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Reactivity feedback mechanisms in aqueous fissile solutions

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**REACTIVITY FEEDBACK MECHANISMS IN AQUEOUS
FISSILE SOLUTIONS**

by

Drew Edward Kornreich

A Thesis Submitted to the Faculty of the
DEPARTMENT OF NUCLEAR AND ENERGY ENGINEERING

In Partial Fulfillment of the Requirements

For the Degree of

MASTER OF SCIENCE
WITH A MAJOR IN NUCLEAR ENGINEERING

In the Graduate College
THE UNIVERSITY OF ARIZONA

1992

STATEMENT BY THE AUTHOR

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APPROVAL BY THESIS DIRECTOR

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David L. Hetrick
Dr. David L. Hetrick
Professor of Nuclear Engineering

29 May 1992
Date

to Mom, Dad, and Brad

the love and support of a true family can never be measured

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ABSTRACT

Solutions of fissile materials are often encountered during spent-fuel reprocessing. In order to estimate the hazards from accidental criticalities in these solutions, models have been developed to understand better the dynamics involved. Accurate representation of reactivity feedback mechanisms are a crucial part of such models.

Reactivity feedback from uniform volumetric solution expansion is studied. For faster transients, density redistribution may also occur due to a variation of nuclear energy as a function of position in the assembly. Neutronic spectral temperature reactivity effects are studied using two methods: cross section corrections via a Maxwellian flux weighting and creation of temperature dependent cross sections from ENDF/B-VI data.

The volumetric and temperature reactivity feedback coefficients are determined for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* solution assemblies. Spectral temperature coefficients are also calculated for poisoned, unpoisoned, and reflected plutonium solutions. Feedback coefficients are seen to be functions of geometry and isotopic contents of the assemblies. Results for plutonium solutions agree with British calculations reported in 1991, confirming the possibility of autocatalytic excursions in large, dilute solutions.

CHAPTER 1

INTRODUCTION

When nuclear fuel materials from power or production reactors are reprocessed, the reprocessing means are almost invariably chemical separation techniques. The fuel, which is usually in oxide form (e.g. UO_2), is first dissolved with some type of acid, such as nitric, sulfuric, or hydrofluoric acid. This results in the fuel being in an aqueous solution form. The presence of fissile isotopes and water in these solutions immediately leads to concerns regarding accidental criticalities with the solutions. When transported through pipes and stored in vessels, different geometric configurations may also affect the multiplicative state of these fissile solutions.

Several experiments have been conducted with fissile solutions. The United States first began significant aqueous fissile solution studies with the *KEWB* set of experiments (Kinetic Experiments on Water Boilers) (Dunenfeld and Stitt, 1963). *KEWB* examined uranium sulfate solutions in both spherical and cylindrical geometries. The study also considered the effects of various reflectors on the systems' dynamics. The *KEWB-5* experiment examined cylindrical geometry with no reflector. The French have conducted experiments in two assemblies: *CRAC* and *SILENE*. The *CRAC* series of experiments (Consequences Radiologiques d'un Accident de Criticité) (Lécorché and Seale, 1973) investigated a wide range of uranium concentrations in uranyl nitrate solutions, in 300 and 800 mm. diameter tanks. The series included both critical experiments and multiple pulse experiments. *SILENE*, (Barbry) which is still operational, also uses uranyl nitrate, but at a lower concentration. It is a burst assembly and can be used for dose measurements and calibrations.

Since the *KEWB* experiments were discontinued in the early 1960's, the United States did very little with supercritical experiments on fissile solutions until the early 1980's when the Department of Energy funded construction of the *SHEBA* (Solution High-Energy Burst Assembly) critical assembly at Los Alamos National Laboratory. *SHEBA* used uranyl fluoride at low enrichment and was intended for dosimetry and criticality alarm measurements. The system is presently being modified for use in a new vessel which has a slightly larger diameter, but will use the same uranyl fluoride solution. The modified system will be able to perform super-prompt critical bursts.

The four previously mentioned solution assemblies studied uranium solutions. Plutonium solutions are also of interest, especially since they are frequently encountered in reprocessing fuel for defense purposes in the United States and for commercial purposes overseas. Critical experiments have been performed on plutonium solutions at the Hanford site (Lloyd, et al., 1972), as well as in France (Paxton and Pruvost, 1987). The French studied the effects of various reflectors on the plutonium solutions' criticality. However, to date, there has been very little study of plutonium solutions in supercritical states.

Accidents have been postulated regarding low concentration plutonium at nuclear waste disposal sites (Stratton, 1983). Given a concentration of plutonium in the soil and a sudden moderator input (such as rain), the possibility for a supercritical excursion was investigated. There have also been several criticality accidents involving both plutonium and uranium solutions, one of which resulted in a fatality at Los Alamos Scientific Laboratory (Stratton, 1967). In order to understand better the situations which lead to such accidents (which should lead to a better understanding of how to avoid accidents) dynamic models of fissile solution excursions have been developed.

Fissile solution excursions are modelled for both neutron power dynamics and system pressure using point reactor kinetics and quasi-static thermodynamic equations of

state, energy, and momentum. In solutions with highly-enriched uranium, reactivity feedback occurs primarily from volumetric expansion. This assembly volumetric expansion may occur as a result of temperature-related expansion or through the evolution of radiolytic gas bubbles. This does not include the effect of spectral neutron temperature feedback. In general, the form of the feedback reactivity is

$$\rho_f(t) = \alpha \Delta T(t) + \phi \Delta V(t) , \quad (1-1)$$

where α is the spectral neutron temperature coefficient ($^{\circ}\text{C}^{-1}$), ϕ is the volumetric feedback coefficient (m^3/m^3), and T and V are the system temperature and volume, respectively. In general, the neutron temperature feedback is necessary for studying plutonium solutions and low enrichment and concentration uranium solutions.

The volumetric feedback coefficient ϕ in Equation 1-1 was obtained for each assembly by matching the modelled and the experimental peak powers. Values for temperature feedback coefficients were assumed or treated as variable parameters when needed. This study examines, in part, the volumetric feedback coefficients for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* solution assemblies in order to evaluate and better understand their magnitudes and relations between the four assemblies. This portion of the study includes the effects of a uniform volumetric expansion and the effects of solution density redistribution within the vessel. Also, recent calculations indicate that low concentration plutonium solutions may exhibit positive temperature coefficients (Suzaki, et al., 1987; Mather, et al., 1991a,b). This study also investigates temperature coefficients for both the uranium solution systems and hypothetical plutonium solutions.

Several computer codes are used to model these systems. Reactivity feedback coefficients are obtained by comparing the absolute reactivity of a reference state with those of geometrically or neutronicallly perturbed states. Generally, effective multiplications are

determined using a discrete ordinates transport code. Temperature dependent cross sections are obtained by correcting available cross sections via a Maxwellian flux distribution and by creating new cross section sets from the latest version of the Evaluated Nuclear Data File (ENDF/B-VI). By calculating and examining these reactivity feedback coefficients, a better understanding of these mechanism will be offered.

CHAPTER 2

VOLUMETRIC EXPANSION REACTIVITY FEEDBACK

In all nuclear systems, a temperature increase will cause materials in the core (fuel, coolant, etc.) to expand. This expansion reduces atomic number densities, thereby also reducing macroscopic cross sections. This may increase neutron leakage, which results in a decrease of the core's neutron population. Such a phenomenon is a negative reactivity feedback mechanism. In solutions of fissile material, this is a primary reactivity feedback. Reactivity feedbacks from volumetric expansion are determined such that the source of the expansion is non-specified. Expansion may occur due to thermal expansion or the appearance of small radiolytic gas bubbles.

2.1 Flux, Energy, and Density Distribution Functions

Using solutions of the diffusion equation in two-dimensional cylindrical geometry, a flux profile is obtained in terms of a cosine and a Bessel function of the first kind, as seen in Equation 2-1. The radius and height are measured from the assembly's center.

$$\phi(r,z) = \phi_0 \cos\left(\frac{\pi z}{H+2\delta z}\right) J_0\left(\frac{2.405r}{R+\delta r}\right) \quad (2-1)$$

In this treatment, δr and δz are the extrapolation distances in the radial and axial directions respectively, R and H are the radius and total height of fissile solution, and ϕ_0 is the central flux, usually determined by the assembly's power level. Given the above flux distribution, it may then be assumed that the nuclear energy is deposited in the solution in a similar fashion. For a nuclear system on a positive period $1/\omega$,

$$\phi(r,z,t) = \frac{\partial}{\partial t} E(r,z,t) ; \quad (2-2a)$$

$$\phi(r,z,t) = \phi_0 \cos\left(\frac{\phi z}{H+2\delta z}\right) J_0\left(\frac{2.405r}{R+\delta r}\right) e^{\omega t} ; \quad (2-2b)$$

$$E(r,z,t) = \frac{\phi_0}{\omega} \cos\left(\frac{\pi z}{H+2\delta z}\right) J_0\left(\frac{2.405r}{R+\delta r}\right) e^{\omega t} . \quad (2-2c)$$

When the energy is deposited, it serves to expand the solution, thereby decreasing the overall density. However, because the energy is not deposited uniformly (which must be assumed in a point-reactor kinetics model) the density change is also non-uniform. Therefore, there will be a functional form for the density change in a form similar to Equations 2-1 and 2-2. Where the energy deposition is high, there will be a large density decrease/large solution expansion, which tends to push the solution away. Clearly this occurs at the center of the assembly. During a slow transient, the solution is pushed out from the center slightly faster than the outer edges of the assembly expand, creating a sort of mixing current. This causes the entire core to expand (solution height to increase) in almost a uniform fashion (see Figure 2-1).

In the fissile solution experiments, the transients of interest are generally super-prompt critical. Time scales are very short (typically 10^{-2} to 10^{-3} sec). During such transients, the solution expands extremely quickly outward from the center. Even though the outer edges are also expanding, the sudden "input" of mass from the center causes the density at the outer edges to increase (see Figure 2-2). Effectively, the solution can not "get out of its own way". The solution height also increases, as the total mass of the system must remain constant, and the average density correspondingly decreases. When the solution moves out from the center, it is removed from the area of highest reactivity worth to one of lower worth. This tends to slow a power rise, giving rise to a negative

Figure 2-1. Schematic comparison of a critical fissile solution, the solution after it has expanded uniformly, and after the density has redistributed.

Figure 2-2. Density redistribution during a fast transient. Shading darkens outward from the center indicating denser regions.

reactivity feedback coefficient associated with solution expansion. Moving the fuel to the edges may also produce a *decrease* in neutron leaking, providing a positive reactivity effect. However, the decrease in density at the center should be more important than the decrease in leakage, providing a negative coefficient overall. In order to gain a better understanding of leakage properties, the effects of radial-only and axial-only leakage are also studied.

It may now be assumed that the solution density is distributed about the original density according to three separate distributions:

$$\delta\rho(r,z) = A \left[C_{1t} - \cos\left(\frac{\pi z}{H+2\delta z}\right) J_0\left(\frac{2.405r}{R+\delta r}\right) \right]; \quad (2-3a)$$

$$\delta\rho(r) = A \left[C_{1r} - J_0\left(\frac{2.405r}{R+\delta r}\right) \right]; \quad (2-3b)$$

$$\delta\rho(z) = A \left[C_{1z} - \cos\left(\frac{\pi z}{H+2\delta z}\right) \right]. \quad (2-3c)$$

In each of these cases, $\delta\rho(\mathbf{r})$ is the density change at any point $\mathbf{r}$ in the assembly, A is the peak-to-trough (total) density change amplitude, and $C_{1(i)}$ is a constant which is determined via conservation of mass constraints.

Equation 2-3a is the most interesting as it contains a density variation throughout the entire assembly, where Equations 2-3b and 2-3c are rather artificial density distributions. These two assume that the density varies in only one direction (axial or radial). They are used to obtain an understanding of the effects on radial and axial leakage. When the density is only axially distributed, there will be minor changes in the radial leakage while the axial leakage will decrease.

2.2 Solution Expansion for Critical Assemblies

As previously noted, C_{1t} is a constant to be determined under the constraint of conservation of mass, or

$$\int_V \delta\rho(r,z) dV = 0 . \quad (2-4)$$

This simply says that all density variations must sum to zero over the entire volume--no mass may be lost. C_{1t} may be derived for the total geometric redistribution case by inserting Equation 2-3a into

$$\int_{-H/2}^{H/2} dz \int_0^R dr 2\pi r \delta\rho(r,z) = 0 , \quad (2-5a)$$

which gives

$$C_{1t} \int_{-H/2}^{H/2} dz \int_0^R dr 2\pi r - 2\pi \int_{-H/2}^{H/2} \cos\left(\frac{\pi z}{H+2\delta z}\right) dz \int_0^R r J_0\left(\frac{2.405r}{R+\delta r}\right) dr = 0 . \quad (2-5b)$$

Performing the integrations shown yields

$$C_{1t} \pi R^2 H - 2 (H+2\delta z) \left[2\sin\left(\frac{\pi H}{2(H+2\delta z)}\right) \right] \left[\frac{(R+\delta r)R}{2.405} J_1\left(\frac{2.405R}{R+\delta r}\right) \right] = 0 , \quad (2-5c)$$

which finally produces the expression for C_{1t} :

$$C_{1t} = \frac{4 (H+2\delta z) (R+\delta r) R}{2.405 \pi R^2 H} \sin\left(\frac{\pi H}{2(H+2\delta z)}\right) J_1\left(\frac{2.405R}{R+\delta r}\right) . \quad (2-6)$$

For the cases of axial or radial density redistribution only, the values for each respective $C_{1(i)}$ may be determined in similar fashions using Equations 2-3b and 2-3c appropriately. Such derivations result in:

$$C_{1r} = \frac{2 (R + \delta r)}{2.405 R} J_1 \left(\frac{2.405 R}{R + \delta r} \right); \quad (2-7)$$

$$C_{1z} = \frac{2 (H + 2 \delta z)}{\pi H} \sin \left(\frac{\pi H}{2(H + 2 \delta z)} \right). \quad (2-8)$$

The primary goal is not only to obtain a value for density redistribution feedback in solution assemblies, but also to compare such feedback values with those given by a uniform density decrease (coupled with an associated increase in solution height). To this end, the average density for each redistributed case is given by the uniformly expanded density, which may be determined from

$$\frac{\rho_u}{\rho_o} = \frac{V_o}{V_u} = \frac{H_o}{H_u}, \quad (2-9)$$

where ρ_u is the uniformly distributed density, and ρ_o is the initial (reference) density. Each case's density is distributed such that

$$\rho(r, z) = \rho_u + \delta \rho(r, z), \quad (2-10)$$

where the solution height is the same as the uniform density decrease case. Integrating Equation 2-10 over the expanded volume and appropriately using Equation 2-4 (conservation of mass) will yield the expression

$$\frac{1}{V} \int_V \rho(r, z) dV = \rho_u. \quad (2-11)$$

The density is distributed uniformly throughout the volume for several cases, determined by the new height, H_u . This requires a uniform reduction in all densities to a fraction, H_o/H_u , of the original density. Again, this is simply a statement of mass conservation (see Equation 2-9):

$$\rho_u = \rho_o \frac{H_o}{H_u} . \quad (2-12)$$

With the uniform case as a reference point, the distributed density may then be analyzed. Again, this method provides a study of the effect of density redistribution *plus* uniform expansion. The term "plus" is used because this is the ultimate effect created. The volumetric average density in the cases of distributed densities is ρ_u , which effectively says that the system first uniformly expands, and then the density distributes within the volume. The amplitude of the redistributed density is determined according to

$$\frac{\Delta V}{V} = \frac{\Delta H}{H} = \frac{\Delta \delta \rho}{\rho} = \frac{A}{\rho} . \quad (2-13)$$

Equation 2-13 states that the density distribution's amplitude is directly proportional to the fractional change in volume, which is directly proportional to the total amount of nuclear energy deposited in the system. The higher the energy input, the higher the volume change and the larger the density distribution amplitude will be. This holds for both thermal expansion and radiolytic gas production; where there is more energy deposition, there is also more expansion or gas production.

Analyzing these cases requires useful input for appropriate computer codes. To this end, Equation 2-3a is discretized with the constraint that

$$\delta \rho_{i(t)} V_i = \int_{V_i} \delta \rho(r,z) dV , \quad (2-14)$$

in order to simulate a functional variance in density (also note the subscript (t) to denote that this is the total density redistribution case). The cylinder is split into N_z equally spaced intervals in the axial (z) direction, and the radial portion is divided into N_r intervals of equal area (see Figure 2-3). Inserting the expression for $\delta \rho(r,z)$ into Equation 2-14 yields

$$\delta\rho_{i(t)} V_i = A \int_{h_{i-1}}^{h_i} dz \int_{r_{i-1}}^{r_i} dr 2\pi r \left[C_{1t} - \cos\left(\frac{\pi z}{H+2\delta z}\right) J_0\left(\frac{2.405r}{R+\delta r}\right) \right]. \quad (2-14a)$$

Figure 2-3. Axial and radial mesh format for density redistribution in cylindrical geometry.

Performing the indicated integrals in Equation 2-14a and noting that

$$V_i = \pi (r_i^2 - r_{i-1}^2) (h_i - h_{i-1}) = \frac{\pi R^2 H}{N_z N_r} \quad (2-15)$$

results in the following equation for the variation in density in the i^{th} region:

$$\delta\rho_{i(t)} = A \left\{ C_{1t} - \frac{2 N_z N_r (H+2\delta z) (R+\delta r)}{2.405 \pi R^2 H} \left[\sin\left(\frac{\pi h_i}{H+2\delta z}\right) - \sin\left(\frac{\pi h_{i-1}}{H+2\delta z}\right) \right] \times \right. \\ \left. \left[r_i J_1\left(\frac{2.405r_i}{R+\delta r}\right) - r_{i-1} J_1\left(\frac{2.405r_{i-1}}{R+\delta r}\right) \right] \right\}. \quad (2-16)$$

Again, performing the same calculation for the axial only and radial only redistribution cases, one obtains

$$\delta\rho_{i(r)} = A \left\{ C_{1r} - \frac{2 N_r (R+\delta r)}{2.405 R^2} \left[r_i J_1\left(\frac{2.405r_i}{R+\delta r}\right) - r_{i-1} J_1\left(\frac{2.405r_{i-1}}{R+\delta r}\right) \right] \right\}; \quad (2-17)$$

$$\delta\rho_{i(z)} = A \left\{ C_{1z} - \frac{N_z (H+2\delta z)}{\pi H} \left[\sin\left(\frac{\pi h_i}{H+2\delta z}\right) - \sin\left(\frac{\pi h_{i-1}}{H+2\delta z}\right) \right] \right\}. \quad (2-18)$$

2.3 Solution Expansion for Assemblies with a Central Thimble

In the above analysis, the limits of integration for the radial coordinate were $(0,R)$. These limits must be altered when considering the *SILENE* and *SHEBA* critical assemblies, as they each have a central control/burst rod shaft. In these cases, the limits are changed to (R_i, R_o) (see Figure 2-4). This introduces a small error in the assumed flux/energy shape (Equations 2-2b and 2-2c) as there is no fissile material in the central shaft. However, the assumed flux shape is a means to obtaining the density redistribution function, and any effects of the new form should be very minor. When the limits are changed, the values for C_{1t} and $\delta\rho_{i(t)}$ are

$$C_{1t} = \frac{4 (H+2\delta z) (R+\delta r)}{2.405 \pi (R_o^2 - R_i^2) H} \sin\left(\frac{\pi H}{2(H+2\delta z)}\right) \times \left[R_o J_1\left(\frac{2.405 R_o}{R+\delta r}\right) - R_i J_1\left(\frac{2.405 R_i}{R+\delta r}\right) \right], \quad (2-19)$$

and with the new value for each volume element,

$$V_i = \pi (r_i^2 - r_{i-1}^2) (h_i - h_{i-1}) = \frac{\pi (R_o^2 - R_i^2) H}{N_z N_r}, \quad (2-20)$$

the new value for the i^{th} volume element's density variation is

$$\delta\rho_{i(t)} = A \left\{ C_{1t} - \frac{2 N_z N_r (H+2\delta z) (R+\delta r)}{2.405 \pi (R_o^2 - R_i^2) H} \left[\sin\left(\frac{\pi h_i}{H+2\delta z}\right) - \sin\left(\frac{\pi h_{i-1}}{H+2\delta z}\right) \right] \times \left[r_i J_1\left(\frac{2.405 r_i}{R+\delta r}\right) - r_{i-1} J_1\left(\frac{2.405 r_{i-1}}{R+\delta r}\right) \right] \right\}. \quad (2-21)$$

Figure 2-4. Axial and radial mesh format for density redistribution in annular geometry.

2.4 Other Considerations or Simplifications

It should also be noted that during a transient, the density redistribution might create a curved top on the system. The greater energy deposition at the center produces more expansion at the center than at the edges, creating a domed shape. The analyses performed will have a small density change amplitude, and it is assumed that at this small level, the effect of the curved top on the effective multiplication of the system is a secondary effect. This is also a motivation for comparing the radial and axial distributions to the combined one. The curved top would affect the axial leakage, which should be less important than the radial leakage, again showing a curved top to be a secondary effect.

CHAPTER 3

VOLUMETRIC EXPANSION REACTIVITY FEEDBACK RESULTS

3.1 Preliminary Considerations for Volumetric Expansion Calculations

The volumetric expansion reactivity feedback effects are calculated given the geometric specifications, diffusion-theory radial and axial extrapolation lengths, and isotopic contents of a solution assembly. The study consists of six actual assemblies and one hypothetical assembly: *CRAC* (61.1, 207, and 320 g U/L); *KEWB-5*; *SILENE*; *SHEBA*; 10.5 g/L plutonium solution. All but *SHEBA* were previously or are presently operational at the time of the study. Therefore, geometric data and isotopic contents are readily available.

All studies are performed using the S_N discrete ordinates transport code TWODANT (Alcouffe, et al., 1990) and the 16-group Hansen-Roach cross section set (Hansen and Roach, 1961). The potential scattering cross section sets for the fissile and fissionable isotopes corrected for resonance self-shielding are calculated according to the Hansen-McLaughlin method (O'Dell, 1990). Given the geometric and material data, a reference state of each assembly is determined. This state is supposedly a critical assembly. In general, the effective multiplications of the reference states are close to unity; however, the important data regard differences in k_{eff} as opposed to values of k_{eff} . The extrapolation distances are obtained from the 16th-group's flux profile (the thermal flux) by taking the flux from the outer two mesh points and linearly extrapolating to zero.

Given the reference states, the height of each solution is increased in increments of 0.1, 0.3, 0.5, 1.0, 2.0, and 3.0 cm. The densities of each isotope in solution must then be

uniformly adjusted according to Equation 2-12 to conserve mass. Obtaining k_{eff} for this configuration allows a determination of the reactivity feedback from the uniform expansion.

For the case of distributed densities, the isotopic densities for the uniformly distributed cases are adjusted such that

$$N_i(r,z) = N_u \left[1 + \frac{\delta\rho_i(r,z)}{\rho_u} \right], \quad (3-1)$$

where N_i is the number density of each isotope in the i^{th} volume element, N_u is the number density in the case of uniform expansion, ρ_u is the density from uniform expansion, and $\delta\rho_i(r,z)$ is the density variation obtained from Equations 2-16, 2-17, 2-18, or 2-21, depending on the situation.

3.2 Numerical Considerations for Volumetric Expansion Calculations

There are several important parameters used by any discrete ordinates code. In order to avoid numerical effects on the effective multiplications, the parameters are held as constant as possible throughout the study.

All TWODANT k_{eff} values in the study have been converged to 10^{-8} . This does not say that the numbers are accurate to this degree (the opposite is most certainly the case), but that no rounding errors should be present. Each calculation uses P₁ Legendre scattering for hydrogen, S₈ angular quadrature, and approximately 100 fine mesh intervals in both radial and axial directions. Again, to obtain differences in k_{eff} only, these are held constant in each run to avoid meshing variance effects. Also, because only differences are desired, the multiplications should not need to be extrapolated to the values for S_∞ or for infinitely fine mesh spacing; the differences should remain constant. Note however, that when the solution height is increased, the number of mesh intervals remains constant. This causes a

small increase in the mesh spacing. It is assumed that with the large number of meshes used, this is a very minor effect and should not significantly affect the results. Also, each discrete density in the distributed cases is defined as a separate material. Thus, there are several different materials in the distributed inputs. To maintain mesh consistency between distributed, uniform, and reference cases, the same input is used for the uniform and reference cases as for the distributed case except that each material is identical. Such efforts should maintain numerical consistency throughout the study. See Appendix A for sample TWODANT inputs.

3.3 CRAC Volumetric Expansion Results

The French *CRAC* series of experiments covered a wide range of uranyl nitrate solutions of various compositions and two different geometries (Lécorché and Seale, 1973). This study only considers Experiments 5, 22, and 25, all of which used a 300 mm. diameter vessel. The experiments contained 61.1, 207, and 320 grams of uranium per liter of solution, respectively. The uranium was enriched to 93.5 % ^{235}U .

Experiment 22 (207 gU/L) was a primary assembly for use in burst experiments. The critical height was 27.0 cm., which corresponds to a solution volume of 18 liters. The solution is contained in a stainless steel vessel with a rounded bottom, but is modelled here as a cylinder. Geometric details of the reference fuel solution, including diffusion extrapolation distances follow (the solution was surrounded by a 3 mm. thick stainless steel shell).

$$\begin{array}{ll} R = 14.7 \text{ cm.} & \delta r = 1.10 \text{ cm.} \\ H = 27.0 \text{ cm.} & \delta z = 1.25 \text{ cm.} \end{array}$$

The geometry described above is considered to be a critical system with the following isotopic constituents (given in atoms/cm³) (Seale, 1991).

$$\begin{array}{ll}
 {}^{235}\text{U} : 4.929 \times 10^{20} & {}^{238}\text{U} : 3.710 \times 10^{19} \\
 \text{H} : 5.955 \times 10^{22} & \text{O} : 3.713 \times 10^{22} \\
 \text{N} : 2.306 \times 10^{21} &
 \end{array}$$

The calculation for this assembly is the only one which examines the effect of radial-only, or axial-only density redistribution. The reference case produced an effective multiplication of 0.971519. Results of the other calculations may be found in Table 3-1. Note that *distributed* refers to the complete density redistribution as obtained from Equation 2-16, *radial-only* refers to density redistribution in the radial direction only (Equation 2-17), and *axial-only* refers to the redistribution in the axial direction only (Equation 2-18).

There are many interesting phenomena which are indicated in Table 3-1. Note that all multiplications are smaller than the reference case. This clearly indicates a negative feedback mechanism from the volumetric expansion, both with and without density redistribution. Also, the radial-only k_{eff} 's are closer to the distributed cases' than are the axial-only k_{eff} 's, indicating the radial distribution is a greater portion of the total distribution than the axial distribution. Because radial redistribution is more "important" than axial redistribution, the effects of a curved top would be lessened. Density amplitudes varied from 0.003 g/cm³ for $H' = 27.1$ cm. to 0.1 g/cm³ for $H' = 30$ cm. Density variations are therefore relatively small, which will also lessen the importance of any geometric uncertainty in the free surface. Figure 3-1 is a graphical representation of Table 1. Note from the figure that the data appear quite linear.

The important data which may be obtained from Table 3-1 are the reactivity effects. By plotting the reactivity differences versus changes in height or volume, where reactivity is defined as

$$\rho = \frac{k_{eff} - 1}{k_{eff}} , \quad (3-2)$$

one may obtain a reactivity feedback coefficient for volumetric expansion as a function of volume change. Figure 3-2 shows the reactivity change from the reference state for the data in Table 3-1. Reactivities are expressed in dollars, and for this system, $\beta_{eff} = 0.00845$ (Lécorché and Seale, 1973). Note how all cases with a distributed density are quite close to each other, but the radial-only is closer to the completely distributed case than is the axial-only case. The fact that the curves appear quite linear with a zero y-intercept is quite reassuring, indicating a constant reactivity feedback coefficient.

Table 3-1. Effective Multiplications from the CRAC (207 gU/L) study

$H' \text{ (cm)}$	<i>uniform</i> k_{eff}	<i>distributed</i> k_{eff}	<i>radial-only</i> k_{eff}	<i>axial-only</i> k_{eff}
27.1	0.969313	0.968823	0.968877	0.968968
27.3	0.964910	0.963517	0.963681	0.963943
27.5	0.960517	0.958234	0.958511	0.958930
28.0	0.949577	0.945129	0.945700	0.946454
29.0	0.927868	0.919357	0.920558	0.921759
30.0	0.906510	0.894171	0.896045	0.897438

Figure 3-3 shows the reactivity differences between each distributed case and the uniformly expanded case. The purpose of this graph is to indicate how much reactivity worth may be attributed to distributing the density throughout the assembly. Recall that the distributed cases are reactivities from a uniform expansion *plus* a density redistribution. Note that even with rather small density amplitudes, a distribution of the density can add up to \$1.8 to the reactivity effect for a 3 cm. height increase.

Figure 3-1. Effective Multiplication versus Height Increase for the CRAC (207 gU/L) assembly using a uniform expansion, complete density redistribution, axial-only redistribution, and radial-only redistribution.

Figure 3-2. Reactivity differences from the reference case versus volume increase for the CRAC (207 g U/L) assembly for a uniform expansion, complete density redistribution, axial-only redistribution, and radial-only redistribution.

Figure 3-4 is simply Figure 3-2 redrawn without the axial-only and radial-only distributions. This graph gives the important data which may be used to obtain the volumetric reactivity feedback coefficients. The best fit line for the data is obtained by using a linear least squares technique. The slope of this line is the reactivity feedback coefficient of volumetric expansion. The least squares analysis yields the results found in Table 3-1. Taking a rough average of these numbers yields a feedback coefficient of about $-4700 \text{ } \$/\text{m}^3$.

Figure 3-3. Reactivity differences from the uniformly expanded case versus volume increase for the CRAC (207 gU/L) assembly for a uniform expansion, complete density redistribution, axial-only redistribution, and radial-only redistribution.

Figure 3-4. Reactivity differences from the critical/reference case versus volume increase for the CRAC (207 gU/L) assembly for a complete density redistribution and a uniformly expanded system.

Table 3-2. Reactivity Feedback Coefficients from the CRAC (207 gU/L) study

Case	Volumetric Feedback Coefficient (\$/cm³)
Uniform/Critical	-4.2945×10^{-3}
Distributed/Critical	-5.1768×10^{-3}

The CRAC experimental series covered many solution concentrations. Two extra are analyzed here to increase the data base with respect to volumetric solution expansion. Experiment 5 used solution with 61.1 grams of uranium per liter of solution. Because of the low concentration, the critical height is considerably larger than for 207 g U/L. The critical dimensions follow.

$$\begin{array}{ll}
 R = 14.7 \text{ cm.} & \delta r = 0.50 \text{ cm.} \\
 H = 69.05 \text{ cm.} & \delta z = 0.68 \text{ cm.}
 \end{array}$$

This system is considered to be a critical system with the following isotopic constituents (given in atoms/cm³) (Seale, 1991).

$$\begin{array}{ll}
 {}^{235}\text{U} : 1.459 \times 10^{20} & {}^{238}\text{U} : 1.097 \times 10^{19} \\
 \text{H} : 6.281 \times 10^{22} & \text{O} : 3.577 \times 10^{22} \\
 \text{N} : 1.580 \times 10^{21} &
 \end{array}$$

The effective multiplication for this reference case is 0.991975. Effective multiplications from the systems with uniform and nonuniform density distributions are found in Table 3-3 and Figure 3-5.

Table 3-3. Effective Multiplications from the CRAC (61.1 gU/L) study

$H' \text{ (cm)}$	<i>uniform</i> k_{eff}	<i>distributed</i> k_{eff}
69.15	0.990980	0.990815
69.35	0.988992	0.988500
69.55	0.987006	0.986186
70.05	0.982051	0.980419
71.05	0.972184	0.968954
72.05	0.962370	0.957582

As before, the effective multiplications show a linear trend and converge on the reference effective multiplication as the height increase approaches zero. Reactivity feedbacks may be seen in Figure 3-6. For this assembly, $\beta_{eff} = 0.00774$. Extracting the volumetric expansion feedback coefficient from the slopes in Figure 3-6 yields the values seen in Table 3-4. A rough average of these numbers is -2100 $\$/\text{m}^3$.

Figure 3-5. Effective Multiplication versus Height Increase for the CRAC (61.1 gU/L) assembly using a uniform and distributed density distribution.

Figure 3-6. Reactivity differences from the critical/reference case versus volume increase for the CRAC (61.1 gU/L) assembly for a uniform and distributed density distribution.

Table 3-4. Reactivity Feedback Coefficients from the CRAC (61.1 gU/L) study

Case	Volumetric Feedback Coefficient (\$/cm ³)
Uniform/Critical	-1.9681 x 10 ⁻³
Distributed/Critical	-2.2980 x 10 ⁻³

Experiment 25 used solution with 320 grams of uranium per liter of solution. Even with this high concentration, the critical height is slightly larger than for 207 g U/L. Apparently the extra fuel is providing relatively more absorption than in the 207 g U/L system, giving rise to an increase in required solution amount. The critical dimensions are shown.

$$\begin{array}{ll}
 R = 14.7 \text{ cm.} & \delta r = 0.44 \text{ cm.} \\
 H = 27.47 \text{ cm.} & \delta z = 0.52 \text{ cm.}
 \end{array}$$

This system's critical isotopic contents follow (given in atoms/cm³) (Seale, 1991).

$$\begin{array}{ll}
 {}^{235}\text{U} : 7.617 \times 10^{20} & {}^{238}\text{U} : 5.733 \times 10^{19} \\
 \text{H} : 5.628 \times 10^{22} & \text{O} : 3.855 \times 10^{22} \\
 \text{N} : 3.180 \times 10^{21} &
 \end{array}$$

The effective multiplication for this reference case is 0.969662. Effective multiplications from the systems with uniform and nonuniform density distributions are found in Table 3-5 and Figure 3-7.

Again, the effective multiplications show a linear trend and converge on the reference effective multiplication as the height increase approaches zero. Reactivity feedbacks may be seen in Figure 3-8. For this assembly, $\beta_{eff} = 0.00854$. Note that the effective delayed neutron fractions have generally increased with decreasing critical height. As the system size increases, the fast fission neutrons have less chance to leak from the

system, leading to a smaller relative delayed neutron fraction. Extracting the volumetric expansion feedback coefficient from the slopes in Figure 3-8 yields the values seen in Table 3-6. A rough average of these numbers is $-4600 \text{ } \$/\text{m}^3$.

Table 3-5. Effective Multiplications from the CRAC (320 gU/L) study

H' (cm)	<i>uniform</i> k_{eff}	<i>distributed</i> k_{eff}
27.57	0.967498	0.967046
27.77	0.963175	0.961830
27.97	0.958863	0.956639
28.47	0.948130	0.943763
29.47	0.926868	0.918453
30.47	0.905896	0.893731

Table 3-6. Reactivity Feedback Coefficients from the CRAC (320 gU/L) study

Case	Volumetric Feedback Coefficient ($\$/\text{cm}^3$)
Uniform/Critical	-4.1779×10^{-3}
Distributed/Critical	-5.0423×10^{-3}

It is somewhat interesting to note that this volumetric feedback is slightly less than that for the 207 g U/L system. This may indicate that geometry is a primary factor in this feedback (the 320 g U/L system has a slightly *larger* critical height than the 207 g U/L system).

Figure 3-7. Effective Multiplication versus Height Increase for the CRAC (320 gU/L) assembly using a uniform and distributed density distribution.

Figure 3-8. Reactivity differences from the critical/reference case versus volume increase for the CRAC (320 gU/L) assembly for a uniform and distributed density distribution.

3.4 KEWB-5 Volumetric Expansion Results

The *KEWB-5* (Dunenfild and Stitt, 1963) and *CRAC* experiments are very similar. Both used a stainless steel cylindrical vessel, the lower portion of which is an elliptical shell. However, *KEWB-5* used uranyl sulfate instead of nitrate. Also, the inner geometric details of this assembly are much more complex than *CRAC*'s. *CRAC* was simply a large test tube, with no internal devices; *KEWB-5* contained two asymmetric burst rod shafts and approximately 110 feet of water-filled cooling coils. These geometric anomalies are ignored in the modelling, and *KEWB-5* is assumed to be a cylinder with square lower edges. Also, the stainless steel shell is approximately twice as thick as that for *CRAC*.

Geometric details of the *KEWB-5* reference fuel solution, including diffusion extrapolation distances follow (the solution is surrounded by a 0.25 inch thick stainless steel shell).

$$\begin{array}{ll} R = 14.6 \text{ cm.} & \delta r = 0.625 \text{ cm.} \\ H = 35.8 \text{ cm.} & \delta z = 0.88 \text{ cm.} \end{array}$$

This system contains approximately 24 liters of solution. This determines the critical height specified above, which contains the following isotopic constituents (given in atoms/cm³) (Smith, 1989).

$$\begin{array}{ll} {}^{235}\text{U} : 4.839 \times 10^{20} & {}^{238}\text{U} : 3.322 \times 10^{19} \\ \text{H} : 5.993 \times 10^{22} & \text{O} : 3.066 \times 10^{22} \\ \text{S} : 5.170 \times 10^{20} & \end{array}$$

The effective multiplication for this reference state is 1.040410. It is somewhat interesting that *KEWB*'s k_{eff} is much higher than that for *CRAC* (207 gU/L) when the isotopic constituents and modelling geometries are quite similar. This is a direct result of the reference height (or solution volume) being so much higher than *CRAC*'s (35.8 cm. as opposed to 27.0 cm.). Even with similar solutions, part of this difference is attributable to

the differences in the isotopic constituents. Performing critical axial dimension searches on the two assemblies yields a critical height for *KEWB* which is 3 cm. higher than *CRAC*'s. Therefore, the small differences in uranium and hydrogen concentrations can account for approximately one-third of the difference. The extra steel around *KEWB* also accounts for about 0.3 cm., which still leaves unaccounted a 5.5 cm. difference in solution heights. This is probably due to the geometric anomalies in the *KEWB* vessel. Absorption in the extra steel and added moderation from the water-filled cooling coils certainly will create uncertainties which are not modelled here, and perhaps explain the differences in critical volumes between the two systems.

The results from the expanded volumes are found in Table 3-7. Again note that all multiplications are lower than the reference, indicating the expected negative effect. Density changes here range from 0.0028 g/cm³ for the 0.1 cm. height increase to 0.0773 g/cm³ for the 3 cm. increase. These are smaller density increases than those for *CRAC* because the higher reference volume makes constant increases relatively smaller. The data in Table 3-7 is seen graphically in Figure 3-9. Again note the linear nature of the data indicating a constant reactivity feedback coefficient.

Table 3-7. Effective Multiplications from the *KEWB*-5 study

$H' \text{ (cm)}$	<i>uniform</i> k_{eff}	<i>distributed</i> k_{eff}
35.9	1.038581	1.038250
36.1	1.034929	1.033936
36.3	1.031286	1.029630
36.8	1.022213	1.018903
37.8	1.004228	0.997615
38.8	0.986460	0.976562

Figure 3-9. Effective Multiplication versus Height Increase for the *KEWB-5* assembly for a uniform expansion and a density redistribution.

Reactivity effects are presented in Figure 3-10. For *KEWB-5*, $\beta_{eff} = 0.008$ (Dunenfild and Stitt, 1963). Note also that these least squares linear fits reassuringly intercept near zero. Table 3-8 contains the slopes of the lines in Figure 3-10, which correspond to the volumetric expansion reactivity feedback coefficients for the *KEWB-5* assembly. Note that these feedback coefficients are much smaller (by about 25%) than those reported for *CRAC* in Table 3-2. A coarse value for the *KEWB-5* volumetric feedback is $-3600 \text{ } \$/\text{m}^3$.

Figure 3-10. Reactivity differences from the critical/reference case versus volume increase for the *KEWB-5* assembly for a complete density redistribution and a uniformly expanded system.

Table 3-8. Reactivity Feedback Coefficients from the *KEWB-5* study

Case	Volumetric Feedback Coefficient (\$/cm ³)
Uniform/Critical	-3.2708×10^{-3}
Distributed/Critical	-3.9110×10^{-3}

This difference in the feedback coefficients may be partially attributed to the stainless steel liner. All studies are performed with the containers intact. As previously mentioned, the reactivity effect from the extra steel accounts for a significant amount of solution. Vacuum boundary conditions are applied on all TWODANT runs. This prohibits escaping neutrons from reflecting back into the assembly. Thus, given a reference state with no external materials, one may place any material (even boron) around the system and

the effective multiplication will increase. No matter how absorbant the external material is, some neutrons will be reflected back into the system. This is another way of saying that a vacuum boundary condition is the same as placing an infinitely absorbant, zero scattering material outside the system.

In the context of the *KEWB-5* assembly, the extra steel actually enhances the reflection of neutrons back into the solution, increasing k_{eff} . However, the steel also reduces the effect of a volumetric expansion. A primary effect of the expansion is to increase the surface area through which neutrons may leak. When the steel is present, some of those neutrons which leak will be reflected back into the system, decreasing the net leakage, which in turn decreases the reactivity effect of an expansion. When the steel is removed, the volumetric reactivity feedbacks are enhanced (see Table 3-9). The data in Table 3-9 is taken only from a 1 cm. height increase. It is assumed that the effect here is linear as previously seen. These feedback coefficients are approximately 11% higher than those reported in Table 3-8, again showing the importance of the stainless steel in the system.

Table 3-9. Reactivity Feedback Coefficients from the *KEWB-5* study with no stainless steel liner

Case	Volumetric Feedback Coefficient ($\$/\text{cm}^3$)
Uniform/Critical	-3.6367×10^{-3}
Distributed/Critical	-4.3482×10^{-3}

3.5 SILENE Volumetric Expansion Results

Like the *CRAC* series of experiments, *SILENE* is a French assembly using a uranyl nitrate solution of enriched to 93.5% ^{235}U (Barbry). However, this is a low uranium concentration system (71 g U/L of solution), which also contains a central control rod/burst rod cylinder. Thus its geometry is annular. Also, the bottom of the tank is flat, where *CRAC*'s and *KEWB*'s are rounded.

Geometric details of the reference fuel solution, including diffusion extrapolation distances follow. The solution is surrounded by a 4 mm. thick stainless steel shell on the outside and the central rod cylinder is 3 mm. thick stainless steel. Radii given are for the fuel solution; thus, R_i is the inside radius of the fuel, or outer radius of the central cylinder.

$$\begin{array}{ll} R_o = 18.0 \text{ cm.} & \delta r = 0.55 \text{ cm.} \\ R_i = 3.8 \text{ cm.} & \delta z = 0.96 \text{ cm.} \\ H = 38.0 \text{ cm.} & \end{array}$$

This system contains approximately 37 liters of solution. The geometry described above is considered to be a critical system with the following isotopic constituents (given in atoms/cm³) (Barbry).

$$\begin{array}{ll} ^{235}\text{U} : 1.686 \times 10^{20} & ^{238}\text{U} : 1.170 \times 10^{19} \\ \text{H} : 6.258 \times 10^{22} & \text{O} : 3.576 \times 10^{22} \\ \text{N} : 1.569 \times 10^{21} & \end{array}$$

The effective multiplication for this reference state is 0.995328, which is quite close to actual criticality. This lends some credence to the given values for geometric details and isotopic contents. The effective multiplications for the increased height cases may be found in Table 3-10, which may also be found graphed in Figure 3-11. Once again the data appear quite linear and tend to intercept the y-axis at the reference state's effective multiplication.

Table 3-10. Effective Multiplications from the *SILENE* study

H' (cm)	<i>uniform</i> k_{eff}	<i>distributed</i> k_{eff}
38.1	0.993863	0.993645
38.3	0.990939	0.990286
38.5	0.988017	0.986934
39.0	0.980729	0.978584
40.0	0.966223	0.962017
41.0	0.951818	0.945631

Figure 3-11. Effective Multiplication versus Height Increase for the *SILENE* assembly for a uniform expansion and a density redistribution.

Reactivity data ($\beta_{eff} = 0.00794$) as a function of volume increase may be found in Figure 3-12, which contains the same general features as the previous assemblies. The volumetric reactivity feedback coefficients are listed in Table 3-11. Note that these

feedback coefficients are much smaller than those from the previous assemblies, with a value of about $-2100 \text{ } \$/\text{m}^3$. This system is much larger, with a radius of 18 cm. as opposed to approximately 15 cm. for *CRAC* and *KEWB*. The distributed density amplitude varied from 0.0026 g/cm^3 for the 0.1 cm. increase and 0.073 g/cm^3 for the 3 cm. increase. These are similar to those seen previously, so the difference in feedback coefficients may be attributed primarily to the size differences. With *SILENE*'s larger system, the leakage becomes relatively less important to the leakage from *CRAC* or *KEWB*, which in turn makes the volumetric expansion less important to the system's reactivity.

Figure 3-12. Reactivity differences from the critical/reference case versus volume increase for the *SILENE* assembly for a complete density redistribution and a uniformly expanded system.

Table 3-11. Reactivity Feedback Coefficients from the *SILENE* study

Case	Volumetric Feedback Coefficient (\$/cm ³)
Uniform/Critical	-1.9840 x 10 ⁻³
Distributed/Critical	-2.2809 x 10 ⁻³

3.6 *SHEBA* Volumetric Expansion Results

SHEBA is very different from the assemblies discussed thus far. Like *SILENE*, *SHEBA* uses an annular geometry with a flat bottom plate. However, this assembly uses uranyl fluoride as the fuel solution with the ²³⁵U enriched to only 5%.

Geometric details of the reference fuel solution, including diffusion extrapolation distances are shown below. The solution is surrounded by a 0.5 inch thick stainless steel shell on the outside and the central rod cylinder is 0.25 inch thick stainless steel. Radii given are for the fuel solution; thus, R_i is the inside radius of the fuel, or outer radius of the central cylinder.

$$\begin{array}{ll}
 R_o = 24.13 \text{ cm.} & \delta r = 0.67 \text{ cm.} \\
 R_i = 3.175 \text{ cm.} & \delta z = 1.02 \text{ cm.} \\
 H = 46.8 \text{ cm.} &
 \end{array}$$

This is a very large system containing approximately 84 liters of solution. As *SHEBA* is not presently in operation due to modifications, the critical height is not known. Therefore, the approximate critical configuration is determined via a critical height search. The fuel solution presently exists; only the geometry is new (the previous version of *SHEBA* used the same solution in a different diameter vessel). The critical isotopic constituents are shown (given in atoms/cm³) (Anderson, 1990).

$$\begin{array}{ll}
 {}^{235}\text{U} : 1.319 \times 10^{20} & {}^{238}\text{U} : 2.499 \times 10^{21} \\
 \text{H} : 6.354 \times 10^{22} & \text{O} : 3.210 \times 10^{22} \\
 \text{F} : 5.334 \times 10^{21} &
 \end{array}$$

The effective multiplication for this reference state is 1.001990. Effective multiplication results from the uniform expansions and density redistributions may be found in Table 3-12 and Figure 3-13.

Table 3-12. Effective Multiplications from the *SHEBA* study

H' (cm)	uniform k_{eff}	distributed k_{eff}
46.9	1.001190	1.001048
47.1	0.999591	0.999167
47.3	0.997992	0.997287
47.8	0.993992	0.992591
48.8	0.985992	0.983225
49.8	0.977993	0.973893

Figure 3-13. Effective Multiplication versus Height Increase for the *SHEBA* assembly for a uniform expansion and a density redistribution.

Again note that the effective multiplications in Figure 3-13 approach the reference case as ΔH approaches zero. The reactivity feedbacks associated with these expanded solutions are found in Figure 3-14. Here, β_{eff} is assumed to be 0.007. The linear least squares fits in Figure 3-14 are found in Table 3-13. These feedback coefficients are even smaller than *SILENE*'s (about -700 \$/m³). However, *SHEBA* is a much larger system than *SILENE*, which reduces the leakage effect on reactivity feedbacks. Also, like *KEWB-5*, significant amounts of steel surround the vessel, further reducing the leakage. The combined effects of the large system and the 0.25 inch outer steel shell will decrease the volumetric reactivity feedback for the *SHEBA* assembly.

Figure 3-14. Reactivity differences from the critical/reference case versus volume increase for the *SHEBA* assembly for a complete density redistribution and a uniformly expanded system.

Table 3-13. Reactivity Feedback Coefficients from the *SHEBA* study

Case	Volumetric Feedback Coefficient (\$/cm ³)
Uniform/Critical	-6.4905×10^{-4}
Distributed/Critical	-7.6310×10^{-4}

Table 3-14 contains a summary of typical values for the volumetric feedback coefficients for the four assemblies studied. In all cases, for both uniform and distributed densities, the feedback coefficients for volumetric solution expansions are linear. With this data, the parameters for solution expansion, independent of temperature, are determined.

Table 3-14. Typical Volumetric Feedback Coefficients for Each Assembly

Assembly	Volumetric Feedback Coefficient (\$/m ³)
<i>CRAC</i> (61.1 gU/L)	-2100
<i>CRAC</i> (207 gU/L)	-4700
<i>CRAC</i> (320 gU/L)	-4600
<i>KEWB-5</i>	-3600
<i>SILENE</i>	-2100
<i>SHEBA</i>	-700

3.7 Dilute Plutonium Solution Volumetric Expansion Results

It is desirable to investigate the volumetric expansion coefficient for a dilute plutonium solution for comparison with other reactivity feedback data. This is a hypothetical assembly consisting of plutonium mixed with unit density water. As this is a hypothetical assembly, two separate geometries are investigated. There is no steel surrounding the fuel solution, which has the following two configurations.

$R = 40.0 \text{ cm.}$	$\delta r = 0.72 \text{ cm.}$
$H = 64.1 \text{ cm.}$	$\delta z = 1.08 \text{ cm.}$
$R = 35.0 \text{ cm.}$	$\delta r = 0.66 \text{ cm.}$
$H = 87.3 \text{ cm.}$	$\delta z = 1.31 \text{ cm.}$

The dilute nature of the fuel, makes this the largest system studied thus far, containing approximately 322 and 336 liters of solution for the 40 cm. and 35 cm. radius systems, respectively. Both approximate critical heights are determined via critical height searches. The plutonium is enriched to 5% in ^{240}Pu . The critical isotopic constituents are shown (given in atoms/cm³).

$^{239}\text{Pu} : 2.512 \times 10^{19}$	$^{240}\text{Pu} : 1.322 \times 10^{18}$
$\text{H} : 6.685 \times 10^{22}$	$\text{O} : 3.343 \times 10^{22}$

The effective multiplication for the reference state in the 40 cm. radius cylinder is 1.004182. Effective multiplication results from the uniform expansions and density redistributions are found in Table 3-15 and Figure 3-15. The effective multiplication for the reference state in the 35 cm. radius cylinder is 1.004290. These results are found in Table 3-16 and Figure 3-15.

Table 3-15. Effective Multiplications for Volumetric Expansion in a Dilute Plutonium Solution in a 40 cm. Radius Cylinder

$H' \text{ (cm)}$	<i>uniform</i> k_{eff}	<i>distributed</i> k_{eff}
64.2	1.003931	1.003865
64.4	1.003428	1.003231
64.6	1.002923	1.002595
65.1	1.001660	1.001005
66.1	0.999116	0.997811
67.1	0.996553	0.994599

Table 3-16. Effective Multiplications for Volumetric Expansion in a Dilute Plutonium Solution in a 35 cm. Radius Cylinder

$H' \text{ (cm)}$	<i>uniform</i> k_{eff}	<i>distributed</i> k_{eff}
87.4	1.004056	1.004008
87.6	1.003587	1.003442
87.8	1.003116	1.002876
88.3	1.001939	1.001459
89.3	0.999575	0.998615
90.3	0.997200	0.995758

As in the other cases, the data properly approaches the reference cases' values of k_{eff} . The reactivity feedbacks ($\beta_{eff} = 0.0022$) associated with these expanded solutions are found in Figure 3-16, and the linear least squares fits are found in Table 3-17. The feedback coefficients from these extremely large system are the smallest yet encountered. The density amplitudes vary from 0.0011 to 0.033 g/cm³ for the 35 cm. radius system, and 0.0016 to 0.045 g/cm³ for the 40 cm. radius system. The size of these assemblies reduces the relative importance of leakage on the systems' effective multiplications; thus, when uniform expansion or density redistribution occurs, the leakage is not changed very much, leading to the small volumetric expansion coefficients seen in Table 3-17. As seen with the

radial-only and axial-only redistribution studies performed with the *CRAC* assembly, the volumetric expansion feedback is greater for the tall/thin assembly than for the shorter assembly. Again, the radial leakage is the more important factor. A rough average of the data in Table 3-17 yields a volumetric feedback coefficient for these dilute plutonium systems of $-280 \text{ } \$/\text{m}^3$. Table 3-17 also contains the volumetric feedback coefficients from an infinite cylinder of this solution. This is obtained by using the radial-only density redistribution and calculating new densities based on "effective" height changes, that is, based on density amplitudes. The infinite cylinder coefficients should be the limiting value for volumetric feedbacks as the system heights increase. Note that the limiting feedback is more than double those seen in the finite cylinders ($-570 \text{ } \$/\text{m}^3$ versus $-280 \text{ } \$/\text{m}^3$).

Figure 3-15. Effective Multiplication versus Height Increase for hypothetical 10.5 g/L plutonium/unit density water solutions in 35 and 40 cm radius cylinders for a uniform expansion and a density redistribution.

Figure 3-16. Reactivity differences from the critical/reference case versus volume increase for hypothetical 10.5 g/L plutonium/unit density water solutions in 35 and 40 cm radius cylinders for a complete density redistribution and a uniformly expanded system.

Table 3-17. Reactivity Feedback Coefficients for Hypothetical 10.5 g/L Plutonium/Unit Density Water Solutions in 35 and 40 cm Radius Finite Cylinders and a 30.1 cm Radius Infinite Cylinder

Case	Volumetric Feedback Coefficient (\$/cm³)
Uniform/Critical (R = 35 cm)	-2.7885×10^{-4}
Distributed/Critical (R = 35 cm)	-3.3599×10^{-4}
Uniform/Critical (R = 40 cm)	-2.2991×10^{-4}
Distributed/Critical (R = 40 cm)	-2.8932×10^{-4}
Infinite Cylinder (R = 30.1)	
Uniform/Critical	-5.4500×10^{-4}
Distributed/Critical	-5.9726×10^{-4}

As a final consideration in this study, the source of variation in the volumetric feedback coefficients is investigated. It has been seen throughout each separate assembly that the volumetric feedback decreases as the system size increase. Again, the volumetric expansion primarily affects the leakage, which is relatively more important in smaller systems. These observations lead to the conclusion that the volumetric feedback is primarily linked to geometry, or more specifically, the size of the system. By taking the data from uranium and plutonium solutions (Tables 3-14 and 3-17) and plotting them versus system volume, the variation in the volumetric feedback coefficients as a function of geometry may be seen. At low system volumes, small changes in volume may create large variations in the volumetric feedback. Note that this is a rather incomplete data set, and that by using both uranium and plutonium solutions it is assumed that the primary factor for determining volumetric expansion feedback coefficients is the geometry.

Figure 3-17. Volumetric feedback coefficients as a function of system volume for uranium and plutonium solutions.

CHAPTER 4

16-GROUP NEUTRON TEMPERATURE REACTIVITY FEEDBACK

When a critical system's temperature increases, two primary mechanisms occur. First, the system volumetrically expands, decreasing number densities thereby affecting leakage and macroscopic interaction cross sections. This is discussed in Chapters 2 and 3. Second, a temperature rise in a very thermal system (one where the energy spectrum of the neutrons is dominant in the thermal range) such that

$$E_{neutron} \approx kT , \quad (4-1)$$

causes the thermal neutrons' energies to increase. Assuming the neutrons are in thermal equilibrium with the system, the average thermal energy therefore increases. By pushing the neutron spectrum up in energy, the neutrons "see" different thermal cross sections. This clearly can affect the system's reactivity. If the thermal neutrons are in the $1/v$ region, a temperature increase shifts the spectrum up in energy where the reaction cross sections are lower. Depending on which cross sections are affected (fission, absorption, etc.), the system's reactivity may increase or decrease.

4.1 Flux-Weighted Temperature-Dependent Cross Sections

Temperature feedback is modelled by adjusting cross sections for a given temperature rise. The reactivity feedback from spectrum "hardening" may be determined by adjusting cross sections while maintaining the geometry.

In a multi-group formulation of the transport equation, the flux-weighted absorption cross section for the g^{th} group is given by (Duderstadt and Hamilton, 1976)

$$\sigma_g = \frac{\int_{E_g} \sigma(E) \phi(E, T) dE}{\int_{E_g} \phi(E, T) dE}, \quad (4-2)$$

where the integration is carried over the energy range for the g^{th} group, the cross section is considered to be a function of energy only, and the flux is a function of both energy and temperature. Note that when Doppler-broadened resonances are discussed, it is assumed that the cross section is temperature dependent. For the purposes of this analysis, only low energy cross sections are important (well away from the crowded resonance region) and only small temperature increases will be used.

In the thermal region, the neutron flux may be approximated by a Maxwellian distribution in energy and temperature, i.e.

$$\phi(E, T) = C \frac{E^{1/2}}{T^{3/2}} e^{-E/kT}, \quad (4-3)$$

where C is a constant, T is the absolute temperature, and k is Boltzmann's constant. By inserting the thermal flux from Equation 4-3 into Equation 4-2, the flux-weighted average cross section for the g^{th} group may be determined for any temperature. Clearly, using the thermal Maxwellian flux assumes that only thermal group cross sections will be calculated via this method.

4.2 Temperature Corrections for Thermal Cross Sections

This study uses as its cross section set the Hansen-Roach 16-group Library (Hansen and Roach, 1961). This set has been widely used and benchmarked for many systems, including those both fast and thermal. The Hansen-Roach set does not include

upscatter and allows for six downscatter cross sections (one in-group and five higher groups cross sections). Recall that group 1 is traditionally the fastest group, and as energy decreases the group number increases. The 15th and 16th groups have the following energy bounds:

Table 4-1. Energy Boundaries for Groups 15 and 16 of the Hansen-Roach Cross Section Library

Group	Low Energy	High Energy
15	0.025 eV	0.1 eV
16	0.1 eV	0.4 eV

It is assumed that for small temperature rises, it would be adequate to adjust the 15th and 16th group cross sections by using curve fits of the continuous cross sections and the Maxwell-Boltzmann flux distribution as seen in Equation 4-3. For purposes here, the basic temperature for the Hansen-Roach cross sections is assumed to be 20 °C, and the new cross section sets are "evaluated" at two higher temperatures, 25 °C and 30 °C. For both low energy groups (15 and 16), the corrected cross sections are given by

$$\sigma_g' = \frac{\int_{E_g} \sigma(E) \phi(E, T) dE}{\int_{E_g} \phi(E, T) dE}, \quad (4-4)$$

and

$$\sigma_{go} = \frac{\int_{E_g} \sigma(E) \phi(E, 20^\circ\text{C}) dE}{\int_{E_g} \phi(E, 20^\circ\text{C}) dE}, \quad (4-5)$$

where the prime indicates a corrected cross section and the zero subscript denotes the original cross section as given in the library.

4.3 Numerical Representation of Isotopic Thermal Cross Sections

Total, absorption, and fission cross sections plots are readily available throughout the literature. Most data here is taken from BNL-325. Cross sections are represented in the range covered by the 15th and 16th group cross sections in the Hansen-Roach Library. Cross sections in the $1/\nu$ regions are simply line fits (note that a $1/\nu$ cross section is linear on a log-log scale) using the 0.0253 eV cross sections. When the cross section is clearly not $1/\nu$ (this usually occurs when the tail of a resonance at higher energy affects the cross section), two points are used to create a modified $1/\nu$ cross section, where this is given by

$$\sigma(E) = \frac{A + B E}{\sqrt{E}} = \frac{A}{\sqrt{E}} + B\sqrt{E} . \quad (4-6)$$

²³⁹Pu has an absorption cross section resonance centered at 0.3 eV, making this resonance an important factor in the 15th group ²³⁹Pu cross sections. This is modelled with the standard Breit-Wigner form of a resonance:

$$\sigma(E) = \sigma_o \sqrt{\frac{E_o}{E}} \frac{1}{\left[1 + \frac{4}{\Gamma^2} (E - E_o)^2 \right]} , \quad (4-7)$$

where σ_o is the peak value of the resonance, E_o is the energy of the peak, and Γ is the full-width at half-maximum. By using this, the modified $1/\nu$ and standard $1/\nu$ cross section forms, it is possible to obtain reasonable numerical fits to most low energy cross sections.

The numerical fit for the low energy cross section of ^{239}Pu is given by a "spline" of a corrected $1/\nu$ and a Breit-Wigner distribution to model the 0.3 eV absorption resonance. The result for the ^{239}Pu cross section fitting is

$$^{239}\text{Pu}: \quad \sigma_f(E) = \begin{cases} \frac{108.3 + 354.5 E}{\sqrt{E}} & "0" \leq E < 0.12 \text{ eV} \\ \frac{1752.7}{\sqrt{E}[1 + 330.6 (E-0.3)^2]} & 0.12 < E \leq 0.4 \text{ eV} \end{cases} \quad (4-8)$$

Note that the cross section used for ^{239}Pu is the fission cross section. The fission and absorption cross sections are of the same form, and appear quite similar, as would be expected. It is assumed that correcting the fission cross section is basically the same as correcting the absorption cross section. The fission cross sections are used only for the fissile isotopes. The cross sections for ^{240}Pu , ^{235}U , and ^{238}U are simply corrected $1/\nu$ cross sections.

$$^{240}\text{Pu}: \quad \sigma_a(E) = \frac{44.04 + 82.49 E}{\sqrt{E}} \quad (4-9)$$

$$^{235}\text{U}: \quad \sigma_f(E) = \frac{93.19 + 55.89 E}{\sqrt{E}} \quad (4-10)$$

$$^{238}\text{U}: \quad \sigma_a(E) = \frac{0.4046 + 1.170 E}{\sqrt{E}} \quad (4-11)$$

The other isotopes of interest in the solution assemblies are the constituents of the various salts and water: H, O, N, S, and F. All absorption cross sections for these isotopes are assumed to be $1/\nu$. The cross section fits used for these isotopes follow.

$$\text{H}: \quad \sigma_a(E) = \frac{0.0525}{\sqrt{E}} \quad (4-12)$$

$$\text{O}: \quad \sigma_a(E) = \frac{3.18 \times 10^{-5}}{\sqrt{E}} \quad (4-13)$$

$$\text{N:} \quad \sigma_{\alpha}(E) = \frac{0.299}{\sqrt{E}} \quad (4-14)$$

$$\text{S:} \quad \sigma_{\alpha}(E) = \frac{0.52}{\sqrt{E}} \quad (4-15)$$

$$\text{F:} \quad \sigma_{\alpha}(E) = \frac{0.001}{\sqrt{E}} \quad (4-16)$$

All numerical values used in the cross section fits are such that E is in eV and σ is in barns.

4.4 Correction Factors for Isotopic Thermal Cross Sections

With the above cross section fits, Equations 4-4 and 4-5 can be numerically integrated to obtain the corrected and reference cross sections. This is done using the integrating package *DESIRE* (Korn, 1989), employing a fourth order Runge-Kutta integration rule. The results (see Tables 4-2 and 4-3) of the integrations produced the temperature-corrected factors which are used to create corrected cross section sets at 25 °C and 30 °C.

In Tables 4-2 and 4-3, some numerical uncertainties are identified. By looking at all isotopes which have $1/v$ cross sections, it is apparent that the correction factors for each isotope are close to each other, but are not the same for all of these isotopes. In fact, they should be constant, and the constant in the $1/v$ equations should cancel out during the numerical integrations. The closeness of these numbers to each other indicate that the integration technique is performing adequately, even when constants that have a large range of magnitude are introduced in the calculations. Also note that correction factors are magnified with increasing temperature, as expected.

Table 4-2. Correction factors for the 15th and 16th groups of each isotope at 25 °C

	σ'/σ_0 (Gp. 15)	σ'/σ_0 (Gp. 16)
²³⁹ Pu	1.0055	0.9969
²⁴⁰ Pu	0.9975	0.9966
²³⁵ U	0.9978	0.9960
²³⁸ U	0.9987	0.9968
H	0.9988	0.9961
O	0.9982	0.9961
N	0.9984	0.9961
S	0.9977	0.9961
F	0.9980	0.9961

Table 4-3. Correction factors for the 15th and 16th groups of each isotope at 30 °C

	σ'/σ_0 (Gp. 15)	σ'/σ_0 (Gp. 16)
²³⁹ Pu	1.0117	0.9939
²⁴⁰ Pu	0.9962	0.9933
²³⁵ U	0.9946	0.9920
²³⁸ U	0.9965	0.9937
H	0.9957	0.9923
O	0.9952	0.9923
N	0.9958	0.9923
S	0.9946	0.9924
F	0.9933	0.9924

It is rather interesting to note that the 15th group correction factor for ²³⁹Pu is greater than one, while all others are less than one. A temperature increase causes the energy of the thermal neutrons to increase as seen from Equation 4-1. Generally, this

causes the thermal neutron flux to shift upward in energy where the cross sections are smaller due to their $1/v$ nature. This gives rise to correction factors less than one for the isotopes which exhibit $1/v$ cross sections. However, for the 0.3 eV resonance in ^{239}Pu , the high energy tail of the thermal flux is shifted up in energy where the absorption and fission cross sections are higher, creating an increase in the fission reaction rate in this group.

Past calculations indicate plutonium solutions may have a positive temperature coefficient (Suzaki, et al., 1987; Mather, et al., 1991a,b). The correction factors for ^{239}Pu seen in Tables 4-2 and 4-3 seem to indicate a source for such a claim. However, there is a competing effect for ^{239}Pu . The vast majority of the thermal flux is in the 16th group, which has a correction factor less than one. For a positive temperature coefficient to be seen, the increase in absorption in the 15th group must outweigh the flux shifting to areas of lower absorption in the 16th group.

4.5 Corrected Cross Sections and Scattering Considerations

Specific cross sections in the standard 16-group Hansen-Roach library are multiplied by the factors in Tables 4-2 and 4-3 to obtain temperature corrected cross section libraries. These libraries are simply edited versions of the original library and therefore are of the same format to be read by the transport code TWODANT. The first three positions in the Hansen-Roach library contain the absorption (σ_a), fission ($\nu\sigma_f$), and transport (σ_{tr}) cross sections. The transport cross section contains terms for the total cross section and the scattering cross section.

In general, correcting the cross sections for the "minor players" in the systems (O, N, S, F, and to some extent ^{240}Pu and ^{238}U) results in minor changes in k_{eff} . However, indiscriminately correcting hydrogen's transport cross section results in extreme variations

in k_{eff} . The hydrogen scattering (and therefore transport) cross section plays a major role in all aqueous systems. Clearly, the amount of hydrogen present and its importance as a moderator make it a primary nuclide in the analysis. Changing hydrogen's transport cross section by a tenth of a percent results in k_{eff} variations from 1.3 to 0.8 when the system should be critical.

Clearly the hydrogen scattering can not be treated in the manner indicated above. Scattering is a much different process from absorption. There is no indication that scattering can be corrected via Equations 4-4 and 4-5 (in fact, it has been seen from data in Chapter 5 that the scattering cross section of hydrogen increases with increasing temperature). By correcting the transport cross section with the factors in Tables 4-2 and 4-3, the scattering portion of the transport cross section is also changing. To rectify this situation, a new treatment which corrects only the absorption portion of the transport cross sections is developed. The transport cross section is given by

$$\sigma_{tr} = \sigma_t - \bar{\mu}\sigma_s . \quad (4-17)$$

Inserting the form of the total cross section and noting that the subscript zero again refers to the reference cross section and the prime denotes the corrected cross section, one obtains

$$\sigma_{tro} = \sigma_{ao} + \sigma_{so} - \bar{\mu}\sigma_{so} , \quad (4-18)$$

and

$$\sigma_{tr}' = \alpha\sigma_{ao} + \sigma_{so} - \bar{\mu}\sigma_{so} , \quad (4-19)$$

where α is the correction factor and σ_{tr}' is now only corrected for absorption. By subtracting Equation 4-18 from 4-19, evaluation of the mean cosine of the scattering angle is avoided, and the corrected transport cross section is written in terms of known quantities:

$$\sigma_{lr}' = \alpha\sigma_{ao} + (\sigma_{lro} - \sigma_{ao}) . \quad (4-20)$$

Using this to correct the transport cross sections (especially hydrogen's) results in a great improvement of the systems' behavior at different temperatures.

4.6 Temperature Reactivity Feedbacks for Solution Assemblies

Neutron temperature reactivity feedback coefficients for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* solution assemblies are calculated. The effective multiplications of the reference state (standard Hansen-Roach library at 20 °C) and two states at higher temperatures (corrected libraries at 25 °C and 30 °C) are obtained using TWODANT. By comparing the reactivities of each state, a temperature reactivity coefficient may be determined. The multiplication eigenvalues are converged to 8 and 6 decimal places for two-dimensional and one-dimensional (infinite cylinders) systems, respectively.

The reactivity feedback coefficients are obtained in the same manner as in Chapter 3. Plotting the reactivities versus temperature and performing a linear least-squares analysis on the data to obtain the slope yields the feedback coefficient. In general, all feedbacks are very linear, with correlation coefficients greater than 0.99. Data for the four solution assemblies may be seen in Tables 4-4 and 4-5.

Table 4-4. Effective multiplications for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* solution assemblies at 20, 25, and 30 °C

Assembly	k_{eff} (20 °C)	k_{eff} (25 °C)	k_{eff} (30 °C)
<i>CRAC</i> (207 g U/L)	0.971485	0.971402	0.971326
<i>KEWB-5</i>	1.040410	1.040328	1.040254
<i>SILENE</i>	0.995328	0.995098	0.994882
<i>SHEBA</i>	1.001990	1.001768	1.001560

Table 4-5. Neutron temperature reactivity feedback coefficients for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* solution assemblies

Assembly	Temperature Feedback Coefficient ($\Delta k/k/^\circ\text{C}$)	Temperature Feedback Coefficient ($\beta/^\circ\text{C}$)
<i>CRAC</i> (207 g U/L)	-1.685×10^{-5}	-0.1994
<i>KEWB-5</i>	-1.441×10^{-5}	-0.1801
<i>SILENE</i>	-4.505×10^{-5}	-0.5674
<i>SHEBA</i>	-4.278×10^{-5}	-0.6112

Note in Table 4-4 that the differences in k_{eff} are quite small. These correspond to the small temperature feedback coefficients seen in Table 4-5. The *CRAC* and *KEWB-5* assemblies have quite similar temperature coefficients, as do the *SILENE* and *SHEBA* assemblies. Again, *CRAC* and *KEWB* are very similar, both in geometry and composition, leading to the similarity seen in Table 4-5. *SILENE* and *SHEBA* are somewhat similar in geometry (they are both annular), but *SHEBA* is a much larger system with respect to both radius and solution height. Even though both systems have vastly different ^{235}U enrichments (5% for *SHEBA*, 93.5% for *SILENE*), they both have approximately the same amount of hydrogen and ^{235}U in solution. However, *SHEBA*'s temperature coefficient arises from ^{238}U absorption while *SILENE*'s is due to its lower uranium concentration. The similarity in temperature coefficients for these two assemblies is coincidental.

The *CRAC* series of experiments consisted of solutions of various uranium concentration (from approximately 50 g U/L to 383 g U/L). By performing the previous calculations on six of these experiments, reactivity feedback coefficients as a function of uranium concentration are obtained. Such calculations have also been performed using the British code WIMS for similar solution of 93 % enriched uranyl nitrate (Mather, et al., 1991a,b). The temperature coefficients are calculated for systems with the following

uranium content: 61.1, 91.8, 153.2, 207 (as before), 320, and 383 g U/liter of solution. Results may be seen in Figure 4-1. They are compared with those obtained by Mather. Mather's data points have been visually extracted from a figure in the previously mentioned reference.

Figure 4-1. Neutron Temperature reactivity feedback coefficient as a function of uranium concentration using the 16-group temperature corrections compared to data obtained by D. Mather.

There is a definite trend for both data sets to have a larger reactivity effect for the lower concentration solutions. However, the 16-group corrected values are smaller in magnitude than Mather's. Also, the data seem to converge at higher concentrations. Mather used 69-group sets evaluated at different temperatures to obtain his data. The convergence at high concentration and the large difference at low concentrations may indicate that the treatment of hydrogen in the 16-group corrections is inadequate. The

hydrogen certainly plays a more crucial role in the systems with low uranium concentration.

As previously mentioned, dilute plutonium solution calculations have indicated positive temperature coefficients. Infinite cylinders of plutonium (5% enriched with ^{240}Pu) of various density are mixed with unit density water and examined for effective multiplication values. Plutonium concentrations of 10.5, 20, 30, 40, 50, 60, 100, 200, 300, and 400 g Pu/liter of solution are investigated. Critical radii for each system determined from the original cross section set may be found in Table 4-6. Results of the study may be seen in Figure 4-2.

Table 4-6. Critical Radii for Infinite Cylinders of Plutonium and Water for Several Plutonium Concentrations using Hansen-Roach Cross Section Sets

Pu Concentration (g Pu/L)	Critical Radius (cm)
10.5	30.1
20	17.4
30	14.9
40	13.9
50	13.3
60	13.0
100	12.5
200	12.2
300	12.1
400	11.8

The data in Figure 4-2 clearly shows that many concentrations of plutonium solutions have positive neutron temperature coefficients. At 10.5 g Pu/L, the reactivity coefficient is $1.069 \times 10^{-4} \Delta k/k/^{\circ}\text{C}$, which corresponds to $4.86 \text{ } \phi/^{\circ}\text{C}$ ($\beta = 0.0022$). The graph crosses over to negative coefficients between 100 and 200 g Pu/L. Mather reported a

zero coefficient around 30 g Pu/L. His graph also tends much further negative after crossing to negative coefficients. Again, the 16-group temperature corrected results have smaller magnitudes than Mather's results.

Figure 4-2. Neutron Temperature reactivity feedback coefficient as a function of plutonium concentration mixed with unit density water in infinite cylinders using the 16-group temperature corrections.

Clearly, this method of correcting cross sections for temperature is inadequate. The scattering cross sections should not be corrected by the previous methods for they do not follow the same patterns as the absorption or fission cross sections. Another means of correcting the scattering cross sections is not readily apparent. This lack of understanding regarding such a temperature-dependent cross section correction has prompted the use of cross sections which have been evaluated at different temperatures, starting from the

original evaluated nuclear data files (ENDF). These include scattering effects for hydrogen at each temperature, making cross section corrections like those above unneeded.

CHAPTER 5

MANY-GROUP NEUTRON INTERACTION CROSS SECTION SETS

Data from Chapter 4 demonstrated that correcting the 16-group Hansen-Roach cross sections via Maxwellian flux-weightings is not completely adequate to describe temperature related phenomena with respect to reactivity feedbacks. However, trends in that data are readily apparent and agree in some form with previously obtained data. The next step is to study neutron temperature reactivity feedbacks by returning to the sources of cross section data and creating new cross section sets which are evaluated at different temperatures. This will avoid correction techniques to obtain temperature dependent cross sections as each cross section set will already be available for each temperature.

5.1 Background and History of Cross Section Generation

Nuclear cross sections have been and are continually being experimentally evaluated. Such evaluations include scattering properties, absorption, fission, and production cross sections. The experimental data is produced in point-wise form as a function of energy. The interpolated functional forms of the cross sections include low energy, epi-thermal, resonance, and fast regions of the neutron energy spectrum. This comprises a vast amount of data, which also requires much storage.

Much time and money has been allocated for proper evaluation of nuclear cross sections. Because such studies must be done for each isotope over the entire energy range, cross sections are evaluated by numerous parties throughout the world. In order to provide continuity and ease of technology transfer, the ENDF (Evaluated Nuclear Data File) format was created by H. Honeck at Brookhaven National Laboratory in the middle 1960's

(Koppel and Houston, 1978). The ENDF is divided into two parts: ENDF/A, which primarily includes data from private industry and laboratories *as it becomes available*; ENDF/B, which is comprised of data that is complete for all reactions of interest (Duderstadt and Hamilton, 1976). As experimental techniques improve and more accurate data is obtained, new versions of the Evaluated Nuclear Data File are produced. The latest version in use is ENDF/B-VI (Rose and Dunford, 1990).

Cross section evaluation of the heavier elements primarily involves absorption, isotopic production, and fission when appropriate. Neutron scattering from these elements is generally simple. However, for elements which moderate neutrons, such as hydrogen and carbon, the scattering properties are of primary importance. Not only is the scattering from the individual nuclei important, but when these atoms are bound in molecular forms, neutron scattering is altered. The bound nature of an atom influences the scattering properties, especially at low neutron energies. In order to account for this phenomenon, codes were developed to calculate the scattering properties given experimental data regarding the bound nature of the atoms.

5.2 Theory of the Scattering Law and Hydrogen in Water Scattering

The primary purpose of hydrogen or graphite in a nuclear system is to moderate the neutrons to thermal energies where the fissile isotopes' absorption cross sections are quite large. When the neutron energy is large (10's of eVs) the bound nature of molecules is unimportant. The neutron only sees the various nuclei as it travels through the medium. However, when the neutrons approach the thermal region as they slow down, the bound nature of the molecules becomes important. Quantum mechanically, the neutron may be treated as a travelling wave. When the neutron energy is low, certain wave properties may interact or interfere with the molecular structure, creating a form of scattering from the

molecule itself. For instance, if neutrons are travelling through a graphite lattice, the neutron waves may interfere after scattering off multiple carbon nuclei, especially if the neutron's energy/wavelength is of the same order as the distance between the carbon nuclei. As electromagnetic radiation scatters according to Bragg's law, so can discrete interference laws be applied to neutron waves (Egelstaff, 1966). Also, thermal neutrons are at thermal equilibrium with the surroundings; thus, upscatter and downscatter are continually occurring to preserve this equilibrium.

Neutron scattering, like any other wave, has two scattering components: incoherent and coherent. As the terms imply, coherent scattering is such that neutron waves from different scattering occurrences interfere with each other, and incoherent scattering assumes that the waves do not interfere. Each scattering component may also be divided into elastic and inelastic scattering. Thermal elastic scatter involves no energy loss, as the scattering is from the "infinite" mass of the lattice material (MacFarlane, 1988a,b). Inelastic scatter involves neutron energy loss, which is transferred to the lattice in the form of phonons, vibrations, or recoil. Generally, the coherent and incoherent inelastic scattering portions are combined, and the coherent and incoherent elastic cross sections are important for crystalline or hydrogenous solids (MacFarlane, 1988a,b). As the assemblies of interest in this study are hydrogenous systems, the inelastic scattering of neutrons from hydrogen in water is of primary concern.

The following is a rudimentary presentation of the mathematical expressions used to calculate the scattering properties of an inelastic scattering material (MacFarlane, 1988a,b). For the low energy neutron spectrum, and for inelastic scatter, the scattering cross section is given as:

$$\sigma(E \rightarrow E', \mu) = \frac{\sigma_b}{2kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S(\alpha, \beta) , \quad (5-1)$$

where μ is the cosine of the scattering angle, T is the absolute temperature of the system, E and E' are the incident and resultant neutron energy, and σ_b is the material's bound scattering cross section. The primary information for inelastic scatter comes from the scattering law, $S(\alpha, \beta)$, where α is the momentum transfer and β is the energy transfer given by:

$$\alpha = \frac{E' + E - 2\sqrt{E'E}\mu}{2kT} ; \quad (5-2)$$

$$\beta = \frac{E' - E}{kT} . \quad (5-3)$$

The experimental input to the calculation comes from the frequency spectrum of molecular excitations, given as a sum of different excitation modes:

$$\rho(\beta) = \sum_{i=1}^N w_i \rho_i(\beta) . \quad (5-4)$$

The spectra of the individual modes, $\rho_i(\beta)$, are weighted by the w_i 's, such that the overall frequency spectrum is normalized. For hydrogen in water, there are three important modes which comprise the basis for the scattering law:

1. As water is a liquid, neutrons are interacting with a material which has no lattice-type structure. Thus, *diffusive* behavior of the H_2O molecules is considered.
2. Water molecules have *discrete* frequencies of internal vibrations which may affect neutron scattering.
3. Water molecules may rotate or translate in a *continuous* fashion (as a function of energy transfer), given by a continuous frequency spectrum, called a solid-spectrum.

Thus, the scattering law is comprised of a continuous distribution of rotations, discrete oscillators, and molecular diffusive behavior.

Given the form of the continuous distribution and its overall weight, the discrete oscillator energies and their weights, and the diffusion parameters, the scattering law may be calculated. The portion of the scattering law from each excitation mode is calculated separately, and then added (convolved) to produce the final form. The continuous (solid-spectrum) form of the scattering law is given by

$$S_s(\alpha, \beta) = e^{-\alpha\lambda} \sum_{n=0}^{\infty} \frac{1}{n!} \left[\alpha \int_{-\infty}^{\infty} P_s(\beta) d\beta \right]^n T_n(\beta) , \quad (5-5)$$

where the following definitions apply:

$$T_0(\beta) = \delta(\beta) ; \quad (5-6a)$$

$$T_1(\beta) = \frac{P_s(\beta)}{\int_{-\infty}^{\infty} P_s(\beta') d\beta'} ; \quad (5-6b)$$

$$T_n(\beta) = \int_{-\infty}^{\infty} T_{n-1}(\beta') T_1(\beta - \beta') d\beta' , \quad n > 1 ; \quad (5-6c)$$

$$\lambda = \int_{-\infty}^{\infty} P_s(\beta) e^{-\beta/2} d\beta ; \quad (5-6d)$$

$$P_s(\beta) = \frac{\rho_s(\beta)}{2\beta \sinh(\beta/2)} . \quad (5-7)$$

Given the continuous distribution, Equation 5-7 is specified and the integrals in the sum are numerically evaluated. For discrete oscillators whose energies, and weights, w_i , are provided, the scattering law is given in terms of a modified Bessel's function by

$$S_i(\alpha, \beta) = e^{-\alpha \lambda_i} \sum_{n=-\infty}^{\infty} I_n \left[\frac{w_i \alpha}{\beta_i \sinh(\beta_i/2)} \right] \delta(\beta - n \beta_i) , \quad (5-8)$$

where,

$$\lambda_i = w_i \frac{\coth(\beta_i/2)}{\beta_i} , \quad (5-9)$$

and β_i is the normalized energy of the discrete oscillator. Finally, the diffusive component's scattering law is explicitly given in terms of a modified Bessel's function:

$$S_d(\alpha, \beta) = \frac{2d\alpha}{\pi} e^{2dc\alpha} \frac{\sqrt{c^2+0.25}}{\sqrt{\beta^2+4d^2\alpha^2}} K_1 \left\{ \sqrt{c^2+0.25} \sqrt{\beta^2+4d^2\alpha^2} \right\} , \quad (5-10)$$

and the frequency spectrum is also explicitly given in terms of two necessary parameters c (the diffusion constant) and d (approximately given by $w_d c$):

$$\rho_d(\beta) = \frac{4d}{\pi\beta} \sqrt{c^2+0.25} \sinh(\beta/2) K_1 \left\{ \sqrt{c^2+0.25} \beta \right\} . \quad (5-11)$$

The previous equations are numerically integrated and manipulated in the code LEAPR (MacFarlane, 1989). With the appropriate input parameters, LEAPR produces the thermal range scattering law in ENDF/B-IV format for use by a cross section generation code.

5.3 Hydrogen in Water for the LEAPR Code

The majority of the necessary input for the LEAPR code is available in the General Atomics (GA) thermal scattering data (Koppel and Houston, 1978), which contains input

parameters for the older counterpart to LEAPR, GASKET (Koppel, et al., 1967). The overall frequency spectrum weights for each portion are listed in Table 5-1.

There are two discrete oscillators, whose energies are 0.205 eV and 0.48 eV, with corresponding weights 0.166667 and 0.333333, respectively. Note that these w_i 's sum to the total discrete weight given in Table 5-1. The discrete w_i 's and β_i 's are then used in Equations 5-8 and 5-9 to compute the discrete form of the scattering law.

Table 5-1. Weights for Each Excitation Mode for Hydrogen in Water Thermal Neutron Scattering

Excitation Mode	weight
Continuous Spectrum	0.4444444
Discrete Oscillators	0.5
Diffusive	0.0555556

Note that the diffusive mode's weight in Table 5-1 is equal to $1/M$, where M is the mass of the molecule. LEAPR requires the translational weight (0.0555556) and the diffusion constant c , as seen in Equations 5-10 and 5-11. The GASKET code does not require the diffusion constant as input; therefore, it must be determined. By treating c as a free parameter, executing LEAPR for each different c , and then roughly comparing LEAPR's $S(\alpha, \beta)$ output to that from GASKET, the diffusion constant is determined. Sample results are shown in Figure 5-1.

Figure 5-1. $S(\alpha, \beta)$ as a function of the diffusion constant, c . $\alpha = 0.05$, $\beta = 0.0$; the desired value of $S(\alpha, \beta)$ is approximately 5.1.

The asymptotic behavior of Figure 5-1 may be derived from Equation 5-10. For β equal to zero and c large, Equation 5-10 reduces to

$$S_d(\alpha, 0) \approx \frac{c}{\pi} e^x K_1(x) , \quad (5-12)$$

where the substitution $x = 2dc\alpha$ has been made. As c grows, so does x ; however, for large x ,

$$\frac{d}{dx} [e^x K_1(x)] \approx 0 . \quad (5-13)$$

This tends to zero faster than c in Equation 5-12 diverges; thus, the asymptotic slope is zero. The asymptotic value is quite close to the reference value of $S(\alpha, \beta)$ as obtained by GASKET. The value for c which seems to adequately match the old data is $c = 120$.

The final required input is the form of $\rho_s(\beta)$, for use in Equations 5-5 through 5-7. The GASKET code allows for variable energy widths (the width is smaller in the region of a peak), while LEAPR does not. The data provided in the GA thermal scattering data book is therefore linearly interpolated where necessary to provide constant energy widths. The continuous energy spectrum is plotted in Figure 5-2.

Figure 5-2. Continuous frequency spectrum, $\rho_s(\beta)$, as a function of β .

The LEAPR output consists simply of some isotopic information and the scattering law data. Some sample $S(\alpha, \beta)$ data curves are plotted in Figure 5-3. Note that at low α , there is an upward trend in $S(\alpha, \beta)$. This is a result of the water molecule's diffusive behavior. Without the diffusive component, all curves peak and then turn downward at low α (MacFarlane, 1988a,b).

Figure 5-3. Sample LEAPR output of $S(\alpha, \beta)$ as a function of α for three values of β .

5.4 Creation of Temperature-Dependent Cross Section Sets

Any computer code which attempts to model the behavior of neutrons in a certain medium must have available to it the neutron interaction probabilities. Thus, cross sections must be input to the code in some format. In general, the continuous-energy form of the cross sections is far too unwieldy to be used in a timely fashion by a computer code. Thus, by using the multi-group approximation to discretize the energy spectrum, convenient forms of the cross sections become available.

Given the thermal scattering law data from LEAPR and the experimental or point-wise data from the ENDF/B files, neutron cross sections may be created using the NJOY code (MacFarlane, et. al., 1982), developed at Los Alamos National Laboratory. NJOY is a modular code, where each module performs specific operations on the cross sections. A general schematic of the cross section creation process is shown in Figure 5-4.

Figure 5-4. Schematic diagram displaying the important steps in the creation and use of neutron cross section sets. Parentheses indicate modules of NJOY.

The process begins primarily in the BROADR module, where the resonance cross sections are Doppler-broadened for each temperature desired from their reference condition at 0 K. Next, for isotopes where self-shielding is important, the UNRESR (not shown in Fig. 5-4) module corrects for self-shielding effects. The primary module for thermal systems is THERMR. The thermal scattering matrices from LEAPR are used for the bound systems, such as H in H₂O or C in graphite, and a free gas approximation is used for those isotopes where molecular binding is unimportant. Cross section grouping is performed by the GROUPE module. Grouped cross sections are calculated by assuming a group structure (several kinds may be defaulted) and a weighting flux. Finally, the cross sections are output in an intermediate *matxs* file by the MATXSR module. This file uses a format based on the CCCC (Committee on Computer Code Coordination) convention. By using appropriate interfacing codes, these cross sections are then made readable by a transport code.

Table 5-2 contains some selected parameters used as input to NJOY. In the THERMR module, the *iinc* parameter determines how the $S(\alpha, \beta)$ is to be formed; 1 denotes compute as a free gas (used for all isotopes except hydrogen) and 4 denotes read $S(\alpha, \beta)$ from a data file (provided by LEAPR). The maximum energy for thermal treatment is 4.6 eV. The primary group structure information may be found in the GROUPE section. Several group structures were investigated, but the one which adequately modelled both the high and low energy portions of the spectrum was the 69-group EPRI-CPM structure (*ign* = 9). The weighting flux (*iwt* = 6) for the group constant calculations was a combination of a thermal flux, a $1/E$, and a fission/fusion fast region. Cross sections for Legendre orders P_0 through P_5 were also calculated (*lord* = 5). Sample NJOY inputs may be found in Appendix C. The PLOTR module in NJOY also plots cross sections; sample cross section plots may be found in Appendix D.

Table 5-2. Selected input parameters for various modules in NJOY

BROADR		GROUPR	
errthn	0.002	ign	9
THERMR		iwt	6
nbin	8	lord	5
iinc	1 or 4	MATXSR	
icoh	0	npart	1
tol	0.01	ntype	2
emax	4.6	ngrp	69

Once the grouped cross sections are created and output by the MATXSR module, they still must be converted to a format readable by a transport code. The TRANSX code (MacFarlane, 1992) is the vehicle through which the formatted cross sections are transferred. The cross sections are read in from the *matxs* file and produced in *goxs* (group-ordered binary) format. By renaming the *goxs* file to *macrxs* and *snxedt*, the cross sections are then readable by TWODANT. A Bell-Hansen-Sandmeier transport correction is applied (consistent with past inputs), and P_1 scattering is assumed. Upscatter is allowed in the lowest 20 groups, and the thermal treatments can extend up through the lower 40 groups. Self-shielding calculations use a constant escape cross section (as opposed to a heterogeneous option). For this calculation, the assembly's mean chord length must be provided. This is given by (Lamarsh, 1966)

$$chord = \frac{4V}{A_s}, \quad (5-14a)$$

where V is the system's volume and A_s is the surface area. All geometries studied are of a cylindrical form. For an infinite cylinder, this is simply

$$chord = 2R; \quad (5-14b)$$

for a finite cylinder, the mean chord length is given by

$$chord = \frac{2RH}{R + H} , \quad (5-14c)$$

where the surface area is assumed to be both circular ends of the cylinder plus the round sides. Some assemblies have a central cylinder for a control/burst rod. It is assumed that this affects only the volume--most neutrons entering an empty void in the middle will pass through and reenter the solution. The mean chord length for such assemblies with outer radius R_o and inner radius R_i is then

$$chord = \frac{2 (R_o^2 - R_i^2) H}{(R_o^2 - R_i^2) + R_o H} . \quad (5-14d)$$

The cross sections may be evaluated at one or several temperatures. Two such temperature sets have been investigated: 300, 350, and 400 K; 293, 303, 313, 323, 333, 343, 353, 363, and 373 K.

5.5 General Results for Various Cross Section Sets

The standard cross section libraries available from Los Alamos National Laboratory are evaluated at 300 K and 400 K. Clearly, this is an extremely coarse temperature grid, and better resolution in this range is desired. The H in H₂O data calculated by GASKET is available at 300, 350, and 400 K. Even this seems somewhat coarse. A "reasonable" grid for such studies would be 10 °C increments.

The first method used to calculate the temperature dependent cross sections involves a single execution of LEAPR which calculates the scattering law data for each temperature (293, 303, 313, 323, 333, 343, 353, 363, 373). This produces one file containing the thermal scattering law data for each temperature. By then running NJOY for all isotopes at

these same temperatures, a grouped cross section file may be generated containing all isotopic cross sections at each temperature. In order to compare results to the old data, the cross sections have also been evaluated at 300, 350, and 400 K. This adds only the 350 K temperature to the existing grid. The data obtained from these 10 °C incremental temperatures is dubious.

Figure 5-5 contains the effective multiplication data for the *KEWB-5* assembly obtained from TWODANT using cross sections generated with 50 °C and 10 °C increments (note that these 10 °C increments are from 300 K to 380 K). It is known from experiments that this assembly has a negative temperature feedback coefficient. Clearly the data using 10 °C increments is not properly modelling the effective multiplication as a function of temperature. There is no initial positive temperature coefficient which then becomes negative in this assembly. However, note that the *general* trend of the 10 °C data is negative. Also, the oscillations appear to be converging in some sense at higher temperatures.

Several attempts have been made to eliminate the instability in the effective multiplications. Tightening convergence criteria, reducing grid spacings in LEAPR, and calculating 5 °C temperature increments do not alleviate the problem. However, it is noted that when the temperatures are calculated with different initial temperatures (e.g. 293 K and 300 K), even though the oscillations were present in both sets, the initial two points appeared to be numbers appropriate for use in temperature coefficient calculations. That is, the effective multiplication at 293 K was slightly higher than 300 K. This might indicate that the decoupling of the scattering law calculations may be a more effective means of obtaining temperature coefficients. Thus cross section sets are calculated at each temperature separately and saved in separate files--one cross section file for each

temperature. The results for the *KEWB-5* assembly using these new cross section sets may be found in Figure 5-6.

Figure 5-5. Effective multiplications for the *KEWB-5* assembly as a function of temperature using 50 and 10 °C temperature increments.

The data shown in Figure 5-6 is an extreme improvement over that seen in Figure 5-5. The effective multiplications appear quite linear as a function of temperature, but the absolute values of k_{eff} are quite different (1.030 as opposed to 1.015 for a 1.5 % difference). The reason for this discrepancy is not apparent. However, the linear nature of this data combined with the oscillatory nature of the coupled cross section sets seems to indicate that the decoupled sets are more suitable for temperature coefficient calculations. Again, the difference in k_{eff} is relatively small, and only slopes are desired.

Assuming that the data obtained using the decoupled cross section sets is more appropriate than the coupled sets, the previous analysis seems to indicate that LEAPR has

difficulty calculating multiple temperature scattering laws accurately. Testing LEAPR at 300, 350, and 400 K against the established cross sections from GASKET seemed to provide agreement between LEAPR and GASKET. However, this indicates that the problems may occur at low temperature spacings. Again, the decoupled sets appear to be adequate for calculating temperature coefficients, and are the best alternative seen thus far.

Figure 5-6. Effective multiplications for the *KEWB-5* assembly as a function of temperature using the 10 °C decoupled temperature increments.

5.6 Effects of Legendre Scattering Order on Calculations

The cross sections created by TRANSX are such that P_5 scattering may be used. However, throughout the study only P_1 scattering is used. In order to test the effect of the Legendre scattering order, test cases using the *KEWB-5* assembly are performed using P_1 and P_3 scattering. The 50 °C temperature grid is used for simplicity. A plot of the effective

multiplication versus temperature may be seen in Figure 5-7. The least squares line fits for each curve are

$$P_1: \quad k_{eff} = -2.2335 \times 10^{-5} T + 1.0224 ; \quad (5-15a)$$

$$P_3: \quad k_{eff} = -2.2348 \times 10^{-5} T + 1.0231 . \quad (5-15b)$$

Figure 5-7 seems to indicate that the difference in the effective multiplication is much more discernable than the difference in the slopes. The slopes and intercepts in Equations 5-15a and 5-15b both differ by 0.06 %, which is considered to be negligible. Because the P_3 calculations require significantly more computer execution time than the P_1 calculations, and the effects of using the higher Legendre order are rather insignificant, all calculations will continue to use P_1 scattering.

Figure 5-7. Effective multiplications for the *KEWB-5* assembly as a function of temperature using P_1 and P_3 Legendre order scattering.

CHAPTER 6

69-GROUP NEUTRON TEMPERATURE REACTIVITY FEEDBACK

Having established the 69-group structure as adequate for modelling the low energy portion of the cross section sets, the first step in calculating temperature feedback coefficients is complete. It is also assumed that the 10 °C incremental temperature cross section sets (293 K to 373 K) are the best available and are able to accurately describe the behavior of neutrons at these temperatures. With these two points in mind, temperature feedback coefficients are calculated.

6.1 Temperature Coefficients for the Solution Assemblies

As in Chapter 4, the temperature reactivity feedback coefficients for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* fissile solution assemblies are calculated. In these calculations all steel is removed so that only the solution itself is being analyzed. As in the other studies using TWODANT, an angular quadrature order S₈ is used consistently, and all k_{eff} values have been converged to 1×10^{-8} . Effective multiplications for each assembly may be found in Table 6-1.

Note from Table 6-1 that in each case except *CRAC*, the effective multiplications are slightly below those seen in Table 4-4 (k_{eff} 's for 16-group corrections). *CRAC*'s effective multiplication is slightly higher than in Table 4-4, but it is still quite close. Without the steel outer shell to reflect some neutrons back into the system, the effective multiplications should be lower. Also note that the *SHEBA* effective multiplications are significantly lower than those in Table 4-4. The cross section sets created do not include the isotope ¹⁹F (the data has not been converted to ENDF/B version VI as of this study).

The smaller multiplications for *SHEBA* are due to the steel being removed and the small amount of moderation lost due to the absence of fluorine. Comparison with the old 50 °C incremental data, which includes fluorine (from ENDF/B-V), does not indicate any loss of accuracy by this assumption.

Table 6-1. Effective multiplications for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* assemblies using cross section sets evaluated at every 10 °C increment between 293 K and 373 K

Temperature	<i>CRAC</i> (207) k_{eff}	<i>KEWB-5</i> k_{eff}	<i>SILENE</i> k_{eff}	<i>SHEBA</i> k_{eff}
293	0.973368	1.032155	0.985423	0.971384
303	0.973302	1.032062	0.984953	0.970694
313	0.972929	1.031695	0.983817	0.969169
323	0.972677	1.031449	0.982925	0.967974
333	0.972424	1.031201	0.981992	0.966619
343	0.972011	1.030798	0.980889	0.965381
353	0.971718	1.030512	0.979921	0.964101
363	0.971372	1.030171	0.978946	0.962943
373	0.971061	1.029860	0.977997	0.961646

An important consideration for evaluating the effectiveness or accuracy of any cross section set is benchmarking. The 16-group Hansen-Roach cross section set is widely used throughout the nuclear industry, and has been rather strenuously tested for applicability in both fast and thermal systems. Assuming that the Hansen-Roach cross sections have been adequately benchmarked leads to the supposition that the results obtained using the Hansen-Roach cross sections are accurate. By comparing the reference cases' effective multiplications obtained with the 69-group sets with those obtained using Hansen-Roach, a crude and simple method for benchmarking the new cross section sets is possible. Noting the effect of the steel casings and that the same general geometries and mesh formats have

been preserved, it is apparent that the excellent agreement between the data in Tables 6-1 and 4-4 supports the claim that the 69-group cross section sets are applicable to these systems and allow accurate calculations of critical eigenvalues. The 69-group cross section set has effectively been benchmarked against the 16-group Hansen-Roach set.

By evaluating reactivities at each temperature and calculating the best fit line using least squares techniques, the neutron temperature coefficient is obtained from the slope of that line. In general, correlation coefficients are at or above 0.99, indicating that the curves are near linear. With the 10 °C temperature grid, the least squares correlation coefficients decrease as the temperature coefficients decrease. However, this is not surprising as the closer the slope is to zero, the smaller the differences in k_{eff} must be. Table 6-2 contains the temperature reactivity feedback coefficients for the assemblies of interest. The appropriate effective delayed neutron fractions are used as in Chapter 3.

Table 6-2. Neutron temperature coefficients for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* assemblies using cross section sets evaluated at 10 °C increments between 293 and 373 K

Assembly	Temperature Feedback Coefficient ($\Delta k/k/^{\circ}\text{C}$)	Temperature Feedback Coefficient ($\beta/^{\circ}\text{C}$)
<i>CRAC</i> (61.1 g U/L)	-1.046×10^{-4}	-1.3514
<i>CRAC</i> (207 g U/L)	-3.192×10^{-5}	-0.3778
<i>CRAC</i> (320 g U/L)	-1.817×10^{-5}	-0.2128
<i>KEWB-5</i>	-2.801×10^{-5}	-0.3501
<i>SILENE</i>	-9.951×10^{-5}	-1.2533
<i>SHEBA</i>	-1.337×10^{-4}	-1.9096

An important consideration regarding the temperature coefficients in Table 6-2 is how they compare to the volumetric expansion coefficients obtained in Chapter 3. A differential change in volume is related to a differential change in temperature by

$$\frac{dV}{V} = \beta dT , \quad (6-1)$$

where β is the system's volume expansion coefficient. Thus, the volumetric expansion coefficient may be converted into a temperature coefficient. This simply determines what the coefficient would be if it were a temperature coefficient. For water at 20 °C, a typical value for β is $210 \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$. By multiplying the expansion coefficients by βV , the units $\$/\text{m}^3$ may be converted to $\$/^\circ\text{C}$. Table 6-3 contains the volumetric coefficients reported in Table 3-10, the temperature coefficients with adjusted units, and the sum of the two effects for an overall temperature coefficient. The total effect has been experimentally determined for the *CRAC* (Barbry, 1973), *KEWB-5* (Dunenfeld and Stitt, 1963), and *SILENE* (Barbry) assemblies. These comparisons may be seen in Table 6-4.

Table 6-3. Comparison of Volumetric and Neutronic Temperature Feedback Coefficients for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* assemblies

Assembly	Volumetric Feedback Coefficient ($\$/^\circ\text{C}$)	Temperature Feedback Coefficient ($\$/^\circ\text{C}$)	Total Feedback Coefficient ($\$/^\circ\text{C}$)
<i>CRAC</i> (61.1 g U/L)	-2.067	-1.351	-3.418
<i>CRAC</i> (207 g U/L)	-1.777	-0.378	-2.155
<i>CRAC</i> (320 g U/L)	-1.805	-0.213	-2.018
<i>KEWB-5</i>	-1.814	-0.350	-2.164
<i>SILENE</i>	-1.632	-1.253	-2.885
<i>SHEBA</i>	-1.235	-1.910	-3.145

Note in Table 6-4 that there is a significant discrepancy between the experimental and calculated temperature coefficient values. It is not apparent which portion of the temperature feedback is responsible for the error, what the geometric effects may be, or how accurate the experimental values are.

Table 6-4. Calculated and Experimental Temperature Feedback Coefficients for the *CRAC*, *KEWB-5*, and *SILENE* assemblies

Assembly	Total Feedback Coefficient ($\beta/^\circ\text{C}$)	Experimental Feedback Coefficient ($\beta/^\circ\text{C}$)
<i>CRAC</i> (61.1 g U/L)	-3.418	-4.4
<i>CRAC</i> (207 g U/L)	-2.155	-4.0
<i>CRAC</i> (320 g U/L)	-2.018	-3.7
<i>KEWB-5</i>	-2.164	-5.3
<i>SILENE</i>	-2.885	-6.4

The second important calculation involving the uranium-fueled solution assemblies involves a larger study of the various *CRAC* experiments which varied uranium content. Temperature coefficients are obtained for the same experiments listed in Chapter 4: 61.1, 91.8, 153.2, 207, 320, and 383 g U/liter of solution, plus those at 166 and 211 g U/L and a fictitious assembly at 122.5 g U/L (the data for this assembly is interpolated between that for the 91.8 and 153.2 g U/L assemblies). Temperature reactivity coefficients along with the least-squares correlation coefficient are listed in Table 6-5. Note that the temperature coefficient for *SILENE* (at 71 g U/L) in Table 6-2 will clearly be in agreement for a uranium solution at this concentration. This indicates that the spectral temperature coefficients are primarily dependent on the solution's composition rather than geometry (as expected).

As the reactivity feedback coefficients grow smaller, the correlation coefficients also grow smaller, indicating a degradation in the linear properties of the data. Again, this shows how smaller slopes require smaller differences in k_{eff} to accurately fit the data. However, even at the high concentrations, the data fits are still quite linear. These temperature coefficients are plotted in Figure 6-1 and are compared to Mather's data in Figure 4-1 (Mather, et al., 1991a,b).

Table 6-5. Neutron temperature reactivity feedback coefficients and least squares correlation coefficients for 8 *CRAC* experiments

<i>CRAC</i> Assembly (g Uranium/Liter)	Temperature Feedback Coefficient ($\Delta k/k/^\circ\text{C}$)	Linear Least Squares Correlation Coeff. (R^2)
61.1	-1.046×10^{-4}	0.9969
91.8	-7.784×10^{-5}	0.9963
122.5	-5.368×10^{-5}	0.9947
153	-4.202×10^{-5}	0.9931
166	-4.182×10^{-5}	0.9931
207	-3.192×10^{-5}	0.9909
211	-2.964×10^{-5}	0.9907
320	-1.817×10^{-5}	0.9830
383	-1.492×10^{-5}	0.9780

Figure 6-1 clearly indicates a strong agreement between the data obtained using 69-group cross section sets and data previously obtained by Mather. There seems to be slight discontinuities in the data near 150 and 200 g U/L, but these are small in magnitude and the general trends in the data are quite well preserved. These coefficients are a vast improvement over the temperature coefficients derived from flux-weighted correction factors. Note that the 69-group data has the same general shape as Mather's data, but all values are shifted so that they are farther negative. Again, these temperature coefficients are for actual *CRAC* experiments, where Mather's are for similar uranyl nitrate solutions.

As with Table 6-1, the data in Tables 6-2 and 6-5 is readily compared to its counterpart data in Table 4-5 and Figure 4-1. First, it is apparent that the 69-group temperature coefficients are consistently higher than the 16-group temperature coefficients. Second, they differ by varying degrees. For Table 6-2, the *CRAC* and *KEWB-5* assemblies have 69-group temperature coefficients 89% and 94% higher than those in Table 4-5, respectively. *SILENE* and *SHEBA* differ from the data in Table 4-5 by 121%

and 213%, respectively. This phenomenon is quite interesting if analyzed from a certain perspective. By plotting the percent difference versus the hydrogen concentration in each assembly, an interesting trend appears (see Figure 6-2).

Figure 6-1. Neutron temperature reactivity feedback coefficient as a function of uranium concentration in the CRAC series of experiments using the 69-group cross section sets and comparing to data obtained by Mather.

Figure 6-2 lends further credence to the hypothesis that the primary deficiency with the flux-weighted cross section corrections for the 16-group Hansen-Roach set is their inability to correct the hydrogen scattering cross sections. Clearly, as the hydrogen amount in the system increases, the importance of proper treatment of hydrogen in water is magnified. Also note from Appendix D that the scattering cross section for hydrogen *increases* with increasing temperature. The correction techniques in Chapter 4 would have assumed just the opposite if used on the scattering cross sections.

Figure 6-2. Percent difference in temperature coefficients versus hydrogen concentration between the 69 and 16-group evaluations.

6.2 Temperature Coefficients for Plutonium Infinite Cylinders

In Figure 4-2, it is seen that at low concentration, infinite cylinders of plutonium mixed with unit density water exhibit a strongly positive temperature reactivity effect. The temperature coefficient tapers off as the plutonium concentration increases, finally becoming negative around 200 g Pu/L. The same calculations were performed for the 69-group cross section sets. Each solution is comprised only of unit density water and plutonium, enriched to 5% in ^{240}Pu . The critical radius of each cylinder is determined using the reference cross section set (293 K), so that all data are referred to a critical state, primarily for aesthetic reasons. (It is noted that the temperature coefficients are not very dependent on the reference state.) Critical radii used may be seen in Table 6-6. More confidence is placed on these calculations, so more sample assemblies are studied. The results of these temperature reactivity coefficients may be found in Figure 6-3.

Table 6-6. Critical Radii for Infinite Cylinders of Plutonium and Water for Several Plutonium Concentrations

Pu Concentration (g Pu/L)	Critical Radius (cm)	Pu Concentration (g Pu/L)	Critical Radius (cm)
10.5	32.5	60	13.1
15	21.3	80	12.8
20	17.7	100	12.6
25	16.1	150	12.5
30	15.1	200	12.4
35	14.5	250	12.4
40	14.0	300	12.4
45	13.7	350	12.4
50	13.5	400	12.4

Figure 6-3. Temperature reactivity feedback coefficient of a hypothetical mixture of plutonium (5% ²⁴⁰Pu) and unit density water in critical infinite cylinders using 69-group cross section sets.

A similar graph presented by Mather appears both quantitatively and qualitatively similar. In Figure 4-2, the last data point (400 g Pu/L) turned upwards slightly. In Figure 6-3, the higher concentration solutions become less negative as plutonium concentration increases. Again, this furthers the notion that trends seen in the corrected 16-group cross sections may be accurate, but that the actual magnitudes of the feedback coefficients are reduced with respect to the 69-group coefficients. A comparison of the data found in Figure 6-3 and the 16-group Hansen-Roach cross sections temperature coefficients may be found in Figure 6-4. The plutonium temperature coefficient becomes negative near 20 g Pu/L (Mather's graph becomes negative around 30 g Pu/L), with a peak feedback coefficient of $1.583 \times 10^{-4} \Delta k/k/^{\circ}\text{C}$ ($7.19 \phi/^{\circ}\text{C}$) at 10.5 g Pu/L. The relative extremum seen in the negative region occurs around 80 g Pu/L, with a spectral temperature feedback coefficient of $-9.113 \times 10^{-5} \Delta k/k/^{\circ}\text{C}$ ($-4.14 \phi/^{\circ}\text{C}$).

Figure 6-4. Comparison of temperature coefficients using the 69-group cross sections and the 16-group Hansen-Roach flux-weighted cross sections.

It is also possible to compare the spectral temperature coefficient to volumetric expansion for the system at 10.5 g Pu/L. A typical volumetric expansion coefficient (derived from two specific systems with volumes of 322 and 336 L) is $-280 \text{ } \$/\text{m}^3$, which corresponds to $-1.93 \text{ } \phi/^{\circ}\text{C}$ using Equation 6-1. Even though the spectral temperature coefficient is determined with different geometries, this feedback is almost geometry independent. As previously mention, the spectral temperature coefficient for 10.5 g Pu/L solution is $7.19 \text{ } \phi/^{\circ}\text{C}$, which is significantly higher in magnitude than the system's volumetric expansion feedback coefficient. However, as seen in Table 6-4, there are significant discrepancies in the calculated and experimental temperature coefficient values, and if this discrepancy is primarily due to the volumetric feedback portion, the positive effect seen in this dilute plutonium system may not be so great.

6.3 Temperature Coefficients for Poisoned Infinite Cylinders

These positive temperature coefficients for low concentration plutonium solutions have been seen in diffusion calculations (Suzaki, et al., 1987). In this same paper, the effect of a soluble poison is shown to *enhance* the positive effect. Gadolinium is the primary poison used in plutonium nitrate solutions due to its excellent solubility properties and compatibility during separation or extraction processes (Lloyd, et al., 1972). By placing some gadolinium in the already existing solutions, the effect of a soluble poison such as gadolinium on the temperature reactivity feedback may be studied.

Lloyd performed critical experiments on cylinders containing plutonium nitrate and dissolved Gd_2O_3 . The lowest concentration of plutonium was 116 g Pu/liter, which allowed large amounts of gadolinium to be placed in solution without extremely increasing the critical dimensions. In this study, only 0.1 g Gd/L is added to the solutions. This is to prevent the low concentration solution data from being enormously affected by the presence of the poison.

Gadolinium has seven stable isotopes. To simplify the calculations only the two "poisonous" isotopes are added to the plutonium solutions. ^{155}Gd and ^{157}Gd have thermal absorption cross sections of 61,000 and 255,000 barns, respectively, and each comprises about 15% of natural gadolinium. The largest cross section of any other isotope is 80 barns (^{154}Gd). Thus, the actual amount of gadolinium in the solutions is less than 0.1 g Gd/L; however, the effects of the poison should be the same as if all isotopes were present. Figure 6-5 shows the critical radii of infinite cylinders of poisoned and unpoisoned plutonium solutions. The 10.5 g Pu/L poisoned assembly's effective multiplication is below k_{∞} .

As expected, the effect of the gadolinium poison weakens as the plutonium concentration increases. However, all trends seen in Figure 6-3 are maintained. The temperature feedback for the poisoned system is graphed along with the data from Figure 6-3 in Figure 6-6. The poisoned system exhibits divergent positive temperature coefficients at low plutonium concentrations, eventually crossing to negative, and then turning slightly upward (yet remaining negative) as the plutonium concentration increases. However, it is readily apparent that the presence of the poison causes the temperature feedback coefficients to shift upward (more positive/less negative).

Figure 6-5. Critical radii of hypothetical mixtures of poisoned and unpoisoned plutonium solutions in infinite cylinders using 69-group cross section sets.

Appendix D contains a plot of ^{157}Gd 's total cross section. Thermal energies are very near a region where the cross section appears $1/v$ below thermal energies and then it

immediately drops off rapidly at higher energies (much faster than $1/v$). As the temperature of the system increases, gadolinium's absorption cross section decreases faster than would be expected from a $1/v$ absorbing isotope (such as ^{10}B), giving rise to a net positive effect on system reactivity. Suzuki noted that using a poison such as ^{10}B does not appreciably affect the spectral temperature coefficient of the plutonium solutions. Therefore, this effect is primarily due to the non- $1/v$ nature of gadolinium.

The poisoned system certainly exhibits general properties similar to the unpoisoned one, but the positive reactivity coefficients are increased, and the negative ones become less so. The temperature coefficient becomes negative between 50 and 60 g Pu/L. At 10.5 g Pu/L (subcritical), the temperature coefficient is $5.124 \times 10^{-4} \Delta k/k/^{\circ}\text{C}$ ($23.3 \phi/^{\circ}\text{C}$). The relative minimum in the negative region occurs in the vicinity of 150-200 g Pu/L at $-5.511 \times 10^{-5} \Delta k/k/^{\circ}\text{C}$ ($-2.50 \phi/^{\circ}\text{C}$). As the plutonium concentration increases, the relative effect of the gadolinium decreases, and the two plots converge into each other. However, this convergence is such that the poisoned system consistently exhibits greater (less negative) temperature feedback coefficients.

Generally, such phenomena exhibited here seem most counter-intuitive. As plutonium concentration decreases, the severity of an accidental criticality becomes a very important issue. Then, by poisoning the system with a certain element, the deleterious effects are enhanced. However, the addition of the poison also makes the possibility of criticality less probable.

Figure 6-6. Comparison of temperature reactivity feedback coefficients in poisoned and unpoisoned plutonium solutions in critical infinite cylinders using 69-group cross section sets.

6.4 Temperature Coefficients for Plutonium in Finite Cylinders

Having studied the neutronic temperature coefficients of infinite cylinders of aqueous plutonium, the next logical step is to investigate plutonium solution assemblies of finite geometry, especially when criticality experiments have been performed on such systems.

LA-10860-MS is a data base-like collection of critical experiments for systems containing fissile isotopes (Paxton and Pruvost, 1987). Included in this document is a series of French experiments with plutonium nitrate ($\text{Pu}(\text{NO}_3)_4$) in water-reflected cylinders. Critical heights and specific compositions are listed in Table 6-7.

Table 6-7. Critical Dimensions and Compositions for Finite Cylinders of Plutonium Nitrate

H/Pu Ratio	Pu Density (g Pu/L)	NO ₃ Density (g NO ₃ /L)	Critical Height (cm)
540	45.5	177	26.3
650	38.2	176	29.0
750	33.3	168	32.7
830	30.1	161	35.6
890	28.0	152	38.5
980	25.7	146	43.7
1070	23.4	145	51.6

The plutonium consists of 98.5% ²³⁹Pu and 1.5% ²⁴⁰Pu. The cylinder containing the fissile solution has a 33.0 cm. outside diameter, with a stainless steel liner 3 mm. thick. The reflector is 40 cm. thick, and is assumed to be on the lateral surface only. In the studies, the stainless steel liner is neglected (thus, the outside diameter of the fuel becomes 32.4 cm.). A schematic diagram of the geometry may be seen in Figure 6-7. The solution and reflector always have the same height in each experiment.

Figure 6-7. Geometry used for finite cylinders of aqueous plutonium solutions surrounded by a water reflector.

All concentrations are determined from the data in Table 6-7. The nitrate concentration specifies nitrogen concentration, regardless if it came from the metal salt or nitric acid. The plutonium concentration is given, and the hydrogen concentration is obtained from the H/Pu ratio. Assuming that oxygen is only found in water or in the nitrate, it too is then completely specified.

Given the geometry in Figure 6-7, the study actually consists of three different geometries. The first portion uses the critical assemblies at various heights with the water reflector in place. Second, these assemblies are also analyzed for temperature feedback coefficients at the reflected critical height with the reflector removed. Clearly these will be subcritical. Finally, the unreflected systems are analyzed at their critical heights. This should test the effect of the water reflector as well as the effect of criticality on the temperature coefficient (this latter effect should be primarily geometric).

Because these are somewhat more complicated geometries and are large systems, the computational times become rather large for these systems. Therefore, the data is converged to 1×10^{-6} instead of the previously standard 1×10^{-8} . For the critical systems, all effective multiplications are close to unity (between 0.98 and 1.02). For the subcritical unreflected systems, effective multiplications are near 0.90. The water reflector clearly has a significant effect on the systems' criticality. Table 6-8 contains the temperature feedback coefficients for each plutonium concentration and each geometry. The data is also plotted in Figure 6-8. The critical reflected system is denoted by *Reflected*, the unreflected critical system is denoted by *Critical*, and the unreflected subcritical system by *Subcritical*.

Table 6-8. Temperature Reactivity Feedback Coefficients for Finite Cylinders of Plutonium Nitrate with the Reflector (Critical) and without the Reflector (Critical and Subcritical)

H/Pu ratio	Reflected $\Delta k/k/^\circ\text{C}$	Critical $\Delta k/k/^\circ\text{C}$	Subcritical $\Delta k/k/^\circ\text{C}$
540	-2.903×10^{-5}	-7.499×10^{-5}	-9.010×10^{-5}
650	-1.710×10^{-5}	-6.580×10^{-5}	-8.012×10^{-5}
750	-4.037×10^{-6}	-5.630×10^{-5}	-6.896×10^{-5}
830	6.379×10^{-6}	-4.800×10^{-5}	-6.134×10^{-5}
890	1.477×10^{-5}	-4.209×10^{-5}	-5.555×10^{-5}
980	2.672×10^{-5}	-3.206×10^{-5}	-4.405×10^{-5}
1070	4.105×10^{-5}	$-2.319 \times 10^{-5} \dagger$	-3.307×10^{-5}

$\dagger$ This system is near or below the critical radius of an infinite cylinder and is therefore modelled as an infinite cylinder.

Figure 6-8. Temperature reactivity feedback coefficients for finite cylinders of plutonium nitrate with the reflector (critical) and without the reflector (critical and subcritical).

The most interesting feature in Figure 6-8 is that some of the reflected systems have positive temperature coefficients. Again, these are actual systems on which critical experiments have been performed. The temperature coefficient crosses from positive to negative around 32 g Pu/L; this is significantly higher than the concentration for the infinite cylinders. The most plausible explanation for this is that the water reflector makes the plutonium concentration appear less than it actually is. A 32 g Pu/L system with a water reflector may correspond neutronically to a 20 g Pu/L unreflected system. For the unreflected systems, the curves extrapolate to 17 or 18 g Pu/L where the temperature coefficient changes sign. This corresponds well with the data obtained using infinite cylinders. Also, all three curves have the same general shape, and would correspond to the area between the relative minimum and the divergence in the infinite cylinder graphs.

The second feature in Figure 6-8 is the closeness between the two unreflected systems. The critical systems have the same radius as the subcritical assemblies, but they also have much larger heights. Because the subcritical assemblies are so much smaller than their critical counterparts, neutron leakage should be more important. Since both data sets correspond to the same radius, the primary phenomenon responsible for the difference in temperature coefficients is the difference in axial leakage. In the small systems the axial leakage is more important, creating a more negative temperature coefficient, as seen in the figure. In general, the finite geometry plutonium solutions have temperature coefficients which agree well with the infinite systems, in both magnitudes and shapes.

CHAPTER 7

SUMMARY AND CONCLUSIONS

The volumetric feedback coefficients for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* solution assemblies have been calculated. These were assumed to be decoupled from neutronic temperature coefficients as the source of the volumetric expansion could come from thermal expansion or radiolytic gas bubble production. The effect of a uniformly distributed density on the criticality of these systems was determined. During slow transients (sub-prompt critical), this is the most likely form of volumetric feedback as there is time for mixing currents to be established which uniformly mix the solution as density changes. During fast transients, the rate of energy deposition may be so great that mixing can not occur. Therefore, the effect of density redistribution throughout the assembly was studied. The effect of radial and axial leakage on the feedbacks was also studied by considering density redistribution separately in the axial and radial directions. As expected, the radial effects were more important. The magnitude of the feedbacks varied throughout the assemblies due to geometric effects and solution properties. All volumetric feedback coefficients were constants, as reactivities as functions of volume increases were linear. In general the method used for calculating the volumetric feedback coefficients seemed to be effective for this purpose.

Volumetric expansion coefficients were calculated for three of the *CRAC* experiments. In order to expand the data base for dynamics calculations, expansion coefficients for other *CRAC* experiments should be calculated. Also, primarily uranium solutions were studied for expansion feedback. Only one plutonium solution was examined for volumetric expansion feedback. Because different plutonium solutions will be studied further, expansion coefficients for such systems will also need to be calculated.

Two methods were used for calculating neutronic temperature coefficients. The first used a flux-weighted Maxwellian temperature correction for the 16-group Hansen-Roach cross section library. By correcting cross sections for temperature increases and not affecting the geometry (as would be required for thermal expansion), the reactivity effect from neutron spectral shifts upward in energy due to temperature increase could be studied. Only the absorption and fission cross sections (where applicable) were corrected via this method. Methods for correcting scattering cross sections were not investigated. In general, the shapes of the temperature coefficients for uranium solutions were consistent with past numerical experiments, but the magnitudes of the temperature coefficients were smaller than expected. The plutonium solutions exhibited positive temperature coefficients at low concentration, and again were smaller in magnitude than past calculations. The primary pitfall in this correction technique was the inability to correct for hydrogen scattering. This prompted the creation of cross section sets at various temperatures from original ENDF/B-IV data for use in temperature coefficient calculations. This method will avoid having to correct cross sections for temperature increases.

An area for further study regarding the cross section temperature corrections may be to determine a proper way to correct the scattering cross sections for temperature increases. The temperature corrections currently used qualitatively exhibit the proper behavior, but are not accurate in quantitative respects. However, the fact that the 16-group cross section corrections did so well with such a crude correction model is impressive. Also, the 16-group library is convenient and calculations are rather timely.

Neutronic temperature coefficients were then calculated with 69-group cross sections sets created by the NJOY code. This involved compiling appropriate input parameters for the LEAPR code, which evaluated the thermal scattering law for hydrogen in water at various temperatures. Every other isotope in the assemblies used a free gas

scattering approximation. The cross sections for use in temperature coefficient calculations were evaluated at 10 °C increments between 293 K and 373 K, inclusive. Cross sections were prepared for use by TWODANT with the TRANSX code. When LEAPR was used to calculate the thermal scattering law for each temperature in one execution, the effective multiplications as a function of temperature were oscillatory, especially at low temperature. By calculating the thermal scattering law for each temperature separately, the effective multiplications as functions of temperature became quite linear.

Temperature coefficients were again calculated for the *CRAC*, *KEWB-5*, *SILENE*, and *SHEBA* solution assemblies. They were also calculated for several different *CRAC* experiments. These results agreed with British calculations qualitatively and quantitatively. Generally, temperature coefficients were primarily dependent on the solution's composition. Plutonium solutions exhibited positive temperature coefficients at low concentration. These results also agreed well with previous studies. The positive temperature effect seen in these solutions was enhanced by the addition of a gadolinium soluble poison, due to its non- $1/v$ nature. Concentrations with negative temperature coefficients saw their coefficients shifted upward so that they were less negative. Some French experiments using water-reflected plutonium solutions were studied for the effect of the reflector on the temperature coefficients. Because of the water reflector, the effective concentration of the plutonium solutions was decreased, giving rise to positive temperature coefficients in these assemblies. No mention of such temperature coefficients in these or any other actual plutonium solution assemblies has been seen in literature thus far. In general, the results from these temperature coefficient calculations seem to be accurate in modelling this feedback mechanism. Experimentally, this is surely an area suited for further research.

It was noted that the temperature coefficients were primarily composition dependent. The effect of various isotopes (especially ^{238}U and ^{240}Pu) on these coefficients may be readily seen by removing them from the system and noting the change in the temperature coefficient. For low enrichment systems like *SHEBA*, the removal of ^{238}U may affect the system greatly, while removal of ^{238}U from high enrichment solutions may not appreciably change the temperature coefficients. Also, in order to gain a complete understanding of the various other parameters which affect reactivity feedback coefficients, it may be desirable to continue this study by creating a data base where geometry and composition are the adjustable parameters. This was begun in this study--temperature coefficients for the *CRAC* series were obtained for different critical heights, and for the plutonium solutions at different critical radii. By extending the study to include the effects of height, radius, and concentration, a complete data base of neutron temperature and volumetric expansion feedback coefficients may be obtained.

Further study should be made regarding the LEAPR code and its ability to calculate thermal scattering laws for several temperatures at one time. This study was able to avoid the difficulties here, but any such problems in the primary computer code for generating cross section libraries may result in questioning the libraries produced.

The volumetric and temperature coefficients calculated here are generally much smaller (by about a factor of 2) than those obtained by matching peak powers. In the past, the modelled shape of the power pulse did not drop off as rapidly as expected from the experiment, even with the negative feedback from radiolytic gas production, which primarily occurs after the peak of the pulse. This may indicate that another more powerful negative feedback is present. It has been seen in recent work with multi-region models (Hetrick and Kimpland, 1992) that this feedback may be an extension of the volumetric expansion. Beyond the uniform and distributed density feedback models, the energy input

from these super-prompt critical bursts may be so swift and localized that the solution disassembles. This could provide the great density decreases necessary to remove reactivity from the system and drop the power pulse after peak. Such a feedback may be modelled by transport codes (e.g. TWODANT) by separating sections of the assembly various distances and determining the reactivity feedback from such a mechanism. This may replace or enhance the effect from uniform or redistributed density changes. Further study of this mechanism may be desirable.

Such studies on the disassembly of the solution may also provide a mechanism for analyzing multiple pulses as performed in the *CRAC* series. By determining the reactivity effect from various separations of solution regions, the shutdown mechanism is determined. However, after the assembly has disassembled, gravity will bring it back together. By knowing the negative feedbacks from disassembly and temperature increase feedbacks, the reactivity input from reassembly should also be known.

APPENDIX A

SAMPLE TWODANT INPUTS FOR VOLUMETRIC REACTIVITY
FEEDBACK STUDIESA.1 CRAC TWODANT Input for the Reference Case

```

      3      0      0
Crac reactor using a 3mm stainless steel liner
Dim: r=15 cm h=27 cm assume UO2(93.5) (NO3)2:6H2O
207 gU/Liter, using Dr. Seale's concentrations
/      cross sections: from standard xslib (118 isos)
/*****BLOCK I*****/
      igeom=r-z
      ngroup=16
      isn=8
      niso=118
      mt=2      nzone=2
      im=6      it=85
      jm=8      jt=115
      maxscm=500000
      maxlcm=5000000      t
/*****BLOCK II*****/
      xmesh=0.0,6.57404,9.297096,11.38657,13.1481,14.7,15.0
      xints=15,15,15,15,15,10
      ymesh=0.0,0.3,4.157,8.014,11.871,15.729,19.586,23.443,27.3
      yints=10,15,15,15,15,15,15
      zones=2,2,2,2,2,2;1,1,1,1,1,2;1,1,1,1,1,2;1,1,1,1,1,2;
              1,1,1,1,1,2;1,1,1,1,1,2;1,1,1,1,1,2;1,1,1,1,1,2      t
/*****BLOCK III*****/
      lib=xslibb      t
/*****BLOCK IV*****/
      matls= fuel1, "238-14" 2.821e-5 "238-13" 8.891e-6
              "235-9r" 3.327e-4 "23510r" 1.602e-4
              "o16" 3.7132e-2 "n" 2.306e-3 "h" 5.955e-2;
      steel, "cr" 1.6471e-2 "ni" 6.4834e-3 "fe" 6.036e-2
              "si" 1.694e-3 "c" 3.1691e-4
      assign= matls      t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 oitm=50 t

```

A.2 CRAC TWODANT Input for a Uniformly Expanded Case

```

      3      0      0
Crac reactor using a 3mm stainless steel liner
Dim: r=15 cm h=27 cm assume UO2(93.5)(NO3)2:6H2O
207 gU/Liter, using Dr. Seale's concentrations
/      cross sections: from standard xslib (118 isos)
/*****BLOCK I*****/
      igeom=r-z
      ngroup=16
      isn=8
      niso=118
      mt=2      nzone=2
      im=6      it=85
      jm=8      jt=115
      maxscm=500000
      maxlcm=5000000      t
/*****BLOCK II*****/
      xmesh=0.0,6.57404,9.297096,11.38657,13.1481,14.7,15.0
      xints=15,15,15,15,15,10
      ymesh=0.0,0.3,4.3,8.3,12.3,16.3,20.3,24.3,28.3
      yints=10,15,15,15,15,15,15
      zones=2,2,2,2,2,2;1,1,1,1,1,2;1,1,1,1,1,2;1,1,1,1,1,2;
              1,1,1,1,1,2;1,1,1,1,1,2;1,1,1,1,1,2;1,1,1,1,1,2      t
/*****BLOCK III*****/
      lib=xslibb      t
/*****BLOCK IV*****/
      matls= fuel1, "238-14" 2.72025e-5 "238-13" 8.57346e-6
              "235-9r" 3.2081786e-4 "23510r" 1.544786e-4
              "o16" 3.580586e-2 "n" 2.223643e-3 "h" 5.742321e-2;
      steel, "cr" 1.6471e-2 "ni" 6.4834e-3 "fe" 6.036e-2
              "si" 1.694e-3 "c" 3.1691e-4
      assign= matls      t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 oitm=50 t

```

A.3 CRAC TWODANT Input for a Distributed Density Case

```

      3      0      0
Crac reactor using a 3mm stainless steel liner
Dim: r=15 cm h=27 cm assume UO2(93.5) (NO3)2:6H2O
207 gU/Liter, using Dr. Seale's concentrations
/      cross sections: from standard xslib (118 isos)
/*****BLOCK I*****/
      igeom=r-z
      ngroup=16
      isn=8
      niso=118
      mt=21      nzone=21
      im=6      it=85
      jm=8      jt=115
      maxscm=500000
      maxlcm=5000000      t
/*****BLOCK II*****/
      xmesh=0.0,6.57404,9.297096,11.38657,13.1481,14.7,15.0
      xints=15,15,15,15,15,10
      ymesh=0.0,0.3,4.3,8.3,12.3,16.3,20.3,24.3,28.3
      yints=10,15,15,15,15,15,15
      zones=21,21,21,21,21,21;1,2,3,4,5,21;6,7,8,9,10,21;
            11,12,13,14,15,21;16,17,18,19,20,21;
            11,12,13,14,15,21;6,7,8,9,10,21;1,2,3,4,5,21      t
/*****BLOCK III*****/
      lib=xslibb      t
/*****BLOCK IV*****/
      matls= fuel1, "238-14" 2.72523e-05 "238-13" 8.58917e-06
            "235-9r" 3.21405e-04 "23510r" 1.54761e-04
            "o16" 3.58714e-02 "n" 2.22772e-03 "h" 5.75284e-02;
      fuel2, "238-14" 2.73222e-05 "238-13" 8.61119e-06
            "235-9r" 3.22229e-04 "23510r" 1.55158e-04
            "o16" 3.59634e-02 "n" 2.23343e-03 "h" 5.76759e-02;
      fuel3, "238-14" 2.73833e-05 "238-13" 8.63045e-06
            "235-9r" 3.22950e-04 "23510r" 1.55505e-04
            "o16" 3.60439e-02 "n" 2.23842e-03 "h" 5.78049e-02;
      fuel4, "238-14" 2.74364e-05 "238-13" 8.64719e-06
            "235-9r" 3.23577e-04 "23510r" 1.55807e-04
            "o16" 3.61138e-02 "n" 2.24276e-03 "h" 5.79170e-02;
      fuel5, "238-14" 2.74822e-05 "238-13" 8.66161e-06
            "235-9r" 3.24116e-04 "23510r" 1.56067e-04
            "o16" 3.61740e-02 "n" 2.24651e-03 "h" 5.80136e-02;
      fuel6, "238-14" 2.69546e-05 "238-13" 8.49533e-06
            "235-9r" 3.17894e-04 "23510r" 1.53071e-04
            "o16" 3.54795e-02 "n" 2.20338e-03 "h" 5.68999e-02;
      fuel7, "238-14" 2.70991e-05 "238-13" 8.54086e-06
            "235-9r" 3.19598e-04 "23510r" 1.53891e-04
            "o16" 3.56697e-02 "n" 2.21519e-03 "h" 5.72048e-02;
      fuel8, "238-14" 2.72254e-05 "238-13" 8.58069e-06
            "235-9r" 3.21088e-04 "23510r" 1.54609e-04
            "o16" 3.58360e-02 "n" 2.22552e-03 "h" 5.74716e-02;
      fuel9, "238-14" 2.73352e-05 "238-13" 8.61529e-06
            "235-9r" 3.22383e-04 "23510r" 1.55232e-04

```



```

    "o16" 3.59806e-02 "n" 2.23449e-03 "h" 5.77034e-02;
fuel10, "238-14" 2.74299e-05 "238-13" 8.64512e-06
    "235-9r" 3.23499e-04 "23510r" 1.55770e-04
    "o16" 3.61051e-02 "n" 2.24223e-03 "h" 5.79031e-02;
fuel11, "238-14" 2.67534e-05 "238-13" 8.43191e-06
    "235-9r" 3.15521e-04 "23510r" 1.51928e-04
    "o16" 3.52147e-02 "n" 2.18693e-03 "h" 5.64751e-02;
fuel12, "238-14" 2.69482e-05 "238-13" 8.49333e-06
    "235-9r" 3.17819e-04 "23510r" 1.53035e-04
    "o16" 3.54712e-02 "n" 2.20286e-03 "h" 5.68865e-02;
fuel13, "238-14" 2.71187e-05 "238-13" 8.54706e-06
    "235-9r" 3.19830e-04 "23510r" 1.54003e-04
    "o16" 3.56956e-02 "n" 2.21679e-03 "h" 5.72464e-02;
fuel14, "238-14" 2.72668e-05 "238-13" 8.59374e-06
    "235-9r" 3.21577e-04 "23510r" 1.54844e-04
    "o16" 3.58905e-02 "n" 2.22890e-03 "h" 5.75590e-02;
fuel15, "238-14" 2.73945e-05 "238-13" 8.63397e-06
    "235-9r" 3.23082e-04 "23510r" 1.55569e-04
    "o16" 3.60586e-02 "n" 2.23934e-03 "h" 5.78285e-02;
fuel16, "238-14" 2.66823e-05 "238-13" 8.40952e-06
    "235-9r" 3.14683e-04 "23510r" 1.51525e-04
    "o16" 3.51212e-02 "n" 2.18112e-03 "h" 5.63252e-02;
fuel17, "238-14" 2.68950e-05 "238-13" 8.47655e-06
    "235-9r" 3.17191e-04 "23510r" 1.52732e-04
    "o16" 3.54011e-02 "n" 2.19851e-03 "h" 5.67741e-02;
fuel18, "238-14" 2.70810e-05 "238-13" 8.53519e-06
    "235-9r" 3.19385e-04 "23510r" 1.53789e-04
    "o16" 3.56460e-02 "n" 2.21371e-03 "h" 5.71668e-02;
fuel19, "238-14" 2.72427e-05 "238-13" 8.58613e-06
    "235-9r" 3.21292e-04 "23510r" 1.54707e-04
    "o16" 3.58587e-02 "n" 2.22693e-03 "h" 5.75080e-02;
fuel20, "238-14" 2.73820e-05 "238-13" 8.63004e-06
    "235-9r" 3.22935e-04 "23510r" 1.55498e-04
    "o16" 3.60421e-02 "n" 2.23832e-03 "h" 5.78021e-02;
steel, "cr" 1.6471e-2 "ni" 6.4834e-3 "fe" 6.036e-2
    "si" 1.694e-3 "c" 3.1691e-4
assign= matls t
/*****BLOCK V*****/
ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 t
/*****BLOCK VI*****/

```

A.4 KEWB-5 TWODANT Input for the Reference Case

```

      2      0      0
KEWB-5 reactor including stainless stell liner
Dim: ri=14.605 cm h=35.8 cm density redistribution study
/      cross sections: from H-R 16 group xslib (118 isos)
/*****BLOCK I*****/
      igeom=r-z ngroup=16 isn=8 niso=118
      mt=2      nzone=2
      im=6      it=85
      jm=8      jt=115
      maxscm=500000
      maxlcm=5000000      t
/*****BLOCK II*****/
      xmesh=0.0,6.53155,9.23701,11.31298,13.06311,14.605,15.24
      xints=15,15,15,15,15,10
      ymesh=0.0,0.635,5.749285714,10.86357143,15.97785714,
      21.09214286,26.20642857,31.32071429,36.435
      yints=10,15,15,15,15,15,15,15
      zones=2,2,2,2,2,2;1,1,1,1,1,2;1,1,1,1,1,2;
      1,1,1,1,1,2;1,1,1,1,1,2;
      1,1,1,1,1,2;1,1,1,1,1,2;1,1,1,1,1,2      t
/*****BLOCK III*****/
      lib=xslibb      t
/*****BLOCK IV*****/
      matls= fuel1, "238-14" 3.10564e-05 "238-13" 2.15897e-06
      "235-9r" 3.25183e-04 "23510r" 1.58720e-04
      "o16" 3.06600e-02 "sulfur" 5.17000e-04 "h" 5.99266e-02;
      steel, "cr" 1.6471e-2 "ni" 6.4834e-3 "fe" 6.036e-2
      "si" 1.694e-3 "c" 3.1691e-4
      assign= matls      t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 oitm=50      t

```

A.5 SILENE TWODANT Input for the Reference Case

```

3      0      0
SILENE reactor using a 3mm stainless steel liner and central thimble
Dim: ro=3.8 cm Ri=18 cm hsoln=38.0 cm assume UO2(93.5) (NO3)2:6H2O
Information obtained from draft copy of Barbry letter 28 Dec 88
/      cross sections: from standard xslib (118 isos)
/*****BLOCK I*****/
      igeom=r-z ngroup=16 isn=8 niso=118
      mt=2
      nzone=2
      im=8
      it=90
      jm=8
      jt=110
      maxscm=170000
      maxlcm=1500000 t
/*****BLOCK II*****/
      xmesh= 0.0,3.5,3.8,8.737963149,11.75857134,14.1483568,
              16.18913216,18,18.4
      xints= 5,5,15,15,15,15,15,5
      ymesh= 0.0,3.6,9.028571429,14.45714286,19.88571429,
              25.31428571,30.74285714,36.17142857,41.6
      yints= 5,15,15,15,15,15,15,15
      zones= 0,2,2,2,2,2,2,2;0,2,1,1,1,1,1,2;
              0,2,1,1,1,1,1,2;0,2,1,1,1,1,1,2;
              0,2,1,1,1,1,1,2;0,2,1,1,1,1,1,2;
              0,2,1,1,1,1,1,2;0,2,1,1,1,1,1,2 t
/*****BLOCK III*****/
      lib=xslibb t
/*****BLOCK IV*****/
      matls= fuel1, "238-16" 1.17000e-05
              "23511r" 8.18258e-05 "23512r" 8.67742e-05
              "o16" 3.57600e-02 "n" 1.56900e-03 "h" 6.25800e-02;
              steel, "cr" 1.661e-2 "ni" 8.178e-3 "fe" 5.922e-2
              "si" 1.709e-3 "c" 1.200e-4
      assign= matls t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 oitm=50 t

```

A.6 SHEBA TWODANT Input for the Reference Case

```

      2      0      0
SHEBA reactor using soln data obtained from R. Anderson (N-2)
Dim: ro=1.25 in Ri=9.5 in hsoln=44.0 cm assume UO2(5)F2
/      cross sections: from standard xslib (118 isos)
/*****BLOCK I*****/
      igeom=r-z ngroup=16 isn=8 niso=118
      mt=2
      nzone=2
      im=8
      it=90
      jm=8
      jt=110
      maxscm=170000
      maxlcm=1500000 t
/*****BLOCK II*****/
      xmesh= 0.0,2.54,3.175,11.15866838,15.45804435,
             18.79857415,21.62918503,24.13,25.4
      xints= 5,5,15,15,15,15,15,5
      ymesh= 0.0,2.54,9.225714286,15.91142857,22.59714286,
             29.28285714,35.96857143,42.65428571,49.34
      yints= 5,15,15,15,15,15,15,15
      zones= 0,2,2,2,2,2,2,2;0,2,1,1,1,1,1,2;
             0,2,1,1,1,1,1,2;0,2,1,1,1,1,1,2;
             0,2,1,1,1,1,1,2;0,2,1,1,1,1,1,2;
             0,2,1,1,1,1,1,2;0,2,1,1,1,1,1,2 t
/*****BLOCK III*****/
      lib=xslibb t
/*****BLOCK IV*****/
      matls= fuel1, "238-6r" 1.73097e-03 "238-7r" 7.68030e-04
             "23511r" 4.14485e-05 "23512r" 9.04515e-05
             "o16" 3.21000e-02 "f19" 5.33400e-03 "h" 5.35400e-02;
             steel, "cr" 1.7384e-2 "ni" 7.6994e-3 "fe" 5.9205e-2
      assign= matls t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 oitm=50 t

```

APPENDIX B

SAMPLE LEAPR INPUT FOR HYDROGEN IN H₂O THERMAL
SCATTERING LAW CALCULATION

```

h in h2o, endf model
80 80 0 0 0/
0.050406 0.100812 0.151218 0.201624 0.252030 0.302436 0.352842
0.403248 0.453654 0.504060 0.554466 0.609711 0.670259 0.736623
0.809349 0.889061 0.976435 1.072130 1.177080 1.292110 1.418220
1.556330 1.707750 1.873790 2.055660 2.255060 2.473520 2.712950
2.975460 3.263080 3.578320 3.923900 4.302660 4.717700 5.172560
5.671180 6.217580 6.816500 7.472890 8.192280 8.980730 9.844890
10.79190 11.83030 12.96740 14.21450 15.58150 17.07960 18.72080
20.52030 22.49220 24.65260 27.02160 29.61750 32.46250 35.58160
38.99910 42.74530 46.85030 51.34960 56.28130 61.68680 67.61050
74.10280 81.21920 89.01800 97.56480 106.9310 117.2040 128.4550
140.7840 154.3030 169.1220 185.3530 203.1560 222.6530 244.0360
267.4640 293.1410 321.2880/
0.000000 .0806495 0.161299 0.241949 0.322598 0.403248 0.483897
0.564547 0.645197 0.725846 0.806496 0.887145 0.967795 1.048440
1.129090 1.209740 1.290390 1.371040 1.451690 1.532340 1.612990
1.693640 1.774290 1.854940 1.935590 2.016240 2.096890 2.177540
2.258190 2.338840 2.419490 2.500140 2.580790 2.669500 2.767090
2.874450 2.992500 3.122350 3.265300 3.422470 3.595360 3.785490
3.994670 4.224730 4.477870 4.756310 5.062580 5.399390 5.769970
6.177660 6.626070 7.119240 7.661810 8.258620 8.915110 9.637220
10.43200 11.30510 12.26680 13.32430 14.48670 15.76600 17.17330
18.72180 20.42450 22.29760 24.35720 26.62340 29.11650 31.85860
34.87590 38.19360 41.84400 45.85830 50.27490 55.13310 60.47710
66.35540 72.82150 79.93380/
1/
293/
.00255 66 1/
0 .0005 .001 .002 .0035 .005 .0075 .01 .013 .0165 .02 .0245
.029 .034 .0395 .045 .0506 .0562 .0622 .0686 .075 .083 .091
.099 .107 .115 .1197 .1214 .1218 .1195 .1125 .1065 .1005 .09542
.09126 .0871 .0839 .0807 .07798 .07574 .0735 .07162 .06974
.06804 .06652 .065 .0634 .0618 .06022 .05866 .0571 .05586
.05462 .0535 .0525 .0515 .05042 .04934 .04822 .04706 .0459
.04478 .04366 .04288 .04244 .042/
0.05555556 120. 0.5 0 0/
2/
.205 .48/
.166667 .333333/
1 1001. 0.9992 20.36 2 0 2/
h in h2o/
endf model with extended alpha and beta grids/

```

APPENDIX C

SAMPLE NJOY, TRANSX, AND TWODANT INPUTS FOR 69-GROUP NEUTRON
TEMPERATURE COEFFICIENT CALCULATIONSC.1 NJOY Input for Hydrogen-1 at 293 K

```

0
6
*moder*
20 -21
*reconr*
-21 -22
*pendf tape for endf/b-vi 1-h-1b*/
125 5 0 /
.001 0. 7 /
*1-h-1b corrected endf/b-vi tape 120*/
*processed with the njoy nuclear data processing system*/
*see original endf/b-vi tape for details of evaluation*/
*the following reaction types are added*/
*   mt222   h in h2o thermal scattering*/
0/
*broadr*
-22 -23
125 1/
.001/
293 /
0/
*thermr*
30 -23 -24
1 125 8 1 4 0 2 222 0 /
293 /
.005 4.6 /
groupr
-21 -24 0 -25
125 9 0 6 5 1 1 1
*1-h-1 69 group set from endf/b-vi*/
293 /
1.e10
3/ *cross sections*/
3 222 *h in water thermal scattering*/
3 251 *mubar*/
3 252 *xi*/
3 253 *gamma*/
3 259 *1/v*/
6/ *matrices*/
6 222 *h in water thermal scattering*/
0 /
0 /
*stop*

```

C.2 NJOY Input for Uranium-235 at 293 K through 373 K

```

0
6
moder
20 -21
reconr
-21 -22
*pendf tape for endf/b-vi u-235a*/
9228 5 0 /
.002 0. 7 /
*92-u-235a from endf/b-vi tape 121 (ornl/lanl) */
*processed with the njoy nuclear data processing system*/
*see original endf/b-vi tape for details of evaluation*/
*the following reaction types are added*/
*   mt221   free thermal scattering*/
0/
broadr
-22 -23
9228 9 0 1/
.002/
 293 303 313 323 333 343 353 363 373 /
0/
unresr
-21 -23 -24
9228 9 7 1
 293 303 313 323 333 343 353 363 373 /
1e10 1e4 1e3 300 100 30 10
0/
thermr
0 -24 -26
0 9228 8 9 1 0 1 221 0 /
 293 303 313 323 333 343 353 363 373 /
.01 4.6 /
groupr
-22 -26 0 -27
9228 9 0 6 5 9 7 1
*92-u-235a 69 group set from endf/b-vi*/
293 303 313 323 333 343 353 363 373 /
1e10 1e4 1e3 3e2 1e2 3e1 1e1/
3/
3 221 *free*/
3 251 *mubar*/
3 252 *xi*/
3 253 *gamma*/
3 259 *1/v*/
3 455 *delayed nubar*/
5 455 *delayed neutron spectra*/
6/
6 221 *free*/
0/
3   1 *total*/

```

```

3  2 *elastic*/
3 18 *total fission*/
3 102 *(n,g)*/
3 221 *free*/
6  2 *elastic*/
6 221 *free*/
0/
.
.
. (same array for other 6 temperatures)
.
.
3  1 *total*/
3  2 *elastic*/
3 18 *total fission*/
3 102 *(n,g)*/
3 221 *free*/
6  2 *elastic*/
6 221 *free*/
0/
0/
*stop*

```


C.3 NJOY (MATXS) Input for All Isotopes at 293 K

```

0
6
matxsr
-25 0 26 /
0 12 *uofa drew njoy*/
1 2 5 10/
*matxs9 69-group thermal library*/
*march 1992*/
*69-group epri-cpm neutron structure*/
*thermal--1/e--fission+fusion weighting*/
*endf/b-vi*/
n /
69 /
nscat ntherm /
1 1 /
1 1 /
h1      125/
o16     825/
n14     725/
s32     1625/
u235a   9228/
u238a   9237/
pu239   9437/
pu240a  9440/
gd155   6434/
gd157   6440/
stop

```

C.4 TRANSX and TWODANT Input for CRAC (207 gU/L)

(note this is a COSMOS/batch type file)

```

*mass get wait=on matxs:/108972/libraries/matxs293
*mass get wait=on transx:/108972/transx/transx
*mass get wait=on tdn:/108972/twodant/tdn
*file name=input
temperature feedback from critical crac
0 5 0 1 1 1 0 3 0 0
69 2 93 20 40 1 1 5 1 0
crac/
crac 293. 1. 1 19.036/
1 1 h1 5.955e-2 h2o/
1 1 o16 3.7132e-2 free/
1 1 n14 2.306e-3 free/
1 1 u235a 4.929e-4 free/
1 1 u238a 3.7101e-5 free/
chi/
stop
*transx
*switch goxs macrxs
*copy macrxs snxedt
*file name=tdnin
      2      0      0
Crac reactor using Dr. Seale's concs 207 gU/l
Dim: ro=14.7 cm h=27 cm
/*****BLOCK I*****/
      igeom=r-z ngroup=69 isn=-8 niso=1 mt=1
      nzone=1
      im=1
      it=50
      jm=1
      jt=50
      maxlcm=10000000 maxscm=100000
      t
/*****BLOCK II*****/
      xmesh=0.0,14.7 xints=50
      ymesh=0.0,27.0 yints=50
      zones=1 t
/*****BLOCK III*****/
      lib=macrxs t
/*****BLOCK IV*****/
      assign= matls t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 oitm=50 t
*tdn i=tdnin o=output
*mass store wait=on output:/108972/newout/207.293o

```

C.5 TRANSX and TWODANT Input for SILENE

```

*mass get wait=on matxs:/108972/libraries/matxs293
*mass get wait=on transx:/108972/transx/transx
*mass get wait=on tdn:/108972/twodant/tdn
*file name=input
temperature feedback from critical SILENE
0 5 0 1 1 1 0 3 0 0
69 2 93 20 40 1 1 5 1 0
SILENE/
SILENE 293. 1. 1 23.679/
1 1 h1 6.258e-2 h2o/
1 1 o16 3.576e-2 free/
  1 1 n14 1.569e-3 free/
1 1 u235a 1.686e-4 free/
1 1 u238a 1.17e-5 free/
chi/
stop
*transx
*switch goxs macrxs
*copy macrxs snxedt
*file name=tdnin
  2      0      0
SILENE reactor using data obtained from letter from F.Barbry 28Dec88
Dim: ro=3.8 cm Ri=18 cm hsoln=38.0 cm assume UO2(93.5) (NO3)2:XH2O
/*****BLOCK I*****/
  igeom=r-z ngroup=69 isn=-8 niso=1 mt=1
  nzone=1
  im=2
  it=50
  jm=1
  jt=50
  maxlcm=10000000 maxscm=100000
  t
/*****BLOCK II*****/
  xmesh=0.0,3.8,18.0  xints=5,45
  ymesh=0.0,38.0  yints=50
  zones=0,1  t
/*****BLOCK III*****/
  lib=macrxs  t
/*****BLOCK IV*****/
  assign= matls  t
/*****BLOCK V*****/
  ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-8 oitm=50  t
*tdn i=tdnin o=output
*mass store wait=on output:/108972/newout/sil293o

```

C.6 TRANSX and TWODANT Input for Gadolinium Containing Plutonium Solution

```

*mass get wait=on matxs:/108972/libraries/matxs293
*mass get wait=on tdn:/108972/twodant/tdn
*mass get wait=on transx:/108972/transx/transx
*file name=input
temperature feedback from critical pu soln
0 5 0 1 1 1 0 3 0 0
69 2 93 20 40 1 1 6 1 0
pusoln/
pusoln 293. 1. 1 200/
1 1 h1 6.68546e-2 h2o/
1 1 o16 3.34273e-2 free/
1 1 pu239 2.51231e-5 free/
1 1 pu240a 1.32227e-6 free/
1 1 gd155 5.6678e-8 free/
1 1 gd157 5.9933e-8 free/
chi/
stop
*transx
*switch goxs snxedt
*copy snxedt macrxs
*file name=tdnin
      2      0      0
Infinite cylinder of 10.5 g/L of 95 Pu-239, 5 Pu-240
Cross section set used is xslibb (20 C)
/*****BLOCK I*****/
      igeom=cylinder ngroup=69 isn=8 niso=1 mt=1 nzone=1
      im=1
      it=50
      maxscm=7000
      maxlcm=80000      t
/*****BLOCK II*****/
      xmesh=0.0,100      xints=50
      zones=1      t
/*****BLOCK III*****/
      lib=macrxs      t
/*****BLOCK IV*****/
      assign= matls      t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 epsi=1e-6 oitm=130      t
*tdn i=tdnin o=output
*mass store wait=on output:/108972/infcylnew/10.5293o

```

C.6 TRANSX and TWODANT Input for Water-Reflected Plutonium Solution

```

*mass get wait=on matxs:/108972/matxs293
*mass get wait=on transx:/108972/transx/transx
*mass get wait=on tdn:/108972/twodant/tdn
*file name=input
temperature feedback from critical pu soln
0 5 0 1 1 1 0 3 0 0
69 2 93 20 40 2 2 7 1 0
pu980 water/
pu980 293. 1. 1 23.637/
water 293. 1. 1 51.565/
1 1 h1 6.344293e-2 h2o/
1 1 o16 3.59754e-2 free/
1 1 n14 1.41798e-3 free/
1 1 pu239 6.37666e-5 free/
1 1 pu240a 9.710652e-7 free/
2 2 h1 6.685e-2 h2o/
2 2 o16 3.34273e-2 free/
chi/
stop
*transx
*switch goxs macrxs
*copy macrxs snxedt
*file name=980r.tdn
      2      0      0
LANL Report LA-10860-MS Table 13 with Reflector
H/Pu=980 Dim: Ro=16.2 cm H= 43.7 cm
/*****BLOCK I*****/
      igeom=r-z ngroup=69 isn=-8 niso=2 mt=2
      nzone=2
      im=2
      it=70
      jm=1
      jt=50
      maxlcm=10000000 maxscm=100000
      t
/*****BLOCK II*****/
      xmesh=0.0,16.2,56.2  xints=50,20
      ymesh=0.0,43.7  yints=50
      zones=1,2  t
/*****BLOCK III*****/
      lib=macrxs  t
/*****BLOCK IV*****/
      assign= matls  t
/*****BLOCK V*****/
      ievt=1 isct=1 ibr=0 ibt=0 ibb=0 epsi=1e-6 oitm=50 t
*tdn i=980r.tdn
*switch odnout 980r293o
*mass save wait=on 980r293o:/108972/puout/980r293o

```

APPENDIX D

SAMPLE CONTINUOUS ENERGY AND MULTI-GROUP CROSS SECTION PLOTS

D.1 Continuous and Grouped H-in-Water Total Cross Sections

D.2 Continuous H-in-Water Neutron Emission Distribution

H IN H₂O
NEUTRON EMISSION DISTRIBUTION

D.3 Grouped H Thermal Scattering Cross Sections at Various Temperatures

D.4 Continuous and Grouped U-235 Total Cross Sections

D.5 Continuous and Grouped Pu-239 Total Cross Sections

D.6 Continuous and Grouped Gd-157 Total Cross Sections

GD-157 TOTAL CROSS SECTIONS (300K, ENDF/B-VI)
CONT'S ENERGY AND 69-GP EPRI-CPM STRUCTURE

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