right] N_{in}^{\alpha}(t) , \quad (25)$$

where

$N_{in}^{\alpha}(t)$ = time-dependent intact particle inventory of nuclide i in local region n in particle type α , $\alpha = T(\text{TRISO})$ or $B(\text{BISO})$,

f_n^{α} = time-dependent failure fraction in local region n for particle type α , and

$N_{in}^{\alpha}(t)$ = time-dependent total particle inventory of nuclide i in local region n in particle type α , $\alpha = T(\text{TRISO})$ or $B(\text{BISO})$.

The time rate of change of the retained particle inventory is given by

$$\frac{dN_{in}^{\alpha}(t)}{dt} = \left[1 - f_n^{\alpha}(t) \right] \frac{dN_{in}^{\alpha}(t)}{dt} - N_{in}^{\alpha}(t) \frac{df_n^{\alpha}(t)}{dt} . \quad (26)$$

The first term on the right-hand side in Eq. (25) accounts for the inventory variation in the intact particles due to changes in failed fraction and production. This term is included in the first and second terms of Eq. (20). The last term accounts for the inventory loss brought about by the failure of particles at the given instant in time.

By substituting Eqs. (22) and (23) into the last term of Eq. (25), the burst release, $R_{in}^{\alpha P}(t)$, from a local region is obtained by

$$R_{in}^{\alpha P}(t) = N_{in}^{\alpha}(t) \frac{df_n^{\alpha}(t)}{dt} . \quad (27)$$

These terms appear in Eq. (20). At this point, the vector $\vec{G}(t)$ has been defined with the exception of the local release fractions, $g_i^\alpha(t)$.

It has been stated that $g_i^\alpha(t)$ is experimentally measured, based on the fuel rods or compacts. For calculational purposes, the local release fraction for rods is converted to an equivalent sphere. This transformation is valid if it is assumed that the fuel rod matrix and the fuel block graphite offer minimal resistance to fission gas release.

The release rate from a spherical particle is just the product of the flux of a given nuclide across the particle boundary and the surface area of the particle. This is divided by the birth rate within the same volume to give the release fraction. A solution to this problem has been published⁵ for a single homogeneous material neglecting precursor effects, and the result is repeated here.

$$g_i(t) = 3\sqrt{\frac{D_i'}{\lambda_i}} \left(\coth \sqrt{\frac{\lambda_i}{D_i'}} \cdot \sqrt{\frac{D_i'}{\lambda_i}} \right) - 6e^{-\lambda_i t} \sum_{n=1}^{\infty} \frac{e^{-(n^2 \pi^2 D_i' t)}}{n^2 \pi^2 + \frac{\lambda_i}{D_i'}}. \quad (28)$$

The solution for $\lambda = 0$ is given by⁵

$$g_i(t) = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{e^{-(n^2 \pi^2 D_i' t)}}{n^2}. \quad (29)$$

In Eqs. (28) and (29), λ_i is the decay constant of the nuclide of interest and D_i' is an effective diffusion coefficient, D_i/a^2 , (D = diffusion coefficient and a = effective particle radius), for nuclide i .

The diffusion coefficients have been fitted to an Arrhenius relation above a threshold temperature.⁶ From the graphical data available an empirical relation can be developed.

$$D_i'(T) = D_i'(\text{REF}) \left(\sqrt{\frac{D_i'(0)}{D_i'(\text{REF})}} + \left(1 - \sqrt{\frac{D_i'(0)}{D_i'(\text{REF})}} \right) \exp \left(\frac{Q}{Rg} \left(\frac{1}{T_{\text{REF}}} - \frac{1}{T} \right) \right) \right), \quad (30)$$

where

Q = activation energy (kcal/mole),

R_g = gas constant (1.987 cal/mole-K), and

$D_{\chi}^*(T)$ = effective diffusion coefficient at temperature T in K
($0 = 0$ K, REF = Reference temperature).

V. FUEL FAILURE MODELS

The HTGR fuel particles are expected to experience a small degree of failure during operation. The onset of failure is statistical in nature due to fabrication uncertainties of the large number of particles in the system. For a given collection of fuel particles at a given temperature, a predictable fraction of the collection is assumed to be failed after irradiation for any selected time.

Three fuel failure models are incorporated in the SUVIUS code. These models allow the circulating activity to be calculated for a fuel environment like that of the Fort St. Vrain reactor, the GASSAR reactor, or the General Atomic Company 3000-MW(t) reactor most probable fuel failure model.

The analytic fits for the first two models were developed in connection with work of Carruthers and Lee on the LARC-1 code.⁷ For completeness, the analytic fits are repeated for these two failure models in Tables I and II.⁷ The TRISO and BISO failure as a function of time for a single fuel region for these models is illustrated in Figs. 4 to 7.

The third fuel failure model is based on information reported by Shenoy and McEachern⁸ for the first seven years of operation of a 3000-MW(t) HTGR. The total TRISO and BISO failure fraction as a function of time for each of four regions was determined by summing the reported results for failure due to amoeba effect, pressure vessel effect, and manufacturing defects, Figs. 8 and 9. It is generally accepted that years 3 through 7 represent a near equilibrium period. Upon this assumption, the four regions were averaged over years 3 to 7 using volume fraction weighting. The TRISO and BISO fractions generated by this procedure as a function of time have been taken to be the most probable TRISO and BISO failure model for an average fuel region, Figs. 10 and 11. Analytic fits were obtained for these models using a spline fit to the data in Table III.

TABLE I
FORT ST. VRAIN FUEL FAILURE MODEL

$$0 \leq t \leq 0.15 \text{ y}$$

$$f = A + BT$$

TYPE	A	B
TRISO	-13.2725	7.14286
BISO	-13.2725	7.14286

$$0.15 \text{ y} \leq t \leq 4 \text{ y}$$

$$f = \frac{T(t) - T_0(t)}{T_1(t) - T_0(t)}$$

where

$$T_i(t) = \frac{\ln(t) - \ln(\alpha_i)}{\beta_i} = \left(\frac{1}{\beta_i} \right) \ln(t/\alpha_i)$$

TYPE	$\alpha_i(K)$	$\beta_i(y^{-1})$	$\alpha_1(K)$	$\beta_1(y^{-1})$
TRISO	5.07494×10^3	-5.61267×10^{-3}	4.80245×10^7	-9.8012×10^{-3}
BISO	3.13835×10^4	-6.5932×10^{-3}	2.075834×10^6	-8.2291×10^{-3}

TABLE II
GASSAR FUEL FAILURE MODEL

TRISO FUEL

$$f \leq f_0$$

$$f(t) = \alpha e^{BT}$$

$$f > f_0$$

$$f(T) = A + BT$$

GASSAR TRISO FAILED FRACTION PARAMETERS

Age (yr)	$\Delta T(K)$	$10^3 \alpha$	$10^3 \beta(K)^{-1}$	ΔT	A	$10^2 \beta(K)^{-1}$
1	<1941.15	1.57		1941.15 < T < 2273.15	5.8361	0.300732
2	<1894.15	0.99966	0.915323	1894.15 < T < 2273.15	4.9638	0.262359
3	<1888.15	1.2240	1.08109	1888.15 < T < 2273.15	4.8593	0.257762
4	<1873.15	1.17176	1.19064	1873.15 < T < 2273.15	4.6209	0.24728

(TABLE II cont)

BISO FUEL

$$f \leq f_o$$

SPLINE FIT

$$f > f_o$$

$$f(T) = A + BT$$

Age = 1 yr		2 yr		3 yr		4 yr	
f	T(K)	f	T(K)	f	T(K)	f	T(K)
0.00179	T<2073.15	0.00377	T<2073.15	0.00526	T<1690.15	0.00718	T<1673.15
0.282	2143.15	0.282	2143.15	0.0059	1743.15	0.0079	1697.15
1.0	2273.15	1.0	2273.15	0.0071	1793.15	0.010	1733.15
				0.0116	1873.15	0.021	1793.15
				0.0185	1917.15	0.0557	1853.15
				0.046	1973.15	0.10	1893.15
				0.057	2000.0	0.222	1973.15
				0.0815*	2073.15	0.4039*	2073.15
				0.10	2083.15	0.649	2153.15
				0.23	2113.15	1.0	2273.15
				1.0	2273.15		

* Linear fit above this fraction and temperature, spline fit below.

GASSAR BISO FAILED FRACTION PARAMETERS

Age (yr)	f_o	A	$10^3 B(K)^{-1}$
1	0.00179	-10.3454	4.99105
2	0.00377	-10.3229	4.98115
3	0.0815	- 9.4394	4.5925
4	0.4039	- 5.7751	2.9805

TABLE III
3000-MW (C) MOST PROBABLE FAILURE MODEL

TRISO

Time (Years)	Failed Fraction
0.0	0.0
0.5	4.856×10^{-4}
1.0	1.05×10^{-3}
1.5	1.775×10^{-3}
2.0	2.675×10^{-3}
2.5	3.676×10^{-3}
3.0	4.7×10^{-3}
3.5	5.727×10^{-3}
4.0	6.76×10^{-3}

RIISO

Time (Years)	Failed Fraction
0.0	0.0
0.2	1.62×10^{-4}
0.4	3.365×10^{-4}
0.7	6.3×10^{-4}
0.8	7.422×10^{-4}
0.9	8.570×10^{-4}
2.0	2.128×10^{-3}
3.0	3.284×10^{-3}
4.0	4.440×10^{-3}

Fig. 4. Fort St. Vrain TRISO failure model.

Fig. 5. Fort St. Vrain BISO failure model.

Fig. 6. GASSAR TRISO failure model.

Fig. 7. GASSAR BISO failure model.

Fig. 8. 3000-MW(t) most probable TRISO failure by region.

Fig. 9. 3000-MW(t) most probable BISO failure by region.

Fig. 10. 3000-MW(t) most probable TRISO failure model.

Fig. 11. 3000-MW(t) most probable BISO failure model.

VI. SOLUTION OF THE ANALYTIC MODEL

The matrix equations, Eqs. (2) and (12), describing the analytic model incorporated in the SUIVUS code, have the form

$$\frac{d\vec{X}}{dt} = \vec{S}(t) + A(t) \vec{X}(t). \quad (31)$$

This equation has been solved and evaluated by Lee⁹ using the Volterra Calculus¹⁰ and matrix operator techniques for the special case that the matrix $A(t)$ is constant in a time interval (t_0, t) ,

$$\vec{X}(t) = e^{A(t-t_0)} \vec{X}(t_0) + e^{A(t-t_0)} \int_{t_0}^t d\tau e^{-A(\tau-t_0)} \vec{S}(\tau). \quad (32)$$

When the linear source term, Eq. (1), is submitted for the time-dependent source in Eq. (32), the solution form required by SUIVUS is obtained by

$$\begin{aligned} \vec{X}(t) = & e^{A(t-t_0)} \vec{X}(t_0) - (A^{-1}) \left(I - e^{A(t-t_0)} \right) \vec{S}_0 \\ & + \left(-(A^{-1})t - (A^{-2}) \right) + \left((A^{-1})t_0 + A^{-2} \right) e^{A(t-t_0)} \vec{S}_1. \end{aligned} \quad (33)$$

The restraint that A must be constant is less stringent computationally than the time step control required by the assumption of a linear time-dependent source arising from the birth rate equations.

Although the matrix operator $e^{A(t-t_0)}$ can be explicitly evaluated by a uniformly convergent series, it can become a lengthy process due to the large number of terms which must be kept to obtain reasonable significance. This difficulty is avoided by defining two new matrix operators^{9,11} for which recursion relations have been developed that are utilized in an algorithm.

$$e^{A\tau} = \sum_{n=0}^{\infty} \frac{(A\tau)^n}{n!}. \quad (34)$$

$$D(A\tau) = (A\tau)^{-1} (e^{A\tau} - I) = \sum_{n=0}^{\infty} \frac{(A\tau)^n}{(n+1)!}. \quad (35)$$

$$Z(A\tau) = (A\tau)^{-1} (D(A\tau) - I) = \sum_{n=0}^{\infty} \frac{(A\tau)^n}{(n+2)!} \quad (36)$$

These operators exist even if A is singular.

Substitution of these operators, Eqs. (35) and (36), into Eq. (33) presents the SUVIUS solution in the simplified form that is implemented in the code.

$$\begin{aligned} \vec{x}(t) = & \left[I + A(t-t_0) D(A(t-t_0)) \right] \vec{x}(t_0) + (t-t_0) D(A(t-t_0)) \vec{S}_0 \\ & + (t-t_0)^2 Z(A(t-t_0)) \vec{S}_1 \quad (37) \end{aligned}$$

The recursion relations necessary for the evaluation of $D(A\tau)$ and $Z(A\tau)$ are discussed in Appendix A.

VII. PROGRAM STRUCTURE

A. Role and Function of Subroutines

The SUVIUS program consists of a driver routine, SUVIUS, and thirty-three functions and subroutines. The functions and subroutines can be divided into three classifications: primary, secondary, and graphic. The primary routines are those which are called directly by the controlling routine and perform major tasks. The secondary routines are utility routines called by the primary subroutines that do vector and matrix operations and function evaluation. The graphic routines are available for the generation of plots on 35-mm film. A complete listing of the code is given in Appendix B.

1. Primary Routines. The nine primary routines are discussed in the order in which they are called by SUVIUS.

a. INPA. The subroutine INPA reads and prints the basic nuclear data used in constructing the decay chains. The input is stored locally so that it is readily available for subsequently called routines.

b. INPB. The subroutine INPB reads and prints the problem-dependent and graphic data. The graphic input is handled in such a manner that the graphics package can be deleted without necessitating changes in this routine.

c. RELEAS. The source terms to the fuel and coolant are evaluated in the subroutine RELEAS. This routine evaluates the birth rate and release rate in the fuel using release fraction, fuel failure fraction, and fissions fractional partition between TRISO and BISO fuel of the

estimates obtained from secondary routines (RBCAL, FRAC10, and FRACB0).

d. MAKEA. The decay matrices for the system and the total inventory are assembled in the routine MAKEA for both the operating and shutdown conditions. The input to this routine is derived from INPA and RELEAS.

e. SOLVER. The subroutine SOLVER operates on the matrices generated by MAKEA to calculate the three matrix operators: $D(A\tau)$, $I + A\tau D(A)$, and $Z(A\tau)$. The recursion relations discussed in Appendix A are part of this routine.

f. ESOLVE. The subroutine ESOLVE uses the operators calculated in SOLVER and the source and inventory vectors to calculate the new inventories for the specified time interval. The routine RELEAS, MAKEA, SOLVER, and ESOLVE are evaluated for each time interval specified by INPB.

g. PREP. Upon completion of the calculation for all time intervals, the subroutine PREP prepares the results for display. The calculated results are converted from atoms into curies for radioactive nuclides and into grams for stable nuclides.

h. PAPER and TERM. The results of the SUVIUS calculations are printed by either the subroutine PAPER or TERM. The subroutine PAPER provides a detailed presentation of the results for each time interval in atoms and in curies or grams. The subroutine TERM produces an abbreviated listing for each time interval in atoms. TERM is intended for use when the code is run in the interactive mode.

2. Secondary Routines. There are sixteen secondary routines in SUVIUS.

These routines do utility operations such as vector and matrix operations, sorts, and function evaluation.

a. The general mathematic routines are listed below.

AVG	-	Averages two scalar values
DOTPRO ¹²	-	Evaluates the inner product of two vectors
GENID ¹²	-	Generates an identity matrix
IFACT	-	Evaluates factorials
MATMOV ¹²	-	Equivalences two matrices
MATMPY ¹²	-	Multiplies combinations of vectors and matrices
SCALAR	-	Multiplies a matrix by a scalar
SPL1D1 ¹³	-	Evaluates coefficients for a spline interpolation
SPL1D2 ¹³	-	Evaluates spline interpolation

- b. There are three routines used to estimate fuel behavior.
 - FRACBO - Estimates BISO fuel failure fraction
 - FRACTO - Estimates TRISO fuel failure fraction
 - RBCAL - Estimates the failed and intact release fraction for BISO and TRISO fuel
- c. The SUVIUS utility routines are given.
 - PRIM - Prints a matrix
 - PRIV - Prints a vector
 - QQSORT¹² - Sorts a table into ascending order
 - SEARCH¹² - Searches a monotonic table for a given value

3. Graphics. The graphic routines generate 35-mm film output in the form of plots of the calculated results for the last year in the problem. Since graphics packages do not readily transfer between computer centers, these routines can be deleted without affecting the remainder of the code. Use is made of system routines available at LASL, some of which are not listed.

- DRAW - Controls the plotting of time-dependent results
- PLOPB¹² - Produces plots under the control of DRAW
- DLNLNT¹² - Draws linear-linear tick marks on a grid
- DLNLGT¹² - Draws linear-logarithmic tick marks on a grid
- SBLG¹² - Scales logarithmically on plot
- SBLN¹² - Scales linearly on top or bottom of plot
- SLLN¹² - Scales linearly on left of plot
- SRLN¹² - Scales linearly on right of plot

B. Program Flow

The flow of the SUVIUS program is illustrated by Fig. 12. The name of the primary subroutine involved in a given step is given in all capitals.

C. SUVIUS Input Instructions

The SUVIUS input is contained in fourteen cards, which are divided into five sets. The first set consists of card 0, which establishes the print and restart options. The second set consists of cards 1 and 2 and defines the nuclear decay chains. Cards 3 and 4 compose the third card set, which contains the multigroup cross-section data. The fourth set, cards 5 to 12, defines the physical makeup of the system being evaluated. The last set contains the graphic data.

The specific data for the five sets are detailed in Table IV. The user should note that if words 3 and/or 4 of card 1A are negative, one or two

Fig. 12. SUVIUS program flow.

TABLE IV
SDV105 INPUT INSTRUCTIONS

<u>CARD</u>	<u>WORD</u>	<u>FORMAT</u>	<u>SYMBOL</u>	<u>DESCRIPTION</u>
0	1	I4	NSKIP	0/1 unabridged/abridged output
	2	I4	STRIP	0/1 initial/restart problem
	3	I4	KX	number of neutron energy groups
1A	1	A6	NANMAT(I,1)	Alphanumeric nuclide name
	2	I4	NANMAT(I,2)	ID number
	3	I4	NANMAT(I,3)	Decay parent No. 1, negative if branching ratio involved
	4	I4	NANMAT(I,4)	Decay parent No. 2, negative if branching ratio involved
	5	I4	NANMAT(I,5)	Capture parent No. 1
	6	I4	NANMAT(I,6)	Capture parent No. 2
	7	I4	NANMAT(I,7)	n - 2 n parent
	8	I4	NANMAT(I,8)	n - α parent
	9	I4	NANMAT(I,9)	n - p parent
	10	E12.5	ANMAT(I,1)	Nuclear decay constant (s^{-1})
	11	E12.5	ANMAT(I,2)	Plateout rate constant (s^{-1})
	12	E12.5	ANMAT(I,3)	^{235}U fission yield
	13	E12.5	ANMAT(I,4)	^{233}U fission yield
	14	E12.5	ANMAT(I,5)	D' failure fuel, $D' = \frac{D}{a^2}$
	15	E12.5	ANMAT(I,6)	D' intact fuel, $D' = \frac{D}{a^2}$
	16	E12.5	ANMAT(I,7)	Activation energy (kcal/mole)
	17	E12.5	ANMAT(I,8)	ratio of g(0) to g (ref)
	18	E12.5	ANMAT(I,9)	Mass (g)
2	1	E12.5	BRV(M)	Branching ratio associated with first negative decay parent, if applicable
2	1	E12.5	BRV(M+1)	Branching ratio associated with second negative decay parent, if applicable

TABLE IV
(cont)

CARD	WORD	FORMAT	SYMBOL	DESCRIPTION
Blank	A blank card must follow the last pair of cards 1 and 2.			
3	1	A6	NXSEC(11,1)	cross section title No. 1
	2	A6	NXSEC(11,2)	cross section title No. 2
	3	I4	NXSEC(11,3)	number of groups
4	1	E12.5	XSEC(11,EX,1)	microscopic σ_f cross sections (cm ²)
	2	E12.5	XSEC(11,EX,2)	microscopic σ_{2n} cross section (cm ²)
	3	E12.5	XSEC(11,EX,3)	microscopic σ_a cross section (cm ²)
	4	E12.5	XSEC(11,KX,4)	microscopic σ_p cross section (cm ²)
Blank	A blank card must follow the last set of KX cross sections.			
5	1	I12	NR	number of core regions
	2	I12	MFUEL	Fuel Model MFUEL-1 GA-A-12462 MFUEL-2 GA-A-13200 MFUEL-3 GA-A-12985
	3	E12.5	PAVG	Average reactor power (watts)
	4	E12.5	LAMDAP	Purification rate constant (s ⁻¹)
	5	E12.5	PIF	Power fraction in region No. 1
6	.	.	.	.
	.	.	.	.
	.	.	.	.
	NR	E12.5	PIF(NR)	Power fraction in region No. NR.

TABLE IV
(cont)

CARD	WORD	FORMAT	SYMBOL	DESCRIPTION
7	1	E12.5	VFRAC(NR)	Volume fraction of region No. 1
	.	.	.	.
	.	.	.	.
	.	.	.	.
	NR	E12.5	VFRAC(NR)	Volume fraction of region No. NR
<hr/>				
8	1	E12.5	TEMP1(1)	Temperature in region No. 1 (K)
	.	.	.	.
	.	.	.	.
	.	.	.	.
	NR	NR	TEMP1(NR)	Temperature in region No. NR (K)
<hr/>				
9	1	E12.5	AGE(1)	Age of region No. 1 at beginning of calculation (d)
	.	.	.	.
	.	.	.	.
	.	.	.	.
	NR	E12.5	AGE(NR)	Age of region No. NR at beginning of calculation (d)
<hr/>				
10	1	E12.5	PHI(K,1)	Group K flux in region No. 1 $\frac{\text{neutrons}}{\text{cm}^2\text{-s}}$
	.	.	.	.
	.	.	.	.
	.	.	.	.
	NR	E12.5	PHI(K,NR)	Group K flux in region No. NR $\frac{\text{neutrons}}{\text{cm}^2\text{-s}}$

Supply one card per group if KX > 0

TABLE IV
(cont)

<u>CARD</u>	<u>WORD</u>	<u>FORMAT</u>	<u>SYMBOL</u>	<u>DESCRIPTION</u>
11	1	E12.5	TINT	Time at beginning of calculation (yr)
	2	E12.5	TINC	Number of time steps per year
	3	E12.5	TIMAX	Full power days per year (d)
	4	E12.5	TIDNC	Number of time steps per refueling period
	5	E12.5	TIDN	Refuel time (d)
	6	I4	IYR	Number of years in calculation
	7	I4	ITP	Punt frequency during a year
	8	I4	IPLT	Number of plots
<hr/>				
12A	1	E12.5	TOTIC(1)	Initial inventory of nuclide 1 in system (atoms)
	.	.	.	.
	.	.	.	.
	.	.	.	.
	I	E12.5	TOTIC(I)	Initial inventory of nuclide I in system (atoms)
12B	1	E12.5	XNIC(1)	Initial inventory of nuclide 1 in fuel (atoms)
	.	.	.	.
	.	.	.	.
	.	.	.	.
	I	E12.5	XNIC(I)	Initial inventory of nuclide I in fuel (atoms)

TABLE IV
(cont)

<u>CARD</u>	<u>WORD</u>	<u>FORMAT</u>	<u>SYMBOL</u>	<u>DESCRIPTION</u>
12C	1	E12.5	XNIC(I+1)	Initial inventory of nuclide 1 in coolant (atoms)
	.	.	.	.
	.	.	.	.
	.	.	.	.
	I	E12.5	XNIC(I+I)	Initial inventory of nuclide I in coolant (atoms)
12D	1	E12.5	XNIC(2I+1)	Initial inventory of nuclide 1 in filter (atoms)
	.	.	.	.
	.	.	.	.
	.	.	.	.
	I	E12.5	XNIC(2I+I)	Initial inventory of nuclide I in filter (atoms)
12E	1	E12.5	XNIC(3I)	Initial inventory of nuclide 1 on plateout surfaces(atoms)
	.	.	.	.
	.	.	.	.
	.	.	.	.
	I	E12.5	XNIC(3I+I)	Initial inventory of nuclide I on plateout surfaces (atoms)

Cards 12 are present only if TINT > 0.

TABLE IV
(cont)

<u>CARD</u>	<u>WORD</u>	<u>FORMAT</u>	<u>SYMBOL</u>	<u>DESCRIPTION</u>
13	1	I4	IGRAPH(N,1)	Number of curves on plot N
	2	I4	IGRAPH(N,2)	Type of plot (see below)
	3	I4	IGRAPH(N,3)	ID of nuclide for first curve on plot N
	4	I4	IGRAPH(N,4)	ID of nuclide for second curve on plot N
	5	I4	IGRAPH(N,5)	ID of nuclide for third curve on plot N
	6	I4	IGRAPH(N,6)	ID of nuclide for fourth curve on plot N

IPLT cards are required

Note: Possible values for IGRAPH(N,2)

INVENTORY

<u>PLOT TYPE</u>	<u>ATOMS</u>	<u>CURIES</u>
TOTAL	11	21
FUEL BODY	12	22
COOLANT	13	23
FILTER	14	24
PLATEOUT	15	25

branching ratio cards, card 2, must follow card 1B before the next card 1A. It should also be noted that cards 2 and 3 and cards 4 and 5 are separated by a blank card.

Upon completion of a run the code creates a file, TAPE1, which contains the data necessary to restart the problem at the beginning of the final year of a given calculation. To utilize this file for restarting, word 2 of card 0 should be set to 1 and cards 5 through 12E in the original data deck must be replaced with the new card image file, TAPE 1.

D. Machine Requirements

The SUVIUS code requires special 35-mm film hardware for graphics. The code is structured to avoid the use of LCM.

SUVIUS was designed to operate on the CDC 7600 under the CROS operating system,¹⁴ which was developed at Los Alamos using the CDC RUN compiler. The code is also operational on the CDC 6600 under the NOS operating system.¹⁵

The SUVIUS code less the graphics package also runs under the LTSS operating system¹⁶ on the CDC 7600 using the FTN compiler.

E. Algorithm Validation

The main solution routine, SOLVER, has undergone extensive testing against analytic solutions to validate the algorithm used in the evaluation of D(C) and Z(C).¹¹ The routines which perform algebraic and matrix operations have also been tested to verify their accuracy.

VIII. SUVIUS TEST PROBLEM

As an illustration of the SUVIUS program, the output from a four-nuclide sample problem is presented, Appendix D. The card image input for this test problem is listed in Appendix C. Although the results may be realistic, they are not intended to be used in a comparison with other published results. These results are solely for demonstration purposes.

The decay chain used to construct the SUVIUS sample problem is illustrated in Fig. 13.¹⁷ The physical data used to generate the card image input are presented in Table V. There are four regions in the problem, the reactor thermal power is 3000 MW(t), and the purification rate is $4.27 \times 10^{-5} \text{ s}^{-1}$.

The problem was run for five years at a capacity factor of 0.80 with an annual refueling period of 30 days.

TABLE V
SAMPLE PROBLEM DATA

NUCLIDE	DECAY CONSTANT s^{-1}	Fission Yield		Plate- out Rate (s^{-1})	σ_n, σ (cm^2)	Diffusion Parameter in Fuel at 1100°C (s^{-1})		$g(0)/g(1100)$
		^{235}U	^{233}U			Failed	Intact	
^{135}I	2.924×10^{-5}	.0633	.0486	0.100	~0	2.02×10^{-10}	3.94×10^{-16}	0.210
^{135m}Xe	7.55×10^{-4}	.00161	.00798	0.0	~0	2.02×10^{-10}	3.94×10^{-16}	0.210
^{135}Xe	2.100×10^{-5}	9.31×10^{-4}	5.39×10^{-3}	0.0	2.64×10^{-18}	2.02×10^{-10}	3.94×10^{-16}	0.210
^{136}Xe	0.0	.0627	.0679	0.0	0.0	2.02×10^{-10}	3.94×10^{-16}	0.210

REGION	1	2	3	4
Power fraction	0.18	0.21	0.27	0.33
Volume fraction	0.269	0.244	0.244	0.244
Temperature (K)	1163	1163	1163	1163
Flux (cm^{-2} -sec)	1.0×10^{13}	1.0×10^{13}	1.0×10^{13}	1.0×10^{13}
Age at beginning of problem (d)	0.0	0.0	0.0	0.0

Fig. 13. Sample problem decay chain.

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APPENDIX A

MATRIX OPERATOR RECURSION RELATIONS

The recursion relations for Eqs. (35) and (36) of the text are repeated here without proof. References 9 and 10 discuss the proof by induction of these relations.

The matrix operators $D(C)$ and $Z(C)$ are defined by

$$D(C) = C^{-1}(e^C - I) = \sum_{n=0}^{\infty} \frac{C^n}{(n+1)!} \quad (A-1)$$

and

$$Z(C) = C^{-1}[D(C) - I] = \sum_{n=0}^{\infty} \frac{C^n}{(n+2)!} \quad (A-2)$$

To evaluate these operators, the matrix C is scaled so that the eigenvalues are bounded by $1/2$.

$$H = 2^{-p}C, \quad (A-3)$$

where p is chosen so that $||H|| < 1/2$.

The matrix operators $D(H)$ and $Z(H)$ are approximated by a finite number of terms, M .

$$D(H) \approx \sum_{n=0}^M \frac{H^n}{(n+1)!} . \quad (A-4)$$

$$Z(H) \approx \sum_{n=0}^M \frac{H^n}{(n+2)!} . \quad (A-5)$$

The error in the excluded terms, ϵ , is determined by the value of M ,⁹

$$\frac{1}{2^{M+1}(M+2)} < \epsilon . \quad (A-6)$$

Recurring upward by a power of two in H , $D(C)$ and $Z(C)$ can be evaluated from $D(H)$ and $Z(H)$.

$$D\left(2^{P+1}H\right) = D\left(2^PH\right) \left[I + 1/2 \left(2^PH\right) D\left(2^PH\right) \right] . \quad (A-7)$$

$$Z\left(2^{P+1}H\right) = 1/2 Z\left(2^PH\right) + 1/4 \left[D\left(2^PH\right) \right]^2 . \quad (A-8)$$

APPENDIX B

SUVIUS CODE LISTING (LASL Code LP # 0145)

A microfiche of the SUVIUS code listing is contained in the envelope inside the back cover.

APPENDIX C

The input for the SUVIUS sample problem is given in Figure C-1.

```

      1  0  1
I 135  1  0  0  0  0  0  0  0  2.924 E-05  0.100
6.33336E-02 4.85851E-02 2.02 E-10 3.94 E-15 10800.0 0.210
      135.0
XE135M 2 -1  0  0  0  0  0  0  7.55 E-04  0.0
1.61409E-03 7.93462E-03 2.02 E-10 3.94 E-16 10800.0 0.210
      135.0
      0.147
XE 135  3 -1  2  0  0  0  0  2.100 E-05  0.0
9.31095E-04 5.38956E-03 2.02 E-10 3.94 E-16 10800.0 0.210
      135.0
      0.853
XE 136  4  0  0  3  0  0  0  0.0  0.0
6.27185E-02 6.79339E-02 2.02 E-10 3.94 E-16 10800.0 0.210
      136.0

XE 135      1  3
2.64 E-18      0.0      0.0      0.0

      4      3  3.0 E+09 4.27 E-05
      .18      .21      .27      .33
      .269      .244      .244      .244
      1163.0      1163.0      1163.0      1163.0
      0.0      0.0      0.0      0.0
1.0 E+13 1.0 E+13 1.0 E+13 1.0 E+13
      0.0      16.0      292.2      1.0
30.0 5 1 10

4 11 1 2 3 4
4 21 1 2 3 4
4 12 1 2 3 4
4 22 1 2 3 4
4 13 1 2 3 4
4 23 1 2 3 4
4 14 1 2 3 4
4 24 1 2 3 4
1 15 1
1 25 1

```

Fig. C-1. SUVIUS input.

APPENDIX D

A microfiche of the output generated by the sample data of Appendix C is located in the envelope inside the back cover. Graphic output generated by the same problem is in Figs. D-1 through D-10.

Fig. D-1. Total inventory (curies).

Fig. D-3. Fuel inventory (curies).

Fig. D-2. Total inventory (atoms).

Fig. D-4. Fuel inventory (atoms).

Fig. D-5. Coolant inventory (curies).

Fig. D-7. Coolant trap inventory (curies).

Fig. D-6. Coolant inventory (atoms).

Fig. D-8. Coolant trap inventory (atoms).

Fig. D-9. Plateout inventory (curies).

Fig. D-10. Plateout inventory (atoms).