Hand Calculation Methods for Nuclear Criticality Safety

Douglas G. Bowen
Robert D. Busch

April 2023

![Oak Ridge National Laboratory logo]

Nuclear Energy and Fuel Cycle Division

HAND CALCULATION METHODS FOR NUCLEAR CRITICALITY SAFETY

Douglas G. Bowen
Robert D. Busch

April 2023

CONTENTS

LIST OF FIGURES

LIST OF TABLES

ABSTRACT

This primer provides an overview of the most common hand calculation methods used for criticality safety calculations. The most widely used tools available to a nuclear criticality safety (NCS) practitioner are probably the common Monte Carlo or deterministic criticality safety codes, which can be used to model very complex systems. However, use of these codes can obscure the parameters to which a particular fissile system may be sensitive, whereas the hand calculation methods can be used to delve into the ways each parameter may affect the reactivity of a fissile material system. Furthermore, practitioners must avoid using computer codes as devices that take inputs and simply provide outputs (i.e., a "black box"). Many years ago, pioneers such as Joe Thomas, David Smith, and Hugh Paxton, among others in the field of nuclear criticality safety, took the time before the advent of high-speed desktop computers to create simple hand methods for criticality safety analyses. Some of the methods can be used for single fissile units; others are applicable to fissile units arranged into simple array configurations. This primer discusses the applicability of the various methods, illustrates how they are used, and provides an interpretation of the various results. The NCS practitioner will need to spend time to master the methods that could be most useful; however, they can provide the practitioner with fast and accurate answers to criticality safety problems if they are used correctly and if critical data exist for the problem at hand. Hand calculation methods can be used as a starting point for more advanced calculations, and in many circumstances, they can provide sensitivity and perturbation information more quickly than using a criticality code.

1. INTRODUCTION

The nuclear criticality safety practitioner has many tools to analyze normal case and credible process upsets for criticality safety evaluation development. The most common tools are probably the Monte Carlo or the deterministic criticality safety codes, which can be used to model very complex systems. However, use of these codes can obscure the parameters to which a particular fissile system may be sensitive, and criticality safety practitioners must avoid using computer codes as devices that take inputs and simply provide outputs. Many years ago, pioneers such as Joe Thomas, David Smith, and Hugh Paxton, among others in the field of nuclear criticality safety, took the time before the advent of high-speed desktop computers to create simple hand calculation methods for criticality safety analyses. Some of the methods can be used for single fissile units, whereas others can be used for fissile units arranged into simple array configurations. The following methods are discussed at some length in this primer.

Single Unit Methods

- One-group diffusion theory
- One-group modified diffusion theory
- Buckling conversions
- Core density conversions

Array Unit Methods

- Surface density method
- Density analog method
- Limiting surface density (NB_N^2) method
- Solid angle method

This primer provides some background for each method to describe how each method is applicable and useful and to provide example problems so that the criticality safety practitioner can apply the methods quickly and accurately. These hand calculation methods can provide a first look at a simple system to determine whether more complex calculations are warranted. Furthermore, the hand methods can be used for parametric studies that identify the criticality safety parameters to which a fissile system may be sensitive.

1.1 PURPOSE OF HAND CALCULATION METHODS

Hand calculation methods can take some time to learn and apply, but the time investment is valuable, particularly in gaining insight into the physics of fissile systems. The methods covered in this primer can be easily adapted to scripts, programming languages, and spreadsheets. Once the user has learned the methods, they can easily be used to perform comprehensive parametric calculations on individual parameters (mass, density, volume, concentration, etc.) and perturbation analyses. Furthermore, they can provide a first look at simple single unit and array systems. For example, if diffusion theory is used to examine a worst-case process upset condition and if the infinite multiplication factor, k_∞, for a particular system is much less than unity, there is no further need to perform calculations because a criticality event is not possible under the upset conditions. If the resulting k_∞ is close to unity or exceeds unity, then further calculations are necessary.

Hand calculation methods are useful to provide the analyst with a better understanding of the basic physics of the problem. Computer calculations are convenient and very fast; however, it is sometimes difficult to relate the basic output provided by the codes to the basic physics involved. Thus, hand

calculations can be valuable for new practitioners in developing intuition with respect to neutron transport physics, whereas advanced users can employ hand calculations as a starting point for more advanced calculations.

1.2   CHOOSING THE APPROPRIATE METHOD

The biggest challenge in applying these hand calculation methods to physical problems is choosing the most appropriate or best method. The discussion that accompanies each hand method includes the applicability of the method and its limitations. For example, if a solid chunk of plutonium or uranium metal is being machined in a particular fissile material operation, then the result of the machining could be the generation of small chips or turnings. Assuming that no moderating material is introduced to the machined plutonium or uranium metal, the density of the fissile material has been significantly reduced. Therefore, the best method to use would be the core density method. This primer provides the following information for each method:

- Overview of the method
- Applicability of the method to solve certain problems
- Example problems solved step-by-step

1.3   SINGLE UNIT HAND CALCULATIONS

The methods listed in Table 1-1 are valid for single fissile units only. The methods discussed for single units are the one-group and modified one-group diffusion theories, buckling conversions, and core density conversions. These methods can be used to resolve a wide variety of criticality safety problems, as summarized Table 1-1.

Table 1-1. Single unit methods and applicability summary.

Single Unit Hand Calculation Method	Applicability Summary
One-group and Modified One-Group Diffusion Theories	• Good for large, homogeneous systems with isotopes that have low neutron absorption. • Caution: Diffusion theory is not a good method to use for small systems, near boundaries, or in or near strong neutron-absorbing materials.
Buckling Conversions	• Useful for simple geometries such as spherical, slab, or cylindrical systems. • Can convert the neutron leakage characteristics for a critical simple geometry to another simple geometry that has equivalent leakage characteristics, as long as critical data exist for a particular system.
Core-Density Conversions	• Can be applied to homogeneous, critical systems if the volume or density of the system changes uniformly. • Applicable to bare systems or those with a close-fitting reflector, as long as the reflector density remains constant.

1.4   ARRAY HAND CALCULATIONS

The methods listed in Table 1-2 are valid for fissile units arranged in certain array configurations. The methods discussed in this section are the surface density method, density analog method, the solid angle method, and the limiting surface density method or the NB_N^2 method. These methods can be used to resolve a wide variety of criticality safety problems in which fissile materials are arranged into various multiple-unit configurations.

Table 1-2. Array methods and applicability summary.

Array Hand Calculation Method	Applicability Summary
Surface Density Method	• Useful for determining the subcritical center-to-center spacing for fissile materials stored or staged in finite array configurations where the size of the array is controlled in one direction. • Useful for irregular shapes such as equipment stored on the floor. • Considers 15.5 cm of water reflection on the top and bottom of the array.
Density Analog Method	• Useful for determining the subcritical center-to-center spacing for fissile materials stored or staged in array configurations of any shape. • Useful for irregular shapes such as equipment stored on the floor. • Considers 20.0 cm of water reflection on the top and bottom of the array.
Limiting Surface Density (NB_N^2) Method	• Useful for determining the critical center-to-center spacing for fissile materials stored or staged in array configurations of any shape (>64 units). • Useful for irregular shapes such as equipment stored on the floor. • Data exist for powders, metals, up to an H/X of about 20 for some fissile materials. • Data exist for arrays reflected by concrete instead of water. • Can be used to calculate trends due to a change in unit shape or density. • Considers 20.0 cm of water reflection on the top and bottom of the array.
Solid Angle Method	• Useful for small numbers of moderated fissile units because the basis for this method is experiments with aqueous solutions of fissile materials. • The multiplication factor for any individual unit cannot exceed 0.8, and the unit must be subcritical with a thick close-fitting water reflector. • The minimum separation distance between fissile units should be at least 0.3 m, and the total allowed solid angle should not exceed 6 steradians. • Reflectors that are more effective than a thick water reflector should not be considered for this method. • Concrete reflection on three sides of the fissile material is considered bounded by this method.

1.5   CONFIDENCE IN HAND CALCULATIONS

The analyst may be interested in how useful and practical hand calculations are when there are many comprehensive Monte Carlo and deterministic codes available for criticality safety applications. Many of the example problems herein have been verified using the following code packages and data:

- MCNP5
- SCALE, KENO V.a
- DANTSYS
- Physical Dimensions

Section 9 presents the results of this verification effort. The purpose of this effort is to demonstrate the usefulness and accuracy of the various hand calculation methods and assist the criticality safety practitioner in choosing the appropriate method for a particular problem.

2. ONE-GROUP AND MODIFIED ONE-GROUP DIFFUSION THEORIES

2.1 WHAT YOU WILL BE ABLE TO DO

- Determine how to apply one-group diffusion theory to a simple fissile material system.

- Use one-group diffusion and modified one-group diffusion theory and compare differences between the two methods.

- Calculate the infinite multiplication factor, k_∞, and critical dimensions for simple fissile systems.

- Interpret the results provided by one-group diffusion theory.

2.2 OVERVIEW OF DIFFUSION THEORY

Diffusion theory characterizes the basic neutron physics of a system and is a mathematical statement of the neutron balance. The diffusion equation is derived from the Boltzmann neutron transport equation by applying several assumptions. Because of the assumptions, one-group and modified one-group diffusion theory are good for large, homogeneous systems with isotopes that have low neutron absorption.

CAUTION: Diffusion theory is not a good method to use for small systems, near boundaries, or in or near strong neutron-absorbing materials.

2.2.1 One-Group Diffusion Theory

Rigorous derivations of the one-speed diffusion equation can be found in many textbooks (References 1 and 2). The focus of the discussion in this work is on using the diffusion approximation to solve several example problems. The neutron flux in a critical system can be represented by the time dependent, one-speed diffusion approximation (Reference 1).

$$- \left(-D\nabla^2\phi \right) - \Sigma_a\phi + \nu\Sigma_f\phi = \frac{1}{v}\frac{d\phi}{dt} \tag{1}$$

In this equation, ϕ is the one-group or single energy neutron flux (neutrons/cm²-sec), D is the one-group diffusion coefficient (cm), Σ_a is the macroscopic absorption cross section (cm^{-1}), Σ_f is the macroscopic fission cross section (cm^{-1}), ν is the number of neutrons emitted per fission (unitless), t is time (sec), v is the neutron speed (cm/sec), and $\nabla^2\phi$ is the Laplacian operating on the neutron flux.

To maintain a fission chain reaction within fissile material, the volume-to-mass ratio of fissile material must exceed a critical value that depends on system conditions. The determination of critical size is based on a consideration of the conservation or balance of neutrons in the fissile system. For a fissile system, neutrons are either produced (from an external source or fission reactions in the fissile material) or lost (either leakage from the system or absorption by the materials present in the system).

Thus, a neutron balance equation can be developed based on these production and loss effects, as follows.

Net rate of gain of neutrons per unit volume	=	Rate of production of neutrons by fission per unit volume	−	Rate of loss of neutrons by leakage and absorption per unit volume

Therefore, for the one-group, time-dependent diffusion equation, the neutron balance can also be written in the following form, where n represents the neutron density (neutrons/cm^3).

$$\frac{1}{v}\frac{d\phi}{dt} = v\Sigma_f\phi - \Sigma_a\phi - \left(-D\nabla^2\phi\right)$$
$$\frac{1}{v}\frac{d\phi}{dt} = \frac{dn}{dt} = \text{Production - Absorption - Leakage} \tag{2}$$

The components of the one-speed, time-dependent diffusion approximation, as illustrated in the neutron balance equation shown above, are explained below.

$\frac{1}{v}\frac{d\phi}{dt}$ Represents the rate of change of the neutron density in the system, which is equal to the sum of the terms listed below or the neutron balance for the system.

$v\Sigma_f\phi$ Represents neutron production in the system due to fissions within the fissile material. This term is positive in the diffusion equation, which indicates that there is a net gain of neutrons in the system (neutrons/cm^3-sec).

$\Sigma_a\phi$ Represents the loss of neutrons from the system due to absorption in the system. The negative sign in front of this term in the diffusion equation indicates that there is a net loss of neutrons from the system (neutrons/cm^3-sec).

$-D\nabla^2\phi$ Represents the neutron leakage from the system. The negative sign in front of this term in the diffusion equation indicates that there is a net loss of neutrons from the system (neutrons/cm^3–sec).

For a steady-state fissile system in which the neutron population is constant, such as in a just-critical system, the rate of change of the neutron population is zero or dn/dt = 0. Thus, the neutron balance can be written as

$$\text{- Leakage - Absorption + Production = 0} \tag{3}$$

If the steady-state diffusion equation is rearranged slightly, then

$$v\Sigma_f\phi = \left(-D\nabla^2\phi\right) + \Sigma_a\phi$$

Dividing both sides of this equation by D and combining terms results in the following expression:

$$\nabla^2\phi + \left(\frac{v\Sigma_f - \Sigma_a}{D}\right)\phi = 0 \tag{4}$$

Note this is in the form of $\nabla^2\phi + B^2\phi = 0$, where B^2 is equal to a constant.

$$B^2 = \text{constant} = \left(\frac{v\Sigma_f - \Sigma_a}{D}\right) \tag{5}$$

In this form, the term B^2 is a function of only the material properties of the system; there is dependency on geometry. Thus, changes in the material properties of the system will affect B^2, whereas a change in

the geometry of the system will not. For this reason, B_m^2, as defined above, is known as the material buckling. It describes the curvature of the flux and is based only on material properties.

For a specific geometry, the steady-state diffusion equation can then be solved. However, recall from Eq. (4) that $\nabla^2\phi + B^2\phi = 0$, when the system is critical. Then using the form of the Laplacian appropriate to the geometry of the system, (i.e., for a slab, $\nabla^2\phi = \left(\frac{d^2\phi}{dx^2}\right)$, the steady-state diffusion equation can then be solved. Using Eq. (4) and knowing that $\left[\frac{d^2\phi}{dx^2}\right]$, the diffusion equation for a one-dimensional slab with thickness x, can be rewritten as:

$$\frac{d^2\phi}{dx^2} + B^2\phi = 0 \tag{6}$$

and has a solution, $f(x) = A\cos Bx + C\sin Bx$.

A complete solution for the 1-dimensional slab can be found by considering the possible boundary conditions for the system:

    1. The flux is finite and real,

    2. The current and flux are continuous at the system boundaries,

$$\tag{7}$$

    3. $\left.\frac{d\phi}{dx}\right|_{x=\,\text{centerline}} = 0$ (symmetry condition), and

    4. $\phi(x)|_{x=\,\text{outside edge}} = 0$

$$\tag{8}$$

Boundary conditions 3 and 4 for the 1-dimensional slab are needed to obtain a complete solution to this problem. Figure 2-1 will assist with completing the solution to the 1D slab example.
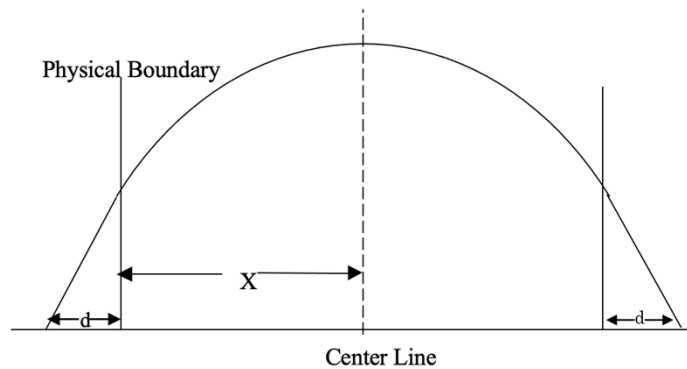
Figure 2-1. Neutron Flux Profile for the 1-D Slab, One-Group Diffusion Theory Approximation.

Appendix A provides an in-depth discussion of the linear extrapolation distance. Based on this discussion of extrapolation distance and vacuum boundary conditions, the following relationship can be defined; it identifies the assumed pseudo-physical location (i.e., the extrapolated boundary) where the mathematical representation of the neutron flux is zero.

7

$$X' = X + d \tag{9}$$

where

X	$=$	one-half of the physical slab thickness and
d	$=$	2D or $0.71\lambda_{tr,}$ as defined and discussed in Appendix A.

The neutron flux vanishes at the extrapolated boundary, which lies approximately $0.71\lambda_{tr}$ beyond the physical boundary. To take advantage of symmetry, we will consider the center of the slab to be at x = 0. To find the solution to the diffusion equation for a slab, we will apply the boundary conditions.

Applying boundary condition #3, $\left.\dfrac{d\phi}{dx}\right|_{x\,=\,\text{centerline}} = 0$;

$$\phi(x) = A\,cos(Bx) + C\,sin(Bx)\,;\text{ then }\frac{d\phi}{dx} = -BA\,sin(Bx) + BC\,cos(Bx)$$

$$\text{so at x} = 0, \frac{d\phi}{dx} = 0. - BA\,sin(B \times 0) + BC\,cos(B \times 0) = 0 \tag{10}$$

$$\text{or } -BA \times 0 + BC \times 1 = 0.\text{ So C } = 0 \text{ and } \phi(x) = A\,cos(Bx).$$

Now, boundary condition #4 can be applied to this system to complete the solution for the 1D slab. This boundary condition is used to determine the value for B.

The boundary condition is expressed as $\phi(X') = 0,\text{ so A}\,cos(BX') = 0.$

$$\text{Now }cos(BX') = 0 \text{ whenever BX}' = \frac{n\pi}{2}. \tag{11}$$

$$\text{Using this to solve for B gives: B } = \frac{n\pi}{2X'}.$$

Usually, the fundamental mode ($n = 1$) is the case of most interest. Thus, B can be rewritten as:

$$B = \frac{\pi}{2X'}\text{ , where, from Figure 2.1, X}' = X + d.$$

$$\text{So }B = \frac{\pi}{2(X+d)}\quad\text{ or }\quad B = \frac{\pi}{(d+2X+d)}. \tag{12}$$

$$\text{Thus, }\phi(x) = A\,cos\!\left(\frac{\pi x}{2X'}\right).$$

The remaining variable to determine is the value for A, the amplitude of the flux, which depends on the power of the fissile system. Until the power of the system is specified or known, A remains undetermined. Note that B determines the flux shape or frequency for the system.

At this point, it appears that we have a problem because two different values for B^2 have been defined.

$$B^2 = \left(\frac{\upsilon\Sigma_f - \Sigma_a}{D}\right) \quad \text{and} \quad B^2 = \left(\frac{\pi}{2X'}\right)^2 \tag{13}$$

These values for B^2 are not incorrect. The first definition is known as the *material buckling*, $\boldsymbol{B_m^2}$, and is dependent only on the materials in the system. The second definition is known as the *geometrical buckling*, B_g^2, and is dependent only on the system geometry. (Note: the buckling is B^2, not B, so it has units of cm^{-2}.)

If the geometric buckling, B_g^2, is the solution to the steady-state diffusion equation, then the definition can only apply when the multiplication factor for the system is 1 (critical). The material buckling, B_m^2, is independent of the multiplication factor; however, if the material buckling is just equal to the geometric buckling, then the system must be critical. This is because the geometric buckling, as defined above, is applicable only to a critical system. Thus, when $B_m^2 = B_g^2$, the multiplication factor is equal to 1, which is a critical system. It is noteworthy that the relationship between the geometric buckling and the material buckling can be used to identify subcritical and supercritical systems as follows.

As previously stated,

$$B_m^2 = B_g^2 \quad \text{then k } = 1 \quad \text{(Critical)}$$

$$B_m^2 > B_g^2 \quad \text{then k } > 1 \quad \text{(Supercritical)}$$

$$B_m^2 < B_g^2 \quad \text{then k } < 1 \quad \text{(Subcritical)}$$

$$\tag{14}$$

In other words, within a fixed geometry containing fissile material, the geometric buckling is constrained. If more fissile material is present than will fill the geometry, then the material buckling exceeds the geometric buckling, and the system is supercritical. If there is less fissile material than needed to fill the geometry, then the system is subcritical.

It is interesting at this point to see how the effective multiplication factor changes with changes in neutron flux. Recall the solution to the steady-state diffusion equation. When the rate of change in the neutron flux is positive ($d\Phi/dt > 0$), then the multiplication factor exceeds 1, which is indicative of a supercritical system. If the rate of change of the neutron flux is negative ($d\Phi/dt < 0$), then the multiplication factor is less than 1, which is indicative of a subcritical system. If the rate of change of the neutron flux is zero ($d\Phi/dt = 0$), then the system is at a critical condition, which indicates that the neutron population is constant and unchanging as a function of time.

If a change to the multiplication factor of a system is desired, then either the material or geometric properties of the system can be changed. Thus, the physical impacts of the material buckling, and geometric buckling can be reviewed.

- Material Buckling (B_m^2) — the material buckling is primarily a function of the absorption and fission cross-sections of a region. Once the moderator is specified, then the diffusion coefficient (D) remains effectively constant even if the quantity of the moderator or fuel is changed.

- Geometric Buckling (B_g^2) — the geometric buckling affects only the leakage of a system. Changing the geometrical properties of a system increases or decreases the neutron leakage.

Thus, a change in the neutron density of a system is equal to the difference of production and losses (absorption and leakage) from the system.

Change in the Neutron Density = Change in (Production – Absorption – Leakage) or

Change in the Neutron Density = Function of $(\boldsymbol{\delta B_m^2}, \boldsymbol{\delta B_g^2})$

2.2.2 Corrections for One-Group Diffusion Theory

For the discussions about diffusion theory, it is beneficial to discuss the difference between the effective multiplication factor (k_{eff}) and the infinite multiplication factor (k_∞). The k_{eff} is the multiplication factor of a finite system and considers neutron leakage, neutron absorption, and neutron production. The k_∞ is the infinite medium multiplication factor, which assumes no neutron losses caused by leakage from the system because a neutron cannot leave a system that is infinite in extent. Thus, the production term in the neutron diffusion equation, $\eta\Sigma_f$, can be written as follows:

$$k_\infty = \left(\frac{\text{Production}}{\text{Absorbtion}}\right) = \left(\frac{\nu\Sigma_f}{\Sigma_a}\right) \quad \text{or} \quad \nu\Sigma_f = k_\infty \times \Sigma_a \tag{15}$$

This relationship can be derived from the four-factor formula as follows:

First, define the fuel utilization factor, f, (often called the thermal utilization factor in thermal systems) as follows:

$$f = \frac{\Sigma_a^{Fuel}}{\Sigma_a^{System}} = \frac{\text{Neutrons absorbed in the fuel}}{\text{Neutrons absorbed in the system}} \tag{16}$$

Now define the neutron reproduction factor, η, as follows:

$$\eta = \frac{\nu\Sigma_f^{Fuel}}{\Sigma_a^{Fuel}} = \frac{\text{Neutrons produced in the fuel}}{\text{Neutrons absorbed in the fuel}} \tag{17}$$

Then the product of the two is:

$$\eta f = \frac{\nu\Sigma_f^{Fuel}}{\Sigma_a^{Fuel}} * \frac{\Sigma_a^{Fuel}}{\Sigma_a^{System}} = \frac{\nu\Sigma_f^{Fuel}}{\Sigma_a^{System}} = \frac{\text{Neutrons produced}}{\text{Neutrons absorbed}} = k_\infty \tag{18}$$

Equation (18) is valid for fast systems (i.e., those without moderation or significant neutron energy loss).

For other systems, corrections are required to account for slowing down and the addition of neutrons from fast fission. Thus, two correction terms, ε and *p,* are included in k_∞ and account for:

- ε   the increase in the number of fissions in the system from fast fissions occurring in a thermal system, and

- p the decrease in the neutrons available in the system for thermal fissions caused by absorptions in the resonance region while neutrons are slowing down.

Thus, ε and p allow for a one-group equation to be generated with correction factors to consider two-group effects. The production term in the one-group diffusion equation should be written with these terms present; however, these terms are usually assumed to be about equal to 1.0 for a fast system. The two terms affect the production of neutrons in a system, so Eq. (15) can be modified as follows:

$$\nu\Sigma_f\varepsilon p = k_\infty\Sigma_a \tag{19}$$

Equation (19) can be rewritten to produce what is known as the four-factor formula for the infinite multiplication factor.

$$\frac{\nu\Sigma_f}{\Sigma_a}\varepsilon p = k_\infty = \eta f\varepsilon p \tag{20}$$

Using Eq. (20), the "corrected" or time-dependent diffusion equation can be written as follows for a finite system:

$$\frac{1}{v}\frac{d\phi}{dt} = k_\infty\Sigma_a\phi - \Sigma_a\phi - (-D\nabla^2\phi) \tag{21}$$

This equation can be simplified as follows and is known as the modified steady-state diffusion equation. Recall that the time rate of change of the neutron flux for a steady-state system is zero (i.e., the neutron population in the system is constant). Therefore,

$$\nabla^2\phi + \frac{\Sigma_a}{D}(k_\infty - 1)\phi = 0 \tag{22}$$

In this equation, Σ_a / D (units of cm^{-2}) is equal to $1/L^2$, where L is the neutron diffusion length. The modified one-group diffusion theory equation can now be rewritten:

$$\nabla^2\phi + \frac{(k_\infty - 1)}{L^2}\phi = 0 \quad \text{or} \quad \nabla^2\phi + B_m^2\phi = 0$$

$$\text{where:} \quad B_m^2 = \frac{(k_\infty - 1)}{L^2} \quad \text{and} \quad L = \sqrt{\frac{D}{\Sigma_a}} \tag{23}$$

Rearranging Eq. (23), we get the following:

$$1 = \frac{k_\infty}{1 + B_m^2 L^2} \tag{24}$$

Equations (23) and (24) represent a critical system where the multiplication factor, k_{eff}, is equal to 1. It is important to note that for a system to be critical, the infinite multiplication factor, k_∞, must be greater than or equal to one. If it is equal to one, then there must be no leakage in a critical system. Thus, the fraction of non-leakage for a critical system is $1/k_\infty$. For example, if $k_\infty = 3/2$, then 2/3 of the neutrons must remain in the system if it is a critical system. If P_{NL} is defined as the non-leakage probability, then for a critical system,

$$P_{NL} = \frac{1}{k_\infty} \quad \text{or} \quad k_\infty P_{NL} = 1 \tag{25}$$

Using the second of the equations in (25) gives a mathematical representation of P$_{NL}$:

$$k_\infty P_{NL} = 1 \quad \text{and} \quad 1 = \frac{k_\infty}{1 + B_m^2 L^2} \quad \text{so} \quad k_\infty P_{NL} = \frac{k_\infty}{1 + B_m^2 L^2} \quad \text{or} \quad P_{NL} = \frac{1}{1 + B_m^2 L^2} \tag{26}$$

The leakage fraction is $P_L = 1 - P_{NL}$ or:

$$P_L = 1 - P_{NL} \quad \text{or} \quad 1 - \frac{1}{1 + B_m^2 L^2} \, \text{so} P_L = \frac{B_m^2 L^2}{1 + B_m^2 L^2} \tag{27}$$

Remember, for a critical system, $\boldsymbol{B_m^2 = B_g^2}$, so the material buckling can be replaced with the geometric buckling to determine the non-leakage probability or the leakage fraction. As this is the case, the critical buckling, $\boldsymbol{B_c^2 = B_m^2 = B_g^2}$ will be used where applicable.

2.2.3 Modified One-Group Diffusion Theory

Even corrected for fast fission and resonance absorption, one-group diffusion theory does not consider moderation as required for thermal systems. In particular, the process of moderation requires some distance for the neutrons to travel while slowing down. In the process of moderation, some neutrons may leak from the system. To account for these effects, one-group diffusion theory is modified by considering the neutron slowing down distance and non-thermal leakage.

The parameter typically used to account for slowing down is τ, known as the neutron age (cm^2). This is analogous to the square of the diffusion length for one-speed neutrons, but it accounts for the range of neutron speeds involved in moderation. When incorporated in the non-thermal non-leakage probability, the neutron age accounts for both the distance required to moderate the neutrons and the leakage of neutrons during moderation.

Using τ, the non-thermal or fast non-leakage probability, P_f, is defined from age diffusion theory as:

$$P_f = e^{-B_c^2 \tau} \tag{28}$$

For large systems, $B_c^2 \tau$ is small, so the fast non-leakage probability, P_f, can be approximated as:

$$P_f = e^{-B_c^2 \tau} \approx 1 - B_c^2 \tau \approx \frac{1}{1 + B_c^2 \tau}, \tag{29}$$

which is analogous to the one-speed non-leakage probability as defined in Eq. (25). Now using the neutron age factor to account for moderation, the production term for a thermal system (one where most of the neutrons have been moderated) can be written as:

$$\text{production} = k_\infty \Sigma_a e^{-B_c^2 \tau} \phi \tag{30}$$

Then the modified, steady-state diffusion equation can be written as:

$$k_\infty \Sigma_a e^{-B_c^2 \tau} \phi - \Sigma_a \phi - (-D\nabla^2 \phi) = 0$$

rearranging and using the definition of L^2

$$\nabla^2 \phi + \frac{k_\infty e^{-B_c^2 \tau} - 1}{L^2} \phi = 0 \quad \text{or} \quad \nabla^2 \phi + B_c^2 \phi = 0 \tag{31}$$

$$\text{so} \quad B_c^2 = \frac{k_\infty e^{-B_c^2 \tau} - 1}{L^2} = B_m^2 \quad \text{and} \quad \frac{k_\infty e^{-B_c^2 \tau}}{1 + B_c^2 L^2} = 1$$

where the last equation is known as the age-diffusion critical equation. Note that neutron age must be determined for the specific moderator used to create a thermal system. Using the definitions of fast and thermal non-leakage probabilities and the four-factor formula from Eq. (20), the age diffusion equation for a critical thermal system can be written in terms of six factors:

$$k_\infty \frac{e^{-B_c^2 \tau}}{1 + B_c^2 L^2} = 1 = \eta f \varepsilon p P_f P_{th} \tag{32}$$

where $P_{th} = \frac{1}{1 + B_c^2 L^2}$ is the thermal non-leakage probability, and $P_{NL} = P_f P_{th}$ is the total non-leakage probability.

If the approximation from Eq. (29) is used for the fast non-leakage probability, then the critical condition can be written as:

$$\frac{k_\infty}{(1 + B_c^2 \tau)(1 + B_c^2 L_{th}^2)} = 1 \quad \text{where} \quad L_{th}^2 = \frac{D_{th}}{\Sigma_{a_{th}}} \tag{33}$$

Doing the indicated multiplication in the denominator and ignoring the fourth-order term in B_c (it was assumed that the buckling was very small, so the square of the buckling will be very, very small), then

$$\frac{k_\infty}{(1 + B_c^2 \tau)(1 + B_c^2 L_{th}^2)} = \frac{k_\infty}{(1 + B_c^2(\tau + L_{th}^2))} = \frac{k_\infty}{(1 + B_c^2 M^2)} = 1 \tag{34}$$

where $M^2 = \tau + L_{th}^2$ is the migration area with units of cm². Equation (34) is the modified one-group expression for a critical thermal system.

2.3 CALCULATION OF PARAMETERS USED IN DIFFUSION THEORY

This section provides equations for calculating corrected cross sections, resonance escape probability, system diffusion length, buckling and flux shape associated with simple geometries, and discussion of calculations in reflected systems.

2.3.1 Corrections to 2,200 m/s Cross Sections

Most tables of thermal neutron cross sections provide values for a single energy (0.0253 eV) or its associated velocity (2,200 m/s). However, in most cases, we will have a distribution of neutron energies, so we will need cross sections for many different energies. At a more advanced level, we can apply what is known as the multigroup treatment to handle this problem. For hand calculations of thermal systems,

we will focus on neutrons that can be described by the Maxwellian distribution. We want to conserve the interaction rate over the range of neutron energies. We will particularly focus on the neutron absorption rate, so

$$\text{Absorptions} = \int n(E)\, v(E)\, \Sigma_a(E)\, dE \tag{35}$$

where Σ_a is the macroscopic absorption cross section as a function of energy, and the integral is evaluated in the thermal region up to about 0.1 eV.

For thermal systems, the neutron absorption cross section varies as $1/v$ at low energies, so we can write the energy variation of the cross section as follows:

$$\Sigma_a(E) = \Sigma_a(E_o)\frac{v_o}{v(E)} \tag{36}$$

where E_o is an energy reference point, and v_o is the velocity associated with E_o. Substituting this expression into the integral of Eq. (35), the $v(E)$ functions cancel out, and we are left with:

$$\text{Absorptions} = \Sigma_a(E_o)v_o \int n(E)\, dE \tag{37}$$

The integral is the total thermal neutron density, n, so the number of absorptions in a thermal system where the cross section is $1/v$ dependent will be:

$$\text{Absorptions} = \Sigma_a(E_o)nv_o = \Sigma_a(E_o)\phi_o \tag{38}$$

Thus, for a $1/v$ absorber, the absorption rate is independent of the energy distribution of the neutrons and is simply based on the absorption cross section at a reference energy. As most neutron cross sections are measured in materials at the ambient temperature, the reference energy, E_o, is taken as 0.0253 eV (20 °C) with a corresponding velocity, v_o, of 2,200 m/s. Cross section tabulations are prepared for 2,200 m/s neutrons. These are often labeled thermal cross sections but are only valid for monoenergetic neutrons with a velocity of 2,200 m/s (thermal neutrons are described in the next section). The product, nv_o, is called the 2,200 m/s flux, or ϕ_o.

Distribution Correction

Using the Maxwellian distribution, it can be shown that the average absorption cross section for a thermal distribution is:

$$\bar{\sigma}_{th} = \frac{\sqrt{\pi}}{2}\sigma_o = \frac{\sigma(2200 \text{ m/sec})}{1.128} = 0.886 \times \sigma(2200 \text{ m/sec}) \tag{39}$$

Thermal Flux

If the flux is given at a temperature (thermal flux) different than 293 K (temperature corresponding to a velocity of 2,200 m/s), then the thermal flux must be converted to the 2,200 m/s flux. This includes the distribution factor shown above and a correction for temperature. The relationship between the two fluxes is as follows:

$$\phi_o = \phi(T)\frac{\sqrt{\pi}}{2}\left(\frac{T_o}{T}\right)^{\frac{1}{2}} = \frac{\phi_o}{1.128}\left(\frac{T_o}{T}\right)^{\frac{1}{2}} \tag{40}$$

where $T_o = 293.16$ K, ϕ_o is the 2,200 m/s flux, and $\phi(T)$ is the thermal flux at absolute temperature T. Because the distribution correction appears in both the thermal cross section and the thermal flux, one needs only to correct either the cross section or the flux, but not both. The correction for thermal flux is often combined with the distribution correction to obtain an average thermal cross section.

$$\overline{\sigma}_{th}(T) = \frac{\sigma(T_o)}{1.128} \times \sqrt{\frac{T_o}{T}} = \frac{\sigma(2200 \text{ m/sec})}{1.128} \times \sqrt{\frac{293.16 \text{ K}}{T}}$$ (41)

This thermal cross section is then multiplied by the thermal flux to get the interaction rate (absorptions per second).

$$\text{Absorptions} = \Sigma_a(E_o)nv_{th} = N\overline{\sigma}_{th}\phi_{th} = N\overline{\sigma}_a(E_o)\phi_o$$ (42)

So, one can either use the thermal flux and thermal cross section or the 2,200 m/s flux and the 2,200 m/s cross section to calculate the absorption reaction rate.

Departure from *1/v* Dependence

For some fissile material and some commonly used absorber materials, the cross-section behavior is not strictly *1/v*. To correct for this, an empirical relationship has been developed, and the correction is characterized by *g(T)*. There are separate correction factors for absorption cross sections and for fission cross sections. Correction factors as a function of system temperature for some commonly used materials are given in Table 2-1 (based on Reference 3). These correction factors are then combined with the temperature and distribution correction factors to give the average microscopic thermal neutron cross section at a given temperature.

$$\overline{\sigma}_{th}(T) = \frac{\sigma(T_o)}{1.128} \times g(T) \times \sqrt{\frac{T_o}{T}} = 0.886 \times \sigma(2200 \text{ m/sec}) \times g(T) \times \sqrt{\frac{293.16 \text{ K}}{T}}$$ (43)

This thermal cross section is then multiplied by the thermal flux and the atom density to give the reaction rate. These results and corrections are strictly applicable to a completely thermalized system in which there is a Maxwell–Boltzmann distribution of neutrons that corresponds to the temperature of the moderator (i.e., the neutrons are in "thermal equilibrium" with the moderator material).

Table 2-1. Non-1/v Factors*.

T (° C)	Cd *ga*	In *ga*	U-235 *ga*	U-235 *gf*	U-238 *ga*	Pu-239 *ga*	Pu-239 *gf*
20	1.3203	1.0192	0.9780	0.9759	1.0018	1.0723	1.0487
100	1.5990	1.0350	0.9610	0.9581	1.0031	1.1611	1.1150
200	1.9631	1.0558	0.9457	0.9411	1.0049	1.3388	1.2528
400	2.5589	1.1011	0.9294	0.9208	1.0085	1.8905	1.6904
600	2.9031	1.1522	0.9229	0.9108	1.0122	2.5321	2.2037
800	3.0455	1.2123	0.9182	0.9036	1.0159	3.1006	2.6595
1000	3.0599	1.2915	0.9118	0.8956	1.0198	3.5353	3.0079

* Based on Reference 3, C.H. Wescott, *Effective Cross Section Values for Well-Moderated Thermal Reactor Spectra,* AECL-1101, January 1962.

2.3.2   Calculation of the Resonance Escape Probability

Resonance Escape Probability

After accounting for fast as well as thermal fissions, there are ε fast neutrons. As these neutrons slow down by interacting with a moderator, some of them may also interact with the U-238 in a uranium system (or Pu-240 in a plutonium system). At energies above 1 eV, U-238 has absorption resonances that dramatically increase the probability of neutron absorption. These resonances have very small energy widths, so a neutron must have a very specific energy to be absorbed in them. The energies of the neutrons will be related to the moderator, its macroscopic scattering cross section, and its average logarithmic energy decrement. To account for absorption in resonances, a parameter called the *resonance escape probability*, *p*, is calculated. The resonance escape probability is the number of neutrons that make it to thermal energies (and are thus absorbed because there is no leakage in an infinite system) divided by the number produced from all fissions (effectively the number of fast neutrons in the system).

$$\varepsilon = \frac{\text{Neutrons produced from all fissions}}{\text{Neutrons produced from thermal fissions}}$$

(44)

$$p = \frac{\text{Thermal neutrons absorbed in the system}}{\text{Neutrons produced from all fissions}}$$

Empirical equations have been derived to calculate resonance escape in U-238. The equation that will be used in this work is the following:

$$p = exp\left\{\frac{-3.06}{\xi}\left(\frac{N_{U238}}{Ns_{modmod}}\right)^{0.528}\right\}$$

(45)

where the units on atom density for U-238 and for the moderator must be the same. The units on the microscopic scattering cross section of the moderator must be barns, and ξ is the average logarithmic energy decrement for the moderator. Depending on the enrichment and fuel to moderator ratio, p will range from 0.3 to 1.0.[1]

Lethargy and "Squiggly (ξ)"

Because the neutron energy in a fissile system covers a wide range (from 10 MeV down to 0.01 eV), it is convenient to express the energy, *E*, in a logarithmic form as a dimensionless quantity called the lethargy, *u*.

---

[1] When using a cross section for hydrogen in a resonance escape calculation or in the determination of "squiggly (ξ)", a scattering cross section of 20.4 b is appropriate. This is the value of the hydrogen scattering cross section in the resonance energy range of 0.1 eV to 10 keV and as such is appropriate to a calculation of the resonance escape probability. (See R.D. O'Dell and R.D. Busch, "Validity of Hansen-Roach Cross Sections in Low-Enriched Systems," LA-UR-91-2347, July 1991 as reproduced as Appendix E of Busch, R.D., "A Primer for Criticality Calculations with DANTSYS," LA-13265, August 1997 (Reference 4). Some references (e.g., References 1, and 2) provide a thermal scattering cross section of 103 barns for water, but due to the bonding behavior of hydrogen in water at thermal energies, this value is higher than the actual value of 44.6 b (=20.4 * 2 + 3.8) over the resonance energy range.

$$u \equiv ln\frac{E_m}{E} \tag{46}$$

where E_m is an arbitrary reference point corresponding to zero lethargy. In most nuclear engineering applications, particularly those involving fission, E_m is usually taken as 10 MeV. Thus, the lethargy of a neutron increases as it slows down; that is, u increases as E decreases. If u_1 is the lethargy corresponding to E_1, the energy before a collision, and u_2 is the lethargy corresponding to E_2, the energy after the collision, then the change in lethargy $u_2 - u_1$ is:

$$\Delta u = u_2 - u_1 = ln\frac{E_1}{E_2} \tag{47}$$

Another useful quantity in neutron slowing down analyses is the average value of the decrease in the natural logarithm of the neutron energy per collision or the *average logarithmic energy decrement per collision*, denoted by ξ.

$$\xi = 1 + \frac{(A-1)^2}{2A} ln\frac{(A-1)}{(A+1)} = 1 + \frac{\alpha}{1-\alpha} ln\, \alpha \;\; where \alpha = \left(\frac{(A-1)}{(A+1)}\right)^2 \tag{48}$$

Note that ξ, often called "squiggly," is independent of the initial energy of the neutron. Except for small values of A (A<4), squiggly is well approximated by:

$$\xi \simeq \frac{2}{A + \frac{2}{3}} \tag{49}$$

For hydrogen, $\xi = 1$, and for deuterium, $\xi = 0.725$.

If the moderator is not a single material but a compound containing k different nuclei, then the effective value of ξ to be used in Eq. (45) is given by:

$$\overline{\xi} = \frac{\sum_{i=1}^{k} N_i \sigma_{s_i} \xi_i}{\sum_{i=1}^{k} N_i \sigma_{s_i}} = \frac{N_1 \sigma_{s_1} \xi_1 + N_2 \sigma_{s_2} \xi_2 + ... + N_k \sigma_{s_k} \xi_k}{N_1 \sigma_{s_1} + N_2 \sigma_{s_2} + ... + N_k \sigma_{s_k}} \tag{50}$$

Note that because moderation is a scattering process, the average logarithmic energy decrement is weighted by the macroscopic scattering cross section, Σ_s, for each nuclide in the system.

2.3.3 Slowing Down and Thermal Diffusion

The neutron leakage from a finite system is a function of the geometry (its size and shape). The size parameter has to do with the average distance traveled from birth to thermalization for a fast neutron and from thermalization to death for a thermal neutron in the system. The first length is called the slowing down length, L_f, whereas the second is known as the diffusion length, L_{th}. In most systems, it is the properties of the moderator that determine the values for the two lengths. Values of fast and thermal properties for typical moderators are given in Table 2-2.

Table 2-2. Values of Fast and Thermal Properties for Selected Moderators*.

Moderator	L_f (cm)	D_f (cm)	τ (cm²)	L_{th} (cm)	D_{th} (cm)
H_2O	5.2	1.13	~27	2.85	0.16
D_2O	11.4	1.29	130	97	0.87

Be	10.1	0.56	102	21	0.50
Graphite	19.2	1.02	368	59	0.84

* Based on Reference 2 and Reference 5.

The D parameters in the table are fast and thermal diffusion coefficients that relate neutron flow to the flux gradient. The slowing down length, neutron age, and thermal diffusion length can be determined from the diffusion coefficients and the macroscopic absorption cross section for the system as

$$L_f = \sqrt{\frac{D_f}{\Sigma_{a-fast}}} \quad \tau = \frac{D_f}{\Sigma_{a-fast}} \quad L_{th} = \sqrt{\frac{D_{th}}{\Sigma_{a-thermal}}} \tag{51}$$

When calculating critical size, the thermal diffusion area of the system is required. This can be calculated from the diffusion coefficient of the system and the macroscopic absorption cross section of the system, or it can also be calculated based on the moderator characteristics.

$$L_{sys}^2 = L_{mod}^{2(1-f)} \tag{52}$$

The leakage probability for fast and thermal neutrons is often characterized by the migration area, M^2, which is the sum of the fast slowing down area and the thermal diffusion area. The greater the value of M^2, the greater the probability that a neutron will leak.

$$M^2 = L_f^2 + L_{th}^2 \quad \text{or} \quad M^2 = \tau + L_{th}^2 \tag{53}$$

2.3.4   Flux Shapes for Critical, Bare, Infinite Geometries

Solutions to the one-group diffusion equation for different geometries are based on the Laplacian for that geometry. For example, in a sphere, the solution to the Laplacian is a function of sine and cosine. After appropriate boundary conditions are applied, the flux in a sphere is as follows:

$\phi(x) = A/r \sin\left(\pi r/\tilde{R}\right)$, whereas the same approach gives the flux in an infinite cylinder as

$\phi(x) = A J_o\left(2.405 r/\tilde{R}\right)$ and for the flux in an infinite slab as $\phi(x) = A \cos\left(\pi x/\tilde{H}\right)$.

In these equations, A is the maximum value of the flux, and the dimensions identified with a ~ include extrapolation distances.

Note that there is an inconsistency in the units between the sphere equation and the other two equations. The last two equations have units associated with the constant A, whereas the sphere has units of those associated with A but divided by units of length. This indicates a normalization problem, so the equations need to be reformed into a consistent set where the value of $\phi(0) = A$.

For the slab and for the cylinder, there is no need for a change in format as both have the value of A at the origin. However, for the sphere, it is necessary to ascertain its value at r = 0. Use of L'Hospital's Rule provides a $\phi(0) = A\left(\pi/\tilde{R}\right)$. So, the equation must be normalized to A by multiplying by $\left(\tilde{R}/\pi\right)$ to give $\phi(x) = A\left(\tilde{R}/\pi r\right)\sin\left(\pi r/\tilde{R}\right)$.

Table 2-3 provides the flux shape and geometric buckling for three simple geometries: a sphere, an infinite cylinder, and an infinite slab.

Table 2-3. Flux Shape and Geometric Buckling for Simple Geometries.

Configuration	Flux Shape for Critical, Bare Reactor	Geometric Buckling, $B_g{}^2$
Sphere of Radius, R	$\frac{\tilde{R}}{\pi r}\sin\left(\frac{\pi r}{R+d}\right)$	$\left(\frac{\pi}{R+d}\right)^2$
Infinite Cylinder of Radius, R	$J_o\left(\frac{2.405r}{R+d}\right)$	$\left(\frac{2.405}{R+d}\right)^2$
Infinite Slab of Thickness, H	$\cos\left(\frac{\pi x}{H+2d}\right)$	$\left(\frac{\pi}{H+2d}\right)^2$

Note: The variable d in each of the expressions for geometric buckling is the extrapolation distance, which is a function of the fissile material present in the system, the shape or geometry, and the materials surrounding the fissile material. Each of the flux shape equations is normalized to a value of 1.0 at the center of the geometry.

The flux shapes are shown in Figure 2-2. The fluxes in Figure 2-2 are normalized to unity at the center. Note that the slab flux is greater than the infinite cylinder flux, which is greater than the flux in a sphere.
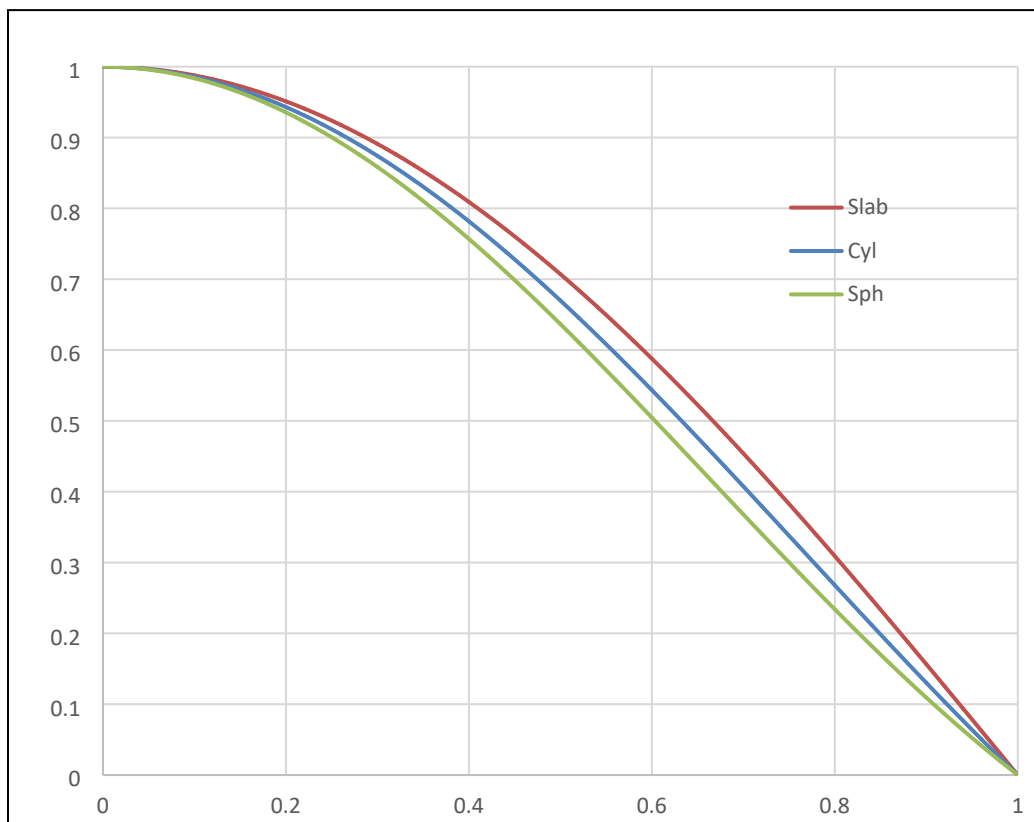
Figure 2-2. Neutron fluxes for the infinite slab, infinite cylinder, and sphere as a function of the fractional distance from their center to the surface.

2.3.5 Reflected Spheres and Slabs

Neutron economy is improved when the core of a reactor is surrounded by a reflector—that is, by a thick, unfueled region of moderator. The neutrons that otherwise would leak from the bare core now pass into the reflector, and some of these diffuse back into the core. The net result is that the critical size, and hence mass of the system, is reduced.

Criticality calculations for reflected reactors are now considered within the framework of the one-group diffusion theory. Recall that this method is applicable to calculations of fast reactors and thermal reactors, such as those moderated by D_2O or graphite for which $\tau_T << L_T^2$. Reflected water reactors are treated separately as $\tau_T >> L_T^2$.

Reflected Sphere

As an example, consider a spherical reactor consisting of a core of radius R and surrounded by an infinite reflector. In the following analysis, parameters that refer to the core and reflector are denoted by the subscripts c and r, respectively.

Solving the diffusion equation in the core gives a flux:

$$\phi_c(r) = A \frac{\sin B\,r}{r} + C \frac{\cos B\,r}{r} \tag{54}$$

where A and C are constants determined from the boundary conditions. The symmetry boundary condition requires $C = 0$. As there is no fuel in the reflector, the flux in that region satisfies the one group diffusion equation:

$$\nabla^2 \phi_r - \frac{1}{L_r^2}\phi_r = 0 \quad \text{whose general solution is} \quad \phi_r(r) = A' \frac{e^{-\frac{r}{L_r}}}{r} + C' \frac{e^{+\frac{r}{L_r}}}{r} \tag{55}$$

where A' and C' are constants determined from the boundary conditions. The boundary condition of a finite flux as r goes to infinity requires $C' = 0$. Applying the continuity of flux and current boundary conditions at the interface between the core and reflector produces the following critical condition for a reflected spherical reactor:

$$BR \cot(BR) - 1 = -\frac{D_r}{D_c}\left(\frac{R}{L_r}\coth\frac{T}{L_r} + 1\right) \tag{56}$$

where T is the thickness of the reflector plus the extrapolation distance. This transcendental equation is solved for R either graphically or using a Goal Seek/Solver approach in a spreadsheet. The B in Eq. (56) is the square root of the critical buckling for the bare system with the same fissile material. Note that the critical radius for a reflected system is less than the critical radius of the bare system for the same material. This means that the reflected system is critical with less fissile material.

Reflected Infinite Slab

As another example, consider an infinite slab of thickness a surrounded on both sides by a reflector of extrapolated thickness, b. In the following analysis, parameters that refer to the core and reflector are denoted by the subscripts c and r respectively.

Solving the diffusion equation in the core gives a flux:

$$\phi_c(r) = A \cos B\, x + C \sin B\, x \qquad \text{(57)}$$

where *A* and *C* are constants determined from the boundary conditions. The symmetry boundary condition requires *C* = 0. As there is no fuel in the reflector, the flux in that region satisfies the one-group diffusion equation:

$$\nabla^2 \phi_r - \frac{1}{L_r^2}\phi_r = 0 \quad \text{general solution}$$

$$\phi_r(r) = A' \sinh\left(\frac{(a/2 + b - |x|)}{L_r}\right) + C' \cosh\left(\frac{(a/2 + b - |x|)}{L_r}\right) \qquad \text{(58)}$$

where *A'* and *C'* are constants determined from the boundary conditions. The boundary condition of flux = 0 at $|x| = a/2 + b$, requires *C'* = 0. Applying the continuity of flux and current boundary conditions at the interface between the core and reflector produces the following critical condition for a reflected infinite slab system:

$$B \tan\left(\frac{Ba}{2}\right) = \frac{D_r}{D_c}\frac{1}{L_r} \coth\left(\frac{b}{L_r}\right) \qquad \text{(59)}$$

This equation can be rearranged to solve for *a* using the critical buckling of the bare system, as the *B* in Eq. (59) is the square root of the critical buckling for the bare system with the same fissile material. Again, note that the critical thickness for a reflected system is less than the critical radius of the bare system for the same material. This means that the reflected system is critical with less material.

Reflected Infinite Cylinder

Calculations for a reflected infinite cylinder are more difficult, as these require I_o, J_o, K_o, *and* Y_o Bessel functions, which are likely unfamiliar to most of us. However, an approximation can be made by assuming similarity to an infinite slab. Notice in Figure 2-2, the flux shape of the infinite slab and infinite cylinder are very similar. As a rough estimate of the thickness of a reflected cylinder, Eq. (59) can be used with the reflected cylinder diameter R_{cyl} replacing *a*.

2.4 APPLICABILITY OF ONE-GROUP DIFFUSION THEORY

Because diffusion theory is derived from the Boltzmann Neutron Transport equation using several assumptions, there are limitations to its application. The one-group diffusion theory method is applicable for fissile material systems with the following characteristics and assumptions.

- All neutrons in the system must have the same energy or velocity (this approximation is more valid for fast, but not thermal, systems).

- It is assumed that neutrons that collide with nuclei in the system do not lose energy, and only their direction of movement changes.

- The medium in which the neutrons are diffusing is homogeneous.

- Neutron scattering is isotropic, meaning that neutrons that scatter will do so in all directions.

- A "close-fitting" neutron reflector does not surround the fissile material.

- The medium in which the neutrons are diffusing is weakly absorbing.

- The neutron flux is a slowly varying function of position in the system, a characteristic which is true at points in the system that are at least a few mean free paths from the system boundaries.

2.5   APPLICABILITY OF MODIFIED ONE-GROUP DIFFUSION THEORY

The modified one-group diffusion approximation has the same applicability and limitations as the one-group diffusion approximation; however, the added correction factors allow this method to be used for homogeneous systems that contain moderating materials.

2.6   EXAMPLE PROBLEMS

The example problems for one-group and modified one-group diffusion theories will illustrate how they can be applied to simple systems to determine the characteristics for the system. Each method will be compared with the others to show the usefulness and limitations of the methods for various systems.

2.6.1   Diffusion Theory Example Problem 1 – Fast System with Uranium

The Godiva critical assembly used for experiments at Los Alamos National Laboratory (LANL) was employed in various critical experiments (see Figure 2-3). Assume the assembly is made from 93.5%[2] enriched U-235 (ρ = 18.74 g/cm^3) and is an unreflected or bare system. Using one-group diffusion theory, estimate the spherical critical radius (cm) for this system with the three fissile pieces fully assembled.

---

[2] Enrichments of uranium are often written in the form of U(93.5) with the value in parentheses indicating the weight percent of U-235.
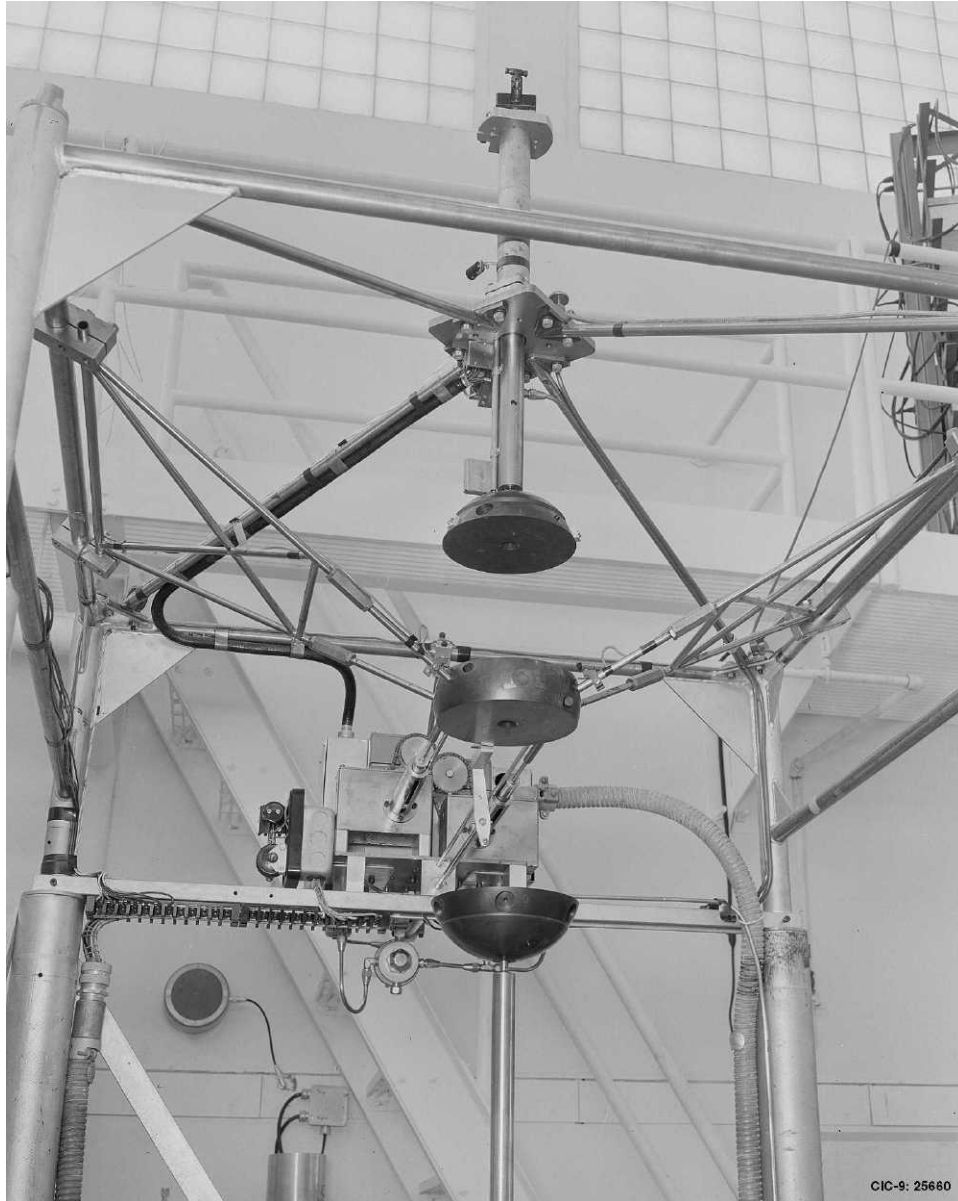
Figure 2-3. The Godiva I Critical Assembly at LANL (Reference 6).

Before starting any calculation of fissile material system properties, one should have an idea what the answer should be—that is, at least an order of magnitude estimate, as well as the expected units of the results. For this case, we are interested in the spherical critical radius in centimeters. There are several handbooks and safety guides that provide information and critical dimensions for fissile systems. For this problem, we are using ARH-600, Vol. II (Reference 7). On page III.B-2, it indicates that the minimum spherical critical mass of U-235 for a bare metal U(93.5) system is 47 kg U-235 at a density of 18.8 g U-235/cc. Using these data, the spherical volume would be 2,500 cc. The associated spherical radius is then 8.42 cm. So, our calculations should give a result around 8.5 cm.

The data relevant for this problem are listed in Table 2-4 below. Note that Godiva is an unmoderated, fast system. Therefore, the first step in solving this problem is to make sure that fast neutron cross section data are used in the calculation.

Table 2-4. Diffusion Theory Example Problem 1 Data.

Constituent	Parameter	Data Value	Reference
^{235}U	σ_a(fast)	1.65 barns	2, Table 6-1, pg. 267
	σ_f(fast)	1.40 barns	2, Table 6.1, pg. 267
	σ_{tr}(fast)	6.80 barns	2, Table 6.1, pg. 267
	ν	2.60	2, Table 6.1, pg. 267
^{238}U	σ_a(fast)	0.255 barns	2, Table 6.1, pg. 267
	σ_f(fast)	0.095 barns	2, Table 6.1, pg. 267
	σ_{tr}(fast)	6.90 barns	2, Table 6.1, pg. 267
	ν	2.60	2, Table 6.1, pg. 267

First, calculate the atom densities for the enriched uranium so that the macroscopic fission and absorption cross sections can be calculated. (Procedures and equations for calculating atom densities can be found in the Appendix of the DANTSYS[3] Primer, Reference 4.)

$$N = \frac{wt.\,\%\ of\ Constituent\ in\ the\ System \times \rho_{mixture} \times N_A}{A_{constituent}}$$

$$N_{235_U} = \frac{(0.935)(18.74\ g/cm^3)(\frac{0.6022\ atoms-cm^2}{mol-b})}{235.04\ g/mol} = 4.489 \times 10^{-2}\ atoms/b-cm$$

$$N_{238_U} = \frac{(0.065)(18.74\ g/cm^3)(\frac{0.6022\ atoms-cm^2}{mol-b})}{238.05\ g/mol} = 3.081 \times 10^{-3}\ atoms/b-cm.$$

Now that the atom densities for U-235 and U-238 have been determined, the macroscopic absorption and fission cross sections can be calculated for this fast system. References 1 and 2 provide good background information about calculating macroscopic cross sections.

$$\Sigma_a^{U-235} = N_{235_U} \times \sigma_a^{235_U}$$

$$\Sigma_a^{U-235} = 4.489 \times 10^{-2}\ atoms/b-cm \times 1.65\ b = 7.407 \times 10^{-2}\ cm^{-1}$$

$$\Sigma_a^{U-238} = N_{238_U} \times \sigma_a^{238_U}$$

$$\Sigma_a^{U-238} = 3.081 \times 10^{-3}\ atoms/b-cm \times 0.255\ b = 7.857 \times 10^{-4}\ cm^{-1}$$

---

[3] DANTSYS (Diffusion Accelerated Neutron Transport code SYStem) was developed at Los Alamos as a modular computer program package designed to solve the time-independent or time-dependent multigroup discrete ordinates form of the Boltzmann transport equation in simple one-, two-, and three-dimensional geometries. It has since been replaced by PARTISN (PARallel, TIme-Dependent SN), which handles the same geometries plus a couple more and has additional features that speed up the solution process. The listed reference for DANTSYS is also applicable to PARTISN. In this document, all further references to the computer code will be to PARTISN.

$$\Sigma_f^{U-235} = N_{235_U} \times \sigma_f^{235_U}$$

$$\Sigma_f^{U-235} = 4.489 \times 10^{-2} \; atoms/b\text{-}cm \times 1.40 \; b = 6.285 \times 10^{-2} \; cm^{-1}$$

$$\Sigma_f^{U-238} = N_{238_U} \times \sigma_f^{238_U}$$

$$\Sigma_f^{U-238} = 3.081 \times 10^{-3} \; atoms/b\text{-}cm \times 0.095 \; b = 2.927 \times 10^{-4} \; cm^{-1}.$$

The infinite multiplication factor, k_∞, can be determined now that the macroscopic cross sections have been calculated. Because it is a small system without moderation, it is dominated by fast neutrons and has a high neutron leakage.

$$k_\infty = \eta = \frac{\nu\Sigma_f^{235_U} + \nu\Sigma_f^{238_U}}{\Sigma_a^{235_U} + \Sigma_a^{238_U}} = \frac{\nu\left(\Sigma_f^{235_U} + \Sigma_f^{238_U}\right)}{\Sigma_a^{235_U} + \Sigma_a^{238_U}},$$

$$k_\infty = \frac{(2.60)[6.285 \times 10^{-2} cm^{-1} + 2.927 \times 10^{-4} cm^{-1}]}{(7.407 \times 10^{-2} cm^{-1}) + (7.857 \times 10^{-4} cm^{-1})} = 2.193.$$

The diffusion coefficient, D, the diffusion length, L^2, and the material buckling, $B_m{}^2$, are now calculated.

$$D = \left(\frac{1}{3\Sigma_{tr}}\right)_{235_U + 238_U} = \left(\frac{1}{3 \times \left[N_{235_U} \times \sigma_{tr}^{235_U} + N_{238_U} \times \sigma_{tr}^{238_U}\right]}\right),$$

D

$$= \left(\frac{1}{3\left[(4.489 \times 10^{-2} \; atoms/b - cm)(6.8 \; b) + (3.081 \times 10^{-3} \; atoms/b - cm)(6.9 \; b)\right]}\right) = 1.021 \; cm$$

,

$$L^2 = \frac{D}{\Sigma_a^{235_U} + \Sigma_a^{238_U}} = \frac{1.021 \; cm}{7.407 \times 10^{-2} \; cm^{-1} + 7.857 \times 10^{-4} \; cm^{-1}} = 13.64 \; cm^2.$$

Now, the material buckling, B_m^2, can be calculated using the results from above:

$$B_m^2 = \frac{k_\infty - 1}{L^2} = \frac{2.195 - 1}{13.64 \; cm^2} = 0.0876 \; cm^{-2}.$$

We can use the process from the last example problem to determine the critical size for this system, knowing that when a system is critical, the material buckling and geometric buckling are equal.

$$B_m^2 = B_g^2 = \left(\frac{\pi}{\overline{R}}\right)^2,$$

$$\overline{R} = \sqrt{\frac{\pi^2}{B_m^2}} = \sqrt{\frac{\pi^2}{0.0876 \; cm^{-2}}} = 10.61 \; cm,$$

$$R = \overline{R} - d = \overline{R} - 2.13 \times D = 10.61 \; cm - 2.13 \times 1.021 \; cm = 8.44 \; cm.$$

The physical radius of Godiva is 8.6 cm. The prediction using this method is very close to the actual system dimensions in this case. Also, note that the predicted radius is well within our estimate from the handbook.

2.6.2   Diffusion Theory Example Problem 2 – Fast System with Plutonium

The Jezebel critical assembly used for experiments at LANL was used to perform various critical experiments (see Figure 2-4). Assume the assembly is made from δ-phase Pu-239 ($\rho = 15.61$ g/cm^3) and is an unreflected or bare system. Using one-group diffusion theory, estimate the spherical critical radius for this system with the three fissile pieces fully assembled.
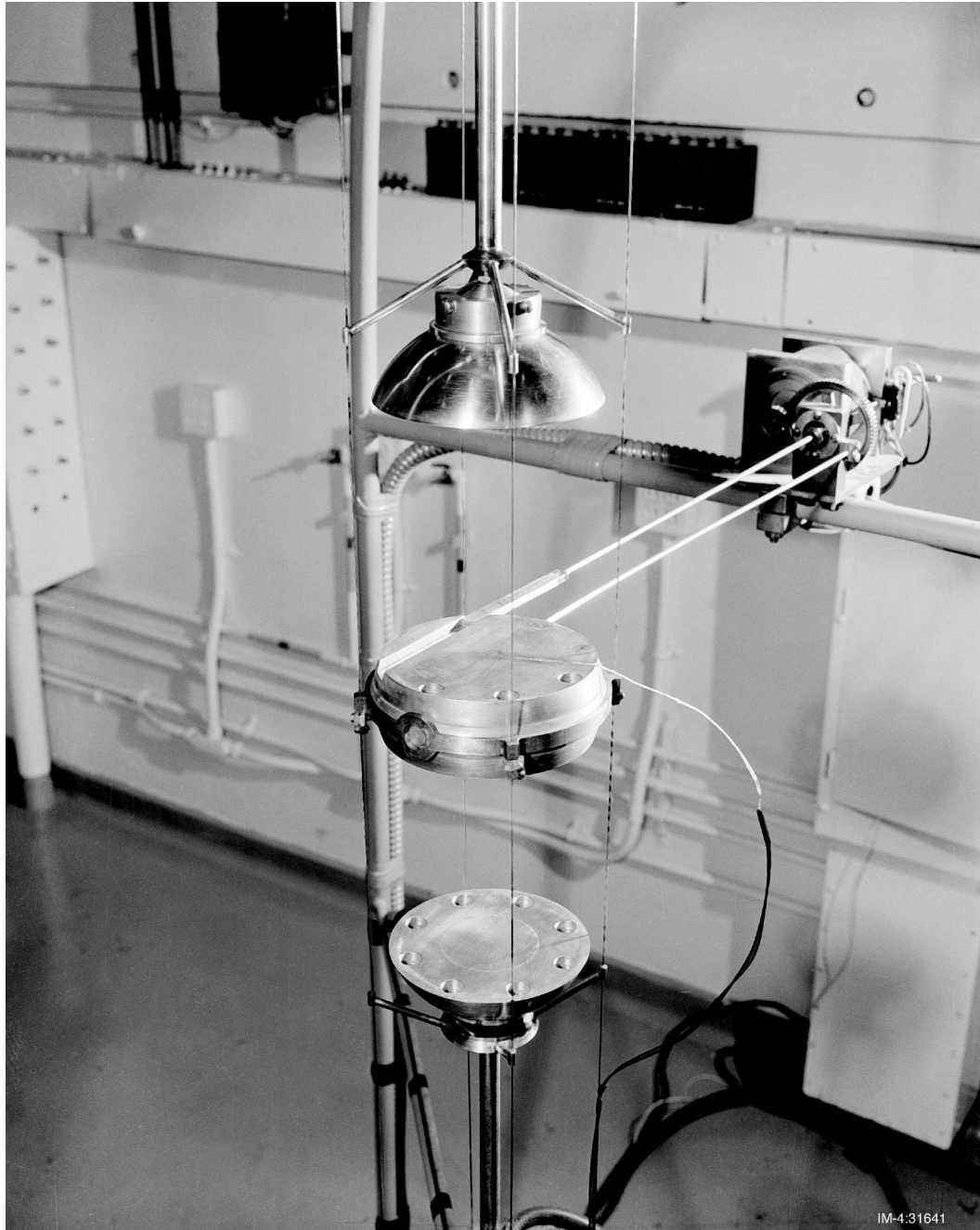
Figure 2-4. The Jezebel Critical Assembly at LANL (Reference 6).

For an estimate of the critical radius (cm), Jarvis et al. (Reference 8), indicate that a sphere of Pu(4.5)[4] has a critical mass of 16.28 kg with an effective density of 15.44 g/cc. Using these data, the spherical critical volume is 1,054 cc with an associated spherical radius of 6.31 cm. So, our one-group calculated radius should be around 6.3 cm. The data relevant for this problem are listed in Table 2-5 below. Note that Jezebel is an unmoderated, fast system. Therefore, the first step in solving this problem is to make sure that fast neutron cross-section data are used in the calculation.

Table 2-5. Diffusion Theory Example Problem 2 Data.

Constituent	Parameter	Data Value	Reference
^{239}Pu	σ_a(fast)	2.11 barns	2, Table 6.1, pg. 267
	σ_f(fast)	1.85 barns	2, Table 6.1, pg. 267
	σ_{tr}(fast)	6.8 barns	2, Table 6.1, pg. 267
	σ_c(fast)	0.26 barns	2, Table 6.1, pg. 267
	ν	2.98	2, Table 6.1, pg. 267

First, calculate the atom densities for the Pu-239.

$$N = \frac{\text{wt. \% Constituent in System} \times \rho_{\text{mixture}} \times N_A}{A_{constituent}}$$

$$N_{239Pu} = \frac{(15.61 \ g/cm^3)(\frac{0.6022 \ atoms-cm^2}{mol-b})}{239.05 \ g/mol} = 3.932 \times 10^{-2} \ atoms/b\text{-}cm.$$

Now that the atom density for Pu-239 has been calculated, the macroscopic absorption and fission cross sections can be determined for this fast system:

$$\Sigma_a^{Pu} = N_{239Pu} \times \sigma_a^{239Pu}$$

$$\Sigma_a^{Pu} = 3.932 \times 10^{-2} \ atoms/b - cm \times 2.11 \ b = 8.298 \times 10^{-2} \ cm^{-1}$$

$$\Sigma_f^{Pu} = N_{239Pu} \times \sigma_f^{239Pu}$$

$$\Sigma_f^{Pu} = 3.932x10^{-2} \ atoms/b - cm \times 1.85 \ b = 7.274 \times 10^{-2} \ cm^{-1}.$$

The infinite multiplication factor, k_∞, can now be calculated. Note that all fissions take place at fast energies and that only Pu-239 is present in the system. The neutron leakage from this kind of system is rather high because the neutrons do not slow down in this type of system.

---

[4] Similar to uranium, the Pu-240 assay of a plutonium mixture is often written in the form of Pu(4.5), with the value in parentheses indicating the weight percent of Pu-240.

$$k_\infty = \eta f = v \times \frac{\Sigma_f^{Pu}}{\Sigma_a^{Pu}} \times \frac{\Sigma_a^{Pu}}{\Sigma_a^{Pu}}$$

$$k_\infty = 2.98 \times \frac{7.274 \times 10^{-2} cm^{-1}}{8.298 \times 10^{-2} cm^{-1}} \times 1 = 2.612.$$

Now, the diffusion coefficient, D, the diffusion length, L^2, and the material buckling, $B_m{}^2$, can be calculated based on the result of the k_∞ calculation.

$$D_{239_{Pu}} = \left(\frac{1}{3\Sigma_{tr}}\right)_{Pu} = \left(\frac{1}{3 \times N_{239_{Pu}} \times \sigma_{tr}^{239_{Pu}}}\right)$$

$$D_{239_{Pu}} = \left(\frac{1}{3 \times 3.932 \times 10^{-2} \ atoms/b - cm \times 6.8 \ b}\right) = 1.247 \ cm$$

$$L^2 = \frac{D_{239_{Pu}}}{\Sigma_a^{Pu}} = \frac{1.247 \ cm}{8.298 \times 10^{-2} \ cm^{-1}} = 15.03 \ cm^2$$

Now calculate the material buckling, $B_m{}^{2:}$

$$B_m^2 = \frac{k_\infty - 1}{L^2} = \frac{2.612 - 1}{15.03 \ cm^2} = 0.1073 \ cm^{-2}.$$

Notice the diffusion length, L, for this system is short—only about 3.9 cm, as most of the neutrons are absorbed in the Pu. The mean free path for this system is as follows:

$$\lambda_t \approx \lambda_{tr} = \frac{1}{\Sigma_{tr}} = \frac{1}{N_{239_{Pu}} \times \sigma_{tr}^{239_{Pu}}} = \left(\frac{1}{3.932 \times 10^{-2} \ atoms/b - cm \times 6.8 \ b}\right) = 3.74 \ cm$$

This is a relatively short distance, so most neutrons in the system will have undergone at least one interaction before leaking or being absorbed. The buckling is needed to determine the critical size. Now, for a critical system, the material and geometric buckling values are equal. The critical dimensions for this system can be calculated as follows:

$$B_m^2 = B_g^2 = \left(\frac{\pi}{\bar{R}}\right)^2$$

$$\bar{R} = \sqrt{\frac{\pi^2}{B_m^2}} = \sqrt{\frac{\pi^2}{0.1073 \ cm^{-1}}} = 9.59 \ cm$$

$$R = \bar{R} - d = \bar{R} - 2.13 \times D = 9.59 \ cm \text{ - } 2.13 \times 1.247 \ cm = 6.93 \ cm.$$

The actual Jezebel system had a density of 15.61 g/cc, was 4.5 wt. % Pu-240, and had a critical radius of 6.385 cm. With the cross sections used and assumption of 100 wt. % Pu-239, this method slightly

over-predicts the critical radius for this type of system. Note also that the calculated radius is within 10% of our initial estimate of 6.31 cm.

Analysis with collapsed H-R Cross Sections: Jezebel was a mixture of Pu-239 (3.7047e-2 atoms/b-cm), Pu-240 (1.7510e-3 atoms/b-cm), Pu-241 (1.17e-4 atoms/b-cm) and Ga (1.375-3 atoms/b-cm). To determine the effect of the mixture on the result, a set of six group cross sections from Reference 9 was collapsed with a typical fast neutron spectrum. The data are listed in Table 2-6 below.

Table 2-6. Diffusion Theory Example Problem 2 Data Set 2.

Constituent	Parameter	Data Value
^{239}Pu	σ_a(fast)	1.92 barns
	$\nu\sigma_f$(fast)	5.62 barns
	σ_{tr}(fast)	6.8 barns
^{240}Pu	σ_a(fast)	1.23 barns
	$\nu\sigma_f$(fast)	3.79 barns
	σ_{tr}(fast)	6.8 barns
^{241}Pu	σ_a(fast)	1.89 barns
	$\nu\sigma_f$(fast)	5.76 barns
	σ_{tr}(fast)	6.0 barns
Ga	σ_a(fast)	0.034 barns
	σ_{tr}(fast)	3.2 barns

Notice that there is much less Pu-239 absorption indicated in this set than in the set given in Table 2-6. The atom densities are given, so we continue to calculate the macroscopic absorption, and fission cross sections can be determined for this nuclear dataset:

$$\Sigma_a^{Pu239} = N_{239Pu} \times \sigma_a^{239Pu}$$

$$\Sigma_a^{Pu239} = 3.7047 \times 10^{-2} \ atoms/b-cm \times 1.92 \ b = 7.113 \times 10^{-2} \ cm^{-1}$$

$$\nu\Sigma_f^{Pu239} = N_{239Pu} \times \nu\sigma_f^{239Pu}$$

$$\nu\Sigma_f^{Pu239} = 3.7047 x 10^{-2} \ atoms/b-cm \times 5.62 \ b = 2.0820 \times 10^{-1} \ cm^{-1}.$$

$$\Sigma_a^{Pu240} = N_{240Pu} \times \sigma_a^{240Pu}$$

$$\Sigma_a^{Pu240} = 1.751 \times 10^{-3} \ atoms/b-cm \times 1.229 \ b = 2.154 \times 10^{-3} \ cm^{-1}$$

$$\nu\Sigma_f^{Pu240} = N_{240Pu} \times \nu\sigma_f^{240Pu}$$

$$\nu\Sigma_f^{Pu240} = 1.751 \times 10^{-3} \ atoms/b-cm \times 3.79 \ b = 6.636 \times 10^{-3} \ cm^{-1}.$$

$$\Sigma_a^{Pu241} = N_{241_{Pu}} \times \sigma_a^{241_{Pu}}$$

$$\Sigma_a^{Pu241} = 1.17 \times 10^{-4} \, atoms/b-cm \times 1.891 \, b = 2.21 \times 10^{-4} \, cm^{-1}$$

$$\nu\Sigma_f^{Pu241} = N_{241_{Pu}} \times \nu\sigma_f^{241_{Pu}}$$

$$\nu\Sigma_f^{Pu241} = 1.17 \times 10^{-4} \, atoms/b-cm \times 5.76 \, b = 6.74 \times 10^{-4} \, cm^{-1}.$$

$$\Sigma_a^{Ga} = N_{Ga} \times \sigma_a^{Ga}$$

$$\Sigma_a^{Ga} = 1.375 \times 10^{-3} \, atoms/b-cm \times 0.034 \, b = 4.7 \times 10^{-5} \, cm^{-1}$$

The infinite multiplication factor, k_∞, can now be calculated by determining η and f.

$$\eta = \frac{\sum \nu\Sigma_f^{Pu}}{\sum \Sigma_a^{Pu}} = \frac{2.0820x10^{-1} + 6.64x10^{-3} + 6.7x10^{-4}}{7.113x10^{-2} + 2.15x10^{-3} + 2.2x10^{-4}}$$

$$\frac{\nu\Sigma_f^{fuel}}{\Sigma_a^{fuel}} = \frac{2.1551x10^{-1}}{7.350x10^{-2}} = 2.932$$

$$f = \frac{\Sigma_a^{fuel}}{\Sigma_a^{fuel} + \Sigma_a^{Ga}} = \frac{7.350x10^{-2}}{7.350x10^{-2} + 5x10^{-5}} = \frac{7.350x10^{-2}}{7.355x10^{-2}} = 0.9993$$

$$k_\infty = \eta f = 2.932 \times 0.9993 = 2.930.$$

Now calculate the macroscopic transport cross section for the system.

$$\Sigma_{tr}^{sys} = \sum \Sigma_{tr} = N_{239_{Pu}} \times \sigma_{tr}^{239_{Pu}} + N_{240_{Pu}} \times \sigma_{tr}^{240_{Pu}} + N_{241_{Pu}} \times \sigma_{tr}^{241_{Pu}} + N_{Ga} \times \sigma_{tr}^{Ga}$$

$$\Sigma_{tr}^{sys} = 3.7047 \times 10^{-2} \, atoms/b-cm \times 6.8 \, b + 1.751 \times 10^{-3} \, atoms/b-cm \times 6.8 \, b +$$
$$1.17 \times 10^{-4} \, atoms/b-cm \times 6.0 \, b + 1.375 \times 10^{-3} \, atoms/b-cm \times 3.16$$
$$= 2.6893x10^{-1} \, cm^{-1}$$

Using the macroscopic system transport cross section, calculate the diffusion coefficient, D, the diffusion length, L^2, and the material buckling, B_m^2.

$$D_{sys} = \left(\frac{1}{3\Sigma_{tr}^{sys}}\right) = \left(\frac{1}{3 \times 2.6893x10^{-1} \, cm^{-1}}\right) = 1.239 \, cm$$

$$L^2 = \frac{D_{sys}}{\Sigma_a^{sys}} = \frac{1.239 \, cm}{7.355 \times 10^{-2} \, cm^{-1}} = 16.85 \, cm^2$$

Now calculate the material buckling, B_m^2:

$$B_m^2 = \frac{k_\infty - 1}{L^2} = \frac{2.930 - 1}{16.85 \; cm^2} = 0.1145 \; cm^{-2}.$$

Notice the diffusion length, L, for this system is a little longer than that of the previous cross sections— about 4.5 cm, as fewer neutrons are absorbed in the Pu.

The mean free path for this system is:

$$\lambda_t \approx \lambda_{tr} = \frac{1}{\Sigma_{tr}^{sys}} = \left(\frac{1}{2.6892 \times 10^{-1} \; cm^{-1}}\right) = 3.72 \; cm$$

There is little change from the mean free path calculated with the first set of cross sections. This is because most of the material is Pu-239, and its transport cross section is very similar to the transport cross section for the mixture. For a critical system, the material and geometric buckling values are equal. The critical dimensions for this system can be calculated as follows:

$$B_m^2 = B_g^2 = \left(\frac{\pi}{\overline{R}}\right)^2$$

$$\overline{R} = \sqrt{\frac{\pi^2}{B_m^2}} = \sqrt{\frac{\pi^2}{0.1145 \; cm^{-1}}} = 9.28 \; cm$$

$$R = \overline{R} - d = \overline{R} - 2.13 \times D = 9.28 \; cm \; - \; 2.13 \times 1.239 \; cm \; = \; 6.64 \; cm.$$

The actual Jezebel system had a critical radius of 6.385 cm. Using the mixture cross sections, the predicted radius is close to the actual value. However, it should be noted that one-group calculations for small, fast systems are highly sensitive to the transport cross sections, so calculated values for fast systems should be used as guidelines or bounding estimates rather than specific physical dimensions.

Calculation of Leakage Fraction. The probability that a neutron will leak out of this material as a critical system can be calculated as follows. The non-leakage probability, P_{NL}, is the probability a neutron will not leak out of the system. The leakage probability is simply equal to 1-P_{NL} and provides the probability that a neutron will leak out of the system. References 1 and 2 provide further detail about this topic. The non-leakage and leakage probabilities can be determined using Eq. (25), which applies to a critical system:

$$P_{NL} = \frac{1}{k_\infty} \quad \text{and} \; P_L \; = \; 1 - P_{NL} = 1 - \frac{1}{k_\infty} = \frac{k_\infty - 1}{k_\infty}$$

For the critical system of this example (the Jezebel critical assembly), the leakage probability (leakage fraction) and nonleakage probability (fraction of neutrons not leaking) can be calculated as:

$$P_L = \frac{k_\infty - 1}{k_\infty} = \frac{2.930 - 1}{2.930} = 0.659 \quad \text{and} \quad P_{NL} = \frac{1}{k_\infty} = \frac{1}{2.930} = 0.341.$$

This provides the analyst with information regarding the probability that a neutron will leak out of the critical system instead of being absorbed within the system materials. Based on this calculation, we know that about 66% of the neutrons will leak out of the system with the remaining 34% absorbed. This calculation illustrates that, for a critical system, the geometry and associated system leakage must be such that the effective multiplication factor is reduced from 2.930 (k_∞) to 1.0.

2.6.3 Diffusion Theory Example Problem 3 – Fast System with Various Densities of Plutonium Oxide Powder

Using one-group diffusion theory, determine the infinite multiplication factor and the critical mass of Pu for a spherical, unreflected configuration of $^{239}PuO_2$ with a density of 1, 3, 5, 7, 9, and 11.46 g/cm^3. Compare these results with an infinite system of ^{239}Pu.

The first step in this problem is to compile the data needed to perform the calculations. As there is no moderator, plutonium oxide is assumed to have a fast neutron energy spectrum; so fast data from Reference 2 and 5 are compiled in Table 2-7.

Table 2-7. Diffusion Theory Example Problem 3 Data.

Constituent	Parameter	Data Value	Reference
^{239}Pu	σ_a(fast)	2.11 barns	2, Table 6.1, pg. 267
	σ_f(fast)	1.85 barns	2, Table 6.1, pg. 267
	σ_{tr}(fast)	6.8 barns	2, Table 6.1, pg. 267
	υ	2.98	2, Table 6.1, pg. 267
	η	2.61	2, Table 6.1, pg. 267
^{16}O	σ_a(fast)	0.022 barns	5, Table 4-30, pg. 298
	σ_{tr}(fast)	3.09 barns	5, Table 3-39, pg. 148

First, calculate the atom densities for the mixture constituents using a bulk density of 1 g/cm^3 (this makes it easy to calculate for the others, as you just multiply the atom density for 1 g/cm^3 by the actual bulk density to get the new atom density):

$$N = \frac{\rho_{\text{mixture}} \times N_A}{A_{constituent}}$$

$$N_{^{239}PuO_2} = \frac{(1 \ g/cm^3)(0.6022 \ atoms-cm^2/mol-b)}{(239.052 \ g/mol + 2 \times 15.9994 \ g/mol)} = 2.222 \times 10^{-3} \text{ molecules PuO}_2\text{/b-cm}$$

$$N_{^{239}Pu} = N_{^{239}PuO_2} = 1 \text{ atom Pu / molecule PuO}_2 \times 2.222 \times 10^{-3} \text{ molecules PuO}_2\text{/b-cm} = 2.222 \times 10^{-3} \text{ atoms Pu/b-cm}$$

$$N_{^{16}O} = 2 \times N_{^{239}PuO_2} = 2 \text{ atoms O / molecule PuO}_2 \times 2.222 \times 10^{-3} \text{ molecules PuO}_2\text{/b-cm} = 4.444 \times 10^{-3} \text{ atoms O/b-cm.}$$

Now that the atom densities have been calculated, the macroscopic cross sections can be determined:

$$\Sigma_a^{Mixture} = \Sigma_a^{239_{Pu}} + \Sigma_a^{O_2} = N_{239_{Pu}} \times \sigma_a^{239_{Pu}} + N_{O_2} \times \sigma_a^{O_2}$$

$$\Sigma_a^{mixture} = 2.222 \times 10^{-3} \text{ atoms Pu/b-cm} \times 2.11 \ b + 4.444x10^{-3} \text{ atoms O/b-cm} \times 0.022 \ b$$

$$\Sigma_a^{mixture} = 4.688 \times 10^{-3} \ cm^{-1} + 9.78 \times 10^{-5} \ cm^{-1} = 4.786 \times 10^{-3} \ cm^{-1}.$$

The infinite multiplication factor can now be calculated. It can be assumed for this type of system that there is no leakage from a system with infinite size and that all fissions occur at thermal energies ($\varepsilon = p = 1$).

$$k_\infty = \eta f = v \frac{\Sigma_f^{fuel}}{\Sigma_a^{fuel}} \times \frac{\Sigma_a^{fuel}}{\Sigma_a^{mixture}} = \eta \times \frac{\Sigma_a^{fuel}}{\Sigma_a^{mixture}} = 2.61 \times \frac{4.688x10^{-3} \text{ cm}^{-1}}{4.786x10^{-3} \text{ cm}^{-1}} = 2.557$$

Now the diffusion length, L^2, can be calculated based on the result of the k_∞ calculation.

$$\Sigma_{tr} = \Sigma_{tr}^{239_{Pu}} + \Sigma_{tr}^{O_2} = N_{239_{Pu}} \times \sigma_{tr}^{Pu} + N_{O_2} \times \sigma_{tr}^{O_2}$$

$$\Sigma_{tr} = (2.222 \times 10^{-3} \text{ atoms Pu/b-cm})(6.8 \ b) + (4.444 \times 10^{-3} \text{ atoms O/b-cm})(3.09 \ b)$$

$$\Sigma_{tr} = 2.884 \times 10^{-2} \ cm^{-1}$$

$$D_{mixture} = \frac{1}{3\Sigma_{tr}} = \left(\frac{1}{3 \times 2.884 \times 10^{-2} \text{ cm}^{-1}}\right) = 11.56 \ cm$$

$$L^2 = \frac{D_{mixture}}{\Sigma_a^{mixture}} = \frac{11.56 \text{ cm}}{4.786 \times 10^{-3} \text{ cm}^{-1}} = 2.415 \text{ x}10^3 \text{ cm}^2.$$

Now calculate the material buckling, B_m^2:

$$B_m^2 = \frac{k_\infty - 1}{L^2} = \frac{2.557 - 1}{2.415 \text{ x}10^3 \text{ cm}^2} = 6.447 \times 10^{-4} \text{ cm}^{-2}.$$

Notice the diffusion length, L^2, is rather large. This indicates the fissile density is low and that there is very little absorption other than in plutonium; this means that neutrons in this system diffuse or travel farther on average between collisions before being absorbed by the materials in this system. Thus, this system will be much larger than a thermal system, such as a mixture of plutonium metal and water. The critical radius can be calculated now that the material buckling is known. Recall that the geometric and material buckling are equal for a critical system.

$$B_g^2 = \left(\frac{\pi}{\bar{R}}\right)^2$$

$$\bar{R} = \sqrt{\frac{\pi^2}{B_g^2}} = \sqrt{\frac{\pi^2}{6.447 \times 10^{-4} \text{ cm}^{-1}}} = 123.7 \ cm$$

$$R = \bar{R} - d = \bar{R} - 2.13 \times D_{mixture} = 123.7 \ cm - 2.13 \times 11.56 \ cm = 99.1 \ cm.$$

Using the critical radius, the spherical critical volume and critical mass can be calculated.

$$R = 99.1 \text{ cm}$$

$$V = \frac{4\pi}{3}R^3 = \frac{4\pi}{3}(99.1)^3 = 4.077 \times 10^6 \text{ cm}^3.$$

The critical mass of PuO_2 can be found by multiplying the critical volume by the density of the material.

$$m = \rho \times V = 1.0 \ \frac{g}{cm^3} \times 4.077 \times 10^6 \text{ cm}^3 \times \frac{kg}{1000 \ g} = 4.077 \times 10^3 \text{ kg.}$$

These calculations can be redone by following the same methodology for the desired densities (i.e., 3, 5, 7, 9, and 11.46 g/cm³). A spreadsheet was used to apply this calculation procedure quickly. The results of these calculations are presented in Table 2-8 for comparison purposes.

Table 2-8. Calculation Results for Diffusion Theory Example Problem 3.

Density of Pu (g/cm³)	Critical Spherical Radius (cm)	Estimated Critical Mass of PuO$_2$ (kg)	PARTISN Estimated Critical Mass of PuO$_2$ (kg)	SCALE 6.1.3 Estimated Critical Mass of PuO$_2$ (kg)
1.0	99.1	4,080	3,540	3,614
3.0	33.0	453	393	404
5.0	19.8	163	142	145
7.0	14.2	83	72.2	73.8
9.0	11.0	50	43.7	44.6
11.46	8.65	31	27.0	27.8

Because this is a fast, unmoderated system, one-group diffusion theory provides a reasonably conservative estimate across the entire density range for the critical dimensions of this system. A series of PARTISN[5] and SCALE[6] calculations was performed to compare the hand calculations with a transport calculation using the 16-group Hansen–Roach cross section set. As seen in Table 2-8, the computer-calculated critical mass values are about 12% less than the values from the hand calculations. Again, this is likely due to the excess absorption present in the fast neutron cross sections for the plutonium isotopes. The hand calculation values are not conservative, but they provide bounding estimates for moving into detailed designs and process analyses. Figure 2-5 shows a comparison between the PARTISN calculated critical masses and those from hand calculations indicating about a 12% difference for all densities considered.

---

[5] As mentioned in footnote 3, PARTISN is a newer version of the DANTSYS deterministic neutron transport system. Version 5.97R with the 16-group Hansen–Roach cross section set was used for all the analyses in this document. See reference 4 for more details on the code package and input requirements.

[6] The SCALE code, version 6.1.3 with continuous energy ENDF/B-VII cross sections was used for all the analyses in this document. See reference 10 for more details on the code package and input requirements.
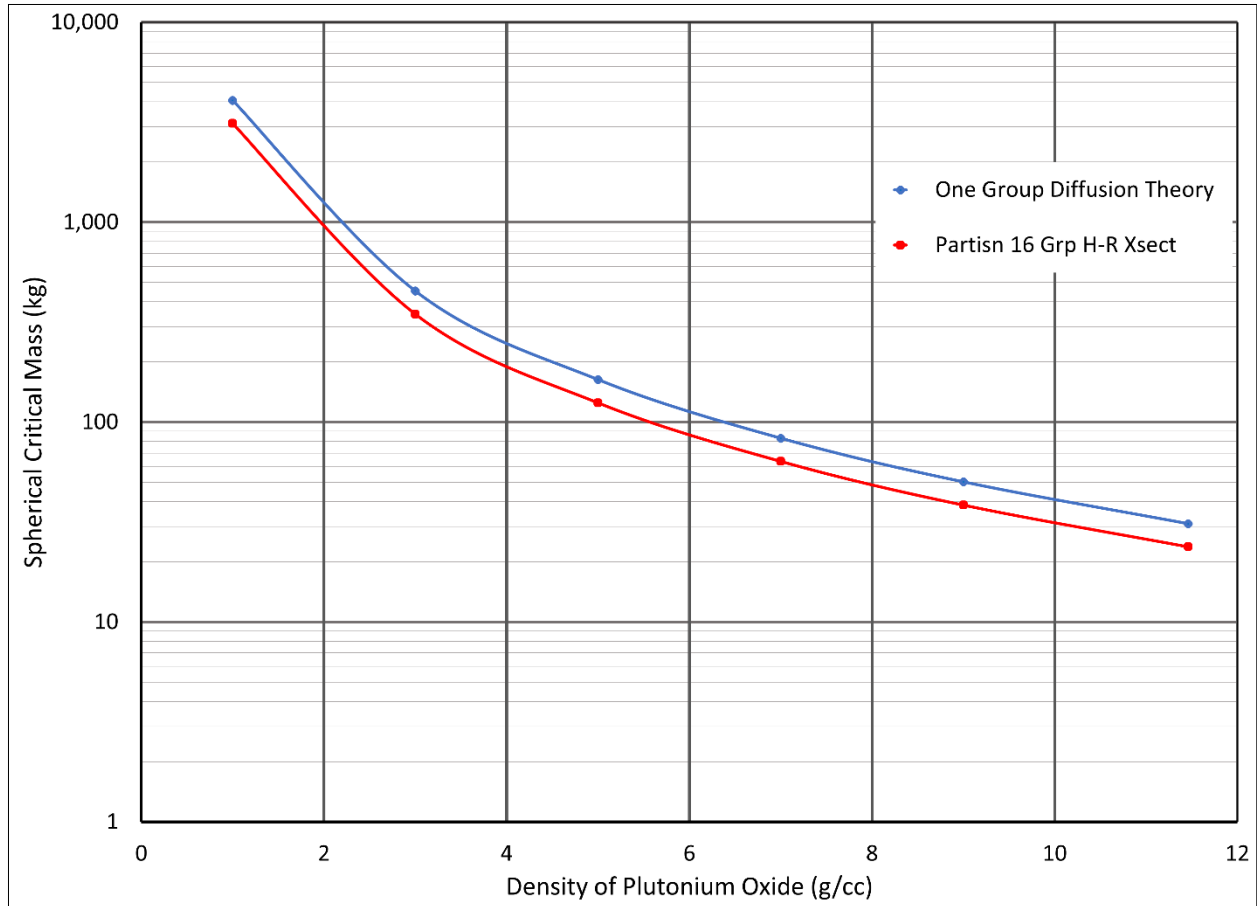
Figure 2-5. Critical Mass Comparison of Results for Diffusion Theory Example Problem 4.

2.6.4   Diffusion Theory Example Problem 4 – Thermal System with Plutonium

Assume a slab tank (Figure 2-6) contains a mixture of water and pure plutonium-239 (^{239}Pu) with a ^{239}Pu concentration of 100 g per liter at 20 °C. Using the data in Table 2-9, determine the following for this system to support the design for a slab tank that will contain a pure ^{239}Pu solution.

1. The infinite multiplication factor, k_∞.
2. The critical slab thickness using one-group diffusion theory.
3. The critical slab thickness for this problem using modified one-group diffusion theory.

36
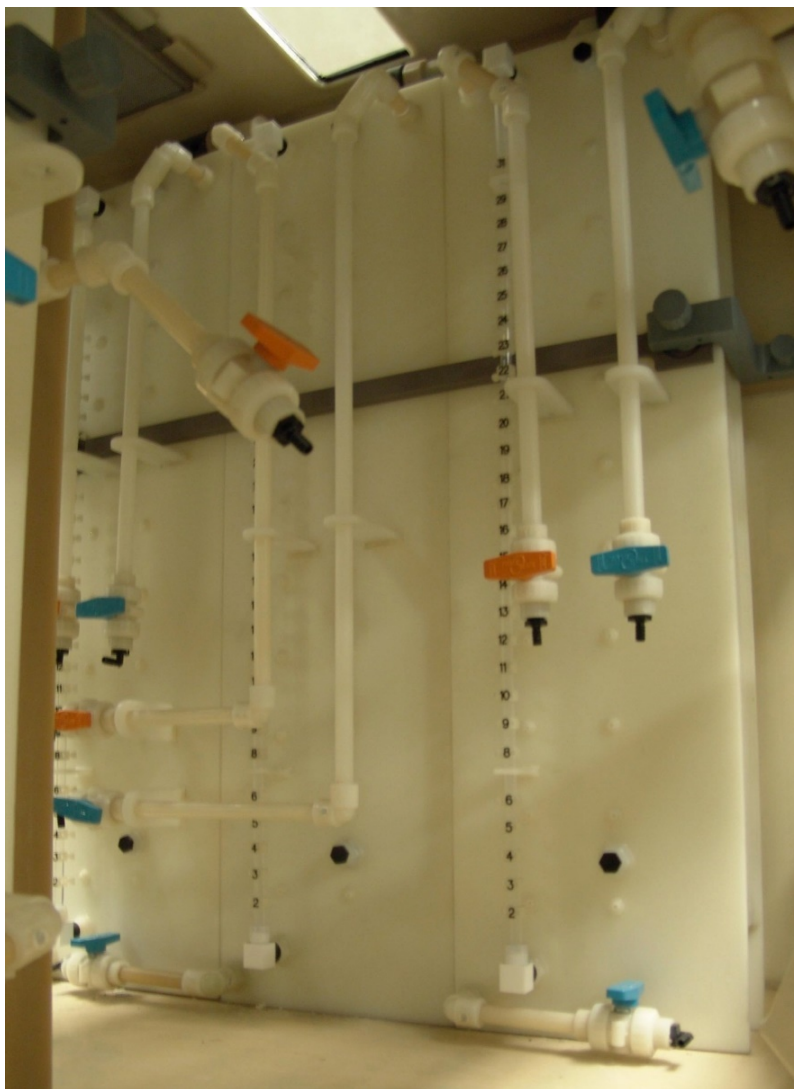
Figure 2-6. Slab Tank Containing a ^{239}Pu Metal-Water Mixture for Diffusion Theory Example Problem 4

Part 1. Before starting any calculation of fissile material system properties, one should have an idea what the answer should be—that is, at least an order of magnitude estimate, and the expected units of the results. For this case, we are interested in the infinite multiplication factor and critical slab thickness in cm. For this problem, we are using ARH-600, Vol. II (Reference 7). On page III.A.10.100.4, it indicates that the infinite multiplication factor for a plutonium (0% Pu-240) water system is 1.78 at a concentration of 100 g Pu-239/liter. The previous page provides useful data on the expected material buckling, 0.0292 cm^{-2}, and extrapolation distance, 2.1 cm, for the system. The graph on page III.A.5-2 shows a critical slab thickness of 5.6 inches (14.2 cm).

Because Pu-239 is a non-1/v absorber in a thermal system, the absorption microscopic cross section must be adjusted using the g_a and g_f factors as listed in Table 2-1. The non-1/v factors are used to adjust the microscopic absorption cross sections for various cross sections that typically have high absorption cross sections. The absorption rate of thermal neutrons with Pu-239 varies as a function of the temperature of the system.

Table 2-9. Diffusion Theory Example Problem 4 Data.

Constituent	Parameter	Data Value	Reference
^{239}Pu	σ_a (2200 m/s)	1020 barns	2, Table II.2, pg. 738
	σ_f (2200 m/s)	749 barns	2, Table II.2, pg. 738
	ν	2.871	2, Table 3.4, pg. 82
	g_a (non-1/v factor) for 20 °C	1.0723	2, Table 3.2, pg. 75 or Table 2-1, this document
	g_f (non-1/v factor) for 20 °C	1.0487	2, Table 3.2, pg. 75 or Table 2-1, this document
Water	*Hydrogen* σ_a (2200 m/s)	0.332 b	2, Table II.3, pg. 740
	Oxygen σ_a (2200 m/s)	0.27 mb	2, Table II.3, pg. 741
	Water σ_a (2200 m/s)	0.6643 b	$= 2 \times 0.332$ b $+ 0.27 \times 10^{-3}$ b
	τ	27 cm^2	2, Table 5.3, pg. 259
	D	0.16 cm	2, Table 5.2, pg. 254
	$D_{mixture} = D_{water}$		The slab tank will contain mostly water with small quantities of ^{239}Pu. Therefore, the diffusion coefficient and neutron age will be approximately that of water.
	$\tau_{mixture} = \tau_{water}$		

Thus, the absorption and fission microscopic cross sections in barns for Pu-239 and water are adjusted as follows.

For Pu-239,

$$\bar{\sigma}_a = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200 \text{ m/sec}) = 0.886 \times 1.0723 \times 1020b \ = \ 969b$$

$$\bar{\sigma}_f = \frac{\sqrt{\pi}}{2} g_f \sigma_f (2200 \text{ m/sec}) = 0.886 \times 1.0487 \times 749b \ = \ 696b$$

For water (H_2O), the cross-section adjustment for hydrogen is expressed as:

$$\bar{\sigma}_{a(hydrogen)} = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200 \text{ m/sec}) = 0.886 \times 1.0 \times 0.332b \ = \ 0.294b$$

Note non-1/v factors are 1.0 for most materials found in fissile material systems other than Cd, In, ^{135}Xe, ^{149}Sm, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu.

And for oxygen, the cross-section adjustment is as follows:

$$\bar{\sigma}_{a(oxygen)} = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200 \text{ m/sec}) = 0.886 \times 1.0 \times 0.27 x 10^{-3}b \ = \ 2.4 x 10^{-4}b$$

The total for water (H_2O) is as follows:

$$\overline{\sigma}_{a(water)} = 2 \times \overline{\sigma}_{a(hydrogen)} + \overline{\sigma}_{a(oxygen)} = 2 \times 0.294b + 1 \times 2.4x10^{-4}b = 0.588b$$

To calculate the macroscopic cross sections, the next step is to calculate the atom densities for Pu-239 and water; knowing the density of ^{239}Pu, ρ_{239}, Avogadro's number, NA, and the atomic weight of Pu-239. Reference 4 contains further information about calculating atom densities for various materials and compositions.

$$N_{Pu} = \frac{\rho_{Pu239}[g/cm^3] \times N_A[\text{atoms - cm}^2/\text{mol - b}]}{A_{Pu239}[g/mol]}$$

$$A_{Pu239}[g/mol] = 239.05[g/mol]; \ \rho \text{ given as } 100 \text{ g/liter} = 0.1 \text{ g/cm}^3$$

$$N_{Pu} = \frac{0.1[g/cm^3] \times 0.6022[\text{atoms - cm}^2/\text{mol - b}]}{239.05[g/mol]} = 2.519x10^{-4}\text{atoms Pu239/b - cm}$$

Now that the Pu-239 atom density is known, calculate the volume fraction for Pu-239 and water to determine the atom density for water.

$$vf_{Pu239} = \frac{\text{Concentration}}{\text{Theoretical Density}} = \frac{0.1 \text{ gPu/cm}^3 \text{ - mix}}{19.75 \text{ gPu/cm}^3 \text{ - Pu}} = 0.00506 \frac{\text{cm}^3 \text{ - Pu}}{\text{cm}^3 \text{ - mix}}$$

$$vf_{Water} = 1 - vf_{Pu239} = 1 - 0.00506 = 0.99494 \frac{\text{cm}^3 \text{ - } H_2O}{\text{cm}^3 \text{ - mix}}$$

Knowing the volume fractions, we can calculate the mixture density.

$$\rho_{mix} = vf_{Pu239} \times \rho_{Pu239} + vf_{Water} \times \rho_{Water}$$

$$\rho_{mix} = 0.00506 \frac{\text{cm}^3 \text{ - Pu}}{\text{cm}^3 \text{ - mix}} \times 19.75 \frac{\text{g - Pu239}}{\text{cm}^3 \text{ - Pu}} + 0.99494 \frac{\text{cm}^3 \text{ - } H_2O}{\text{cm}^3 \text{ - mix}} \times 1.0 \frac{\text{g - } H_2O}{\text{cm}^3 \text{ - } H_2O}$$

$$\rho_{mix} = 1.0949 \text{ g - mix/cm}^3 \text{ - mix}$$

Using the mixture density, can calculate the weight fractions of its two constituents:

$$wf_{Pu239} = \frac{vf_{Pu239} \times \rho_{Pu239}}{\rho_{mix}} = \frac{0.00506 \frac{\text{cm}^3 \text{ - Pu}}{\text{cm}^3 \text{ - mix}} \times 19.75 \text{ gPu/cm}^3 \text{ - Pu}}{1.0949 \text{ g - mix/cm}^3 \text{ - mix}} = 0.0913 \frac{\text{gPu}}{\text{g - mix}}$$

$$wf_{Water} = \frac{vf_{Water} \times \rho_{Water}}{\rho_{mix}} = \frac{0.99494 \frac{\text{cm}^3 \text{ - } H_2O}{\text{cm}^3 \text{ - mix}} \times 1.0 \text{ g}H_2O/\text{cm}^3 \text{ - } H_2O}{1.0949 \text{ g - mix/cm}^3 \text{ - mix}} = 0.9087 \frac{\text{g}H_2O}{\text{g - mix}}$$

Now with the weight fraction of water, can calculate its molecular density in the mixture.

$$\rho_{mix} = 1.0949 [\text{g/cm}^3] \quad A_{Water} = 2 \times 1.00794 + 1 \times 15.9994 = 18.015 [\text{g/mol}]$$

$$N_{Water} = \frac{wf_{Water} \times \rho_{mix}[\text{g/cm}^3] \times N_A [\text{atoms - cm}^2/\text{mol - b}]}{A_{Water}[\text{g/mol}]}$$

$$N_{Water} = \frac{0.9087 \,[\text{g - H}_2\text{O/g - mix}] \times 1.0949[\text{g - mix/cm}^3] \times 0.6022[\text{molecules - cm}^2/\text{mol - b}]}{18.015[\text{g - H}_2\text{O/mol}]} =$$

$$3.3258 x 10^{-2} \text{molecules - H}_2\text{O/b - cm}$$

The macroscopic absorption and fission cross sections can now be determined for Pu-239.

$$\Sigma_a^{Pu239} = N_{Pu239} \times \bar{\sigma}_a = \frac{2.519 x 10^{-4} \text{atoms Pu239}}{\text{b - cm}} \times \frac{969 b}{\text{atom Pu239}} = 0.2441 \text{cm}^{-1}$$

$$\Sigma_f^{Pu239} = N_{Pu239} \times \bar{\sigma}_f = \frac{2.519 x 10^{-4} \text{atoms Pu239}}{\text{b - cm}} \times \frac{696 b}{\text{atom Pu239}} = 0.1753 \text{cm}^{-1}$$

$$\Sigma_a^{Water} = N_{Water} \times \bar{\sigma}_a = \frac{3.3258 x 10^{-2} \text{molecules Water}}{\text{b - cm}} \times \frac{0.588 b}{\text{molecule Water}} = 0.01956 \text{cm}^{-1}$$

$$\therefore \Sigma_a^{mixture} = \Sigma_a^{Pu239} + \Sigma_a^{Water} = 0.2441 \text{cm}^{-1} + 0.01956 \text{cm}^{-1} = 0.2637 \text{cm}^{-1}$$

Next, η, the number of neutrons released in fission per neutron absorbed by a fissile nucleus and f, the thermal utilization factor, can be calculated.

$$\eta = \frac{\nu \times \Sigma_f^{Pu239}}{\Sigma_a^{Pu239}} = \frac{2.871 \times 0.1753 \text{cm}^{-1}}{0.2441 \text{cm}^{-1}} = 2.062$$

$$f = \frac{\Sigma_a^{Pu239}}{\Sigma_a^{Mixture}} = \frac{0.2441 \text{cm}^{-1}}{0.2637 \text{cm}^{-1}} = 0.926$$

Because no fertile material is present (i.e., no Pu-240 or U-238), no corrections are needed for resonance absorption or fast fission, so $k_\infty = \eta f$:

$$k_\infty = \eta \times f = 2.062 \times 0.926 = 1.909$$

This result for k_∞ means that a criticality is possible for this Pu-239 and water system at the stated concentration. To check our value for k_∞, we look at Figure 2-7 from Reference 7. This indicates that the k_∞ for a pure Pu-239 plutonium–water system at a concentration of 0.1 g Pu /cm³ is about 1.78. The difference between the one group k_∞ and that from calculations and handbooks is likely the result of the large Pu-239 resonance at 0.296 eV. Many of the fissile nuclides have resonances in the epithermal range, but the Pu-239 resonance is unusual in that it has a much higher capture to fission ratio than for other neutron energies in Pu-239. (For the thermal cross sections, the capture to fission ratio is 0.392, whereas for the energy range between 0.1 and 0.4 eV, including the resonance, the ratio is 0.494). Inclusion of the effect of this resonance reduces the k_∞ to 1.797, which very close to that found in Figure 2-7.
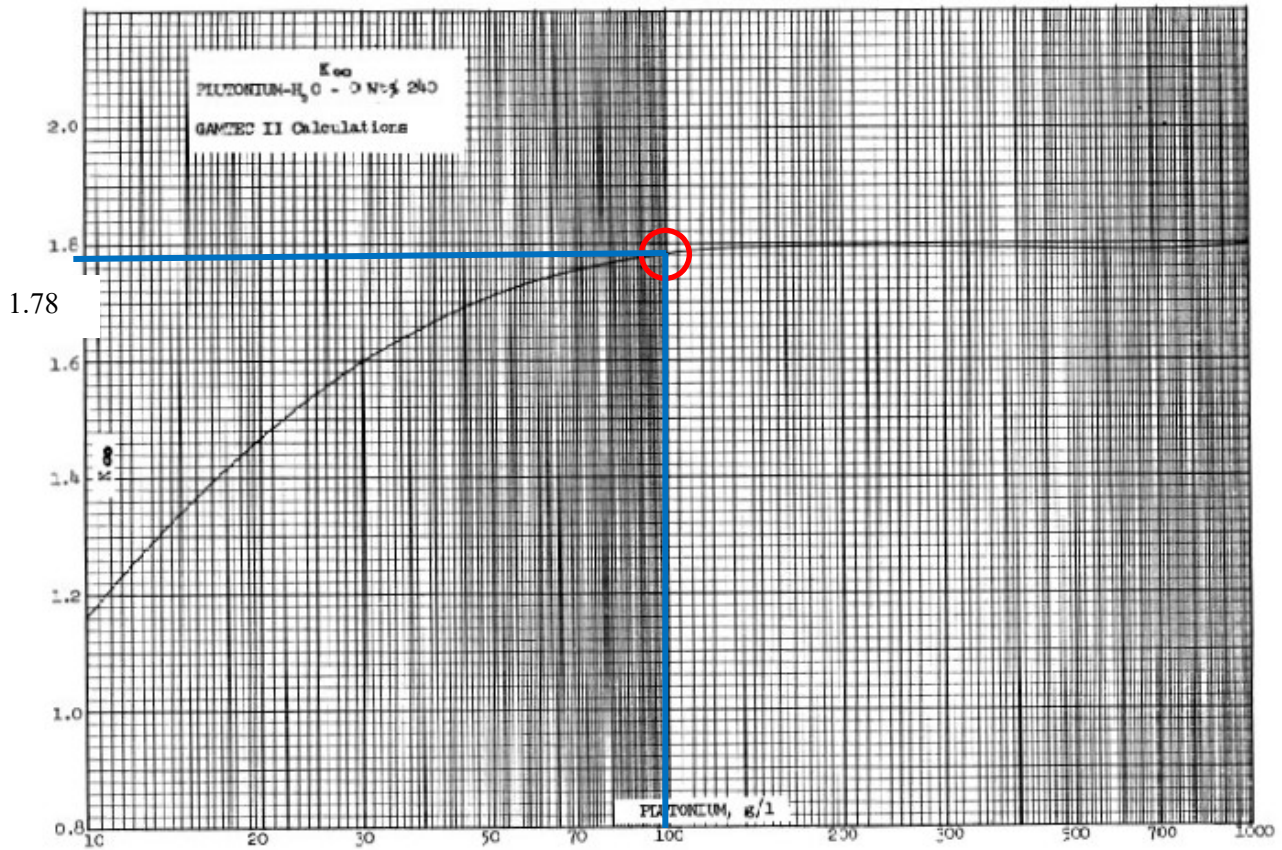
Figure 2-7. k_∞ for a Pu Metal-Water Mixture. (Reference 7, Figure III.A.10-100-4)

With the information provided above, one could determine the concentration required to result in a k_∞ that is less than 1.0, which would provide the "always safe" concentration for an infinite ^{239}Pu–water mixture. Setting up this methodology in a spreadsheet and using the "goal seek" capability provides an answer of 7.6 g Pu per liter (or 0.0076 g Pu/cm³) for an infinite critical system, $k_\infty = 1$.

Part 2. Using one-group diffusion theory, determine the critical slab thickness for the ^{239}Pu–water mixture. The first step is to determine the diffusion length, L^2, and use the result to determine buckling for a critical slab.

$$L^2 = \frac{\overline{D}}{\Sigma_a^{Mixture}} = \frac{0.16\text{cm}}{0.2637\text{cm}^{-1}} = 0.607 \text{ cm}^2$$

$$B^2 = \frac{k_\infty - 1}{L^2} = \frac{1.909 - 1}{0.607\text{cm}^2} = 1.498 \text{ cm}^{-2}$$

From

Table 2-3, the buckling for an infinite slab with a thickness "a" is $B^2 = (\pi/\tilde{a})^2$, where $\tilde{a}$ includes the extrapolation distance. Now that the buckling for this problem is known, the critical slab extrapolated thickness can be determined.

$$B^2 = \left(\frac{\pi}{\tilde{a}}\right)^2 \quad \text{so} \quad \tilde{a} = \sqrt{\frac{\pi^2}{B^2}} = \sqrt{\frac{\pi^2}{1.498 \text{ cm}^{-2}}} = 2.57 \text{ cm}$$

This dimension must be corrected by subtracting two times the extrapolation distance, d (one from each side of the slab). See Appendix A for an overview of extrapolation distance. For this slab and various materials present, $d = 2.13D$.

$$a = \tilde{a} - 2 \times d = \tilde{a} - 2 \times 2.13 \times D = 2.57 \text{ cm} - 2 \times 2.13 \times 0.16 \text{ cm} = 1.89 \text{ cm}$$

Figure 2-8 (from Reference 7, Vol. II) shows that the critical slab thickness for this system, a Pu(0) metal–water mixture and a concentration of 0.1 g/cm^3 (100 gPu/l), is about 5.6 in. (14.2 cm). This result shows that simple one-group diffusion theory **does not** accurately estimate the critical dimensions for the ^{239}Pu–water slab tank. Modified one-group diffusion theory should provide more accurate results.
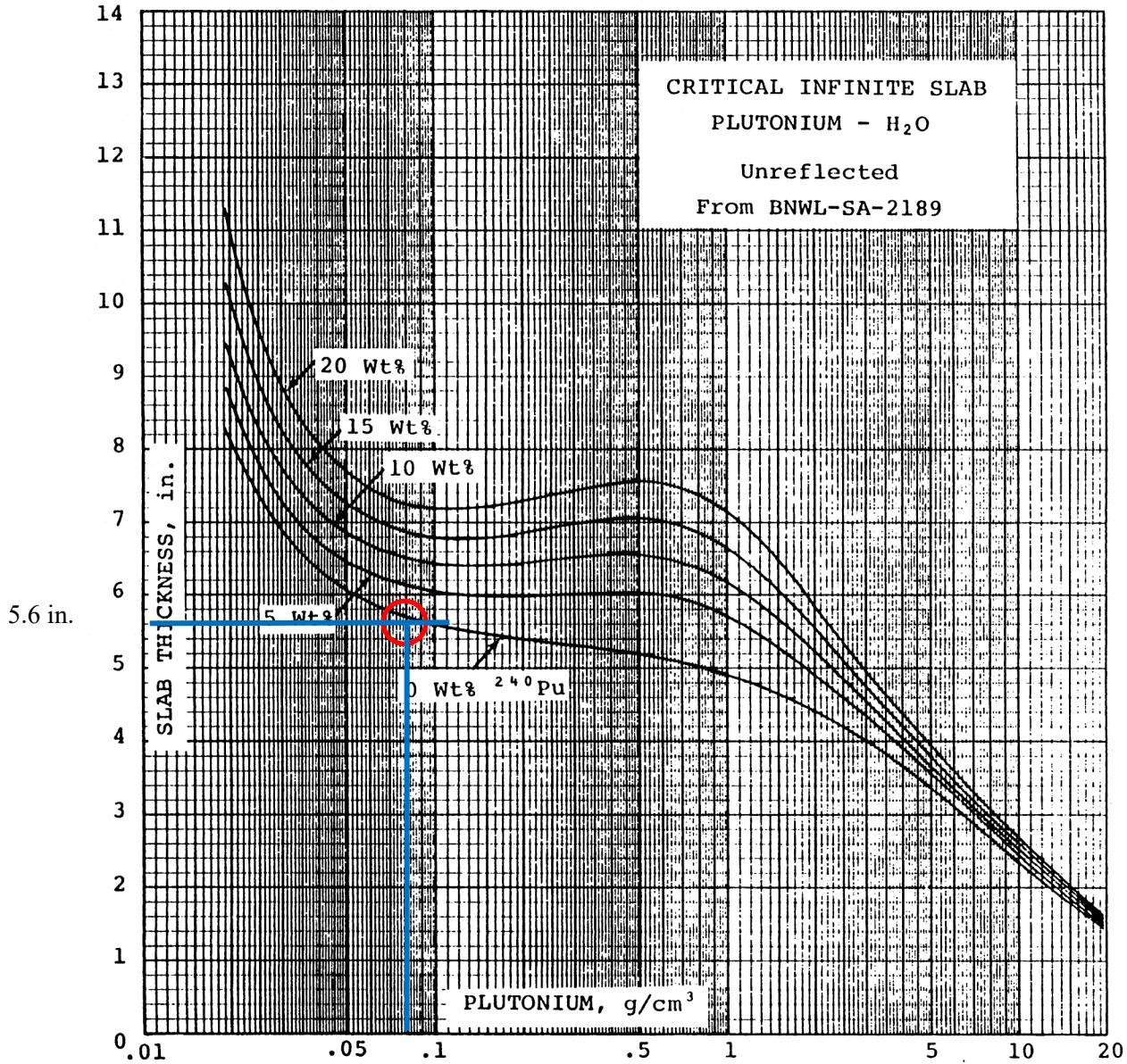
Figure 2-8. Critical Infinite Slab Thickness for a Pu Metal-Water Mixture. (Reference 7, Figure III.A.5-2.)

Part 3. For modified one-group diffusion theory, the thermal migration area, M^2, must be calculated by calculating the sum of L^2 (neutron diffusion area) and τ (neutron age). Then the critical slab height can be determined as follows:

$$B^2 = \frac{k_\infty - 1}{M^2} = \frac{1.909 - 1}{0.607\text{cm}^2 + 27\text{cm}^2} = 0.0329 \text{ cm}^{-2}$$

$$B^2 = \left(\frac{\pi}{\tilde{a}}\right)^2 \quad \text{so} \quad \tilde{a} = \sqrt{\frac{\pi^2}{B^2}} = \sqrt{\frac{\pi^2}{0.0329 \text{ cm}^{-2}}} = 17.32 \text{ cm}$$

Based on Figure 2-8, the extrapolation distance for this type of system is about 2.1 cm.

43

$$a = \tilde{a} - 2 \times d = \tilde{a} - 2 \times 2.1 = 17.32\text{cm} - 2 \times 2.1\text{cm} = 13.12\text{cm}$$

Note that for thermal systems (particularly those containing water), the extrapolation distance is usually around 2 cm, but it is best to use figures such as Figure 2-8 to determine the extrapolation distance for such systems. Based on this result, a ^{239}Pu–water mixture will result in a subcritical configuration if the "infinite" slab tank thickness is less than about 13.12 cm. This result compares well with the infinite slab thickness for a Pu(0) metal–water mixture shown in Figure 2-9.

This data shows that a Pu(0) metal–water mixture at a concentration of 0.1 g/cm^3 (100 gPu/l) has a critical thickness of about 5.6 in. (14.2 cm), which is consistent with the answer. Note that the hand calculation in this case provides a conservative answer: a slab of thickness 13.12 cm has a k_{eff} of about 0.94. Again, the effect of the 0.296 eV Pu-239 resonance would be to decrease the k_∞ to 1.797, which gives a material buckling of 0.0290 cm^{-2} (compare to 0.0282 cm^{-2} from Figure 2-8), and a critical slab thickness of 14.25 cm.

Modified one-group diffusion theory can be used effectively for moderated, thermal problems. Based on the results presented in this example problem, it is recommended that only modified one-group diffusion theory be used for thermal fissile system like this example, as one-group diffusion theory does not consider the effects of moderation.
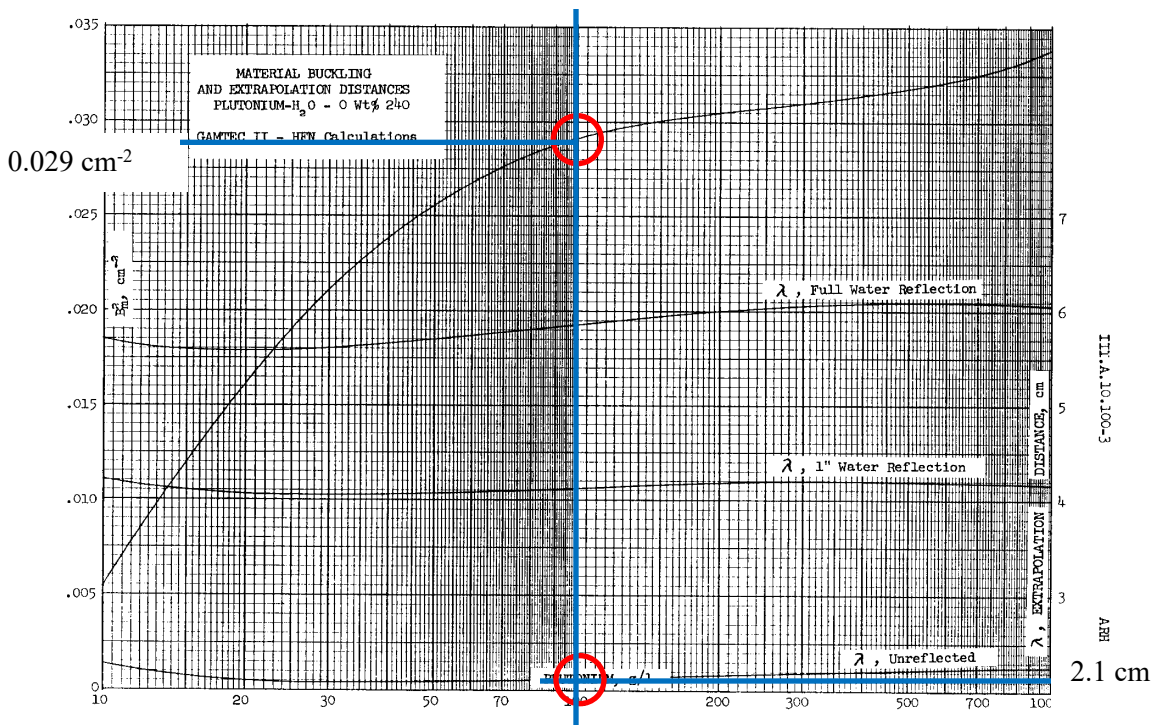
Figure 2-9. Extrapolation Distances and Material Buckling for a Pu Metal-Water Mixture. (Reference 7, Figure III.A.10.100-3.)

2.6.5 Diffusion Theory Example Problem 5 – Thermal System with Uranium

It is proposed to store water solutions of uranyl sulfate ($UO_2SO_4 \cdot 3H_2O$) with a concentration of 30 g ^{235}U/l (0.03 g/cm^3) of the sulfate. Assume the temperature of the solution is 20 °C, and the uranium is fully enriched (i.e., no U-238 is present). Table 2-10 lists the relevant data for this problem.

1. Is this configuration safe when using a tank of unspecified size and shape?
2. If not, calculate the critical cylindrical tank radius using modified one-group diffusion theory.
3. Repeat (2) as if the enrichment were 14.7 wt % U-235 instead of fully enriched U-23.

Before starting any calculation of fissile material system properties, one should have an idea what the answer should be—that is, at least an order of magnitude estimate and the expected units of the results. For this case, we are interested in the infinite multiplication factor and critical infinite cylinder radius in centimeters. We will start with LA-10860, Reference 11. In most cases, the handbooks will have data for uranium–water systems and sometimes for uranium nitrate systems. As we are dealing with a uranyl sulfate solution, we will use the uranium–water data as more conservative (this does not account for the absorption in sulfur). Figure 12 (page 26, reference 11) gives the infinite cylinder diameter of about 34 cm for a U(93.2) water moderated system at a 0.03 g ^{235}U/cm^3 density. This means we should get an infinite cylinder radius of about 17 cm for part 2.

Additional information is obtained from ARH-600, Vol. II (Reference 7). On page III.B.10(100)-2, it indicates that the infinite multiplication factor for a U(100) water system is 1.433 at a concentration of 0.03 g U235/cc. The figure also provides a value of 29.2 cm^2 for the migration area. The previous page, III.B.10(100)-1, provides useful data on the expected material buckling, 0.0147 cm^{-2}, and extrapolation distance, 2.1 cm for the system.

Table 2-10. Diffusion Theory Example Problem 5 Data.

Constituent	Parameter	Data Value	Reference
^{235}U	σ_a(2200 m/s)	687 barns	2, Table II.2, pg. 738
	σ_f(2200 m/s)	587 barns	2, Table II.2, pg. 738
	ν	2.418	2, Table 3.4, pg. 82
	g_a (non-1/v factor) for 20 °C	0.9780	2, Table 3.2, pg. 75 or Table 2-1, this document
	g_f (non-1/v factor) for 20 °C	0.9759	2, Table 3.2, pg. 75 or Table 2-1, this document
O in UO$_2$SO$_4$	σ_a(2200 m/s)	0.27 mb	2, Table II.3, pg. 741
S in UO2SO4	σ_a(2200 m/s)	0.52 b	2, Table II.3, pg. 741
Water	Hydrogen σ_a(2200 m/s)	0.332 b	2, Table II.3, pg. 740
	Oxygen σ_a(2200 m/s)	0.27 mb	2, Table II.3, pg. 741
	Water σ_a(2200 m/s)	0.6643 b	= 2 x 0.332 b + 0.27x10^{-3} b
	τ	27 cm^2	2, Table 5.3, pg. 259
	D	0.16 cm	2, Table 5.2, pg. 254
	$D_{mixture}= D_{water}$		The tank will contain mostly water with small quantities of U-235. Therefore, the diffusion coefficient and neutron age will be approximately that of water.
	$\tau_{mixture} = \tau_{water}$		

Part 1. Because the tank dimensions are not specified in the problem, one must assume that it is effectively infinite in size. Therefore, we must calculate the infinite multiplication factor, k$_\infty$. If the k$_\infty$ has a value less than 1.0, then the system will remain subcritical at the assumed concentration.

As stated in Section 2.3.1, because ^{235}U is a non-1/v absorber, the absorption microscopic cross section must also be adjusted using the g_a and g_f factors as listed in Table 2-1. Thus, the absorption and fission microscopic cross sections in barns for ^{235}U are adjusted as follows.

$$\overline{\sigma}_a = \frac{\sqrt{\pi}}{2} g_a \sigma_a(2200 \text{ m/sec}) = 0.886 \times 0.9780 \times 687b = 595b$$

$$\overline{\sigma}_f = \frac{\sqrt{\pi}}{2} g_f \sigma_f(2200 \text{ m/sec}) = 0.886 \times 0.9759 \times 587b = 508b$$

For sulfur,

$$\bar{\sigma}_a = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200 \text{ m/sec}) = 0.886 \times 1.0 \times 0.52b \;=\; 0.461b$$

For water (H_2O), the cross-section adjustment is expressed as follows:

$$\bar{\sigma}_{a(H_2O)} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(H_2O)} (2200 \text{ m/sec}) = 0.886 \times 1.0 \times 0.6643b \;=\; 0.589b$$

And for Oxygen in uranyl sulfate, it is expressed as follows:

$$\bar{\sigma}_{a(oxy)} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(oxy)} (2200 \text{ m/sec}) = 0.886 \times 1.0 \times 0.28x10^{-3}b \;=\; 0.248x10^{-3}b$$

The next step is to calculate the atom densities for U-235 and water, so the macroscopic cross sections can be determined. Note that the uranium in solution is fully enriched (100 % U-235) and does not contain any U-238.

$$N_{U235} = \frac{\rho_{U235}[\text{g/cm}^3] \times N_A[\text{atoms - cm}^2/\text{mol - b}]}{A_{U235}[\text{g/mol}]}$$

$$A_{U235}[\text{g/mol}] = 235.04[\text{g/mol}]; \; \rho \text{ given as 30 g/liter} \;=\; 0.03 \text{ g/cm}^3$$

$$N_{U235} = \frac{0.03[\text{g/cm}^3] \times 0.6022[\text{atoms - cm}^2/\text{mol - b}]}{235.04[\text{g/mol}]} = \frac{7.686x10^{-5}\text{atoms U235}}{\text{b - cm}}$$

$$N_{U235} = N_U = N_{UO_2SO_4} = 7.686x10^{-5}\text{molecules UO}_2\text{SO}_4/\text{b - cm}$$
Now there are six atoms of oxygen per

atom of uranium, so

$$N_O = 6 \times N_{U235} = 6 \times 7.686x10^{-5}\text{atoms/b - cm} = 4.612x10^{-4}\text{atoms O/b - cm}$$

and one atom of sulfur per atom of uranium:

$$N_S = N_{U235} = 7.686x10^{-5}\text{atoms S/b - cm}$$

Now that the U-235 atom density is known, calculate the volume fractions for U-235 and water to determine the molecular density of water. Note the mixture is uranyl sulfate (U(100)O_2SO_4 •3 H_2O (molecular weight is 417.1 g/mol and density of 3.28 g/cm³ from ARH-600, Vol I, page II.D.2-1, Reference 7) and additional water. First, start by determining the concentration of the uranyl sulfate based on the uranium concentration.

$$\rho_{UO_2SO_4 \cdot 3H_2O} = \frac{\rho_{U235}}{wf_{U235}} = \frac{0.03 \text{ g U(100)}}{\text{cm}^3 \text{ - mix}} \times \frac{417.1 \text{ g } UO_2SO_4 \cdot 3H_2O}{235.04 \text{ g U(100)}} = 0.0532 \frac{\text{g } UO_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - mix}}$$

$$vf_{UO_2SO_4 \cdot 3H_2O} = \frac{\rho_{UO_2SO_4 \cdot 3H_2O}}{\text{Theoretical Density}}$$

$$= \frac{0.0532 \text{ g } UO_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - mix}} \times \frac{\text{cm}^3 \text{ - } UO_2SO_4 \cdot 3H_2O}{3.28 \text{ g } UO_2SO_4 \cdot 3H_2O} = 0.01622 \frac{\text{cm}^3 \text{ - } UO_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - mix}}$$

$$vf_{Water} = 1 - vf_{UO_2SO_4 \cdot 3H_2O} = 1 - 0.01622 = 0.98378 \frac{\text{cm}^3 - H_2O}{\text{cm}^3 \text{ - mix}}$$

Knowing the volume fractions, we can calculate the mixture density.

$$\rho_{mix} = vf_{UO_2SO_4 \cdot 3H_2O} \times \rho_{UO_2SO_4 \cdot 3H_2O} + vf_{Water} \times \rho_{Water}$$

$$\rho_{mix} = 0.01622 \frac{\text{cm}^3 \text{ - } UO_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - mix}} \times 3.28 \frac{\text{g } UO_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - } UO_2SO_4 \cdot 3H_2O}$$

$$+ 0.98378 \frac{\text{cm}^3 - H_2O}{\text{cm}^3 \text{ - mix}} \times 1.0 \frac{\text{g - Water}}{\text{cm}^3 \text{ - mix}} = 1.037 \frac{\text{g - mix}}{\text{cm}^3 \text{ - mix}}$$

Using the mixture density, can calculate the weight fractions of its two constituents:

$$wf_{UO_2SO_4 \cdot 3H_2O} = \frac{vf_{UO_2SO_4 \cdot 3H_2O} \times \rho_{UO_2SO_4 \cdot 3H_2O}}{\rho_{mix}} =$$

$$0.01622 \frac{\text{cm}^3 \text{ - } UO_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - mix}} \times 3.28 \frac{\text{g } UO_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - } UO_2SO_4 \cdot 3H_2O} \times \frac{1 \text{ cm}^3 \text{ - mix}}{1.037 \text{ g - mix}}$$

$$= 0.0513 \frac{\text{g } UO_2SO_4 \cdot 3H_2O}{\text{g - mix}}$$

$$wf_{Water} = \frac{vf_{Water} \times \rho_{Water}}{\rho_{mix}} = 0.98378 \frac{\text{cm}^3 - H_2O}{\text{cm}^3 \text{ - mix}} \times \frac{1 \text{ g } H_2O}{\text{cm}^3 - H_2O} \times \frac{1 \text{ cm}^3 \text{ - mix}}{1.037 \text{ g - mix}}$$

$$= 0.9487 \frac{\text{g } H_2O}{\text{g - mix}}$$

Now with the weight fraction of water, we can calculate its molecular density in the mixture.

$$\rho_{Water} = 1.0 \left[\text{g/cm}^3 \right] \quad A_{Water} = 2 \times 1.00794 + 1 \times 15.9994 = 18.015 \left[\text{g/mol} \right]$$

$$N_{Water} = \frac{wf_{Water} \times \rho_{mix} \left[\text{g/cm}^3 \right] \times N_A \left[\text{atoms - cm}^2/\text{mol - b} \right]}{A_{Water} \left[\text{g/mol} \right]}$$

$$N_{Water} = \frac{0.9487 \, \frac{\text{g } H_2O}{\text{g - mix}} \times 1.037 \, \frac{\text{g - mix}}{\text{cm}^3 \text{ - mix}} \times 0.6022 \, \frac{\text{molecules - cm}^2}{\text{mol - b}}}{18.015 \, \frac{\text{g } H_2O}{\text{mol}}}$$

$$= 3.289 x 10^{-2} \text{molecules Water/b - cm as the solvent}$$

$$N^{H_2O \text{ in } UO_2SO_4 \cdot 3 \, H_2O} = 3 \times N_{U235} = 3 \times 7.686 x 10^{-5} \text{atoms/b - cm}$$

$$= \frac{2.3058 x 10^{-4} \text{molecules } H_2O}{\text{b - cm}} \quad : \text{calculate total Molecules}$$

$$\frac{N_{H_2O} = 3.289 x 10^{-2} \text{molecules Water}}{\text{b - cm}} + \frac{2.3058 x 10^{-4} \text{molecules } H_2O}{\text{b - cm}} =$$

$$= 3.312 x 10^{-2} \text{molecules Water/b - cm}$$

To calculate the macroscopic cross sections, use the atom densities of the constituents as calculated. For U-235:

$$\Sigma_a^{U235} = N_{U235} \times \overline{\sigma}_a = \frac{7.686 x 10^{-5} \text{atoms U235}}{\text{b - cm}} \times \frac{595 b}{\text{atom U235}} = 0.0457 \text{cm}^{-1}$$

$$\Sigma_f^{U235} = N_{U235} \times \overline{\sigma}_f = \frac{7.686 x 10^{-5} \text{atoms U235}}{\text{b - cm}} \times \frac{508 b}{\text{atom U235}} = 0.0390 \text{cm}^{-1}$$

$$\Sigma_a^{S \text{ in } UO_2SO_43 \, H_2O} = N_S \times \overline{\sigma}_a = \frac{7.686 x 10^{-5} \text{atoms S}}{\text{b - cm}} \times \frac{0.461 b}{\text{atom S}} = 0.000035 \text{cm}^{-1}$$

$$\Sigma_a^{O \text{ in } UO_2SO_43 \, H_2O} = N_O \times \overline{\sigma}_a = \frac{4.612 x 10^{-4} \text{atoms O}}{\text{b - cm}} \times \frac{0.248 x 10^{-3} b}{\text{atom O}} = 1.1 x 10^{-7} \text{ cm}^{-1}$$

$$\Sigma_a^{Water} = N_{water} \times \overline{\sigma}_a = \frac{3.312 x 10^{-2} \text{molecules } H_2O}{\text{b - cm}} \times \frac{0.589 b}{\text{molecule } H_2O} = 0.0195 \text{cm}^{-1}$$

$$\therefore \Sigma_a^{mixture} = \Sigma_a^{U235} + \Sigma_a^{S} + \Sigma_a^{O} + \Sigma_a^{Water}$$

$$= 0.0457 \text{cm}^{-1} + 0.000035 \text{cm}^{-1} + 0.00000011 \text{cm}^{-1} + 0.0195 \text{cm}^{-1}$$

$$= 0.0652 \text{cm}^{-1}$$

Next, η, the number of neutrons released in fission per neutron absorbed by a fissile nucleus and f, the thermal utilization factor, can be calculated.

$$\eta = \frac{\nu \times \Sigma_f^{U235}}{\Sigma_a^{U235}} = \frac{2.418 \times 0.0390 \text{cm}^{-1}}{0.0457 \text{cm}^{-1}} = 2.064$$

$$f = \frac{\Sigma_a^{U235}}{\Sigma_a^{Mixture}} = \frac{0.0457 \text{cm}^{-1}}{0.0652 \text{cm}^{-1}} = 0.701$$

Because no U-238 is present, the fast fission factor, ε, is equal to 1. In addition, it can be assumed that the resonance escape probability is equal to 1 because the only resonance material is U-235, and neutron absorption and fission in the resonance region essentially cancel each other out. Thus, the infinite multiplication factor is then $k_\infty = \eta f$, which is equal to the following:

$$k_\infty = \eta \times f = 2.064 \times 0.701 = 1.447$$

Based on the result of this calculation, a tank with infinite dimensions at this concentration of uranyl sulfate solution would **not be safe**. Again, a concentration search could be done in Microsoft Excel to determine the concentration that would result in $k_\infty = 1$. Note that the calculated value of 1.447 compares favorably to our estimated value of 1.443.

Part 2. As this is a thermal system, a one-group analysis is not appropriate, so a modified one-group analysis is done. For modified one-group diffusion theory, the following results can be obtained. For this part the thermal migration area, M^2, needs to be calculated as the sum of L^2 (neutron diffusion length) and τ (neutron age). Then the critical infinite cylinder radius can be determined as follows.

$$L_{th}^2 = \frac{D}{\Sigma_a^{sys}} = \frac{0.16 \text{ cm}}{0.0652 \text{ cm}^{-1}} = 2.454 \text{ cm}^2$$

$$B_m^2 = \frac{(k_\infty - 1)}{M^2} = \frac{(k_\infty - 1)}{(L_{th}^2 + \tau)} = \frac{(1.447 - 1)}{(2.454 \text{ cm}^2 + 27 \text{ cm}^2)} = 0.01518 \text{ cm}^{-2}$$

$$\tilde{R} = \sqrt{\frac{2.405^2}{B_m^2}} = \sqrt{\frac{2.405^2}{0.01518 \text{ cm}^{-2}}} = 19.52 \text{ cm}$$

The extrapolation distance for a cylinder is slightly different than that of a sphere and depends on its height-to-diameter (h/d) ratio. Figure 2-10 (Figure 6 from LA-10860, reference 11) shows the relationship between extrapolation distances for sphere, slabs, and cylinders as a function of (h/d) / (1 + h/d). For an infinite cylinder, this ratio is one. The figure indicates that the extrapolation distance for an infinite cylinder is about 1.03 times the extrapolation distance for a sphere. Using this,

$$R = \tilde{R} - d = 19.52 \text{ cm} - 2.1 \text{ cm} \times 1.03 = 17.36 \text{ cm}$$

a SCALE calculation was performed to determine the radius for a critical, infinite cylinder of this material, which resulted in a cylinder radius of approximately 17.52 cm. Modified one-group diffusion theory provides a reasonable estimate of the critical dimensions for this moderated, thermal system. Note that the calculated values of migration area, material buckling, and critical radius (29.454 cm^2, 0.01518 cm^{-2} and 17.36 cm) compare favorably with our estimates (29.2 cm^2, 0.0147 cm^{-2}, and 17 cm) from the handbooks.

NOTE: As demonstrated in the last example problem, one-group diffusion theory significantly underestimates the critical dimensions of moderated systems and should only be used for fast, unmoderated systems.
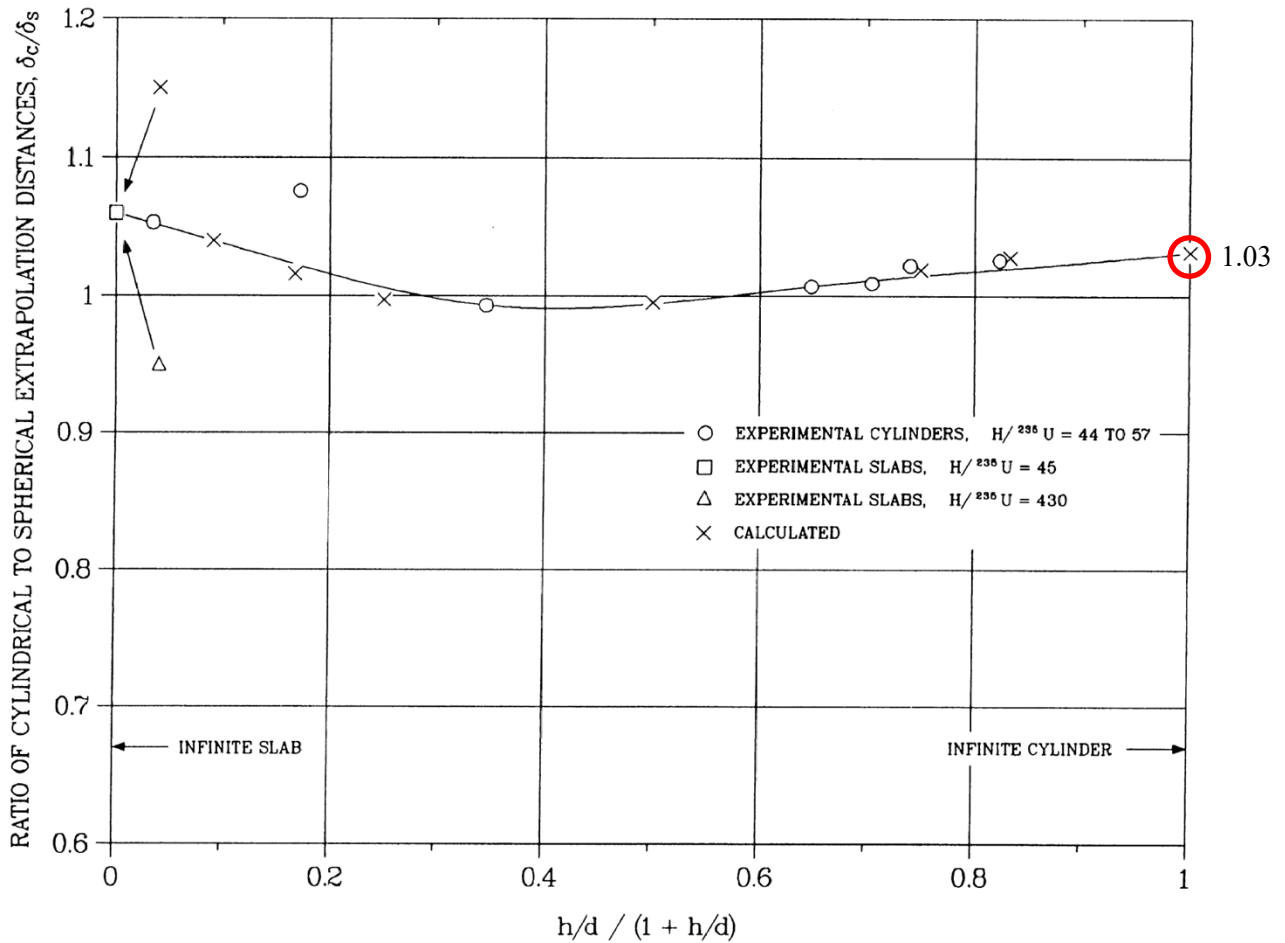
Fig. 6. Ratio of cylindrical extrapolation distance to that of sphere for water reflected U(93)O$_2$F$_2$ solutions. Cylinder height and diameter are h and d respectively.

Figure 2-10. Relationship Between Extrapolation Distances of Sphere, Slabs, and Cylinders. (Reference 11, page 17, Figure 6).

Part 3. Significantly reducing the enrichment from fully enriched U-235 (i.e., 100% ^{235}U) to 14.7 wt. % U-235 involves a corresponding increase in the quantity of U-238 in the system. The increased quantity of U-238 in the system (100 – 14.7 = 85.3 wt. %) will reduce the reactivity of the system compared with Part 2, because there is significant resonance absorption occurring in the U-238. Thus, fewer fissile atoms are present, and the quantity of neutron absorbing nuclides in the system is larger.

First, the atom densities must be modified to reflect the presence of U-238. Data for the new enrichment in this part of the problem are provided in Table 2-11.

Table 2-11. Diffusion Theory Example Problem 5 Additional Data for Part 3.

Constituent	Parameter	Data Value	Reference
^{238}U	σ_a (2200 m/s)	2.73 barns	2, Table II.2, pg. 738
	σ_s (2200 m/s)	9.2 barns	nndc.bnl.gov, ENDF-VIII.0
	g_a (non-1/v factor) for 20 °C	0.9780	2, Table 3.2, pg. 75 or Table 2-3, this document
^{235}U	σ_s (2200 m/s)	14.1 barns	nndc.bnl.gov, ENDF-VIII.0
O in UO_2SO_4	σ_s (2200 m/s)	3.76 b	2, Table II.3, pg. 741
S in UO_2SO_4	σ_s (2200 m/s)	0.975 b	2, Table II.3, pg. 741
H in Water	σ_s (2200 m/s)	49.6 b	=(103 – 3.76)/2
Water	σ_a (2200 m/s)	0.664 b	2, Table II.3, pg. 741
	σ_s (2200 m/s)	103 b	2, Table II.3, pg. 741
	σ_s (slowing down)	44.6 b	=2*20.4+3.8 (Dant app E)
	tτ	27 cm^2	2, Table 5.3, pg. 259
	D	0.16 cm	2, Table 5.2, pg. 254
	$D_{mixture} = D_{water}$		The tank will contain mostly water with small quantities of U. Therefore, the diffusion coefficient and neutron age will be approximately that of water.
	$\tau_{mixture} = \tau_{water}$		

Now, as in the last part of this problem, the atom densities need to be calculated to consider the effects of the U-238 in the system. First, the absorption cross section must be adjusted for U-238 because U-238 is a non-1/v absorber:

$$\overline{\sigma}_{a(U-238)} = \frac{\sqrt{\pi}}{2} g_a \sigma_a(2200) = 0.886 \times 1.0017 \times 2.7 = 2.40\ b$$

The atom density for U-235 remains unchanged as the concentration of U-235 remains the same.

$$N_{U235} = 7.686x10^{-5} \text{atoms U235/b - cm}$$

Knowing the weight fraction of U-235 (14.7 wt %), we can calculate the effective atomic weight of U(14.7).

$$\overline{A} = \left(\frac{wf_1}{A_1} + \frac{wf_2}{A_2}\right)^{-1} = \left(\frac{0.147}{235.04} + \frac{(1-0.147)}{238.05}\right)^{-1} = 237.60\text{g - U(14.7)/mole}$$

To determine the uranium concentration in solution, the concentration of U-235 can be adjusted by dividing by the enrichment, which is equal to 14.7 wt % U-235 in U:

$$C_U = \frac{C_{U235}}{0.147} = \frac{0.03\ \text{g - U235}}{\text{cm}^3} \frac{\text{g - U}}{0.147\ \text{g - U235}} = 0.204\text{g - U /cm}^3$$

With the density of U(14.7) in the solution, we can determine the atom density of U(14.7) and then the atom densities of the constituents.

$$N_{U(14.7)} = \frac{C_{U(14.7)}[g/cm^3] \times 0.6022[\text{atoms - cm}^2/\text{mol - b}]}{A_{U(14.7)}[g/mol]}$$

$$N_{U(14.7)} = \frac{0.204[g/cm^3] \times 0.6022[\text{atoms - cm}^2/\text{mol - b}]}{237.6[g/mol]} = 5.170x10^{-4}\text{atoms U(14.7)/b - cm}$$

$$N_{U238} = N_{U(14.7)} - N_{U235} = 5.170x10^{-4}\text{atoms U(14.7)/b - cm} - 7.686x10^{-5}\text{atoms U235/b - cm}$$

$$N_{U238} = 4.401x10^{-4}\text{atoms U238/b - cm}$$

$$N_O = 6 \times N_{U(14.7)} = 6 \times 5.170x10^{-4}\text{atoms U(14.7)/b - cm} = 3.102x10^{-3}\text{atoms O/b - cm}$$

$$N_S = N_{U(14.7)} = 5.170x10^{-4}\text{atoms S/b - cm}$$

$$N_{waterinUSulf} = 3 \times N_{U(14.7)} = 3 \times 5.170x10^{-4}\text{atoms U(14.7)/b - cm}$$

$$= 1.551x10^{-3}\text{molecules water in USulf/b - cm}$$

The atom densities have changed significantly compared with Part 2 of the problem because of the addition of U-238 to the system. Thus, because the macroscopic cross sections are dependent on the atom densities, they must be recalculated. Recall that the concentration needed for the following calculations must allow for the total uranium content in the system, not only the U-235 content.

The molecular density for water is calculated as follows.

$$\rho_{U(14.7)O_2SO_4 \cdot 3H_2O} = \frac{\rho_{U235}}{\text{wf}_{U235}} = \frac{0.204 \text{ g U(14.7)}}{cm^3 \text{ - mix}} \times \frac{419.7 \text{ g U(14.7)}O_2SO_4 \cdot 3H_2O}{237.60 \text{ g U(14.7)}}$$

$$= 0.3603 \frac{\text{g U(14.7)}O_2SO_4 \cdot 3H_2O}{cm^3 \text{ - mix}}$$

$$vf_{UO_2SO_4 \cdot 3H_2O} = \frac{\rho_{UO_2SO_4 \cdot 3H_2O}}{\text{Theoretical Density}}$$

$$= \frac{0.3603 \text{ g U(14.7)}O_2SO_4 \cdot 3H_2O}{cm^3 \text{ - mix}} \times \frac{cm^3 \text{ - U(14.7)}O_2SO_4 \cdot 3H_2O}{3.28 \text{ g U(14.7)}O_2SO_4 \cdot 3H_2O}$$

$$= 0.1098 \; \frac{\text{cm}^3 \text{ - U}(14.7)O_2SO_4 \cdot 3H_2O}{\text{cm}^3 \text{ - mix}}$$

$$vf_{Water} = 1 - vf_{UO_2SO_4 \cdot 3H_2O} = 1 - 0.1098 = 0.8902 \; \frac{\text{cm}^3 - H_2O}{\text{cm}^3 \text{ - mix}}$$

$$N_{Water} = \frac{vf_{Water}\left[\frac{\text{cm}^3 \text{ - } H_2O}{\text{cm}^3 \text{ - mix}}\right] \times \rho_{water}\left[\frac{\text{g - } H_2O}{\text{cm}^3 \text{ - } H_2O}\right] \times N_A\left[\text{atoms - cm}^2/\text{mol - b}\right]}{A_{Water}[\text{g - } H_2O/\text{mol}]}$$

N_{Water}
$$= \frac{0.8902 \left[\text{cm}^3 \text{ - } H_2O/\text{cm}^3 \text{ - mix}\right] \times 1.0\left[\text{g - } H_2O/\text{cm}^3 \text{ - } H_2O\right] \times 0.6022\left[\text{molecules - cm}^2/\text{mol - b}\right]}{18.015[\text{g - } H_2O/\text{mol}]}$$
$=$

$$N_{Water} = \; 2.976x10^{-2}\text{molecules - } H_2O/\text{b - cm}$$

$$N_{Water}^{total} = \; 1.551x10^{-3} + 2.976x10^{-2} = 3.131x10^{-2}\text{molecules - } H_2O/\text{b - cm}$$

in both U(14.7)O_2SO_4•3H_2O and Water

$$N_O^{total} = \;\; 3.102x10^{-3} + 3.131x10^{-2} = 3.441x10^{-2}\text{atoms - O/b - cm}$$

in both U(14.7)O_2SO_4•3H_2O and Water

Now calculate the macroscopic cross sections for the mixture constituents.

$$\Sigma_a^{U235} = N_{U235} \times \bar{\sigma}_a = \frac{7.686x10^{-5}\text{atoms U235}}{\text{b - cm}} \times \frac{595b}{\text{atom U235}} = 0.0457\text{cm}^{-1}$$

$$\Sigma_f^{U235} = N_{U235} \times \bar{\sigma}_f = \frac{7.686x10^{-5}\text{atoms U235}}{\text{b - cm}} \times \frac{508b}{\text{atom U235}} = 0.0390\text{cm}^{-1}$$

$$\Sigma_a^{U238} = N_{U238} \times \bar{\sigma}_a = \frac{4.401x10^{-4}\text{atoms U238}}{\text{b - cm}} \times \frac{2.40b}{\text{atom U238}} = 0.0011\text{cm}^{-1}$$

$$\Sigma_a^{S \text{ in } UO_2SO_43 H_2O} = N_S \times \bar{\sigma}_a = \frac{5.170x10^{-4}\text{atoms S}}{\text{b - cm}} \times \frac{0.461b}{\text{atom S}} = 0.0002\text{cm}^{-1}$$

$$\Sigma_a^{O \text{ in } UO_2SO_43 H_2O} = N_O \times \bar{\sigma}_a = \frac{3.102x10^{-3}\text{atoms O}}{\text{b - cm}} \times \frac{0.248x10^{-3}b}{\text{atom O}} = 7.7x10^{-7} \text{ cm}^{-1} \approx 0\text{cm}^{-1}$$

$$\Sigma_a^{water \text{ in Usulf}} = N_{WaterU} \times \bar{\sigma}_a = \frac{1.551x10^{-3}\text{molecule water}}{\text{b - cm}} \times \frac{0.589b}{\text{molecule water}} =$$
$$\Sigma_a^{water \text{ in Usulf}} = 0.0009\text{cm}^{-1}$$

$$\Sigma_a^{Water} = N_{water} \times \bar{\sigma}_a = \frac{2.970x10^{-2}\text{molecules H}_2O}{\text{b - cm}} \times \frac{0.589b}{\text{molecule H}_2O} = 0.0175\text{cm}^{-1}$$

$$\therefore \Sigma_a^{UO_2SO_4} = \Sigma_a^{U235} + \Sigma_a^{U238} + \Sigma_a^{S} + \Sigma_a^{O} + \Sigma_a^{waterinUsulf}$$

$$= 0.0457\text{cm}^{-1} + 0.0011\text{cm}^{-1} + 0.0002\text{cm}^{-1} + 0 + 0.0009\text{cm}^{-1}$$

$$= 0.0479\text{cm}^{-1}$$

$$\therefore \Sigma_a^{mixture} = \Sigma_a^{UO_2SO_4} + \Sigma_a^{Water}$$

$$= 0.0479\text{cm}^{-1} + 0.0175\text{cm}^{-1}$$

$$= 0.0654\text{cm}^{-1}$$

Next, η, the number of neutrons released in fission per neutron absorbed by a fissile nucleus and f, the thermal utilization factor, can be calculated for this system. The macroscopic fission cross section for U-238 is very small and can be neglected in this calculation:

$$\eta = \frac{\nu \times \Sigma_f^{235U} + \nu \times \Sigma_f^{238U}}{\Sigma_a^{UO_2SO_4}} = \frac{2.418 \times 0.0390 + 0}{0.0479} = 1.969$$

$$f = \frac{\Sigma_a^{UO_2SO_4}}{\Sigma_a^{mixture}} = \frac{0.0479}{0.0654} = 0.732.$$

Because this system with lower enrichment contains significant quantities of U-238, the resonance escape probability must be calculated. The resonance escape probability is the probability that a neutron will escape being captured by the material resonances as it slows down from fast to thermal energies. In this case, the resonances in the absorption cross-section for U-238 will make fewer neutrons available for subsequent fissions and reduce the system reactivity.

First, calculate the mean lethargy gain per neutron collision, ξ, for the moderator and fuel mixture present in this system.

$$\xi = 1 - \frac{(A-1)^2}{2A} ln \left[\frac{A+1}{A-1} \right]$$

For an atomic weight, A, greater than 10 (A>10), the following approximation can be used:

$$\xi \approx \frac{2}{A + \frac{2}{3}} \quad \text{for } A > 10.$$

We need to calculate ξ for each component of the mixture.

For hydrogen (A=1): $\xi_H = 1 - \frac{(A-1)^2}{2A} ln \left[\frac{A+1}{A-1} \right] = 1 - 0 = 1$ (Reference 2, Table 8 - 1).

For oxygen (A=16): $\xi_O \approx \frac{2}{16 + \frac{2}{3}} = 0.12$.

For sulfur (A=32): $\xi_S \approx \frac{2}{32 + \frac{2}{3}} = 0.061$.

For U-235 (A=235): $\xi_{U235} \approx \frac{2}{235 + \frac{2}{3}} = 0.0085$.

For U-238 (A=238): $\xi_{U238} \approx \frac{2}{238 + \frac{2}{3}} = 0.0084$.

Then the value for the mixture is each individual ξ weighted by the component macroscopic scattering cross section. Note that for this calculation, we use the hydrogen scattering cross section of 20.4 b as appropriate to the slowing down energies of the resonance region.

$$\bar{\xi}_{mixture} = \frac{N_H \sigma_{s_H} \xi_H + N_O \sigma_{s_O} \xi_O + N_S \sigma_{s_S} \xi_S + N_{U235} \sigma_{sU235} \xi_{U235} + N_{U238} \sigma_{sU238} \xi_{U238}}{N_H \sigma_{s_H} + N_O \sigma_{s_O} + N_S \sigma_{s_S} + N_{U235} \sigma_{sU235} + N_{U238} \sigma_{sU238}}$$

$$\bar{\xi}_{mixture} = \frac{(2 \times 3.131x10^{-2} \times 20.4 \times 1) + (3.440x10^{-2} \times 3.76 \times 0.12) + (5.2x10^{-4} \times 0.975 \times 0.061)}{(2 \times 3.131x10^{-2} \times 20.4) + (3.440x10^{-2} \times 3.76) + (5.2x10^{-4} \times 0.975) + (8x10^{-5} \times 14.1) + (4.4x10^{-4} \times 9.2)}$$

$$+ \frac{(8x10^{-5} \times 14.1 \times 0.0085) + (4.4x10^{-4} \times 9.2 \times 0.0084)}{(2 \times 3.131x10^{-2} \times 20.4) + (3.440x10^{-2} \times 3.76) + (5.2x10^{-4} \times 0.975) + (8x10^{-5} \times 14.1) + (4.4x10^{-4} \times 9.2)}$$

$$\bar{\xi}_{mixture} = \frac{1.2930}{1.4125} = 0.915.$$

Note that $\Sigma_s^{\text{moderator}} = (2 \times 3.131x10^{-2} \times 20.4) + (3.440x10^{-2} \times 3.76) = 1.407 cm^{-1}$

Now the resonance escape probability can be calculated from equation 45:

$$p = exp\left\{\frac{-3.06}{\xi}\left(\frac{N_{U238}}{Ns_{modmod}}\right)^{0.528}\right\} = exp\left\{\frac{-3.06}{0.915}\left(\frac{4.40x10^{-4}}{1.407}\right)^{0.528}\right\} = 0.954$$

The fast fission factor, ε, is assumed to be equal to 1.0 for this case to emphasize the importance of the resonance escape probability to this kind of system. Thus, the infinite multiplication factor is then $k_\infty =$ $\eta \varepsilon f p$.

$$k_\infty = \eta\, f \varepsilon p = 1.969 \times 0.732 \times 1.0 \times 0.954 = 1.375\ (Answer\ to\ Part\ 3)$$

When analyzed in PARTISN[7], the k_∞ was 1.37—quite good agreement considering the difference in cross sections and methods. Based on the result of this calculation, a tank with infinite dimensions at this concentration of uranyl sulfate solution **would still not be safe** at the lower uranium enrichment, even with the increased probability for neutron absorption in this kind of fissile system.

Note that even with 85.3% U-238 in the system, the resonance escape probability is close to one. This indicates that only for low-enriched (less than 10%) uranium systems does the resonance escape probability become more than about a 5% correction to the infinite multiplication factor.

Now the critical dimensions for this system can be determined:

---

[7] PARTISN is an upgraded version of the DANTSYS code package and is designed to solve the discrete ordinates form of the Boltzmann transport equation in several different geometries using multigroup cross sections. See Reference 4 for additional information on using PARTISN in nuclear criticality safety calculations.

$$L_{th}^2 = \frac{D}{\Sigma_a} = \frac{0.16 \text{ cm}}{0.0654 \text{ cm}^{-1}} = 2.45 \text{ cm}^2$$

$$B_m^2 = \frac{k_\infty - 1}{M^2} = \frac{k_\infty - 1}{L^2 + \tau} = \frac{1.375 - 1}{2.45 + 27} = 0.01273 \text{ cm}^{-2}$$

$$\overline{R} = \sqrt{\frac{2.405^2}{B_m^2}} = \sqrt{\frac{2.405^2}{0.01273 \text{ cm}^{-2}}} = 21.32 \text{ cm}$$

$$R = \overline{R} - d = 21.32 \text{ cm} - 2.1 \text{ cm} \times 1.03 = 19.16 \text{ cm}.$$

The critical dimensions increased by about 10% compared with the fully enriched case. A larger system than the previous case makes sense because this system has a significantly lower enrichment and more parasitic neutron absorption with the large quantity of U-238 present. When analyzed in PARTISN, the critical radius of an infinite cylinder with 14.7 wt. % U-235 in uranyl sulfate was 19.61 cm.

NOTE on problem complexity and detailed calculation: as indicated, the modified one-group calculations compared quite well with the values from the computer codes. However, in most applications of hand calculations, the detail presented in Part 3 is probably not necessary particularly if one is doing bounding calculations. Let's look at the Part 3 problem and estimate values as appropriate.

We will need to calculate atom densities but will look at only U-235, U-238, and water. We follow the same procedure as above obtaining 7.686×10^{-5} atoms U-235/b-cm, 4.401×10^{-4} atoms ^{238}U/b-cm, and assuming water at nominal density (1.0 g/cm3):

$$N_{Water} = \frac{1.0 [\text{g - H}_2\text{O/cm}^3 \text{ - H}_2O] \times 0.6022 [\text{molecules - cm}^2/\text{mol - b}]}{18.015 [\text{g - H}_2\text{O/mol}]} =$$

$$N_{Water} = 3.3428 x 10^{-2} \text{molecules - H}_2\text{O/b - cm}$$

Then, calculating the macroscopic fission and absorption cross sections,

$$\Sigma_a^{U235} = N_{U235} \times \overline{\sigma}_a = \frac{7.686 x 10^{-5} \text{atoms U235}}{\text{b - cm}} \times \frac{595 b}{\text{atom U235}} = 0.0457 \text{cm}^{-1}$$

$$\Sigma_f^{U235} = N_{U235} \times \overline{\sigma}_f = \frac{7.686 x 10^{-5} \text{atoms U235}}{\text{b - cm}} \times \frac{508 b}{\text{atom U235}} = 0.0390 \text{cm}^{-1}$$

$$\Sigma_a^{U238} = N_{U238} \times \overline{\sigma}_a = \frac{4.401 x 10^{-4} \text{atoms U238}}{\text{b - cm}} \times \frac{2.40 b}{\text{atom U238}} = 0.0011 \text{cm}^{-1}$$

$$\Sigma_a^{water} = N_{Water} \times \overline{\sigma}_a = \frac{3.3428 x 10^{-2} \text{molecules water}}{\text{b - cm}} \times \frac{0.589 b}{\text{molecule water}} = 0.0197 \text{cm}^{-1}$$

$$\Sigma_a^{total} = \Sigma_a^{U235} + \Sigma_a^{U238} + \Sigma_a^{water} = 0.0457 \text{cm}^{-1} + 0.0011 \text{cm}^{-1} + 0.0197 \text{cm}^{-1} = 0.0665 \text{cm}^{-1}$$

Now we note that $\eta f = \frac{\nu \Sigma_f}{\Sigma_a^{total}} = \frac{2.418 \times 0.0390 \text{ cm}^{-1}}{0.0665 \text{cm}^{-1}} = 1.42$

The fast fission factor, ε, is assumed to be equal to 1.0, and we will assume p = 1. This is a reasonable estimate for uranium–water moderated systems with enrichments greater than 10%. (As we calculated earlier, p = 0.954 for this 14.7% enriched case). Thus, the infinite multiplication factor is then $k_\infty = \eta f \varepsilon p$.

$$k_\infty = \eta \, f \varepsilon p = 1.42 \times 1.0 \times 0.954 = 1.355 \; (Estimated \, Answer \; to \; Part \; 3)$$

Now the critical dimensions for this system can be determined:

$$L_{th}^2 = \frac{D}{\Sigma_a} = \frac{0.16 \text{ cm}}{0.0665 \text{ cm}^{-1}} = 2.41 \text{ cm}^2$$

$$B_m^2 = \frac{k_\infty - 1}{M^2} = \frac{k_\infty - 1}{L^2 + \tau} = \frac{1.355 - 1}{2.41 + 27} = 0.01207 \text{ cm}^{-2}$$

$$\bar{R} = \sqrt{\frac{2.405^2}{B_m^2}} = \sqrt{\frac{2.405^2}{0.01207 \, cm^{-2}}} = 21.9 \; cm$$

$$R = \bar{R} - d = 21.9 \; cm - 2.2 \; cm = 19.7 \; cm.$$

The critical dimension from the estimate was about 3% higher than that obtained from the detailed calculation (19.7 cm vs. 19.16 cm). The actual amount of deviation varies depending on the materials in each system. However, a reasonable bounding estimate of size can be obtained through a simplified modified one-group analysis.

2.6.6 Diffusion Theory Example Problem 6 – Thermal System with Uranium

It is proposed to store uranium dioxide–water solutions (U(5)O_2-H_2O) with a concentration of 50 g ^{235}U/l (0.05 g/cm^3) in solution. Assume the temperature of the solution is 20°C, and the uranium is 5 wt %. Table 2-12 lists the relevant data for this problem.

1. What is the H/X for this solution?
2. Calculate the critical spherical radius using modified one-group diffusion theory.
3. Repeat (2) with the sphere reflected by 30 cm of water.

Before starting any calculation of fissile material system properties, one should have an idea what the answer should be—that is, at least an order of magnitude estimate and the expected units of the results. For this case, we are interested in the H/X (hydrogen to fissile atom ratio), the infinite multiplication factor, and the critical spherical radius in centimeters. We will start with ARH-600, Reference 7. Figure III.B.2-6 has H/X ratios for low enriched UO_2 – H_2O solutions. For U(5), the uranium concentration will be 1.0 g U/cm³; this gives an H/X = 470. Figure III.B.10(5)-2 shows k$_\infty$ = 1.39 and the migration area = 28.5 cm². Figure III.B.10(5)-1 shows a material buckling of 0.01375 cm^{-2} and an extrapolation distance for an unreflected system of 2.1 cm. Figure III.B.3-4 gives a bare, critical diameter of 19.5 in. or a critical radius of 24.77 cm.

Table 2-12. Diffusion Theory Example Problem 6 Data.

Constituent	Parameter	Data Value	Reference
^{235}U	σ_a (2200 m/s)	687 barns	2, Table II.2, pg. 738
	σ_f (2200 m/s)	587 barns	2, Table II.2, pg. 738
	v	2.418	2, Table 3.4, pg. 82
	g_a (non-1/v factor) for 20 °C	0.9780	2, Table 3.2, pg. 75 or Table 2-1, this document
	g_f (non-1/v factor) for 20 °C	0.9759	2, Table 3.2, pg. 75 or Table 2-1, this document
	σ_s (2200 m/s)	14.1 barns	nndc.bnl.gov, ENDF-VIII.0
^{238}U	σ_a (2200 m/s)	2.73 barns	2, Table II.2, pg. 738
	σ_s (2200 m/s)	9.2 barns	nndc.bnl.gov, ENDF-VIII.0
	g_a (non-1/v factor) for 20 °C	0.9780	2, Table 3.2, pg. 75 or Table 2-3, this document
O in UO_2	σ_a (2200 m/s)	0.27 mb	2, Table II.3, pg. 741

Table 2-12. Diffusion Theory Example Problem 6 Data (continued).

Constituent	Parameter	Data Value	Reference
Water	Hydrogen σ_a(2200 m/s)	0.332 b	2, Table II.3, pg. 740
	Oxygen σ_a(2200 m/s)	0.27 mb	2, Table II.3, pg. 741
	Water σ_a(2200 m/s)	0.6643 b	= 2 x 0.332 b + 0.27x10^{-3} b
	σ_s (slowing down)	44.6 b	=2x 20.4+3.8 (Ref 4, app E)
	τ	27 cm^2	2, Table 5.3, pg. 259
	D	0.16 cm	2, Table 5.2, pg. 254

Part 1. Calculation of the H/X ratio requires values for atom densities for U-235 and Hydrogen.

As stated in Section 2.3.1, because U-235 is a non-1/v absorber, the absorption microscopic cross section must also be adjusted using the *ga* and *gf* factors as listed in Table 2-1. Thus, the absorption and fission microscopic cross sections in barns for U-235 are adjusted as follows.

$$\bar{\sigma}_a = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200 \text{ m/sec}) = 0.886 \times 0.9780 \times 687b = 595b$$

$$\bar{\sigma}_f = \frac{\sqrt{\pi}}{2} g_f \sigma_f (2200 \text{ m/sec}) = 0.886 \times 0.9759 \times 587b = 508b$$

Note that the uranium in solution is 5 wt %, so it contains 95 wt % U-238. First, the absorption cross section must be adjusted for U-238 because it is a non-1/v absorber:

$$\bar{\sigma}_{a(U-238)} = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200) = 0.886 \times 1.0017 \times 2.7 = 2.40 \ b$$

and for oxygen in UO$_2$, it is expressed as follows:

$$\bar{\sigma}_{a(oxy)} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(oxy)} (2200 \text{ m/sec}) = 0.886 \times 1.0 \times 0.28x10^{-3}b = 0.248x10^{-3}b$$

For water (H$_2$O), the cross section adjustment is expressed as

$$\bar{\sigma}_{a(H_2O)} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(H_2O)} (2200 \text{ m/sec}) = 0.886 \times 1.0 \times 0.6643b = 0.589b$$ The next step is to

calculate the atom densities for UO$_2$ and water, so the macroscopic cross sections can be determined.

$$N_{U235} = \frac{\rho_{U235}[\text{g/cm}^3] \times N_A[\text{atoms - cm}^2/\text{mol - b}]}{A_{U235}[\text{g/mol}]}$$

$$A_{U235}[\text{g/mol}] = 235.04[\text{g/mol}]; \; \rho \text{ given as 50 g/liter} = 0.05 \text{ g/cm}^3$$

$$N_{U235} = \frac{0.05[\text{g/cm}^3] \times 0.6022[\text{atoms - cm}^2/\text{mol - b}]}{235.04[\text{g/mol}]} = 1.281x10^{-4}\text{atoms U235/b - cm}$$

Knowing the weight fraction of U-235 (5 wt %), we can calculate the effective atomic weight of U(5).

$$\overline{A} = \left(\frac{wf_1}{A_1} + \frac{wf_2}{A_2}\right)^{-1} = \left(\frac{0.05}{235.04} + \frac{(1-0.05)}{238.05}\right)^{-1} = 237.90\text{g - U(5)/mole}$$

To determine the uranium concentration in solution, the concentration of ^{235}U can be adjusted by dividing through by the enrichment, which is equal to 5 wt % U-235 in U:

$$C_U = \frac{C_{U235}}{0.05} = \frac{0.05 \text{ g - U235}}{\text{cm}^3} \frac{\text{g - U(5)}}{0.05 \text{ g - U235}} = 1.00\text{g - U(5) /cm}^3$$

With the density of U(5) in the solution, we can determine the atom density of U(5) and then the atom densities of the constituents.

$$N_{U(5)} = \frac{C_{U(5)}[\text{g/cm}^3] \times 0.6022[\text{atoms - cm}^2/\text{mol - b}]}{A_{U(5)}[\text{g/mol}]}$$

$$N_{U(5)} = \frac{1.00[\text{g/cm}^3] \times 0.6022[\text{atoms - cm}^2/\text{mol - b}]}{237.9[\text{g/mol}]} = 2.531x10^{-3}\text{atoms U(5)/b - cm}$$

$$N_{U238} = N_{U(5)} - N_{U235} = 2.531x10^{-3}\text{atoms U(5)/b - cm} - 1.281x10^{-4}\text{atoms U235/b - cm}$$

$$N_{U238} = 2.403x10^{-3}\text{atoms U238/b - cm}$$

$$N_O = 2 \times N_{U(5)} = 2 \times 2.531x10^{-3}\text{atoms U(5)/b - cm} = 5.062x10^{-3}\text{atoms O/b - cm}$$

Now that the U atom density is known, calculate the volume fractions for UO_2 and water to determine the molecular density of water. Note the mixture is uranium dioxide $(U(5)O_2$ (molecular weight is 269.9 g / mole and density of 10.96 g/cm³ from ARH-600, Vol I, page II.D.2-1, Reference 7) and additional water. First, start by determining the concentration of the uranium dioxide based on the uranium concentration.

$$\rho_{UO_2} = \frac{\rho_{U(5)}}{wf_{UO_2}} = \frac{1.00 \text{ g U(5)}}{\text{cm}^3 \text{ - mix}} \times \frac{269.9 \text{ g UO}_2}{237.9 \text{ g U(5)}} = 1.1345 \frac{\text{g UO}_2}{\text{cm}^3 \text{ - mix}}$$

$$vf_{UO_2} = \frac{\rho_{UO_2}}{\text{Theoretical Density}}$$

$$= \frac{1.1345 \text{ g UO}_2}{\text{cm}^3 \text{ - mix}} \times \frac{\text{cm}^3 \text{ - UO}_2}{10.96 \text{ g UO}_2} = 0.1035 \frac{\text{cm}^3 \text{ - UO}_2}{\text{cm}^3 \text{ - mix}}$$

$$vf_{Water} = 1 - vf_{UO_2} = 1 - 0.1035 = 0.8965 \frac{\text{cm}^3 - H_2O}{\text{cm}^3 \text{ - mix}}$$

Knowing the volume fractions, we can calculate the mixture density.

$$\rho_{mix} = vf_{UO_2} \times \rho_{UO_2} + vf_{Water} \times \rho_{Water}$$

$$\rho_{mix} = 0.1035 \frac{\text{cm}^3 \text{ - UO}_2}{\text{cm}^3 \text{ - mix}} \times 10.96 \frac{\text{g UO}_2}{\text{cm}^3 \text{ - UO}_2}$$

$$+ 0.8965 \frac{\text{cm}^3 - H_2O}{\text{cm}^3 \text{ - mix}} \times 0.998 \frac{\text{g - Water}}{\text{cm}^3 \text{ - mix}} = 2.029 \frac{\text{g - mix}}{\text{cm}^3 \text{ - mix}}$$

Using the mixture density, can calculate the weight fractions of its two constituents:

$$wf_{UO_2} = \frac{vf_{UO_2} \times \rho_{UO_2}S}{\rho_{mix}} = 0.1035 \frac{\text{cm}^3 \text{ - UO}_2}{\text{cm}^3 \text{ - mix}} \times 10.96 \frac{\text{g UO}_2}{\text{cm}^3 \text{ - UO}_2} \times \frac{1 \text{ cm}^3 \text{ - mix}}{2.029 \text{ g - mix}}$$

$$= 0.5591 \frac{\text{g UO}_2}{\text{g - mix}}$$

$$wf_{Water} = \frac{vf_{Water} \times \rho_{Water}}{\rho_{mix}} = 0.8965 \frac{\text{cm}^3 - H_2O}{\text{cm}^3 \text{ - mix}} \times \frac{0.998 \text{ g } H_2O}{\text{cm}^3 - H_2O} \times \frac{1 \text{ cm}^3 \text{ - mix}}{2.029 \text{ g - mix}}$$

$$= 0.4410 \frac{\text{g } H_2O}{\text{g - mix}}$$

Now, with the weight fraction of water, we can calculate its molecular density in the mixture.

$$\rho_{Water} = 0.998 \left[\text{g/cm}^3 \right] \quad A_{Water} = 2 \times 1.00794 + 1 \times 15.9994 = 18.015 \left[\text{g/mol} \right]$$

$$N_{Water} = \frac{wf_{Water} \times \rho_{mix} \left[\text{g/cm}^3 \right] \times N_A \left[\text{atoms - cm}^2/\text{mol - b} \right]}{A_{Water} \left[\text{g/mol} \right]}$$

$$N_{Water} = \frac{0.4410 \, \dfrac{\text{g H}_2O}{\text{g - mix}} \times \dfrac{2.029 \, \text{g - mix}}{\text{cm}^3 \text{ - mix}} \times 0.6022 \, \dfrac{\text{molecules - cm}^2}{\text{mol - b}}}{18.015 \, \dfrac{\text{g H}_2O}{\text{mol}}}$$

$$= 2.991 \text{x} 10^{-2} \text{molecules Water/b - cm as the solvent}$$

The H/X ratio is the ratio of hydrogen atoms to fissile atoms (in this case U-235). Knowing there are two hydrogen atoms per molecule of water, we get:

$$\frac{H}{X} = \frac{2 \times 2.991 x 10^{-2} \text{ atoms H}}{1.281 x 10^{-4} \text{ atoms U235}} = 467$$

This compares very well with the value of 470 obtained from the handbook.

Part 2. Calculation of the critical spherical radius using modified one-group diffusion theory.

First, calculate the macroscopic cross sections for the mixture constituents.

$$\Sigma_a^{U235} = N_{U235} \times \overline{\sigma}_a = \frac{1.281 x 10^{-4} \text{atoms U235}}{\text{b - cm}} \times \frac{595 b}{\text{atom U235}} = 0.0762 \text{cm}^{-1}$$

$$\Sigma_f^{U235} = N_{U235} \times \overline{\sigma}_f = \frac{1.281 x 10^{-4} \text{atoms U235}}{\text{b - cm}} \times \frac{508 b}{\text{atom U235}} = 0.0651 \text{cm}^{-1}$$

$$\Sigma_a^{U238} = N_{U238} \times \overline{\sigma}_a = \frac{2.403 x 10^{-3} \text{atoms U238}}{\text{b - cm}} \times \frac{2.40 b}{\text{atom U238}} = 0.0058 \text{cm}^{-1}$$

$$\Sigma_a^{O \text{ in } UO_2} = N_O \times \overline{\sigma}_a = \frac{5.062 x 10^{-3} \text{atoms O}}{\text{b - cm}} \times \frac{0.248 x 10^{-3} b}{\text{atom O}} = 1.3 x 10^{-6} \text{ cm}^{-1} \approx 0 \text{cm}^{-1}$$

$$\Sigma_a^{Water} = N_{water} \times \bar{\sigma}_a = \frac{2.991x10^{-2}\text{molecules } H_2O}{\text{b - cm}} \times \frac{0.589b}{\text{molecule } H_2O} = 0.0176\text{cm}^{-1}$$

$$N_a^{Ototal} = N_{water}^O + N_{UO_2}^O = \frac{2.991x10^{-2}\text{atoms O}}{\text{b - cm}} + \frac{5.062x10^{-3}\text{atoms O}}{\text{b - cm}} = \frac{3.497x10^{-2}\text{atoms O}}{\text{b - cm}}$$

$$\therefore \Sigma_a^{UO_2} = \Sigma_a^{U235} + \Sigma_a^{U238} + \Sigma_a^O$$

$$= 0.0762\text{cm}^{-1} + 0.0058\text{cm}^{-1} + 0$$

$$= 0.0820\text{cm}^{-1}$$

$$\therefore \Sigma_a^{mixture} = \Sigma_a^{UO_2} + \Sigma_a^{Water}$$

$$= 0.0820\text{cm}^{-1} + 0.0176\text{cm}^{-1}$$

$$= 0.0996\text{cm}^{-1}$$

Next, η, the number of neutrons released in fission per neutron absorbed by a fissile nucleus and f, the thermal utilization factor, can be calculated for this system. The macroscopic fission cross section for U-238 is very small and can be neglected in this calculation:

$$\eta = \frac{v \times \Sigma_f^{235U} + v \times \Sigma_f^{238U}}{\Sigma_a^{UO_2}} = \frac{2.418 \times 0.0651 + 0}{0.0820} = 1.920$$

$$f = \frac{\Sigma_a^{UO_2}}{\Sigma_a^{mixture}} = \frac{0.0820}{0.0996} = 0.823.$$

Because this system with lower enrichment contains significant quantities of U-238, the resonance escape probability must be calculated. The resonance escape probability is the probability that a neutron will escape being captured by the material resonances as it slows down from fast to thermal energies. In this case, the resonances in the absorption cross-section for U-238 will make fewer neutrons available for subsequent fissions and reduce the system reactivity.

First, calculate the mean lethargy gain per neutron collision, ξ, for the moderator and fuel mixture present in this system.

$$\xi = 1 - \frac{(A-1)^2}{2A}ln\left[\frac{A+1}{A-1}\right]$$

For an atomic weight, A, greater than 10 (A>10), the following approximation can be used:

$$\xi \approx \frac{2}{A + \frac{2}{3}} \quad \text{for A} > 10.$$

We need to calculate ξ for each component of the mixture.

For hydrogen (A=1): $\xi_H = 1 - \frac{(A-1)^2}{2A}ln\left[\frac{A+1}{A-1}\right] = 1 - 0 = 1$ (Reference 2, Table 8 - 1).

For oxygen (A=16): $\xi_O \approx \dfrac{2}{16 + \frac{2}{3}} = 0.12$.

For ^{235}U (A=235): $\xi_{U235} \approx \dfrac{2}{235 + \frac{2}{3}} = 0.0085$.

For ^{238}U (A=238): $\xi_{U238} \approx \dfrac{2}{238 + \frac{2}{3}} = 0.0084$.

Then the value for the mixture is each individual ξ weighted by the component macroscopic scattering cross section.

$$\bar{\bar{\xi}}_{mixture} = \frac{N_H \sigma_{s_H} \xi_H + N_O \sigma_{s_O} \xi_O + N_{U235} \sigma_{s_{U235}} \xi_{U235} + N_{U238} \sigma_{s_{U238}} \xi_{U238}}{N_H \sigma_{s_H} + N_O \sigma_{s_O} + N_{U235} \sigma_{s_{U235}} + N_{U238} \sigma_{s_{U238}}}$$

$$\bar{\bar{\xi}}_{mixture} = \frac{(2 \times 2.991x10^{-2} \times 20.4 \times 1) + (3.497x10^{-2} \times 3.8 \times 0.12)}{(2 \times 2.991x10^{-2} \times 20.4) + (3.497x10^{-2} \times 3.8) + (1.28x10^{-4} \times 14.1) + (2.403x10^{-3} \times 9.2)}$$

$$+ \frac{(1.28x10^{-4} \times 14.1 \times 0.0085) + (2.403x10^{-3} \times 9.2 \times 0.0084)}{(2 \times 2.991x10^{-2} \times 20.4) + (3.497x10^{-2} \times 3.8) + (1.28x10^{-4} \times 14.1) + (2.403x10^{-3} \times 9.2)}$$

$$\bar{\bar{\xi}}_{mixture} = \frac{1.2365}{1.3771} = 0.898.$$

Note that $\quad \Sigma_s^{moderator} = (2 \times 2.991x10^{-2} \times 20.4) + (3.497x10^{-2} \times 3.8) = 1.353 cm^{-1}$

Now the resonance escape probability can be calculated using Eq. (45):

$$p = exp\left\{ \frac{-3.06}{\xi} \left(\frac{N_{U238}}{Ns_{modmod}} \right)^{0.528} \right\} = exp\left\{ \frac{-3.06}{0.898} \left(\frac{2.403x10^{-3}}{1.353} \right)^{0.528} \right\} = 0.887$$

The fast fission factor, ε, is assumed to be equal to 1.00. Calculating the infinite multiplication factor $k_\infty = \eta \varepsilon f p$:

$$k_\infty = \eta \, f \varepsilon p = 1.920 \times 0.823 \times 1.0 \times 0.887 = 1.402$$

When analyzed in PARTISN, the k_∞ was 1.42; very good agreement considering the difference in cross sections and methods. Based on the result of this calculation, a tank with infinite dimensions at this concentration of uranyl sulfate solution **would still not be safe** at the lower uranium enrichment, even with the increased probability for neutron absorption in this kind of fissile system.

Now the critical dimensions for this system can be determined:

$$L_{th}^2 = \frac{D}{\Sigma_a} = \frac{0.16 \text{ cm}}{0.0996 \text{ cm}^{-1}} = 1.61 \text{ cm}^2$$

$$B_m^2 = \frac{k_\infty - 1}{M^2} = \frac{k_\infty - 1}{L^2 + \tau} = \frac{1.402 - 1}{1.61 + 27} = 0.01405 \text{ cm}^{-2}$$

$$\bar{R} = \sqrt{\frac{\pi^2}{B_m^2}} = \sqrt{\frac{\pi^2}{0.01405 \text{ cm}^{-2}}} = 26.50 \text{ cm}$$

$$R = \bar{R} - d = 26.5 \text{ cm} - 2.1 \text{ cm} = 24.4 \text{ cm}.$$

The critical dimension from the estimate was about a few percent lower than that estimated from the handbook (24.77 cm) and slightly higher than the PARTISN value of 24.30 cm and the SCALE value of 24.39 cm. A reasonable bounding estimate of size can be obtained through a modified one-group analysis.

Part 3. Calculation of the critical spherical radius when reflected by 30 cm of water.

Equation (56) as reproduced below gives the following critical condition for a reflected spherical reactor:

$$BR \cot(BR) - 1 = -\frac{D_r}{D_c}\left(\frac{R}{L_r} \coth\frac{T}{L_r} + 1\right)$$

where T is the extrapolated thickness of the reflector. This transcendental equation is solved for R either graphically or using a goal seek/solver approach in a spreadsheet. The B in Eq. (56) is the square root of the critical buckling for the bare system with the same fissile material.

For a 30 cm water reflector, $Dr = Dc$ and $Lr = 2.85$ cm. Using the square root of the critical buckling $(0.01405 \text{ cm}^{-2})$ from above $= 0.1185 \text{ cm}^{-1}$, then Eq. (56) becomes:

$$0.1185 \text{ cm}^{-1} \times R \times \cot(0.1185 \text{ cm}^{-1} \times R) - 1 = -\frac{0.16 \text{cm}}{0.16 \text{cm}}\left(\frac{R}{2.85 \text{ cm}} \coth\frac{30 \text{ cm}}{2.85 \text{ cm}} + 1\right) \quad \text{OR}$$

$$0.1185 \text{ cm}^{-1} \times R \times \cot(0.1185 \text{ cm}^{-1} \times R) - 1 = \left(\frac{-R}{2.85 \text{ cm}} \times 1 - 1\right)$$

$$0.1185 \text{ cm}^{-1} \times R \times \cot(0.1185 \text{ cm}^{-1} \times R) = \left(\frac{-R}{2.85 \text{ cm}}\right)$$

$$\cot(0.1185 \text{ cm}^{-1} \times R) = \left(\frac{-1}{2.85 \text{ cm}}\right)\left(\frac{1}{0.1185 \text{ cm}^{-1}}\right) = -2.961$$

$$0.1185 \text{ cm}^{-1} \times R = -.3257 \quad \text{or} \; -0.3257 + \pi = 2.816$$

$$R = \frac{2.816}{0.1185 \text{ cm}^{-1}} = 23.76 \text{ cm}$$

Because the reflector and moderator are the same material, the equation can be solved by substitution and algebraic manipulation. The cotangent function returns a negative value but also has a positive value that differs by π, so the positive value is used. The calculated critical reflected core radius seems high compared with the bare radius of 24.4 cm. If the bare radius is approximately B_c / π, then the reflector savings for the case of same moderator and reflector material should be: $\delta = L_r$ (in this case, 2.85 cm). For this example, the calculated bare radius is about 10% less than B_c / π (which is equal to the extrapolated radius, 26.5 cm). As the bare radius is reasonably large compared with the extrapolation distance, we can estimate the reflected radius as 24.4 cm – 2.85 cm = 21.55 cm. This value compares quite well with the estimate of 21.56 cm from Figure 15, LA-10860 (value derived from a critical spherical volume of 42 liters). However, it should be noted that Figure 15 from LA-10860 is for $U(5)O_2F_2$, which has slightly more absorption (due to the presence of the fluorine) than $U(5)O_2$. The modified one-group value of 21.55 slightly larger than the values calculated by PARTISN of 20.44 cm and by SCALE of 20.57 cm.

Note that the reflector savings calculated from PARTISN is 24.30 cm – 20.44 cm = 3.86 cm and as calculated from SCALE is 24.39 cm – 20.57 cm = 3.82 cm. This is larger than the thermal diffusion length in water of 2.85 cm. However, the reflector savings for water-reflected systems is typically in the 3.2 to 4.0 cm range, depending on the fissile material and isotopics. As seen in Figure 2-11, the experimentally measured reflector savings for water thicknesses greater than 15 cm is 3.92 cm. This figure shows the variation of reflector savings with water reflector thickness.
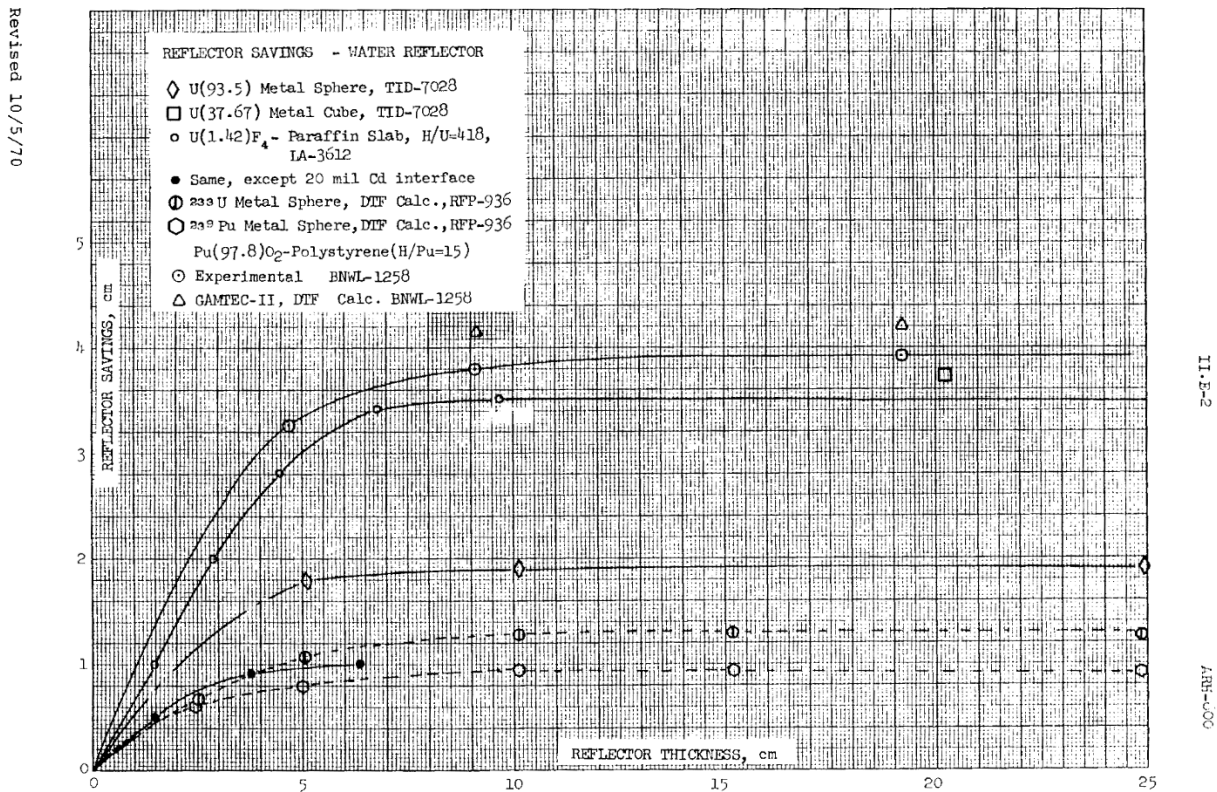
Figure 2-11. Reflector Savings for Various Fissile Materials. (Reference 7, page II.E-2).

Figure 2-12 from reference 12 shows the extrapolation distance for a fully reflected sphere (h/d = 1) to be about 5.9 cm and for a bare sphere to be about 2.1 cm. This gives a reflector savings of 5.9 cm – 2.1 cm = 3.8 cm. Both values compare quite favorably with those from the computer calculations. In most cases, it is easier to use the reflector savings for water-reflected systems than to calculate the reflected critical

radius from an equation like Eq. (56). We will revisit the reflector savings and extrapolation distances in Section 3, on the buckling conversion method.

Fig. 3 – *Effective extrapolation distances for cylinders of U(93.2)O₂F₂ solutions. Cylinder height and diameter are h and d, respectively.*

Figure 2-12. Effective Extrapolation Distances for Cylinders of U(93.2)O₂F₂ Solutions. (Reference 12, page 6, Figure 3).

3. BUCKLING CONVERSION METHOD

3.1 WHAT YOU WILL BE ABLE TO DO

- Use critical data for a fissile system with simple geometries to determine the critical dimensions for other simple geometries.

- Use this method to analyze an upset scenario in which the fissile material changes shape or geometry.

- Use this method to perform comprehensive parametric studies on criticality safety parameters for simple fissile systems.

- Use geometric and material bucklings to determine approximate k_{eff} of a system.

3.2 OVERVIEW OF BUCKLING CONVERSION

This technique is very useful for using critical data for a fissile system with simple geometries to determine the critical dimensions for other geometries. The discussions in Section 2 demonstrate that the geometric buckling is a solution to the neutron diffusion equation and that the material buckling, which is dependent upon the materials in the system, is equal to the geometric buckling for a critical system. The relationship between the geometric and material bucklings can be derived from the critical equation

$$-(-D\nabla^2\phi) - \Sigma_a\phi + \upsilon\Sigma_f\phi = 0, \tag{60}$$

or, after some rearranging,

$$\nabla^2\phi + \frac{\Sigma_a}{D}(k_\infty - 1)\phi = 0. \tag{61}$$

For neutrons with the same energy, the one-group diffusion area, L^2, can be written as:

$$L^2 = \frac{D}{\Sigma_a} \tag{62}$$

After substituting for the diffusion area, the critical one-group diffusion equation becomes

$$\nabla^2\phi + \left[\frac{(k_\infty - 1)}{L^2}\right]\phi = 0, \tag{63}$$

where the term in brackets is the material buckling defined as

$$B_m^2 = \left[\frac{(k_\infty - 1)}{L^2}\right], \tag{64}$$

for simple one-group diffusion theory. For modified one-group diffusion theory, the thermal diffusion area, L^2, is replaced by the migration area, M^2, as given in Eq. (65):

$$B_m^2 = \left[\frac{(k_\infty - 1)}{M^2}\right], \tag{65}$$

Now, for a critical system, the geometric buckling equals the material buckling. In Eq. (63), when the geometric buckling is substituted for the material buckling:

$$\nabla^2 \phi + B_g^2 \phi = 0 \; or \; B_g^2 = -\nabla^2 \tag{66}$$

Notice that the geometric buckling, $B_g{}^2$, is related directly to the neutrons leaking out of a system. Thus, fissile systems that have the **same** geometric buckling have **similar** leakage characteristics—independent of the geometry or the shape of the system. The buckling conversion technique is based on the concept that for critical systems, $B_g^2 = B_m^2$, and uses this to determine the dimensions of different geometric configurations with equivalent leakage.

The neutron balance used to derive the diffusion approximation is as follows:

$$\text{Absorption} \; + \; \text{Leakage} \; = \; \text{Production.} \tag{67}$$

Absorption and production depend on the properties of the materials in the system and not on the geometry of the system. Therefore, for a given critical system, the neutron leakage out of a system must not be changing with time and does not depend on the shape of the system.

According to Lutz (reference 13), "*Geometric buckling refers to the curvature of the neutron flux distribution in a critical unit. In a small body, the neutron flux distribution goes from zero to some maximum in a short distance and, hence, has a large value for its geometric buckling. As the size of any body increases, its geometric buckling decreases. When a system is critical, the geometric buckling, which depends on shape and size, equals the material buckling, which depends only on the nuclear properties of the unit. Buckling calculations allow us to calculate the critical size of different shapes of the same material and to ascertain whether a body is safely subcritical. If we know the material buckling of a fissile material as a function of, say, moderation, we can perform survey calculations in a fast, economical manner. Buckling calculations also help us to understand the relationship between a critically safe infinite slab or cylinder and the corresponding finite critical body.*"

The geometric buckling is the lowest eigenvalue of the Helmholtz equation (equation 66) and as such is only geometry dependent. Equation (66) is the same differential equation that describes wave propagation or molecular diffusion, and it has been solved for many different shapes. In the equations for buckling, each dimension has a physical component and an extrapolation distance.

When calculating the geometric buckling in diffusion theory, the extrapolation distance, *d*, is important, because diffusion theory assumes that the flux is zero at some point, *d*, outside the physical dimensions of the system.[8] Thus, the extrapolation distance must be used to reduce the predicted values for critical size to obtain an accurate estimate for the actual, physical critical dimensions. The value for *d* is usually constant for each type of reflector material that is in close contact with the fissile material (Reference 14). Furthermore, values for *d* are determined from experimental data and calculations; relevant data for various fissile systems can be found in the literature (References 7, 11, 12, 14, 15, and 16). Appendix A provides an in-depth discussion of the linear extrapolation distance.
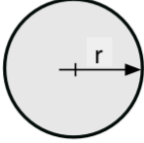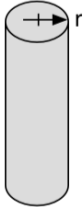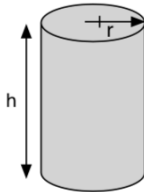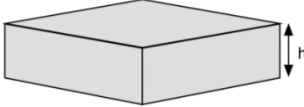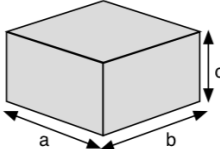
Table 3-1 provides the geometric buckling expressions for five simple geometries: sphere, infinite cylinder, finite cylinder, infinite slab, and rectangular parallelepiped (box). Other references (13, 17, 18, and 19) provide equations for more complex geometries, such as hemispheres, hemicylinders, and cylinders whose cross section is an n-sided polygon. Table 3-2 provides the geometric buckling expressions for hemispheres, infinite hemicylinders, and hemicylinders (Reference 13).

As spherical containers are seldom found in process facilities, one may wonder as to the inclusion of spheres in Table 3-1. Paxton (reference 14) discusses this as follows: "*Of course, the value of the ability*

---

[8] The extrapolation distance is represented by d in this document. Other documents use δ for extrapolation distance.
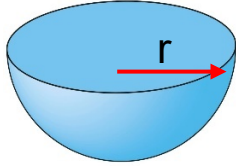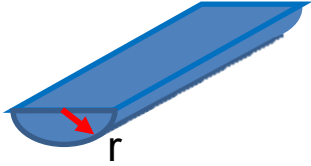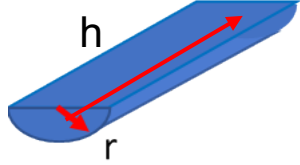
to convert from one critical shape to another is that critical data for a single, simple shape such as a sphere can be applied generally. Thus, the sphere, which appears so seldom in process equipment, represents other more practical shapes. (As an alternative to actual shape conversion, critical masses and volumes of sphere, which are minimum values, may be applied conservatively to other shapes.)"

Table 3-1. Geometric Buckling Expressions for Simple Geometries. (Reference 15 – one of the earliest documents with these relationships and use of the term buckling in the context of nuclear systems.)

Configuration	Geometry Illustration	Geometric Buckling $B_g{}^2$ Relationship
Sphere of Radius, *r*		$\left(\dfrac{\pi}{r+d}\right)^2$
Infinite Cylinder of Radius, *r*		$\left(\dfrac{2.405}{r+d}\right)^2$
Cylinder of Radius, *r*, and Height, *h*		$\left(\dfrac{2.405}{r+d}\right)^2 + \left(\dfrac{\pi}{h+2d}\right)^2$
Infinite Slab of Thickness, *h*		$\left(\dfrac{\pi}{h+2d}\right)^2$
Parallelepiped of Dimensions *a, b,* and *c*		$\left(\dfrac{\pi}{a+2d}\right)^2 + \left(\dfrac{\pi}{b+2d}\right)^2 + \left(\dfrac{\pi}{c+2d}\right)^2$

Note: The variable *d* in each of the expressions for geometric buckling is the extrapolation distance, which is a function of the fissile material present in the system, the shape or geometry, and the materials surrounding the fissile material.

Table 3-2. Bucklings for Other Shapes. (Reference 13)

Configuration	Geometry Illustration	Geometric Buckling B_g^2 Relationship
Hemisphere of Radius, r		$\left(\dfrac{4.49}{r+d}\right)^2$
Infinite Hemicylinder of Radius, r		$\left(\dfrac{3.832}{r+d}\right)^2$
Hemicylinder of Radius, r, and Height, h		$\left(\dfrac{3.832}{r+d}\right)^2 + \left(\dfrac{\pi}{h+2d}\right)^2$

3.3   APPLICABILITY OF THE BUCKLING CONVERSION METHOD

It is important to note that labeling a system as *critical* provides no information about the geometry or the shape of the system. Thus, the buckling conversion method can be applied to a myriad of systems, but there are limitations inherent in the method. The buckling conversion method is applicable for fissile material systems with the following characteristics and assumptions.

- This method allows the conversion among the various geometries mentioned in Table 3-1 if the relevant critical data are available.

- This method can be used for a wide variety of bare and reflected systems including both metal and solution systems.

- Conversion between shapes that are extremely different, such as a sphere and an infinite slab example, does not always give results that are within 5% of actual values due to the difference in leakage from a curved surface versus a flat surface.

- The technique does not guarantee that mass or volume is conserved for critical systems that have different geometries.

- A system can be critical in simple shapes (e.g., a sphere, cylinder, or slab) that have specific expressions for the geometric buckling.

- Bucklings are also available for shapes such as hemicylinder, hemisphere, equilateral triangular cylinder, 45-45-90 triangular cylinder, and 30-60-90 triangular cylinder. (see Reactor Handbook Vol. 1, Physics, 1955, page 614, Table 1.6.8).

- Because the leakage must remain constant and is related to the buckling of a given geometry, the requirements for a critical system can be calculated if the expressions for the geometric bucklings are available.

3.4   BARE VERSUS REFLECTED SYSTEMS

The buckling conversion method when applied to bare systems uses boundaries representing the limits of the fissile material. Table 3-1 provides the geometric buckling for many shapes of bare systems, but to use these equations, accurate values of extrapolation distance are required. It has been assumed that the extrapolation distance is a constant regardless of shape. Experiments have shown that extrapolation distance varies somewhat with shape. The way in which d (also indicated by δ_C in the figures that follow) varies with the elongation of a cylinder (from a very short cylinder that behaves like an infinite slab to a very tall cylinder that is effectively an infinite cylinder) is shown in Figure 3-1 and Figure 3-2. The figures are taken from Figures 3 and 4 in TID-7028, reference 12. In these figures, the shape of each cylinder is characterized by the ratio of its height to its diameter (h/d). From reference 14, "*To avoid infinitely long curves, δ_C appears in the figures as a function of (h/d) / (1+(h/d))*." A value of 0 corresponds to an infinite slab and a value of 1 represents an infinite cylinder.[9]

Notice that the extrapolation distances for the bare (unreflected) systems range from about 2.0 cm to about 2.2 cm. This indicates that a "good" value for extrapolation distance would be about 2.0 cm if no other information is available. According to LA-10860, pg. 16 (Reference 11), "*with 0.13 cm stainless steel reflection, d = 2.2 cm from Stratton's spheres applies universally to the transformation of solution cylinders.*"

---

[9] An infinite cylinder is one that has effectively zero leakage from the top and bottom of the cylinder. Similarly, an infinite slab is one with effectively zero leakage from the ends of the slab.
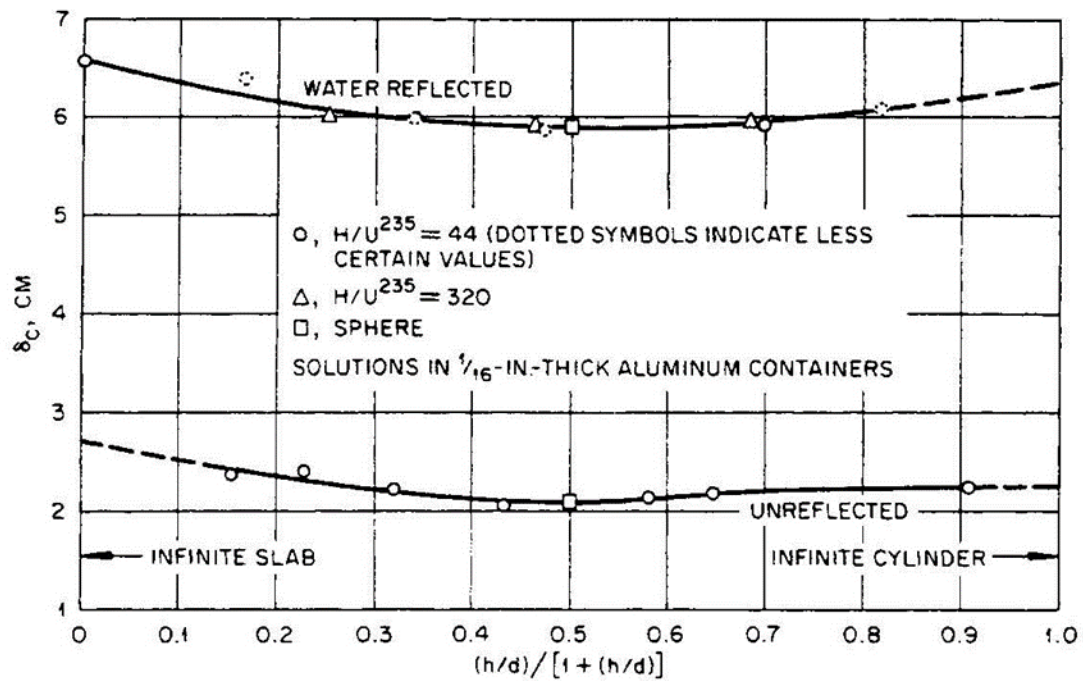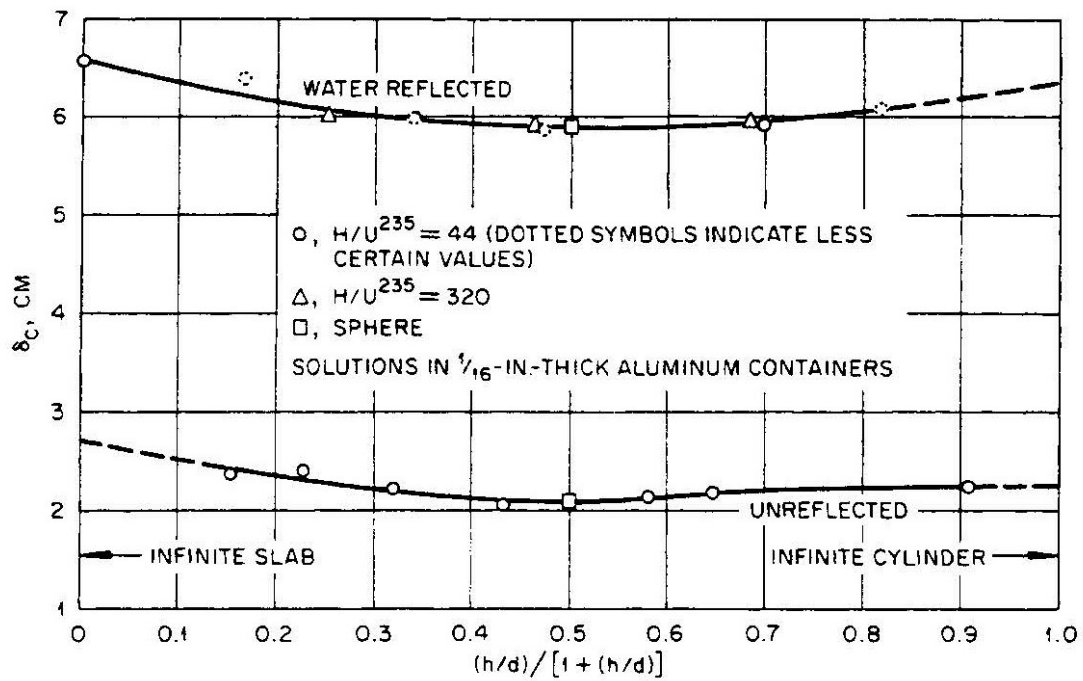
Fig. 3 — Effective extrapolation distances for cylinders of U(93.2)O$_2$F$_2$ solutions. Cylinder height and diameter are h and d, respectively.

Figure 3-1. Extrapolation Distances for High-Enriched Uranium Solution Systems. (Reference 12.)
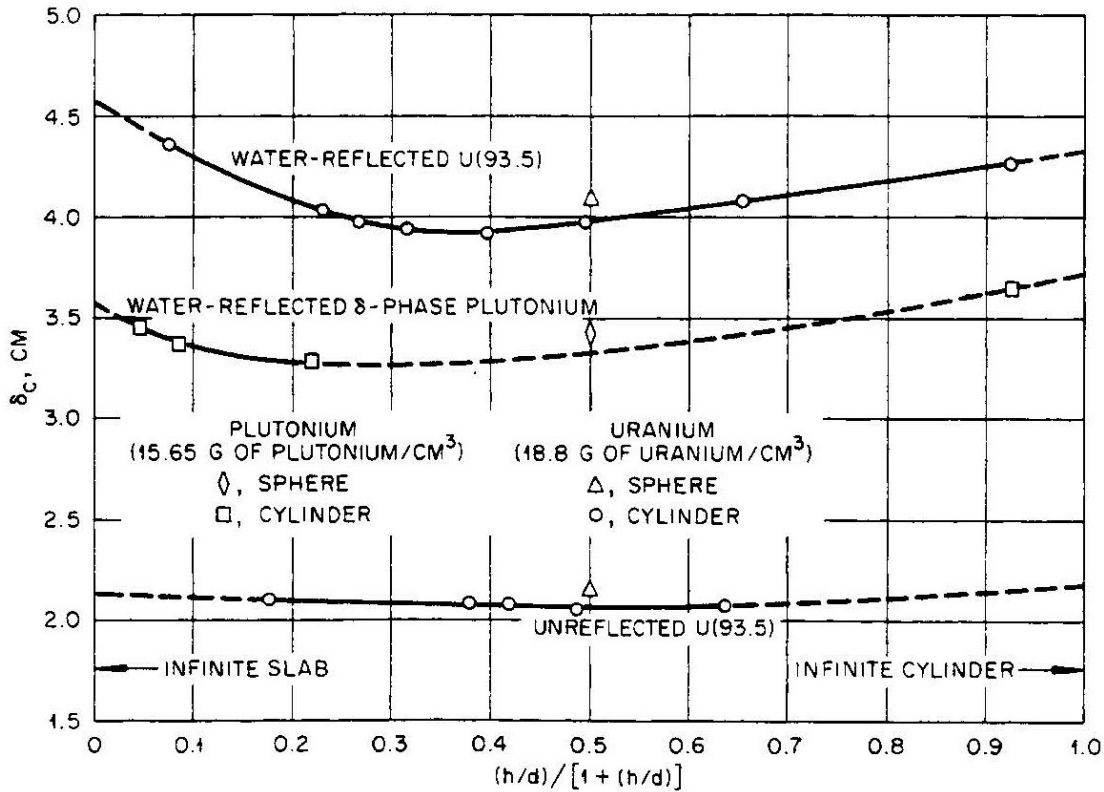
Fig. 4 — Effective extrapolation distances for cylinders of U(93.5) and δ-phase plutonium metal. Cylinder height and diameter are h and d, respectively.

Figure 3-2. Extrapolation Distances for High-Enriched Uranium Metal and delta-phase Plutonium Metal Systems. (Reference 12.)

So now we know how to handle the variation of extrapolation distance with shape, but what about reflected systems? Mathematically, the diffusion equations become more complex with the addition of a reflected zone, so there is not a straightforward derivation of geometric buckling for a reflected system. To evaluate reflected systems, a reflector savings is used based on the given reflector material. The reflector savings is essentially the reduction in critical size between the bare system and the critical size for the system with the reflector added. For a slab and a sphere reactor, the reflector savings, δ_R, is given by:

$$\delta_R = \frac{1}{2}H_0 - \frac{1}{2}H \quad \text{Slab with critical thickness } H_0$$

$$\delta_R = R_0 - R \quad \text{Sphere with critical radius } R_0 \tag{68}$$

Evaluation of the diffusion equations provides the following limiting cases for reflector savings. If the thickness, T, of the reflector is relatively small or the core is relatively large (i.e., δ is very small), then reflector savings can be estimated as follows:

$$\delta_R \approx \frac{D_c}{D_r} \times L_r \times \tanh\frac{T}{L_r} \quad \text{for both a slab and a sphere} \tag{69}$$

78

In Eq. (69), D_c is the diffusion coefficient for the core and D_r is the diffusion coefficient for the reflector. L_r is the thermal diffusion length in the reflector. As noted above, T, is the thickness of the reflector (typically in cm to match units with other parameters).

If the diffusion length, L_r, is appreciably larger than the reflector thickness, T, then the reflector savings can be estimated as:

$$\delta_R \approx \frac{D_c}{D_r} \times T \quad \text{for both a slab and a sphere} \tag{70}$$

For a very thick reflector, then the reflector savings can be estimated as:

$$\delta_R \approx \frac{D_c}{D_r} \times L_r \quad \text{for both a slab and a sphere} \tag{71}$$

Figure 3-1 and Figure 3-2 provide estimates for extrapolation distances for water reflected systems as well as bare systems. These distances are calculated from the sum of the extrapolation distance for a bare system and the reflector savings for the reflector material. For full water-reflected systems, the reflector savings is between 3.5 cm and 4.0 cm, so the reflected "extrapolation distance" is between 5.5 cm and 6.0 cm for water-reflected solution systems. A good default number for full water reflector savings is 3.8 cm. With the bare extrapolation distance of 2.2 cm, the default reflected extrapolation distance would be 6.0 cm. However, it should be noted that if specific data are available, it is strongly encouraged to use those values rather than a default.

3.4.1 Partially reflected systems

In many applications, one or more surfaces may be reflected, creating partial reflection of the geometry. For these surfaces, we add the appropriate reflector savings, δ_R, to the extrapolation distance, d. For example, if a cylinder is sitting on a concrete floor, then the radial and top surfaces are bare, whereas the bottom surface is reflected. In this case, the geometric buckling would take the following form:

$$\left(\frac{2.405}{r+d}\right)^2 + \left(\frac{\pi}{H+d+(d+\delta_R)}\right)^2 \tag{72}$$

Usual values of reflector savings are based on water reflector, but these can be used to account for other reflecting materials. For closely fitting concrete 100 mm or less in thickness, the single unit limits specified in Section 2 for thick water reflection may be used.

3.4.2 Determination of effective multiplication factor from geometric buckling

The multiplication constant can now be written in the form

$$k_{eff} = \frac{k_\infty}{1 + B_g^2 M^2} \tag{73}$$

When $k_{\text{eff}} = 1$, the system is critical and $B_g^2 = B_m^2$, the Eq. (73) becomes:

$$1 = \frac{k_\infty}{1 + B_m^2 M^2} \tag{74}$$

By solving both Eq. (73) and (74) for k_∞ and then setting them equal,

$$k_{eff}\left(1 + B_g^2 M^2\right) = 1 \times \left(1 + B_m^2 M^2\right) \quad or \quad k_{eff} = \frac{\left(1 + B_m^2 M^2\right)}{\left(1 + B_g^2 M^2\right)}$$

<div align="right">(75)</div>

Thus, if we know the material buckling for a system, and we have information about the geometry such that we can determine the geometric buckling, we can determine the effective multiplication factor for the specific materials in a given geometry.

Note that this does require calculation of the migration area, but for water moderated systems, it is reasonable to assume that M^2 is about 28.6 cm^2.[10] The error in the k_{eff} predicted by Eq. (75) increases as the actual k_{eff} decreases. For bare systems, the equation is off by about 1% for a system k_{eff} of 0.9, but it is off by around 18% for a system k_{eff} of 0.5. In all cases, the error is in the conservative direction, with Eq. (75) providing a higher k_{eff} than is actually the case.

This equation also works with water reflected systems if the extrapolation distance used for both the material and geometric bucklings includes the appropriate reflector savings.

EXAMPLE PROBLEMS

3.4.3   Buckling Conversion Example Problem 1

A process criticality accident occurred at the Idaho Chemical Processing Plant in a disengaging head of a solvent extraction column. The head had an $h/d = 1.75$ and a volume of 315.5 liters uranyl nitrate solution $\{U(82)O_2(NO_3)_2\}$ with a mass of 6.08 kg U-235 at critical. Use buckling conversion to determine the equivalent spherical mass involved in the accident. (Assume the head is a bare cylinder.)[11]

Process

This should be a straightforward buckling conversion from a cylinder to a sphere. One must determine the extrapolation distance to be used in the buckling conversions. To use Figure 3-1 (applicable for uranium solutions), we need to determine the ratio $\{H/D\} / (1+\{H/D\})$. For an $H/D = 1.75$, this gives a ratio of 0.64. From Figure 3-1, this provides an extrapolation distance of 2.15 cm for the cylinder. For the sphere, the ratio is 0.5, which gives an extrapolation distance of 2.05 cm.

Now we need the dimensions of the cylinder; given the volume and H/D.

---

[10] As $M^2 = \tau + L^2$, for water systems, $\tau = 27$ cm^2 while L^2 is L^2_{mod} (1-f). For water, $L^2_{mod} = (2.85$ cm$)^2 = 8.12$ cm^2. For most water moderated, thermal systems, f ranges from 0.7 to 0.9 (see example problems 4, 5, and 6 in Chapter 2). Taking the middle ground with $f = 0.8$, $L^2 = 0.2 * 8.12 = 1.6$ cm^2 so an average M^2 would be 28.6 cm^2. Analyses with values of M^2 from 27.8 to 29.5 indicate less than a 0.2% change from results calculated using the 28.6 cm^2 average.

[11] As this is an accident, the k_{eff} of the assembly is greater than 1.0. In this case, the k_{eff} is about 1.041. Thus, the buckling conversion is for a cylindrical system with $k_{eff} = 1.041$ to a spherical system with $k_{eff} = 1.041$. Because the k_{eff} remains constant and the material buckling is constant, consideration of the geometrical buckling will give the proper equivalent spherical mass.

$$V_{cyl} = \frac{\pi D^2}{4} H \Rightarrow \frac{H}{D} = 1.75 \text{ so } H = 1.75 \, D. \text{ Then } V_{cyl} = \frac{\pi D^3 1.75}{4}, \text{ Solve for } D:$$

$$D = \left[\frac{4}{1.75 \, \pi} V_{cyl}\right]^{1/3} = \left[\frac{4}{1.75 \, \pi} (315.5 \text{ L})\left(1000 \, \frac{cm^3}{L}\right)\right]^{1/3} = 61.23 \text{ cm.}$$

$$H = 1.75 D = 1.75 \times 61.23 \text{ cm} = 107.15 \text{ cm.}$$

Now using the equation for the buckling of a cylinder, we need the radius = 61.23 / 2 = 30.62 cm and the extrapolation distance of 2.2 cm.

$$\left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2$$

$$= \left[\frac{2.405}{30.62 \text{ cm} + 2.15 \text{ cm}}\right]^2 + \left[\frac{\pi}{107.15 \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2 = 0.006181 \text{ cm}^{-2}$$

Equating the spherical and cylindrical bucklings,

$$\left[\frac{\pi}{R_{sph} + d}\right]^2 = \left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2 = 0.006181 \text{ cm}^{-2}.$$

$$0.006181 \text{ cm}^{-2} = \left[\frac{\pi}{R_{sph} + d}\right]^2 = \left[\frac{\pi}{R_{sph} + 2.05 \text{ cm}}\right]^2$$

$$R_{sph} + 2.05 \text{ cm} = 39.96 \text{ cm} \Rightarrow R_{sph} = 37.91 \text{ cm}$$

Now to determine the equivalent spherical critical mass, calculate the uranium density and the sphere volume.

$$\text{U density} = \frac{6.08 \text{ kg U235}}{315.5 \text{ liters}} = 0.0193 \, \frac{\text{kg U235}}{\text{liter}}$$

$$V_{sph} = \frac{4}{3} \pi R_{sph}^3 = \frac{4}{3} \pi \, (37.91 \text{ cm})^3 = 228.2 \text{ liters}$$

$$\text{Mass} = 228.2 \text{ liters} \times 0.0193 \, \frac{\text{kg}}{\text{liter}} = 4.4 \text{ kg U235}$$

This value, 4.4 kg, compares favorably with the value of 4.34 kg from the LANL accident report (reference 6, Table 9, pg. 58). That value is derived using a shape factor as found in Figure 3-3 (Figure 4, reference 11).

Based on the *H/D* of 1.75 for the engaging head, Figure 3-3 gives a shape factor of 1.38 for an unreflected system. So, the spherical critical mass is calculated by dividing the cylindrical critical mass by the shape factor. For this situation, $M_{c-sph} = \frac{M_{c-cyl}}{\text{shape factor}} = \frac{6.08 \text{ kg}}{1.38} = 4.41$ kg.

In the accident report (reference 6, Table 9, pg. 58), the shape factor is given as 1.4, which provides a value of 4.34 kg for the spherical critical mass. Shape factors provide a quick way to determine spherical

critical mass when given the cylindrical critical mass or vice versa. However, you may find it difficult to read either curve with much accuracy, so a buckling conversion may give more accurate values.
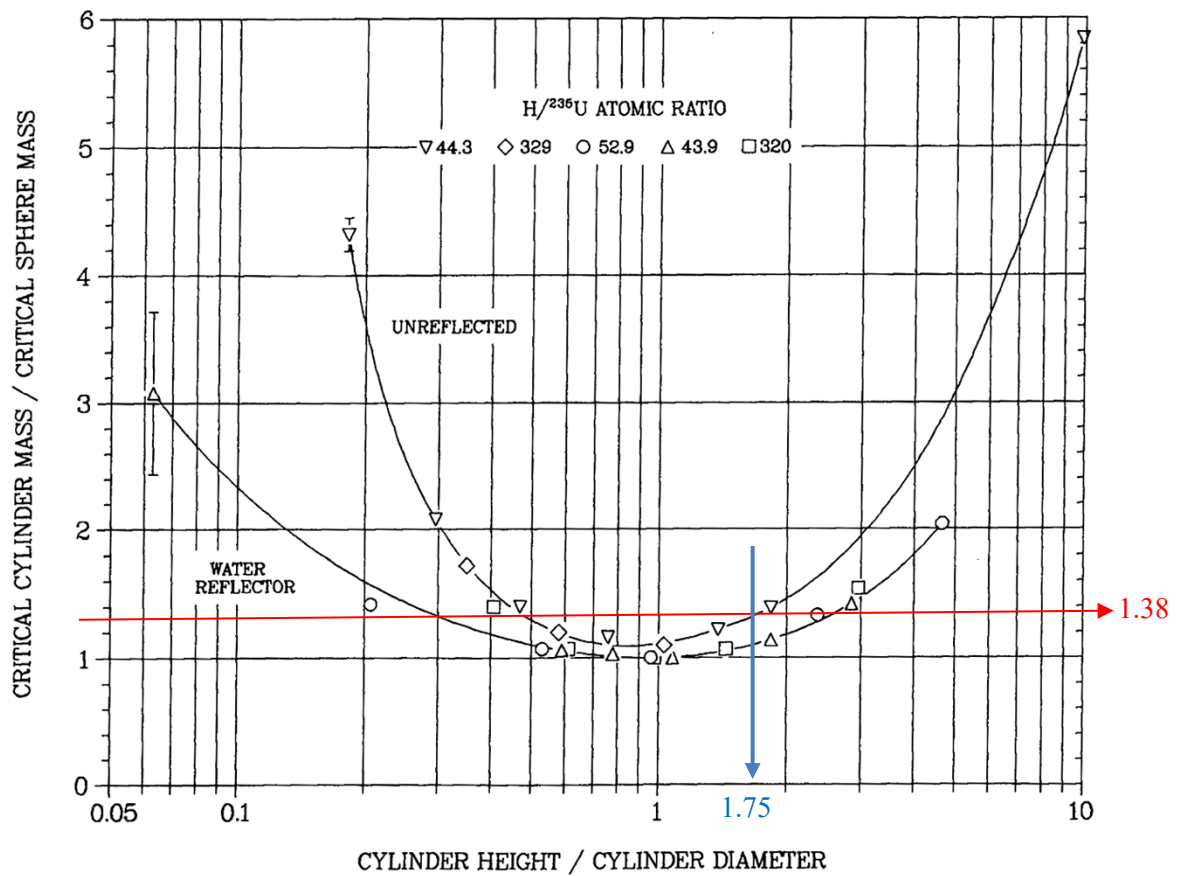
Fig. 4. *The ratio of cylindrical to spherical critical masses of U(93)O$_2$F$_2$ solutions, unreflected and with water reflector, as a function of cylinder height to cylinder diameter ratio.*

Figure 3-3. Shape Factors for Cylinders of Solutions. (Reference 11.)

3.4.4   Buckling Conversion Example Problem 2

1. Calculate the water-reflected, critical radius for a cylindrical tank filled to a height of 20 cm with a 20 gPu/liter Pu(5) metal–water mixture.
2. Compare this resulting critical radius with that of an infinite cylinder.
3. Calculate the relative axial and radial leakage fractions for the cylinder in Part 1 with a height of 20 cm. Do this for both the water-reflected cylinder and for a bare cylinder.
4. Calculate the water-reflected critical height for the cylinder in Part 1 with a radius of 18 cm.
5. Calculate the water-reflected critical height for the cylinder in Part 1 with a diameter of 15 cm.

Part 1.

First, find some data on critical dimensions of a Pu(5) metal-water mixture at 20 gPu/liter. Good starting points include:

- ARH-600, Volume II (has both Pu and ^{235}U data). This is reference 7.

- TID-7028 – Critical Dimensions of Systems Containing ^{235}U, ^{239}Pu, and ^{233}U. This is reference 12.

- LA-10860 - Critical Dimensions of Systems Containing ^{235}U, ^{239}Pu, and ^{233}U, 1986 Revision. This is reference 11.

We will start with ARH-600, and remember that Pu(5) indicates 5 wt % Pu-240. Page III.A-1 provides a table of contents for the Plutonium Systems data along with a description of the numbering system for the figures. The pages that follow provide basic Pu critical parameters and background information on how the data were developed. Figure III.9.95-3 in Volume II shows critical sphere volume for Pu(5)-H$_2$O mixture for a bare (unreflected) system, a system with one-inch (2.54 cm) water reflection, and a system with full water reflection.[12] Looking at 20 g Pu(5)/L on the x-axis intersecting with the full reflection curve gives a critical sphere volume of 36.5 Liters. (see Figure 3-4.)

---

[12] Based on Figures 44 through 47 from TID-7028 (reference 12), full water reflection is anything greater than 3.5 inches (8.9 cm) of water.
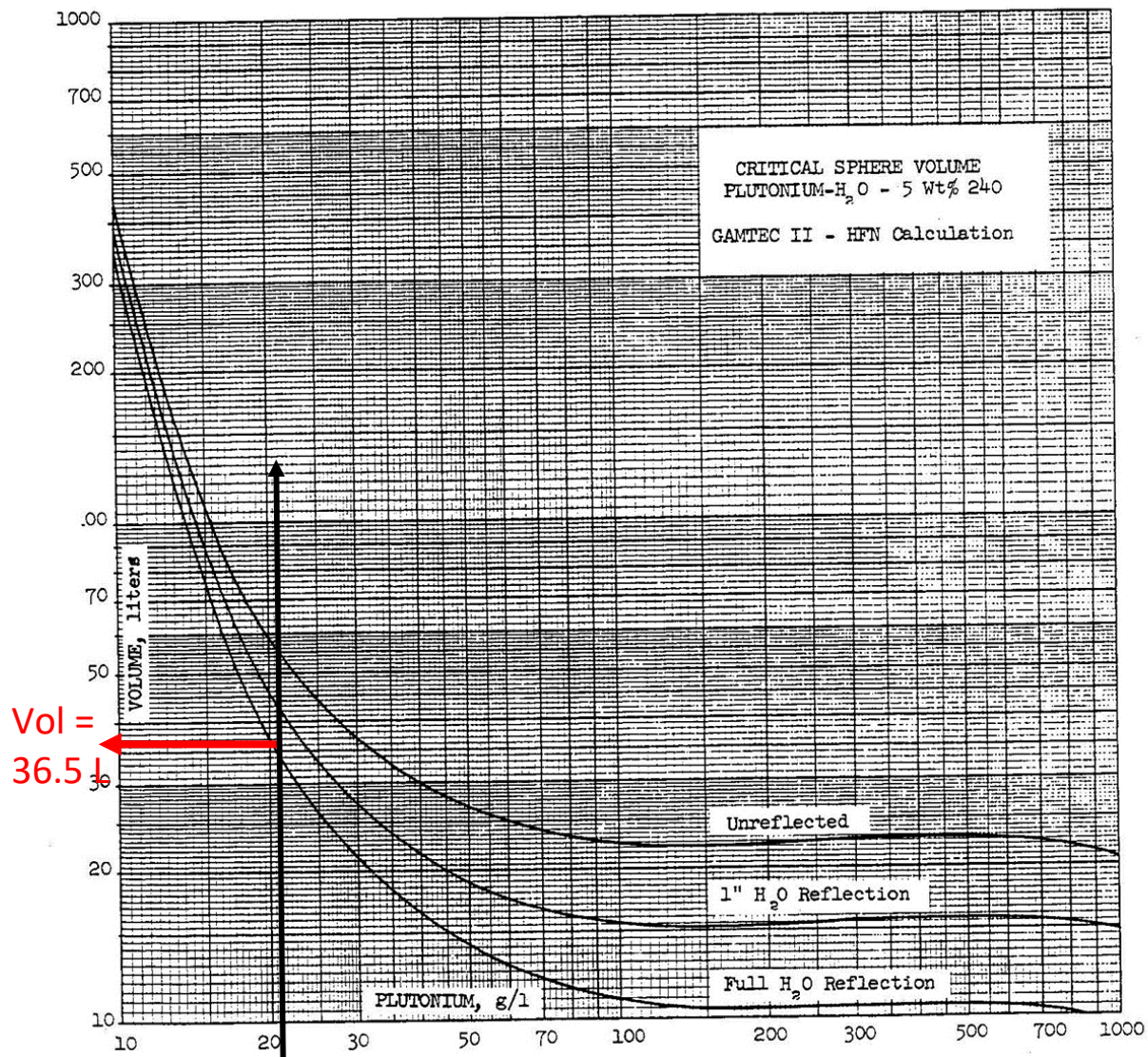
Figure 3-4. Figure III.A.9.95-3 from ARH-600. (Reference 7)

Based on a critical spherical volume of 36.5 liters, we can calculate the critical radius:

$$V_{sph} = \frac{4}{3}\pi R_{sph}^3 \Rightarrow \text{Solve for } R_{sph}: \quad R_{sph} = \left[\frac{3}{4\pi}V_{sph}\right]^{1/3} = \left[\frac{3}{4\pi}(36.5 \text{ L})\left(1000 \frac{cm^3}{L}\right)\right]^{1/3} = 20.58 \text{ cm.}$$

Now that we have the critical radius for the material in a spherical configuration, we can use buckling conversion to determine the critical dimensions for a cylinder.

$$\left[\frac{\pi}{R_{sph} + d}\right]^2 = \left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2.$$

We have R_{sph} = 20.6 cm and H = 20 cm, but we also need the extrapolation distance, d. Using Figure 3-5 (Figure III.A.10.95-3 from ARH-600, Reference 7), we find the full water reflection extrapolation

distance is 5.65 cm (remember this includes the bare distance of 2.15 cm plus the reflector savings of 3.5 cm).
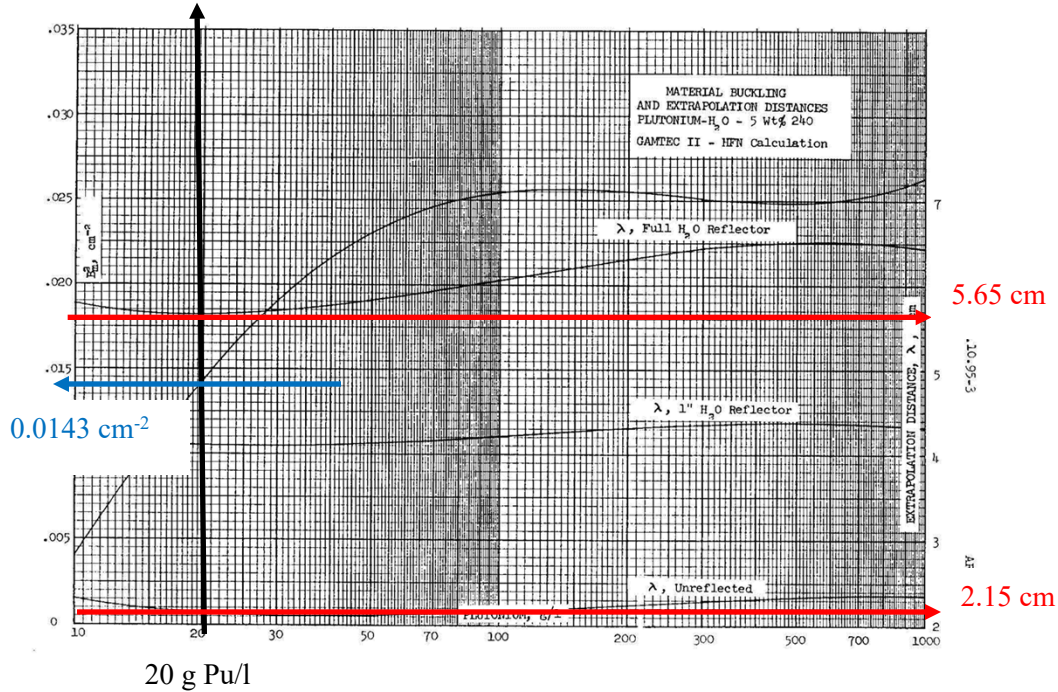
Figure 3-5. Figure III.A.10.95-3 from ARH-600. (Reference 7.)

Notice that Figure 3-5 also provides the material buckling of 0.0143 cm^{-2} for this mixture. We will use this value to check our calculations based on the sphere.

Using the radius of 20.58 cm obtained from the critical volume, calculate the geometric buckling of the sphere.

$$B_g^2 = \left(\frac{\pi}{20.58 + 5.65}\right)^2 = 0.01435 \text{cm}^{-2}$$

This compares favorably with the material buckling of 0.0143 cm^{-2} from Figure 3-5. Now, use buckling conversion to determine the cylindrical radius associated with a mixture height of 20 cm.

$$\left[\frac{\pi}{R_{sph} + d}\right]^2 = \left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2.$$

Inserting known data

$$0.01435 \text{ cm}^{-2} = \left[\frac{2.405}{R_{cyl} + 5.65}\right]^2 + \left[\frac{\pi}{20.0 \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2.$$

85

Solving the equation for R_{cyl} :

$$\left[\frac{2.405}{R_{cyl} + 5.65}\right]^2 = 0.01435 \text{ cm}^{-2} - \left[\frac{\pi}{20.0 \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2$$

$$\left[\frac{2.405}{R_{cyl} + 5.65}\right]^2 = 0.01435 \text{ cm}^{-2} - 0.01007 \text{ cm}^{-2} = 0.00428 \text{ cm}^{-2}$$

$$R_{cyl} = 31.1 \text{ cm.}$$

It should be noted that the same extrapolation distances were used for both the sphere and the cylinder in this calculation. For this cylinder, the height-to-diameter ratio $(H/D) = 20 /(2 \times 31.1) = 0.322$. Figure 3-6 (Figure 6 from LA-10860, reference 11) can be used to determine whether the extrapolation distance used for the cylinder needs to be adjusted. For the cylinder considered in this example, the ratio $(H/D / (1+H/D)) = (0.322 / (1+0.322)) = 0.24$. Figure 3-6 shows the ratio of extrapolation distances for this case is approximately 1, so no adjustment is needed.
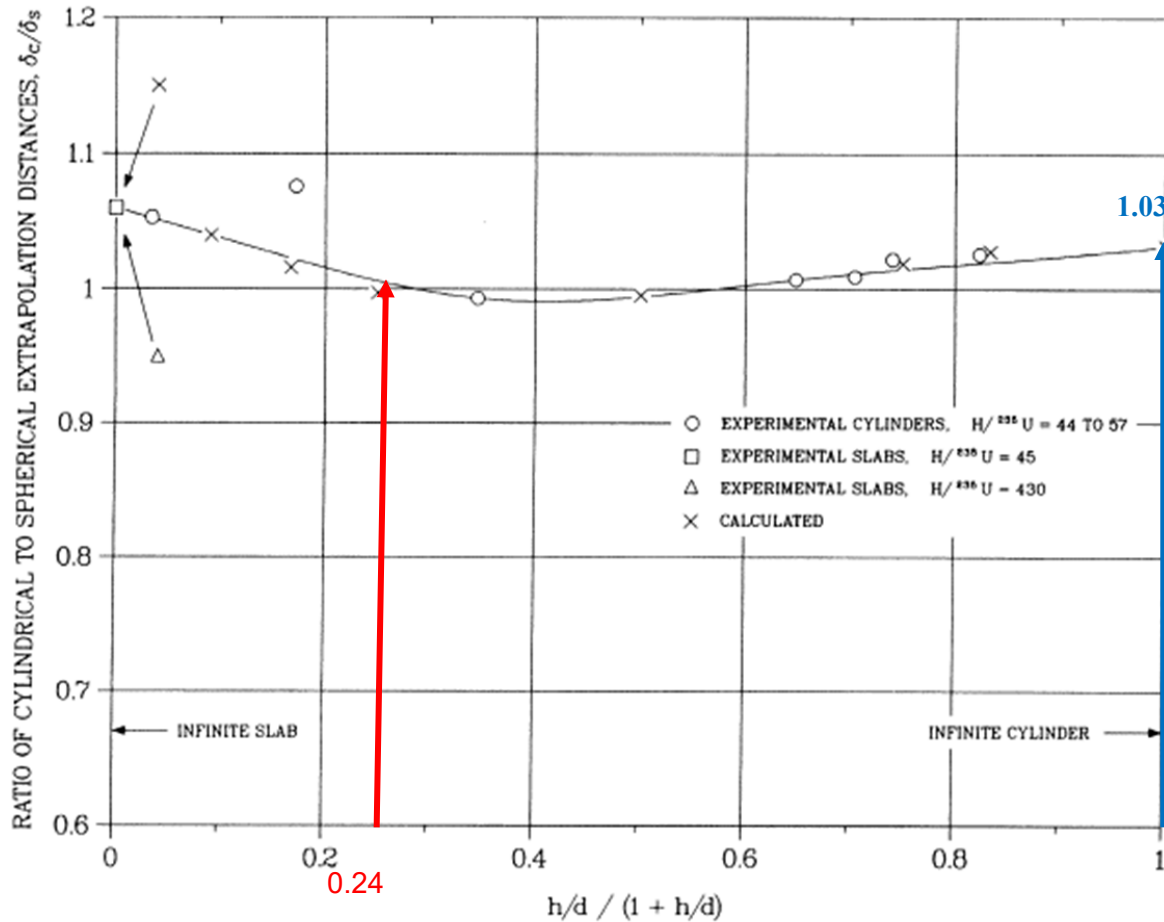
Fig. 6. *Ratio of cylindrical extrapolation distance to that of sphere for water reflected U(93)O$_2$F$_2$ solutions. Cylinder height and diameter are h and d respectively.*

Figure 3-6. Figure 6 from LA-10860. (Reference 11.)

Part 2.

Now the second part of the problem asked how the finite cylinder radius compares with the critical radius of an infinite cylinder. To calculate the infinite cylinder radius, we again use buckling conversion with the calculated material buckling of 0.01435 cm^{-2}. From Figure 3-6, the extrapolation distance for an infinite cylinder is about 1.033 (blue line in Figure 3-6) times that of the sphere, so d = 1.033 * 5.65 cm = 5.84 cm. Putting in the known values and solving for the radius of the fully reflected infinite critical cylinder gives

$$\left[\frac{2.405}{R_{inf\,c\,yl} + 5.84}\right]^2 = 0.01435 \text{ cm}^{-2}$$

$$R_{inf\,c\,yl} = 14.24 \text{ cm.}$$

Notice that the infinite cylinder has a much smaller critical radius (14.24 cm) than a short, finite cylinder (31.1 cm). This result makes sense because a finite cylinder has axial leakage as well as radial leakage, whereas the infinite cylinder only has radial leakage. The critical radius calculation for an infinite cylinder

with Pu(5) solution is comparable to the ANSI/ANS-8.1-2014 subcritical limit of 15.4 cm for a ^{239}Pu(NO$_3$)$_4$ solution at optimum concentration and thick water reflection.

Part 3.

The expression for geometric buckling of a cylinder allows you to calculate the fractional leakage in the axial and in the radial directions. For the water-reflected cylinder, $H = 20$ cm, $R_{cyl} = 31.1$ cm, and $d = 5.65$ cm. Using these values,

$$B_g^2 = \left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2 \quad = \quad \text{radial} + \text{axial}.$$

$$\text{Radial} = \left[\frac{2.405}{R_{cyl} + d}\right]^2 = \left[\frac{2.405}{31.1 + 5.65}\right]^2 = 0.00428 \text{ cm}^{-2}$$

$$\text{Axial} = \left[\frac{\pi}{H + 2d}\right]^2 = \left[\frac{\pi}{20 + 2 \times 5.65}\right]^2 = 0.01007 \text{ cm}^{-2}$$

this indicates that there is 2.35× (= 0.01007 / 0.00428) as much leakage from the ends of the cylinder as from the curved surface. Thus, the radial leakage is 30% (= 0.00428 / 0.01435), whereas the axial leakage is 70% (= 0.01007 / 0.01435). This large axial leakage is why the finite cylinder with a height of 20 cm has a much larger critical radius than that of the infinite cylinder. It is important to note that the leakage fractions are based on the core dimensions and not the system dimensions, which include the reflector. For the reflected system, there is very little leakage either in the radial or the axial directions. What the buckling comparison does provide is a measure of the impact of adding a reflector to a given direction. Because the axial leakage is about 2.33× that of the radial leakage, adding reflection in the vertical direction will have a larger impact on the system k$_{eff}$.

Now repeating the calculation for a bare cylinder, we use buckling conversion to determine the cylindrical radius associated with a mixture height of 20 cm. Remember, the material buckling is independent of reflection conditions. (In this case, the bare critical radius is 24.15 cm with an extrapolation distance of 2.10 cm = 26.25 cm, whereas the reflected critical radius is 20.58 and an extrapolation distance of 5.65 cm = 26.23 cm. Both will give about 0.01434 cm^{-2} when divided into π and then squared.)

Now, determining the bare radius and radial buckling component,

$$0.01435 \text{ cm}^{-2} = \left[\frac{2.405}{R_{cyl} + 2.15}\right]^2 + \left[\frac{\pi}{20.0 \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2.$$

Solving the equation for the radial buckling and R$_{cyl}$:

$$\left[\frac{2.405}{R_{cyl} + 2.15}\right]^2 = 0.01435 \text{ cm}^{-2} - \left[\frac{\pi}{20.0 \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2$$

$$\left[\frac{2.405}{R_{cyl} + 2.15}\right]^2 = 0.01435 \text{ cm}^{-2} - 0.01671 \text{ cm}^{-2} = -0.002364 \text{ cm}^{-2}$$

the radial buckling is negative; what happened? A negative buckling indicates a subcritical situation, so a bare cylinder of Pu(5)-H_2O will not go critical. The issues are basically that when enough material is present to support a chain reaction, there is too much leakage in the axial direction.

Increasing the height to 25 cm, then the radius and associated radial buckling are as follows:

$$0.01435 \text{ cm}^{-2} = \left[\frac{2.405}{R_{cyl} + 2.15}\right]^2 + \left[\frac{\pi}{25.0 \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2.$$

Solving the equation for the radial buckling and R_{cyl} :

$$\left[\frac{2.405}{R_{cyl} + 2.15}\right]^2 = 0.01435 \text{ cm}^{-2} - \left[\frac{\pi}{25.0 \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2$$

$$\left[\frac{2.405}{R_{cyl} + 2.15}\right]^2 = 0.01435 \text{ cm}^{-2} - 0.01150 \text{ cm}^{-2} = -0.002854 \text{ cm}^{-2}$$

$$R_{cyl} = 42.9 \text{ cm}.$$

For the bare cylinder, $H = 25$ cm, $R_{cyl} = 42.9$ cm, the bucklings are as follows:

$$B_g^2 = \left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2 \quad = \quad \text{radial} \ + \ \text{axial}.$$

$$\text{Radial} = \left[\frac{2.405}{R_{cyl} + d}\right]^2 = \left[\frac{2.405}{42.9 + 2.15}\right]^2 = 0.00285 \text{ cm}^{-2}$$

$$\text{Axial} = \left[\frac{\pi}{H + 2d}\right]^2 = \left[\frac{\pi}{25 + 2 \times 2.15}\right]^2 = 0.01150 \text{ cm}^{-2}$$

This indicates that there is 4.04× (= 0.01150 / 0.00285) as much leakage from the ends of the cylinder as from the curved surface. Thus, the radial leakage is 20% (= 0.00285 / 0.01435), whereas the axial leakage is 80% (= 0.01150 / 0.01435). This large axial leakage is why the height had to be increased to attain a critical system. PARTISN calculations give 20.4% radial leakage and 79.6% axial leakage.

Also note that because of the large radius, the geometry of the bare system is close to an infinite slab. Using this, we can determine the thickness of a critical infinite slab of Pu(5)-H_2O at 20 g Pu(5) per liter.

$$0.01435 \text{ cm}^{-2} = \left[\frac{\pi}{x \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2.$$

Solving the equation for the slab thickness:

$$x \text{ cm} + 2 \times 2.15 \text{ cm} = 26.23$$

$$x = 21.9 cm$$

So, as determined above, the slab thickness or height must be greater than 20 cm for a critical system. In this case, where there is no radial leakage (i.e., the radius is greater than 100 cm where $H/D = 20/(2×100) = 0.1$), the height of the solution must be greater than 21.9 cm for a critical system.

Part 4.

To determine the height of a fully reflected critical system with a radius of 18 cm, we again use buckling conversion:

$$0.01435 \text{ cm}^{-2} = \left[\frac{2.405}{18 \text{ cm} + 5.65 \text{ cm}}\right]^2 + \left[\frac{\pi}{H_{cyl} \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2.$$

Solving the equation for H_{cyl}:

$$\left[\frac{\pi}{H_{cyl} \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2 = 0.01435 \text{ cm}^{-2} - \left[\frac{2.405}{18 \text{ cm} + 5.65 \text{ cm}}\right]^2$$

$$\left[\frac{\pi}{H_{cyl} \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2 = 0.01435 \text{ cm}^{-2} - 0.01034 \text{ cm}^{-2} = 0.00401 \text{ cm}^{-2} \text{So, the height is 38.3}$$

$$H_{cyl} = 38.3 \text{ cm}.$$

cm, which makes a cylinder with $H/D = 38.3 / 2 \times 18 = 1.06$. This is just about a right circular cylinder.

Part 5.

To determine the height of a fully reflected critical system with a diameter of 15 cm (about 6 in.), we follow the same process as in Part 4. First, we must convert the 15 cm diameter to a 7.5 cm radius and then use buckling conversion to determine the appropriate height:

$$0.01435 \text{ cm}^{-2} = \left[\frac{2.405}{7.5 \text{ cm} + 5.65 \text{ cm}}\right]^2 + \left[\frac{\pi}{H_{cyl} \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2.$$

Solving the equation for H_{cyl}:

$$\left[\frac{\pi}{H_{cyl} \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2 = 0.01435 \text{ cm}^{-2} - \left[\frac{2.405}{7.5 \text{ cm} + 5.65 \text{ cm}}\right]^2$$

$$\left[\frac{\pi}{H_{cyl} \text{ cm} + 2 \times 5.65 \text{ cm}}\right]^2 = 0.01435 \text{ cm}^{-2} - 0.03345 \text{ cm}^{-2} = -0.01910 \text{ cm}^{-2} \text{ As indicated by the}$$

negative value for buckling, it is not possible for a 15 cm diameter, thick water–reflected cylinder containing a 20 gPu(5)/l solution to attain a critical state. This conclusion could also be reached from the previous analysis in Part 2, where a minimum 28.48 cm (=14.24 cm × 2) diameter is required for a critical infinite cylinder containing the same material. Skinny, long cylinders such as this tend to have more neutron leakage than thick, short cylindrical tanks, which inherently makes them more safe. Figure 3-7 illustrates that, for Pu densities less than about 1 kg/l (the light blue shaded area where plutonium is in solution form), the critical diameter of an infinite cylinder will be greater than 15 cm (about 6 in.) for a water-reflected system. This fact is the main reason that cylindrical Pu solution

storage tanks are designed with this diameter or smaller to ensure, regardless of the Pu concentration or neutron reflectors present, that criticality is not possible.
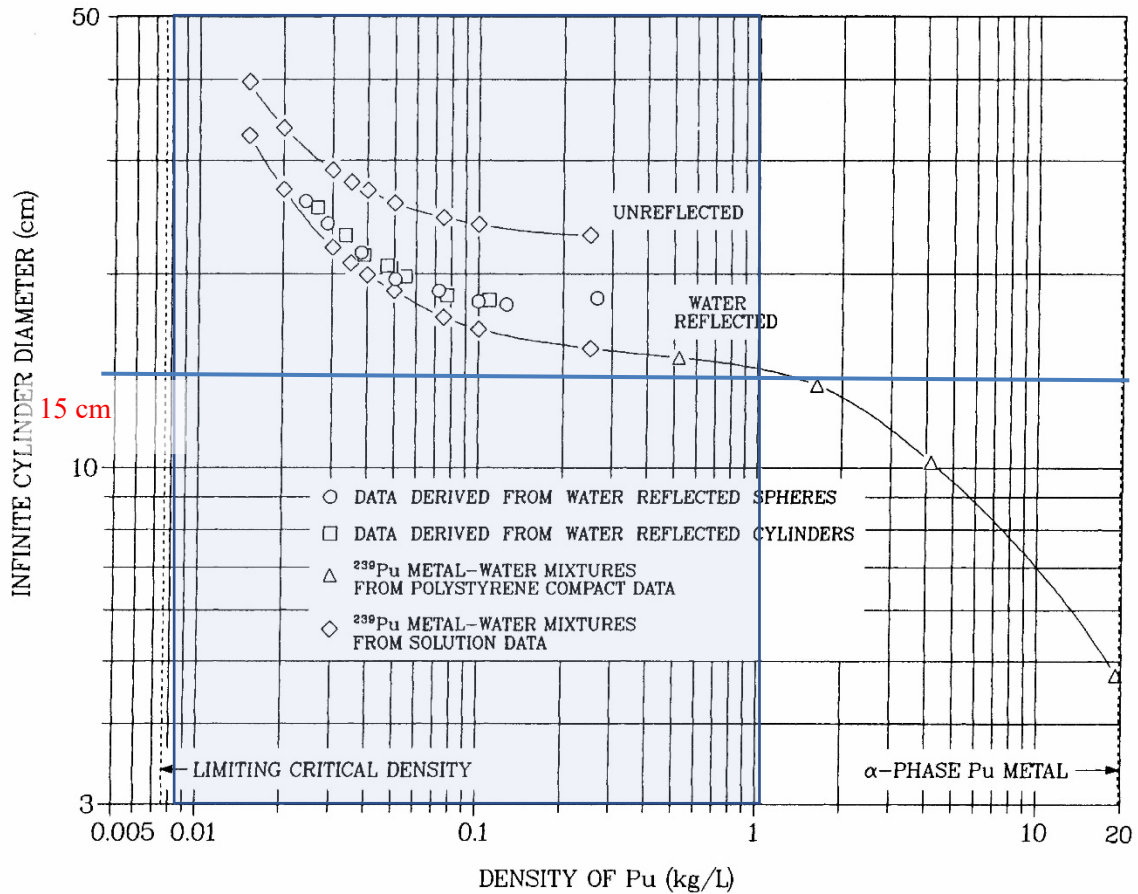
Fig. 33. Estimated critical diameters of infinitely long cylinders of homogeneous water-moderated plutonium. The points suggesting an intermediate curve apply to water-reflected Pu (NO₃)₄ solution with 1 $\underline{N}$ HNO₃ and 3.1% ²⁴⁰Pu content of the plutonium.

Figure 3-7. Estimated Critical Diameters of Infinitely Long Cylinders of Homogeneous Water–moderated Plutonium. (Reference 11, Figure 33.)

NOTE: In Figure 3-7, the units for Pu density (concentration) have changed from grams/liter as used in ARH-600 (Reference 7) to kilograms/liter. Thus, the concentration of 20 g/liter becomes a density of 0.02 kg/liter.

3.4.5   Buckling Conversion Example Problem 3

Deep wells are present in a glovebox (Figure 3-8), where each has a length of 51 in. (129.54 cm), width of 14 in. (35.56 cm), and depth of 6 in. (15.24 cm). Suspended above these wells are 6 in. (15.24 cm) diameter storage tanks, each of which contains 30 liters of Pu solution. (Assume a Pu metal–water mixture with 5 wt % ²⁴⁰Pu.) Assume that a single 30-liter, 6 in. (15.24 cm) diameter storage tank breaks during operations, and its contents are completely drained into a one deep well.

1. Determine the critical solution height in the deep well for a Pu(5) concentration of 200 gPu(5) per liter for an unreflected system. (That is, neglect the effects of neutron reflection from the well steel or other materials in the vicinity of the solution.)
2. Based on the initial volume in the cylindrical storage tank, can a criticality event occur?
3.

Figures are not to scale.

Wells

Deep wells with dimensions 51" L x 14" W x 6" D.
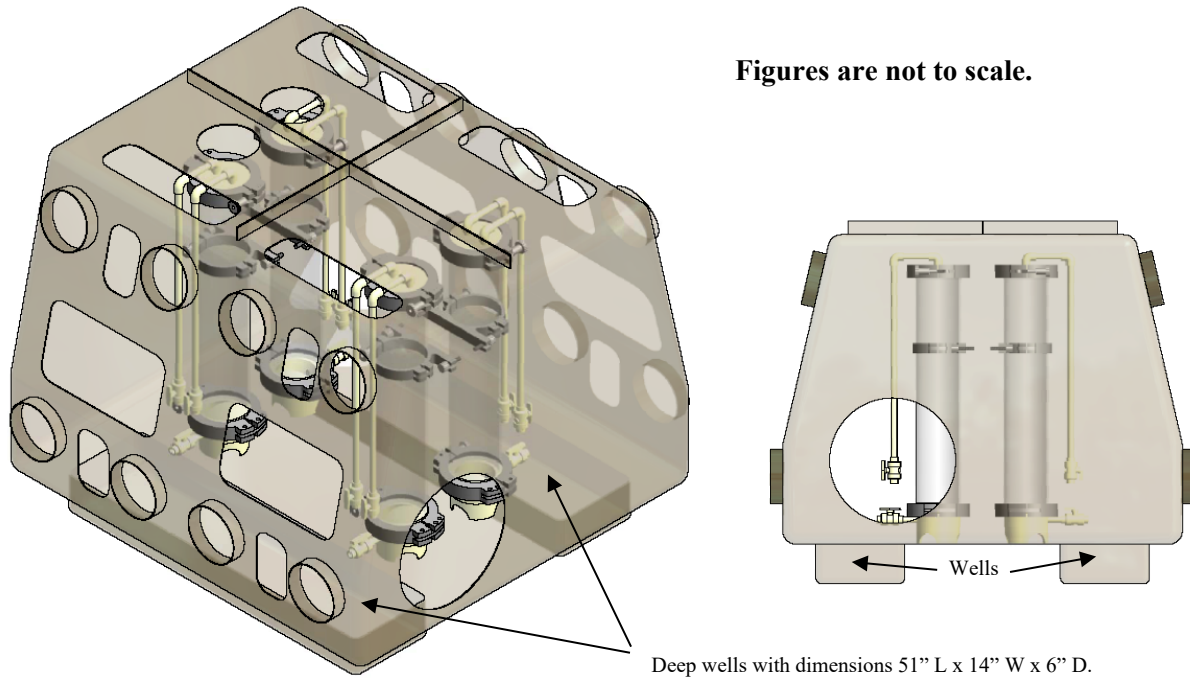
Figure 3-8. Isometric and Elevation Views of Solution Storage Tanks and Glovebox Deep Wells for Buckling Conversion Example Problem 1.

Part 1. The first step in this problem is deciding which of the geometric buckling expressions to use from Table 11. Because the slab is in the shape of a parallelepiped, that expression for buckling would be sufficient for this problem.

The geometric buckling for the parallelepiped that represents the deep well can be equated to that of an unreflected, critical sphere with a known critical radius:

$$\left[\frac{\pi}{R_{sph} + d}\right]^2 = \left[\frac{\pi}{a + 2d}\right]^2 + \left[\frac{\pi}{b + 2d}\right]^2 + \left[\frac{\pi}{c + 2d}\right]^2,$$

Solving this equation for the critical height, c, results in the following expression for the critical solution height in the well.

$$c = \left[\frac{1}{(r_{sph} + d)^2} - \frac{1}{(a + 2d)^2} - \frac{1}{(b + 2d)^2}\right]^{-\frac{1}{2}} - 2d.$$

We know the value for a and b; thus, we need the extrapolation distance, and the critical sphere dimensions for a Pu concentration of 200 gPu/l should be referenced to complete the calculation. Figure 3-9 provides a plot of the extrapolation distances for Pu metal–water mixtures with 5 wt % Pu-240 for various reflection conditions. Figure 3-10 provides volume for a critical sphere for a Pu–metal water mixture for various reflection conditions. These data can be used to determine the spherical dimensions.

The extrapolation distance, d, can be found using Figure 3-9. Notice this graph is specific to Pu-H$_2$O solutions with 5 wt % Pu-240. Selecting 200 g Pu/liter on the x-axis, we find an extrapolation distance of 2.25 cm for an unreflected system. Also, note that the material buckling for the system is found using the top curve and the y-axis values on the left side. For this mixture, the material buckling is 0.026 cm^{-2}.

As we know the material buckling, we can calculate the critical spherical radius from the following:

$$B_m^2 = B_g^2\Big|_{\text{at critical}} = \left(\frac{\pi}{R_{sph} + d}\right)^2 \quad \text{for a sphere}$$

$$0.026 \text{ cm}^{-2} = \left(\frac{\pi}{R_{sph} + 2.25}\right)^2$$

$$19.48 \text{ cm} = R_{sph} + 2.25; R_{sph} = 17.23 \text{cm}$$

We will compare this value with the value we get from the critical spherical volume information in Figure 3-10.
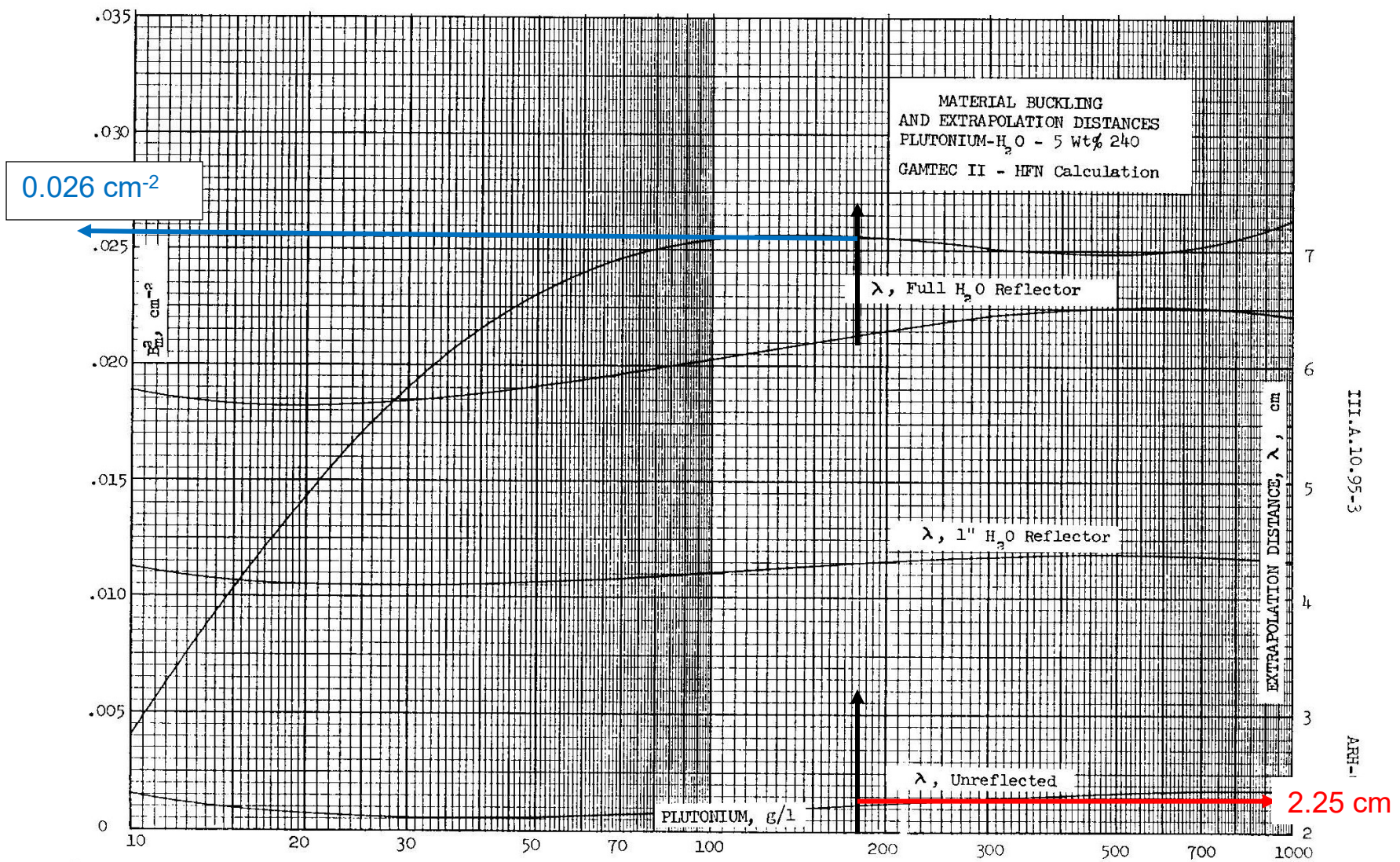
Figure 3-9. Extrapolation Distance Data for Pu Metal–Water Mixtures with 5 Wt % Pu-240. (Reference 7, Figure III.A.10.95-3.)
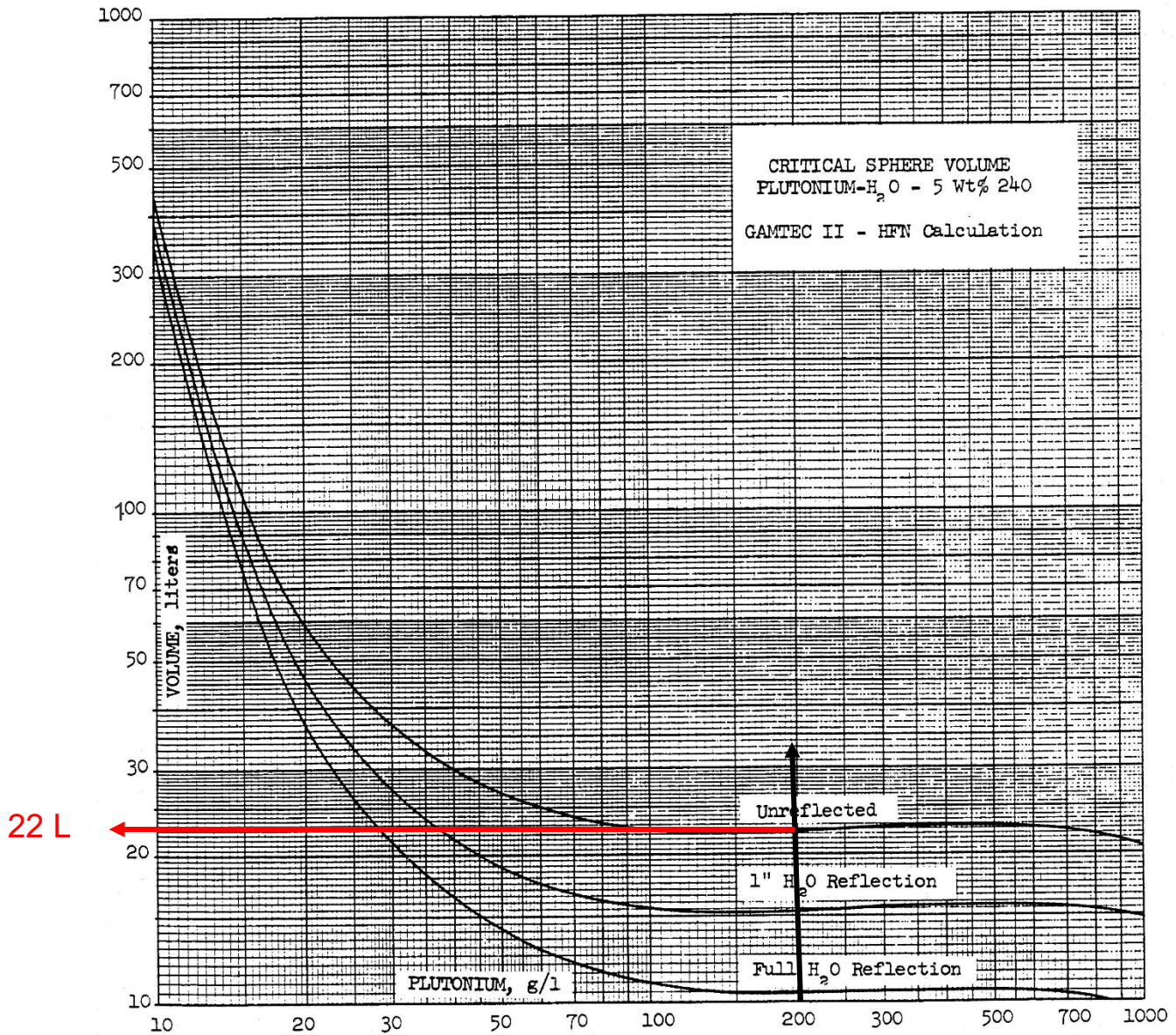
Figure 3-10. Critical Volume for an Unreflected Sphere with a Pu Metal-Water Mixture with 5 Wt. % Pu-240. (Reference 5, Figure III.A.9.95-3.)

From Figure 3-10, the critical unreflected sphere volume for this mixture is 22 liters. Converting to the equivalent spherical radius gives:

$$R_{sph} = \sqrt[3]{\frac{3 \times V}{4 \times \pi}} = \sqrt[3]{\frac{3 \times 22\text{liter} \times 1000\text{cm}^3}{4 \times \pi \times \text{liter}}} = \sqrt[3]{5,252.1\text{cm}^3} = 17.38\text{cm}$$

This compares well with the 17.23 cm calculated from Figure 3-9 and the material buckling.

Now that we have all the values, the critical well height for the Pu metal–water mixture can be determined:

$$c = \left[\frac{1}{(r_{sph} + d)^2} - \frac{1}{(a + 2d)^2} - \frac{1}{(b + 2d)^2} \right]^{-\frac{1}{2}} - 2d.$$

$$c = \left[\frac{1}{(17.38 + 2.25)^2} - \frac{1}{(129.54 + 2 \times 2.25)^2} - \frac{1}{(35.56 + 2 \times 2.25)^2} \right]^{-\frac{1}{2}} - 2 \times 2.25 \text{Note that the depth}$$

$$c = [0.00260 - 0.00006 - 0.00062]^{-\frac{1}{2}} - 4.50$$

$$c = 22.82 - 4.50 = 18.32 \text{ cm}$$

of the well is only 15.24 cm so there is not enough well volume in this configuration to support a critical system.

Part 2. The critical slab height calculated in Part 1 can now be used to calculate the critical solution mass and volume required based on the estimated critical height for the deep well.

Knowing the Pu concentration, ρ, and deep well dimensions a, b, and c, we can calculate the critical volume and mass from the following.

$$V_{\text{crit box}} = a \times b \times c = 129.54 \text{ cm} \times 35.56 \text{ cm} \times 18.51 \text{ cm}$$

$$V_{\text{crit box}} = 85,265 \text{ cm}^3 = 85.3 \text{ liters}$$

The total volume available to the slab tank from a single 6 in. diameter storage tank during an upset of this kind is 30 liters, which is far less than the 85 liters that is needed in the slab tank to result in criticality. If this process upset were to occur, then a criticality event could not occur unless the contents of multiple tanks were to spill into the tank.

3.4.6   Buckling Conversion Example Problem 4

Two isolated cylindrical, non-favorable geometry tanks are being filled with a fissile solution. The first tank is filled with a U(93.5)–water mixture, whereas the second tank is being filled with a Pu metal–water mixture with 5 wt % Pu-240 (Figure 3-11). Both solutions have a fissile concentration of 100 g fissile/L. Assume that the tanks are not externally reflected; the tanks have a 10 in. (25.4 cm) outside radius; the tanks begin filling with solution at the same time; the rate of solution addition to the tank is the same; and no neutron poisons are assumed to be present in the tank.

1. Determine the critical solution height for each tank and compare the results of the two systems.
2. Repeat this calculation with a concentration of 150 g fissile/L.
3. Repeat this calculation with a concentration of 50 g fissile/L.

The first step in the solution to this problem is to compile the data needed for each mixture. Using figures from ARH-600 (reference 7), we can get information about the spherical critical mass (Figure 3-12) = 2 kg, and the spherical critical volume = 20 liters for a bare U(93.5) metal–water mixture.

96

$$R_{U(93.5)} = \left[\frac{3 \times V_{U(93.5)}}{4 \times \pi}\right]^{\frac{1}{3}} = \left[\frac{3 \times 20 \text{ liters} \times 1000 \text{ cm}^3/\text{liter}}{4 \times \pi}\right]^{\frac{1}{3}} = 16.8 \text{ cm}$$

Information for the Pu system is obtained from Figure 3-13 ($m_{crit} = 2.25$ kg) and Figure 3-14 ($V_{crit} = 22.5$ liters).

$$R_{Pu(5)} = \left[\frac{3 \times V_{Pu(5)}}{4 \times \pi}\right]^{\frac{1}{3}} = \left[\frac{3 \times 22.5 \text{ liters} \times 1000 \text{ cm}^3/\text{liter}}{4 \times \pi}\right]^{\frac{1}{3}} = 17.5 \text{ cm}$$

The extrapolation distances for these systems can be found from Figure 3-15 and Figure 3-16 (try to use information from the same dataset for consistency). Figure 3-15 gives the extrapolation distance of 2.05 cm for an unreflected U(93.5)-H_2O system. The material buckling is also found from the chart as 0.028 cm^{-2}. Figure 3-16 gives the extrapolation distance of 2.15 cm for an unreflected Pu(5)-H_2O system. Figure 3-16 also show the material buckling for an unreflected Pu(5)-H_2O system to be 0.0255 cm^{-2}.

The radius of each tank is 25.4 cm

δh

Height U(93.5) & Water

Height Pu Metal & Water
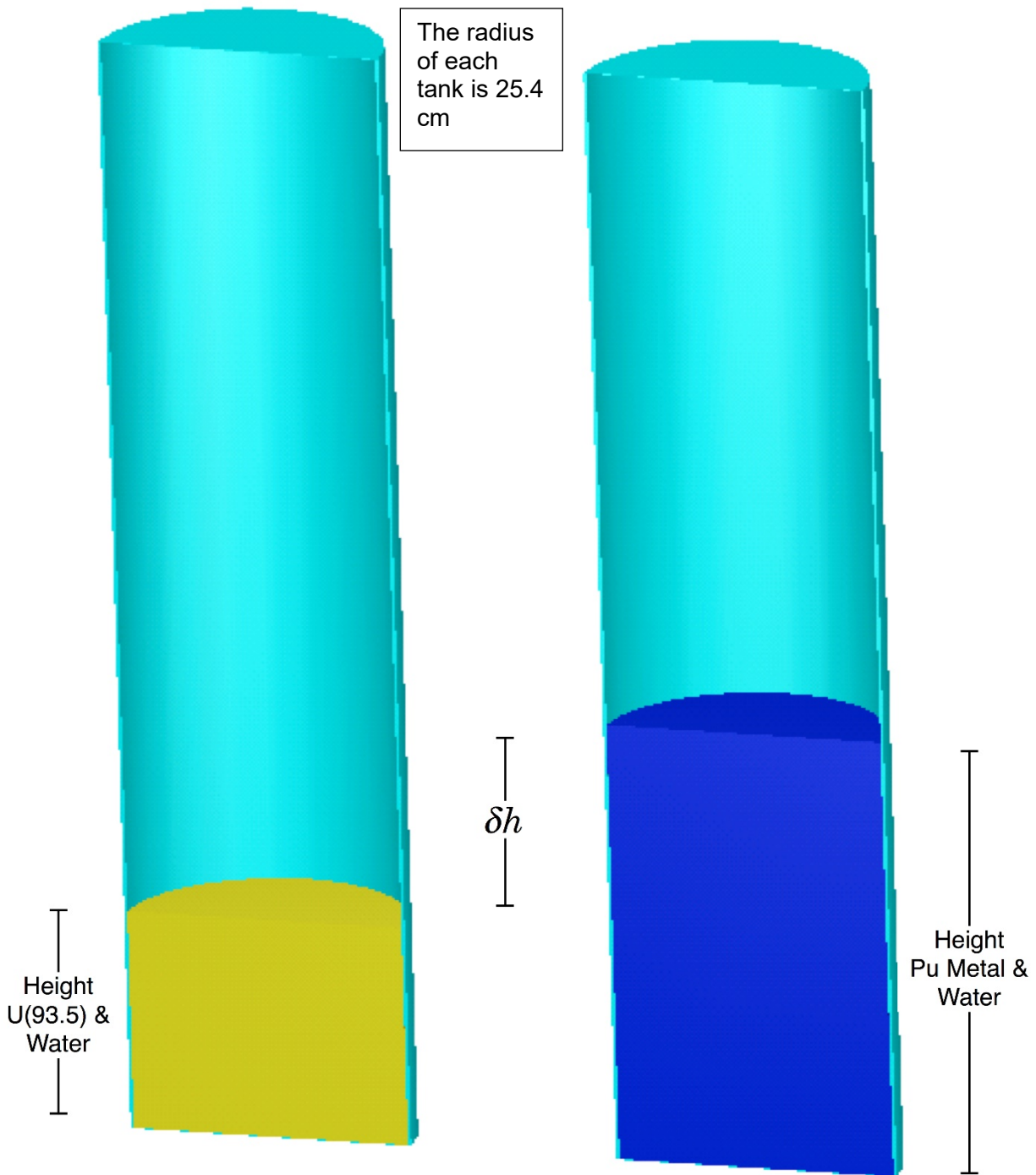
Figure 3-11. KENO 3D Illustration of Tanks for Buckling Conversion Problem 3. (Not to scale.)
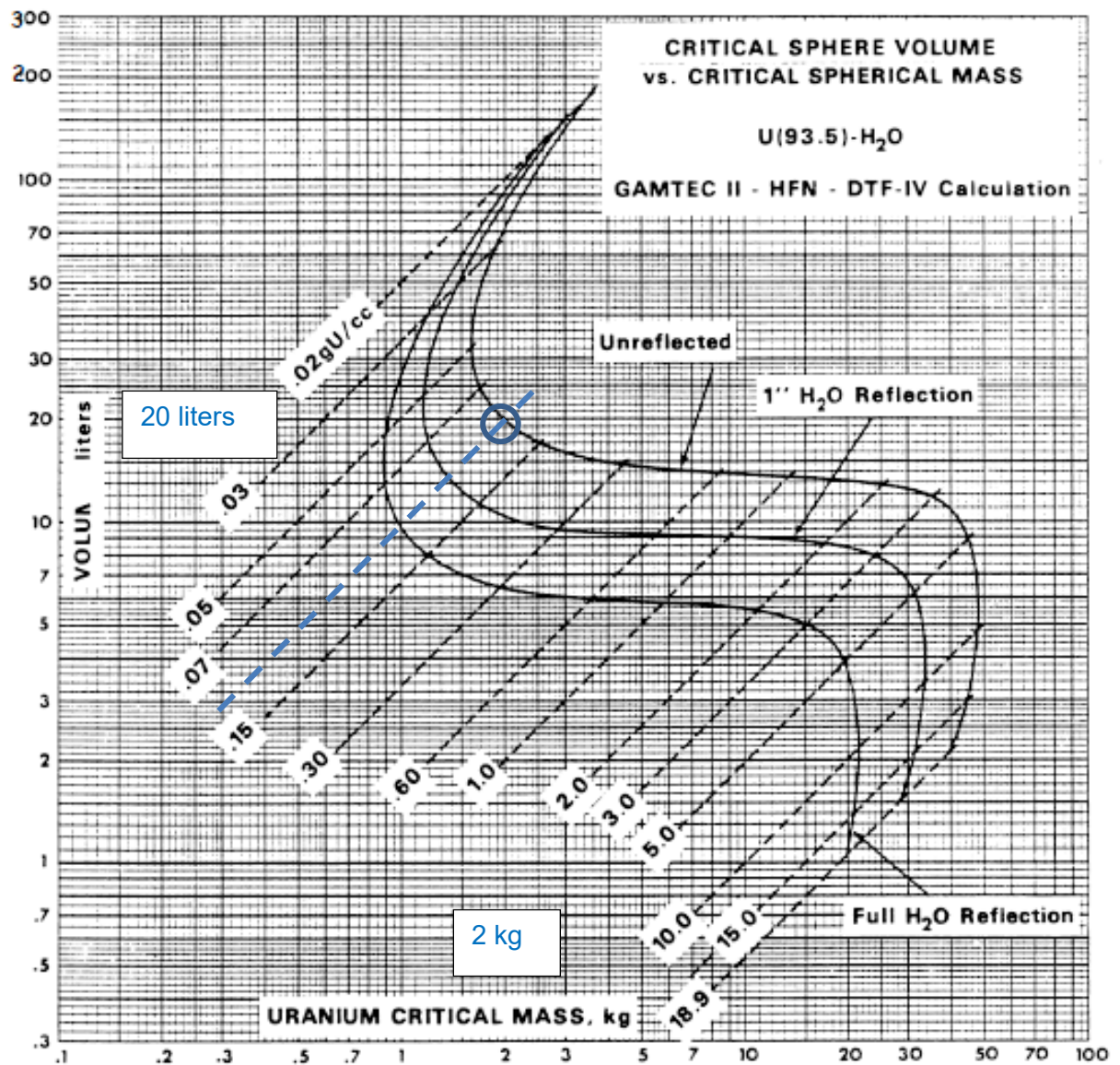
Figure 3-12. Spherical Critical Mass and Volume for a Mixture of U(93.5) and Water. (Reference 7, Figure III.B.9(93.5)-2.)
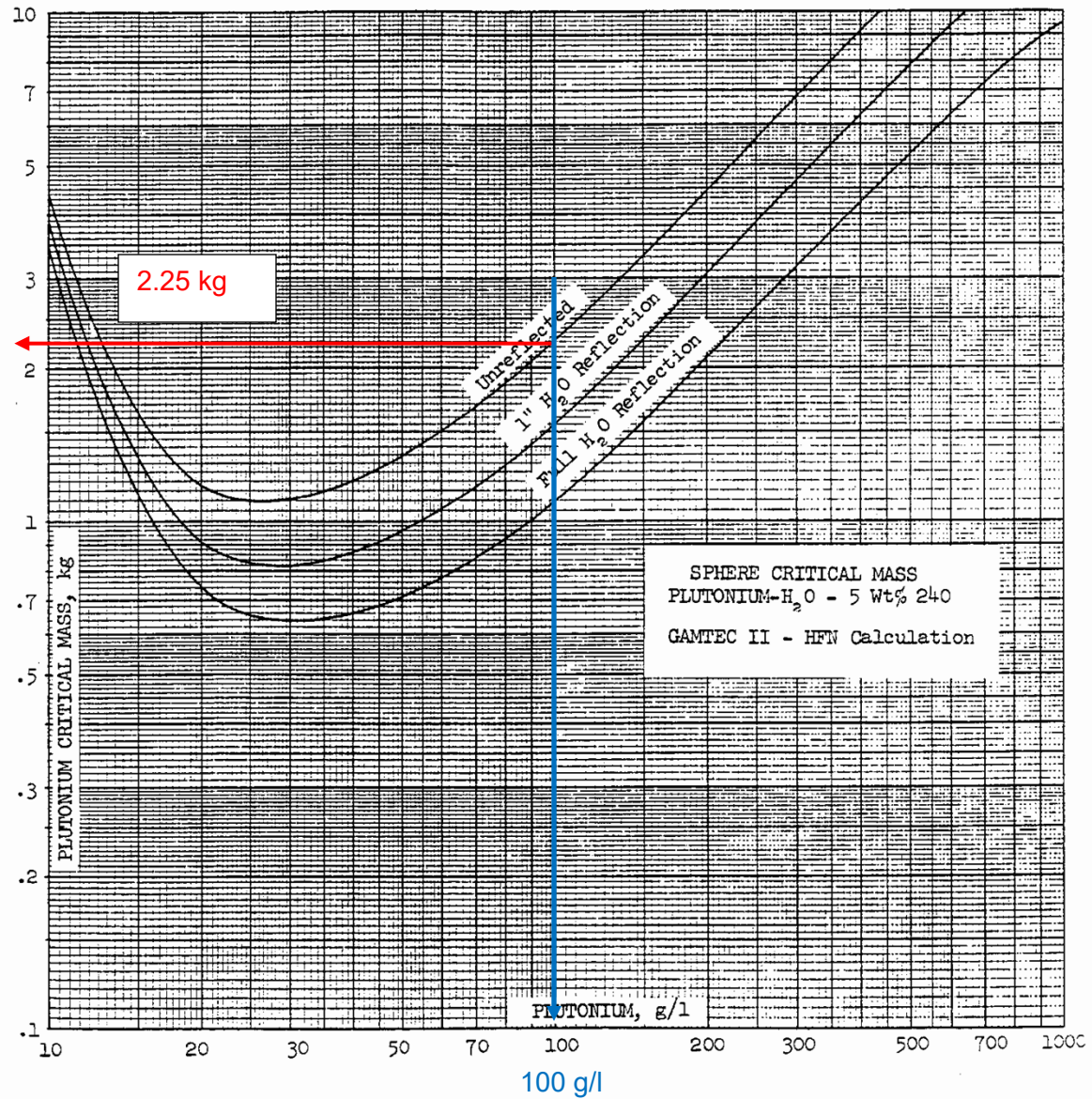
Figure 3-13. Spherical Critical Mass for a Mixture of Pu(5) and Water. (Reference 7, Figure III.A.6.95-3.)
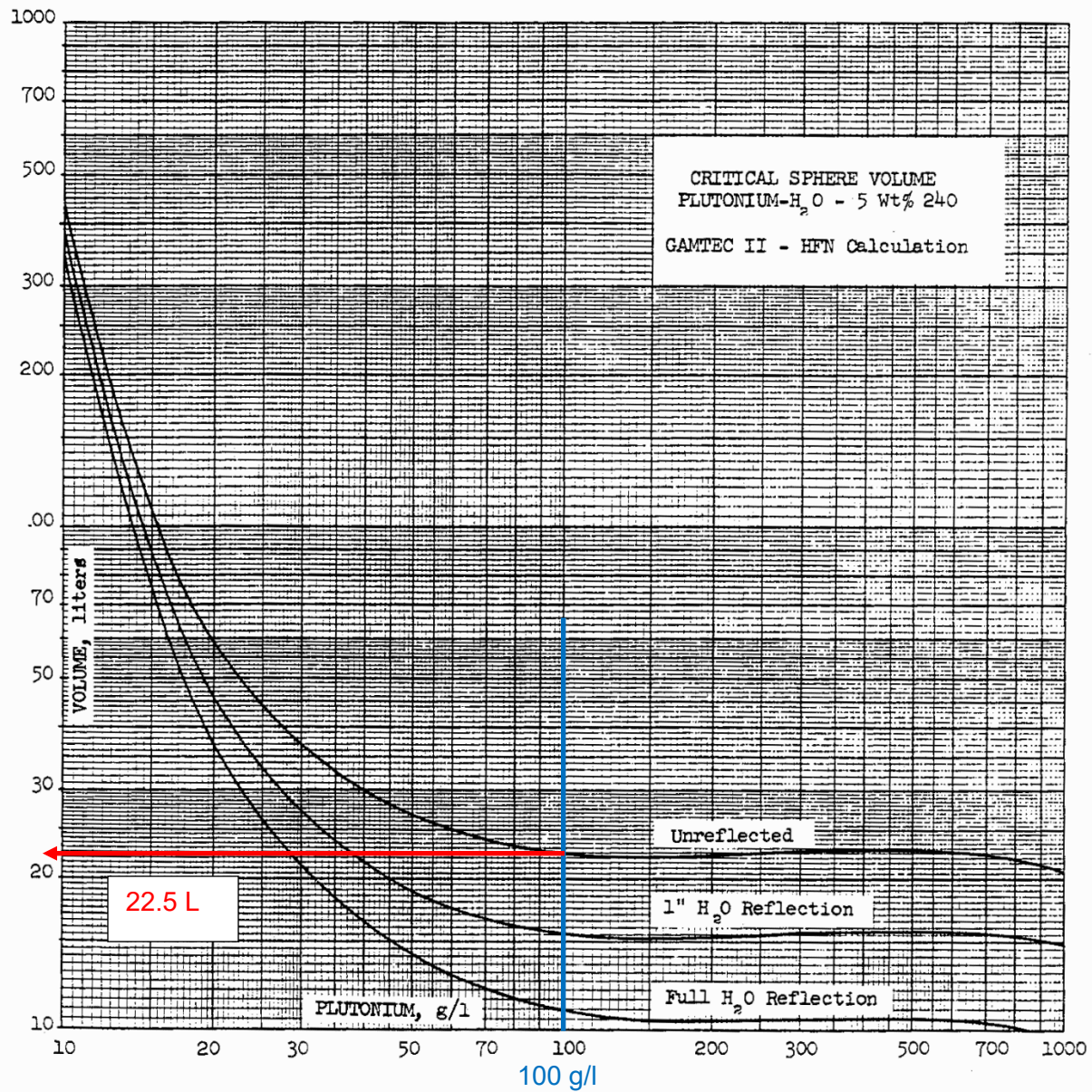
Figure 3-14. Spherical Critical Volume for a Mixture of Pu(5) and Water. (Reference 7, Figure III.A.9.95-3.)
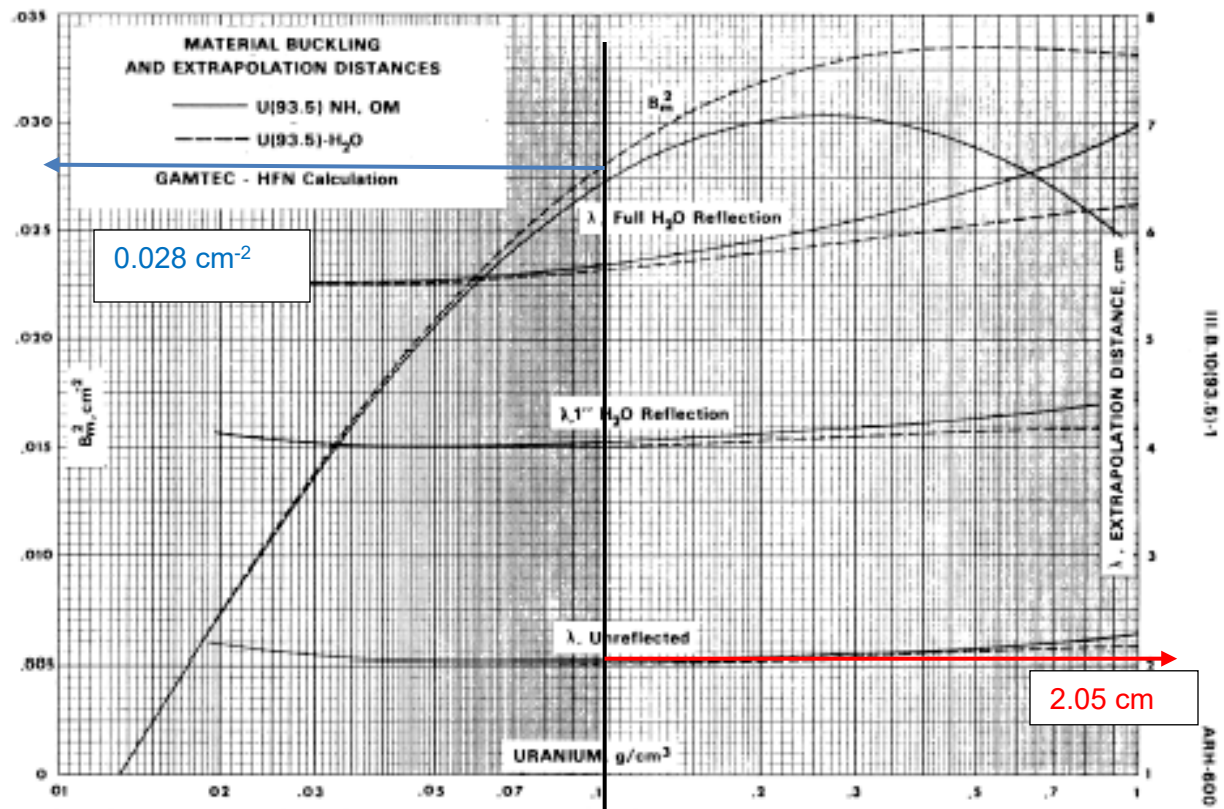
Figure 3-15. Extrapolation Distance and Material Buckling for a Mixture of U(93.5) and Water. (Reference 7, Figure III.B.10 (93.5)-1.)
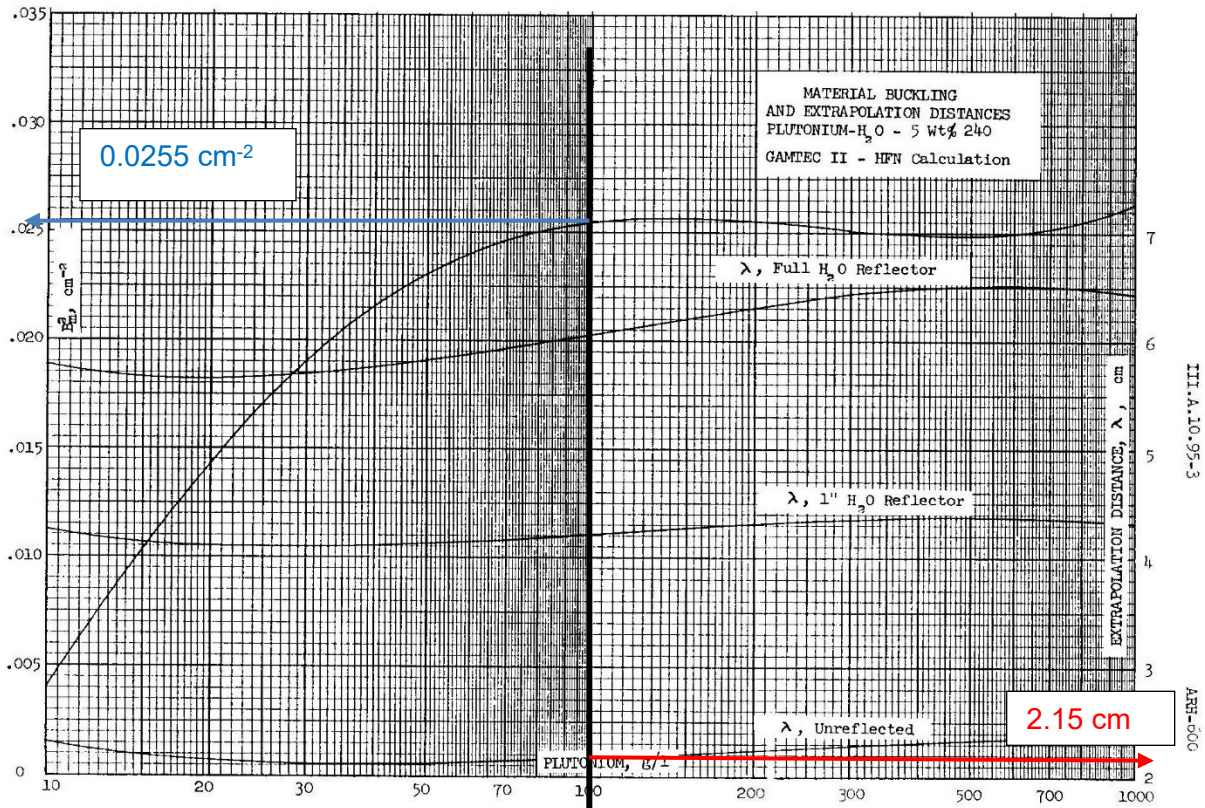
Figure 3-16. Extrapolation Distance and Material Buckling for a Mixture of Pu(5) and Water. (Reference 7, Figure III.A.10.95-3.)

Now, let us check the material bucklings obtained from the critical dimensions with those obtained from Figure 3-15 and Figure 3-16. First, the uranium system with a critical radius of 16.8 cm,

$$B_m^2 = \left[\frac{\pi}{16.8 \text{ cm} + 2.05 \text{ cm}}\right]^2 = 0.02778 \text{ cm}^{-2},$$

which is very close to 0.028 cm^{-2} determined from Figure 3-15. Now, checking the Pu system with a critical radius of 17.5 cm,

$$B_m^2 = \left[\frac{\pi}{17.5 \text{ cm} + 2.15 \text{ cm}}\right]^2 = 0.02556 \text{ cm}^{-2},$$

which is very close to 0.0255 cm^{-2} determined from Figure 3-16. Also note that at critical, the uranium system has more leakage (larger material buckling) than the Pu system. We will discuss this after determining the critical heights of the two systems.

103

Recall that the geometric buckling for a sphere equates to that of a cylinder, as

$$\left[\frac{\pi}{R_{sph} + d}\right]^2 = \left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2.$$

The cylinder radii are both 25.4 cm. We will assume that the extrapolation distance used for spheres is the same as that for cylinders. Then for the U(93.5) solution tank, the height of the solution at critical would be:

$$0.02778 \text{ cm}^{-2} = \left[\frac{2.405}{25.4 \text{ cm} + 2.05 \text{ cm}}\right]^2 + \left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2.$$

Solving the equation for H_U:

$$\left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 = 0.02778 \text{ cm}^{-2} - \left[\frac{2.405}{25.4 \text{ cm} + 2.05 \text{ cm}}\right]^2$$

$$\left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 = 0.02778 \text{ cm}^{-2} - 0.00768 \text{ cm}^{-2} = 0.02010 \text{ cm}^{-2}$$

$$H_U = 18.1 \text{ cm}.$$

Then for the Pu(5) solution tank, the height of the solution at critical would be as follows:

$$0.02556 \text{ cm}^{-2} = \left[\frac{2.405}{25.4 \text{ cm} + 2.15 \text{ cm}}\right]^2 + \left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2.$$

Solving the equation for H_{Pu}:

$$\left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2 = 0.02556 \text{ cm}^{-2} - \left[\frac{2.405}{25.4 \text{ cm} + 2.15 \text{ cm}}\right]^2$$

$$\left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2 = 0.02556 \text{ cm}^{-2} - 0.00762 \text{ cm}^{-2} = 0.01794 \text{ cm}^{-2}$$

$$H_{Pu} = 19.2 \text{ cm}.$$

Although the critical height difference between the plutonium–water and uranium–water mixtures is small (about 1.1 cm), this calculation demonstrates that the uranium–water system will achieve a critical state before the plutonium–water system. Intuition supports this conclusion because the critical mass for an unreflected, spherical system is lower for uranium (2 kg) than for plutonium (2.25 kg) at a fissile concentration of 100 g/l. The height difference can also be inferred from the difference in material bucklings. As the radial buckling for both system is about the same (0.00765 cm⁻²), the larger overall

material buckling for uranium indicates that there must be more axial leakage and thus a smaller height for the uranium system than for the plutonium system.

Part 2.

For 150-g/l fissile concentration, the calculation proceeds as before. Using Figure 3-12 with a uranium concentration of 0.15 g/cm³ (150 g/liter) shows the spherical critical mass as 2.6 kg and a critical spherical volume of 17 liters. Using Figure 3-13 with a plutonium concentration of 150 g/L shows the spherical critical mass as 3.3 kg, whereas Figure 3-14 shows the spherical critical volume to be 22 L. The extrapolation distances change little from 100 g/L to 150 g/L, so we will use 2.05 cm for the uranium extrapolation distance and 2.15 cm for the plutonium extrapolation distance as previously determined.

Determining the critical radii for each solution based on the critical volume. For uranium,

$$R_{U(93.5)} = \left[\frac{3 \times V_{U(93.5)}}{4 \times \pi}\right]^{\frac{1}{3}} = \left[\frac{3 \times 17 \text{ liters} \times 1000 \text{ cm}^3/\text{liter}}{4 \times \pi}\right]^{\frac{1}{3}} = 15.95 \text{ cm.}$$

For the plutonium solution,

$$R_{Pu(5)} = \left[\frac{3 \times V_{Pu(5)}}{4 \times \pi}\right]^{\frac{1}{3}} = \left[\frac{3 \times 22 \text{ liters} \times 1000 \text{ cm}^3/\text{liter}}{4 \times \pi}\right]^{\frac{1}{3}} = 17.4 \text{ cm.}$$

Now, let us check the material bucklings obtained from the critical dimensions with those obtained from Figure 3-15 and Figure 3-16. First, the uranium system with a critical radius of 15.95 cm.

$$B_m^2 = \left[\frac{\pi}{15.95 \text{ cm} + 2.05 \text{ cm}}\right]^2 = 0.03046 \text{ cm}^{-2},$$

which is very close to 0.0306 cm⁻² determined from Figure 3-15. Now, checking the plutonium system with a critical radius of 17.5 cm,

$$B_m^2 = \left[\frac{\pi}{17.4 \text{ cm} + 2.15 \text{ cm}}\right]^2 = 0.02582 \text{ cm}^{-2},$$

which is very close to 0.0258 cm⁻² determined from Figure 3-16. Again, note that at critical, the uranium system has more leakage (larger material buckling) than the plutonium system. This is expected because the critical volume for the uranium solution is less than the critical volume for the plutonium solution.

Calculating the critical height for both solutions, starting with the U(93.5) solution tank, the height of the solution at critical would be

$$0.03046 \text{ cm}^{-2} = \left[\frac{2.405}{25.4 \text{ cm} + 2.05 \text{ cm}}\right]^2 + \left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2.$$

Solving the equation for H_U :

$$\left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 = 0.03046 \text{ cm}^{-2} - \left[\frac{2.405}{25.4 \text{ cm} + 2.05 \text{ cm}}\right]^2$$

$$\left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 = 0.03046 \text{ cm}^{-2} - 0.00768 \text{ cm}^{-2} = 0.02278 \text{ cm}^{-2}$$

$$H_U = 16.7 \text{ cm.}$$

Then for the Pu(5) solution tank, the height of the solution at critical would be

$$0.02582 \text{ cm}^{-2} = \left[\frac{2.405}{25.4 \text{ cm} + 2.15 \text{ cm}}\right]^2 + \left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2.$$

Solving the equation for H_{Pu}:

$$\left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2 = 0.02582 \text{ cm}^{-2} - \left[\frac{2.405}{25.4 \text{ cm} + 2.15 \text{ cm}}\right]^2$$

$$\left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2 = 0.02582 \text{ cm}^{-2} - 0.00762 \text{ cm}^{-2} = 0.01820 \text{ cm}^{-2}$$

$$H_{Pu} = 19.0 \text{ cm.}$$

Notice that at a fissile concentration of 150 g/L, the difference in critical height for these two systems is larger than at 100 g/L. The critical height difference between the two systems has increased from 1.05 cm to 2.30 cm. It can be seen from this problem that a Pu metal–water mixture (5 wt % Pu-240) at 100 or 150 gPu/L requires more volume to achieve a critical state than for a U(93) metal–water system at the same concentration for the equivalent cylindrical system. This argument is also true for spherical systems as is shown in the minimum critical volume data for the unreflected spherical tanks.

Part 3.

For 50 g/L fissile concentration, the calculation proceeds as before. Figure 3-12 shows the spherical critical mass for U(93.5)-H_2O at 0.05 g/cm³ (50 g/liter) as 1.6 kg and a critical spherical volume of 32 liters. Figure 3-13 shows the spherical critical mass for Pu(5)-H_2O at 50 g/liter as 1.35 kg, whereas Figure 3-14 shows the spherical critical volume to be 27 L. Notice the critical volume (and critical mass) for the plutonium solution is now less than that of the uranium solution at 50 g/L. The extrapolation distances change little from 100 g/L to 50 g/L, so we will use 2.05 cm for the uranium extrapolation distance and 2.15 cm for the plutonium extrapolation distance.

Determining the critical radii for each solution based on the critical volume. For uranium,

$$R_{U(93.5)} = \left[\frac{3 \times V_{U(93.5)}}{4 \times \pi}\right]^{\frac{1}{3}} = \left[\frac{3 \times 32 \text{ liters} \times 1000 \text{ cm}^3/\text{liter}}{4 \times \pi}\right]^{\frac{1}{3}} = 19.7 \text{ cm.}$$

For the plutonium solution,

$$R_{Pu(5)} = \left[\frac{3 \times V_{Pu(5)}}{4 \times \pi} \right]^{\frac{1}{3}} = \left[\frac{3 \times 27 \text{ liters} \times 1000 \text{ cm}^3/\text{liter}}{4 \times \pi} \right]^{\frac{1}{3}} = 18.6 \text{ cm.}$$

Now, let us check the material bucklings obtained from the critical dimensions with those obtained from Figure 3-15 and Figure 3-16. First, the uranium system with a critical radius of 19.7 cm:

$$B_m^2 = \left[\frac{\pi}{19.7 \text{ cm} + 2.05 \text{ cm}} \right]^2 = 0.02086 \text{ cm}^{-2} ,$$

which is very close to 0.0208 cm^{-2} determined from Figure 3-15. Now, checking the plutonium system with a critical radius of 18.6 cm,

$$B_m^2 = \left[\frac{\pi}{18.6 \text{ cm} + 2.15 \text{ cm}} \right]^2 = 0.02292 \text{ cm}^{-2} ,$$

which is very close to 0.0230 cm^{-2} determined from Figure 3-16. Note that at critical, the 50 g/L uranium system now has less leakage (smaller material buckling) than the plutonium system. This is as expected because the critical volume for the uranium solution is greater than the critical volume for the plutonium solution at the given fissile density of 50 g/L.

Calculating the critical height for both solutions, starting with the U(93.5) solution tank, the height of the solution at critical would be:

$$0.02086 \text{ cm}^{-2} = \left[\frac{2.405}{25.4 \text{ cm} + 2.05 \text{ cm}} \right]^2 + \left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}} \right]^2 .$$

Solving the equation for H_U :

$$\left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}} \right]^2 = 0.02086 \text{ cm}^{-2} - \left[\frac{2.405}{25.4 \text{ cm} + 2.05 \text{ cm}} \right]^2$$

$$\left[\frac{\pi}{H_U \text{ cm} + 2 \times 2.05 \text{ cm}} \right]^2 = 0.02086 \text{ cm}^{-2} - 0.00768 \text{ cm}^{-2} = 0.01318 \text{ cm}^{-2}$$

$$H_U = 23.3 \text{ cm.}$$

Then for the Pu(5) solution tank, the height of the solution at critical would be:

$$0.02292 \text{ cm}^{-2} = \left[\frac{2.405}{25.4 \text{ cm} + 2.15 \text{ cm}} \right]^2 + \left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}} \right]^2 .$$

Solving the equation for H_{Pu} :

$$\left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2 = 0.02292 \text{ cm}^{-2} - \left[\frac{2.405}{25.4 \text{ cm} + 2.15 \text{ cm}}\right]^2$$

$$\left[\frac{\pi}{H_{Pu} \text{ cm} + 2 \times 2.15 \text{ cm}}\right]^2 = 0.02292 \text{ cm}^{-2} - 0.00762 \text{ cm}^{-2} = 0.01530 \text{ cm}^{-2}$$

$$H_{Pu} = 21.1 \text{ cm.}$$

Notice that at a fissile concentration of 50 g/L, the critical height for the plutonium system is now the smaller value by about 2.2 cm. Thus, at some fissile concentration between 50 g/L and 100 g/L, the critical volumes of these two solutions will be equal. It is left to the reader to verify that the material bucklings and associated solution heights are approximately equal at this concentration.

3.4.7 Buckling Conversion Example Problem 5

For the uranium fissile solution (U(93.5)–water mixture at 100 g fissile/L) in example problem 4, perform a parametric study on *H/D* for an unreflected cylinder. Use *H/D* values of ∞, 10, 5, 2, 1, 0,9238, 0.7, 0.5, 0.25, and 0 (i.e., infinite slab thickness). Determine the critical radius and height for the system along with the critical mass of U-235. Use a constant extrapolation distance of 2.05 cm for all shapes. The first step in the solution to this problem is to compile the data needed. Using Figure 3-12 (from ARH-600, reference 7), we can obtain information about the spherical critical mass = 2 kg, and the spherical critical volume = 20 L for a bare U(93.5) metal–water mixture.

$$R_{U(93.5)} = \left[\frac{3 \times V_{U(93.5)}}{4 \times \pi}\right]^{\frac{1}{3}} = \left[\frac{3 \times 20 \text{ liters} \times 1000 \text{ cm}^3/\text{liter}}{4 \times \pi}\right]^{\frac{1}{3}} = 16.8 \text{ cm},$$

which is the same answer as found in example problem 4. Now, let us check the material buckling obtained from the critical dimensions with that obtained from Figure 3-15 for the uranium system with a critical radius of 15.95 cm:

$$B_m^2 = \left[\frac{\pi}{16.8 \text{ cm} + 2.05 \text{ cm}}\right]^2 = 0.02778 \text{ cm}^{-2},$$

which is very close to 0.0280 cm^{-2} determined from Figure 3-15.

Calculating the critical radius for the infinite cylinder,

Solving the equation for R$_{cyl}$:

$$\left[\frac{2.405}{R_{cyl} \text{ cm} + 2.05 \text{ cm}}\right]^2 = 0.02778 \text{ cm}^{-2}$$

$$R_{cyl} = 14.4 \text{ cm} - 2.05 \text{ cm} = 12.4 \text{ cm.}$$

Now, repeating the calculation for *H/D* = 1 requires iteration or using a program like Excel with its Solver Add-on. Notice that we have replaced the height with (*H/D*) × 2 and are iterating on the radius of the cylinder.

$$0.02778 \text{ cm}^{-2} = \left[\frac{2.405}{R_{cyl} \text{ cm} + 2.05 \text{ cm}}\right]^2 + \left[\frac{\pi}{2 \times (H/D) \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 .$$

For H/D = 10:

$$0.02778 \text{ cm}^{-2} = \left[\frac{2.405}{R_{cyl} \text{ cm} + 2.05 \text{ cm}}\right]^2 + \left[\frac{\pi}{2 \times (10) \times r \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 .$$

Iterating gives $R_{cyl} = 12.4$ cm.

Now that we have the dimensions (i.e., $r = 12.4$ cm and $H = 248.0$ cm), we can calculate the volume and the critical mass of U-235 based on the 0.1 g ^{235}U/L given concentration.

$$V_{sph} = \pi R_{cyl}^2 H = \left[\pi(12.4 \text{ cm})^2(248 \text{ cm})\right] \times \frac{1 \text{ liter}}{1000 \text{ cm}^3} = 119.8 \text{ liters}.$$

$$M_{235} = \frac{0.1 \text{ kg}}{\text{liter}} \times 119.8 \text{ liters} = 12.0 \text{ kg}$$

Continuing the process through the h/d values down to $H/D = 0.25$, we find

For H/D = 0.25:

$$0.02778 \text{ cm}^{-2} = \left[\frac{2.405}{R_{cyl} \text{ cm} + 2.05 \text{ cm}}\right]^2 + \left[\frac{\pi}{2 \times (0.25) \times r \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 .$$

Iterating gives $R_{cyl} = 33.1$ cm.

Now that we have the dimensions (i.e., $r = 33.1$ cm and $H = 16.55$ cm), we can calculate the volume and the critical mass of ^{235}U based on the 0.1 g ^{235}U /liter given concentration.

$$V_{sph} = \pi R_{cyl}^2 H = \left[\pi(33.1 \text{ cm})^2(16.55 \text{ cm})\right] \times \frac{1 \text{ liter}}{1000 \text{ cm}^3} = 56.96 \text{ liters}.$$

$$M_{235} = \frac{0.1 \text{ kg}}{\text{liter}} \times 56.96 \text{ liters} = 5.7 \text{ kg}$$

Then for the infinite slab (i.e., $H/D = 0$), we find a thickness:

Solving the equation for H_{cyl} :

$$\left[\frac{\pi}{H_{cyl} \text{ cm} + 2 \times 2.05 \text{ cm}}\right]^2 = 0.02778 \text{ cm}^{-2}$$

$$H_{cyl} = 18.85 \text{ cm} - 4.1 \text{ cm} = 14.75 \text{ cm}.$$

Tabulation of the results along with the radius values determined from PARTISN is given in Table 3-3 (Dimensions rounded to one decimal place for ease of viewing).

Table 3-3. Parametric Evaluation of *H/D* for 0.1 gU(93.5)/L Solution in Cylinder.

radius (cm)	*H/D*	height (cm)	(*H/D*)/(1+(*H/D*))	mass (kg)	volume (liters)	PARTISN calc. radius (cm)
12.3	100	∞	0.99	∞	∞	12.3
12.4	10	248.0	0.91	11.98	119.8	12.6
12.5	5	125.0	0.83	6.14	61.4	12.7
13.2	2	52.8	0.67	2.89	28.9	13.4
15.2	1	30.4	0.50	2.21	22.1	15.5
15.6	0.9238	28.8	0.48	2.20	22.0	15.8
17.3	0.7	24.2	0.41	2.28	22.8	17.6
20.5	0.5	20.5	0.33	2.71	27.1	20.8
33.2	0.25	16.6	0.20	5.75	57.5	33.6
∞	0	14.8	0.00	∞	∞	14.7

Note that the minimum volume and minimum mass occurs with $H/D = 0.9238$, which comes from differentiating the equation for the volume of a cylinder with a given material buckling. Also, note that there is little difference between $H/D = 0.9328$ and $H/D = 1$, as both have small values of surface area for a given volume. Although $H/D = 1$ seems to imply that the radial buckling should equal the axial buckling, this is not the case. The radial buckling depends on the radius and not the diameter, so $H/D = 1$ is actually $H/r = 2$. This indicates that there should be more leakage in the radial direction than in the axial direction, as the height is larger than the radius. Also, the radial buckling has the 2.405 factor in the numerator, whereas the axial buckling has π in the numerator. This precludes easy quantifiable leakage calculations, but the qualitative conclusions will still hold. PARTISN calculations for the $H.D = 1$ case show a radial buckling of about 0.0192 cm^{-2} and an axial buckling of about 0.0082 cm^{-2}. This indicates that for this uranium solution, the radial leakage is about 2.3× the axial leakage.

The ratio in column 4 of the table can be used with Figure 3-17 to determine the effective extrapolation distance for each shape. Similar figures appear in Reference 14, LA-3366 Rev (Figures 4 and 5) and Reference 11, LA-10860 (Figures 6 and 7).
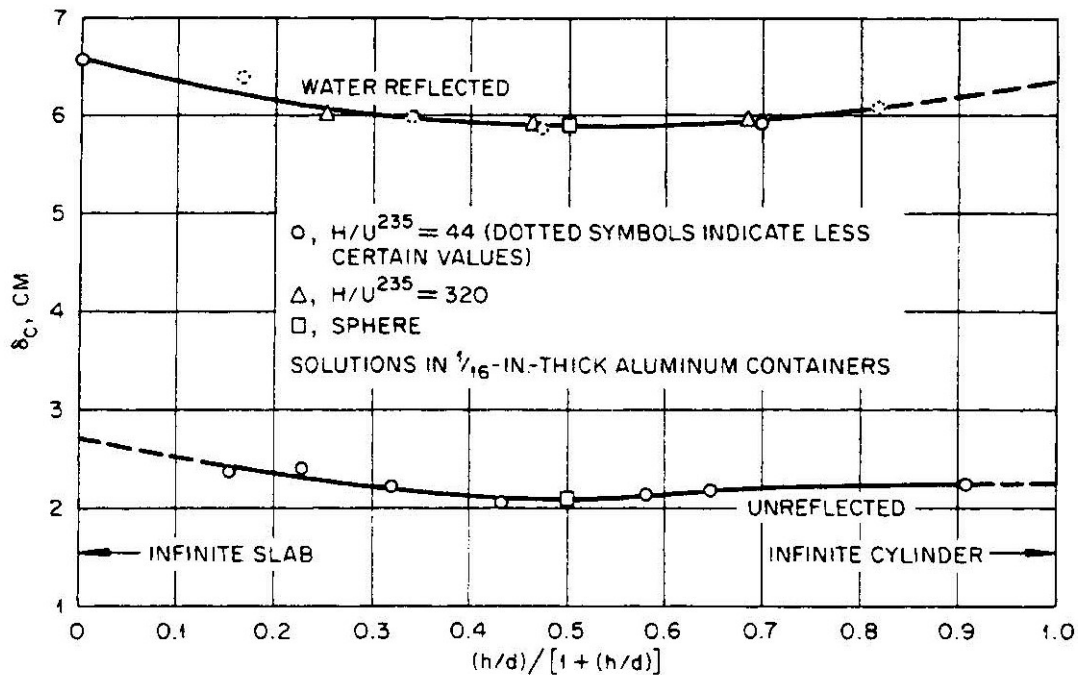
Figure 3-17. Effective extrapolation distances for Cylinders of Uranium Solutions. (Figure 3, page 6, Reference 12.)

3.4.8 Buckling Conversion Example Problem 6

One of the process criticality accidents occurred in January 1958 at the Mayak Enterprise. The accident involved highly enriched uranium solution in a cylinder that was being moved and likely tipped. Use buckling conversion to discuss the variation in effective multiplication factor for the various configurations of solution in the cylinder.

Mayak 1958 accident

This accident involved a high concentration of highly enriched, 418 g $U(90)O_2(NO_3)_2$, uranyl nitrate solution. Figure 3-18 shows the solution in the tank just prior to tipping. Characteristics of the tank are as follows:

- Stainless-steel vessel
  - 750 mm inside diameter with a wall thickness of 2 to 4 mm
  - Approximate capacity of 440 L (~116 gallons)
    - This indicates a vessel height of at least 900 mm
  - >1.5 m from any walls but 600 mm from the control panel shielding slab
  - ~0.8 m above the concrete floor
  - Resting on and bolted to a thick (~8 mm) steel support plate/stand

On January 2, 1958, after removing some of the solution through a filling system, the experimenters judged the remaining solution volume to be highly subcritical. The knowledgeable dedicated team decided to circumvent their procedure and to manually pour the remaining solution from the vessel.
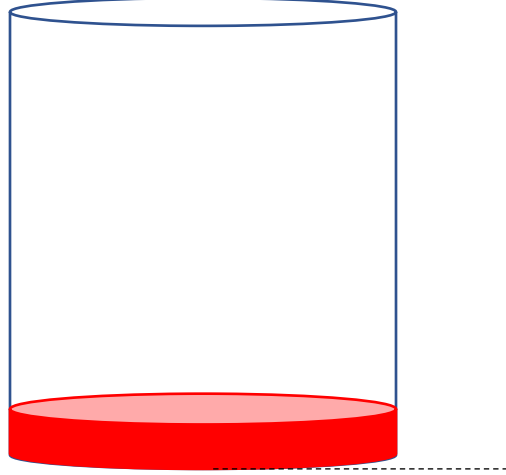
Figure 3-18. Cylindrical Tank with 58.3 L of uranyl nitrate solution.

At the point where the experimenters decided to stop draining into 6 L bottles and to tip the container, there was about 58.3 L of solution (13.2 cm high and 75 cm diameter). Calculations with the PARTISN code indicate a bare, unreflected k_{eff} of 0.88 for this configuration. However, the tank was setting on a stainless-steel pedestal, so there was some bottom reflection. This was modeled as 2.1 cm of water, and the resulting k_{eff} was 0.97.

To calculate the k_{eff} using Eq. (75) (material and geometric bucklings), we need the material buckling for this system. The bare sphere critical volume is 17.5 liters (reference 20). This gives a radius of 16.11 cm, and a geometric buckling of:

$$\left(\frac{\pi}{r+d}\right)^2 = \left(\frac{\pi}{16.11+2.2}\right)^2 = 0.02944 cm^{-2}$$

Because the system is critical, the geometric buckling is equal to the material buckling for this solution. The geometric buckling for the unreflected initial geometry is:

$$\left(\frac{2.405}{r+d}\right)^2 + \left(\frac{\pi}{H+2d}\right)^2 = \left(\frac{2.405}{37.5+2.2}\right)^2 + \left(\frac{\pi}{13.2+2\times2.2}\right)^2 = 0.03553 cm^{-2}$$

Now using the material buckling for the liquid and the geometric buckling for bare initial configuration, Eq. (75) is used to determine k_{eff}:

$$k_{eff} = \frac{\left(1+B_m^2 M^2\right)}{\left(1+B_g^2 M^2\right)} = \frac{1+0.02944 cm^{-2}\times28.6 cm^2}{1+0.03553 cm^{-2}\times28.6 cm^2} = 0.914$$

The value of 28.6 cm^2 is typical of water-moderated systems, as discussed in footnote 10. This value, though higher than the code calculated value of 0.88, gives a reasonable indication of the degree of subcriticality of the system.

Now, let us use the same technique to assess the k_{eff} of the initial configuration with some bottom reflection. As noted in Section 3.4.2, partial reflected conditions can be evaluated using the reflector savings for the reflector material. In this case, we are going to assume that the stainless-steel reflector has

113

the same effect as 2.1 cm of water. The reflector savings for full water reflection is about 3.8 cm (reference 14, LA-3366 Rev, Figure 4, page 16). However, full water reflection requires at least 8 cm of water (reference 11, LA-10860, Figure 42, page 95 shows a linear decrease in critical mass up to 8 cm of water and then is flat with additional water thickness), so we will reduce the reflector savings by (2.1) / 8 to get a value of 1.0 cm for this reflection. Also, remember that the reflection is only on the bottom, so there is no correction for the upper surface. The geometric buckling for the partially reflected case is then

$$\left(\frac{2.405}{r+d}\right)^2 + \left(\frac{\pi}{h+d+\delta+d}\right)^2 = \left(\frac{2.405}{37.5+2.2}\right)^2 + \left(\frac{\pi}{13.2+2.2+1.0+2.2}\right)^2 = 0.03220 cm^{-2}$$

Then, the k_{eff} for the partially reflected case is

$$k_{eff} = \frac{\left(1 + B_m^2 M^2\right)}{\left(1 + B_g^2 M^2\right)} = \frac{1 + 0.02944 cm^{-2} \times 28.6 cm^2}{1 + 0.03220 cm^{-2} \times 28.6 cm^2} = 0.959$$

Again, this value, though lower than the code calculated value of 0.97, gives a reasonable indication of the effect of partial reflection on the system multiplication.

Tipping the tank changes the leakage from the liquid and thus affects the multiplication factor. The following parts of Figure 3-19 (Figure 3-19.a, b, c, and d) show the solution as the tank is tipped from the vertical position (angle = 0°).

Figure 3-19. Condition of Cylindrical Tank at Various Angles of Tilt.

For the unreflected container, the change in surface area with tilt angle is shown in Figure 3-20. The surface area increases up to the point where it just covers the bottom of the tank (tilt angle = 19.39°). With a little further tilting to about 19.8°, the surface area is at a local maximum. This means the bare configuration has the minimum k_{eff} at this point. Continuing to tip the container rapidly decreases the surface and increases the reactivity of the system. This continues to a tilt angle of 47.55° where the surface area is 8.64% less than that of the initial condition.
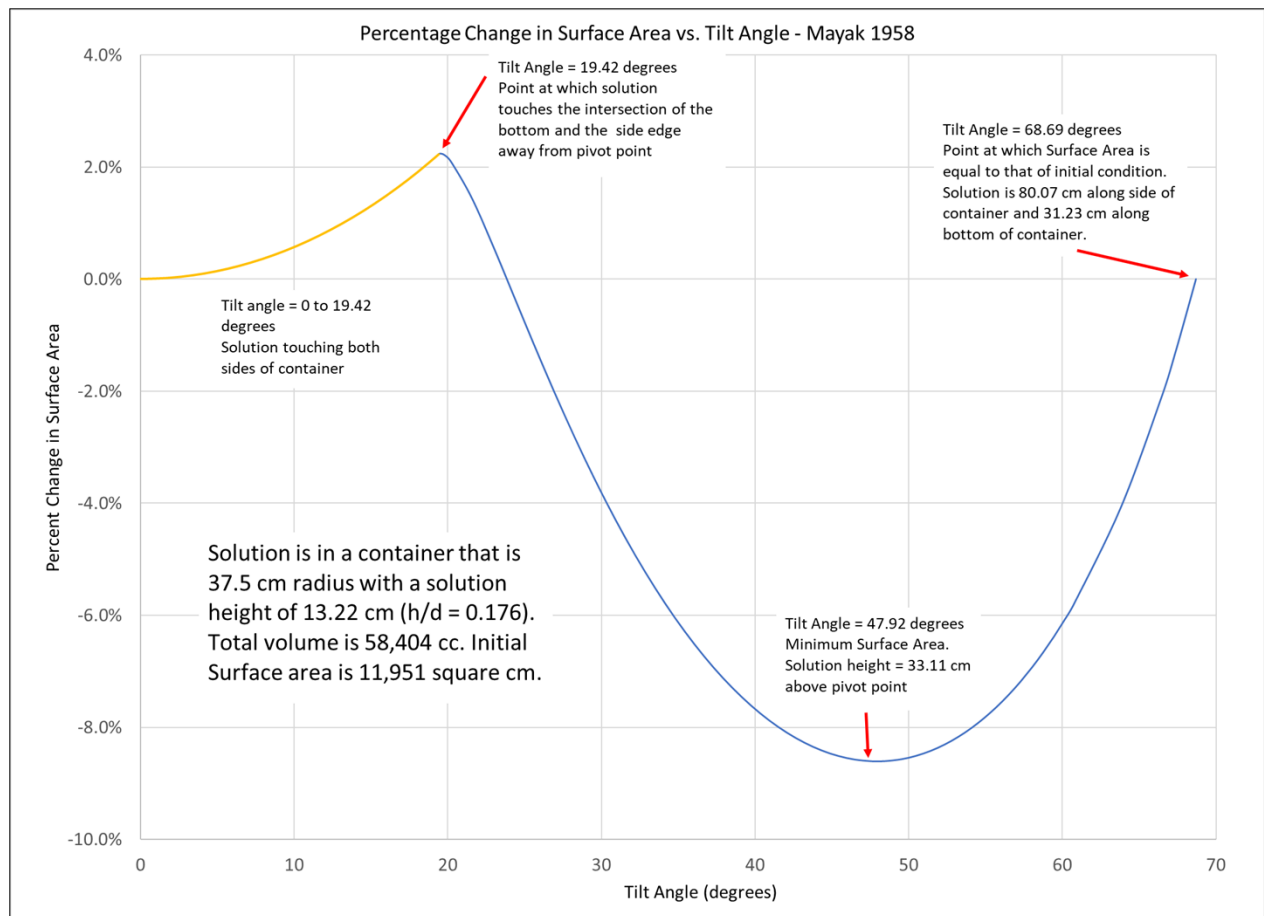
Figure 3-20. Percentage Change in Surface Area as *h/d*=0.176 Container is Tilted.

For a container reflected on the bottom, the surface area behavior does not change. However, the reflection will decrease. As the container is tipped, the bottom reflection diminishes. At the point of maximum reactivity (i.e., minimum surface area for a given volume), there is effectively no bottom reflection. This adds negative reactivity but does not cancel the added positive reactivity from the decrease in surface area. So, the leakage is being reduced due to the "coalescing" of the fluid, but the reflection is also being reduced from tipping. As expected, that the multiplication factor will decrease at first as the reflector "moves" away more quickly than the fluid moves together. Then, the fluid moving together decreases the leakage increasing the multiplication factor.

As the liquid in Figure 3-19c (tipped at 47.55°) is in the most reactive configuration, the liquid surface is effectively a truncated ellipse. The semi-minor axis is the cylinder radius (=37.5 cm), and the semi-major axis = 55.56 cm. The total length of the surface in the truncated direction is 66.4 cm. If we treat the liquid as a hemicylinder with the "height" (from front to back on the flat top liquid surface as viewed in Figure 3-21) equal to two times the semi-minor axis (diameter of container = 75 cm, so *H* = 75 cm), then the radius is determined by conserving the volume of liquid.

116

$$Vol_{hemicyl} = \frac{\pi r^2 H}{2} = 58{,}316 cm^3$$

$$r = \sqrt{\frac{2 \times 58{,}316 cm^3}{\pi \times 75\ cm}} = 22.25 cm$$

So, the flat surface has a width of 44.5 cm in the assumed hemicylinder versus the 66.4 cm of the truncated surface. This makes sense, as seen in Figure 3-21, where the height is smaller to encompass the liquid. Thus, it appears that the assumption of a hemicylinder would be an upper bound on the reactivity configuration of the solution.

47.55°

r = 22.25 cm
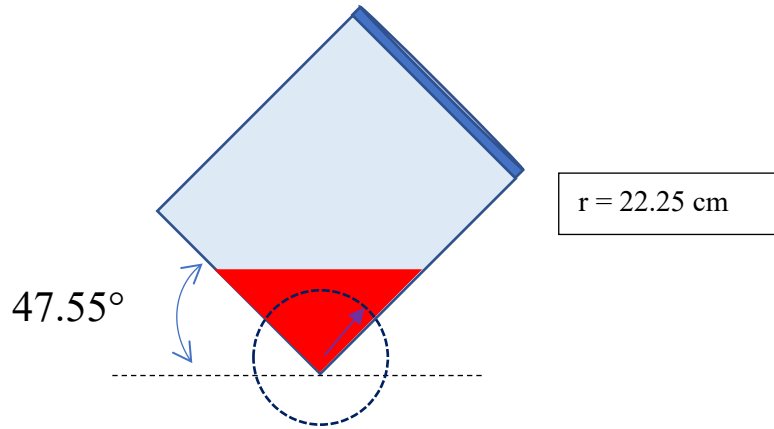
Figure 3-21. Liquid in most reactive position.

From Table 3-2, the geometric buckling for a hemicylinder is

$$\left(\frac{3.832}{r + d}\right)^2 + \left(\frac{\pi}{H + 2d}\right)^2$$

Assuming no reflection and using an extrapolation distance of 2.2 cm, the buckling for the approximated Mayak hemicylinder is

$$\left(\frac{3.832}{r + d}\right)^2 + \left(\frac{\pi}{H + 2d}\right)^2 = \left(\frac{3.832}{22.25 + 2.2}\right)^2 + \left(\frac{\pi}{75 + 2 \times 2.2}\right)^2 = 0.02613 cm^{-2}$$

To use Eq. (75) to determine k_{eff} requires a value for the migration area. As noted in the footnote (repeated below) to the discussion of Eq. (75), it is reasonable to assume that M^2 is about 28.6 cm² for water-moderated systems.[13]

---

[13] As $M^2 = \tau + L^2$, for water systems, $\tau = 27$ cm² while L^2 is L^2_{mod} (1-f). For water, $L^2_{mod} = (2.85\ cm)^2 = 8.12$ cm². For most water moderated, thermal systems, f ranges from 0.7 to 0.9 (see example problems 4, 5, and 6 in Chapter 2). Taking the middle ground with $f = 0.8$, $L^2 = 0.2 * 8.12 = 1.6$ cm² so an average M^2 would be 28.6 cm². Analyses with values of M^2 from 27.8 to 29.5 indicate less than a 0.2% change from results calculated using the 28.6 cm² average.

Now, using the material buckling for the liquid and the geometric buckling for the bare hemicylinder configuration, Eq. (75) is used to determine k_{eff}:

$$k_{eff} = \frac{\left(1 + B_m^2 M^2\right)}{\left(1 + B_g^2 M^2\right)} = \frac{1 + 0.02944 cm^{-2} \times 28.6 cm^2}{1 + 0.02613 cm^{-2} \times 28.6 cm^2} = 1.054$$

Thus, the system will go critical as the container is tipped. Because the tipping process takes some time, the system becomes supercritical and then starts bubbling, etc. This increases the leakage keeping the multiplication factor from getting to the 1.05 value calculated. However, the supercritical condition will result in a decreased multiplication shutting down the reaction. Also, as shown in Figure 3-20, the surface area increases as the container is tipped beyond 47.55°, so the multiplication factor decreases as the container is further tipped.

4. CORE DENSITY CONVERSIONS

4.1 WHAT YOU WILL BE ABLE TO DO

- Determine the critical dimensions of a fissile system caused by changes in the fissile material density or volume for a sphere, infinite cylinder, or infinite slab.

- Determine the critical mass of a fissile system due to changes in the fissile material density or volume for a sphere, infinite cylinder, or infinite slab.

4.2 CORE DENSITY METHOD OVERVIEW

For homogeneous, critical systems, one exact quantitative relationship can be applied if the density of that system changes uniformly. If the dimensions of an assembly are scaled inversely as the density, then any neutron path from one region to another will scale in the same way. If the materials of that system remain unchanged, then there is no change in the neutron processes in that system (Reference 14). Even though the dimensions of the system change, the relative number of neutrons that leak out of the system, are absorbed, or scatter remains the same. For example, if the critical radius of a solid plutonium sphere at 19.75 g Pu/cm^3 is 5 cm, then reducing the density by a factor of two will double the radius. Thus, the system remains at a critical state (Figure 4-1). References 11, 12, 14, 21, and 22 provide much more discussion about this hand calculation method including supporting data.

Critical, Solid Pu
Metal Sphere
R=5 cm at
19.75 g/cc
density.

Critical, Solid Pu
Metal Sphere R=10
cm at 9.875 g/cc
density.
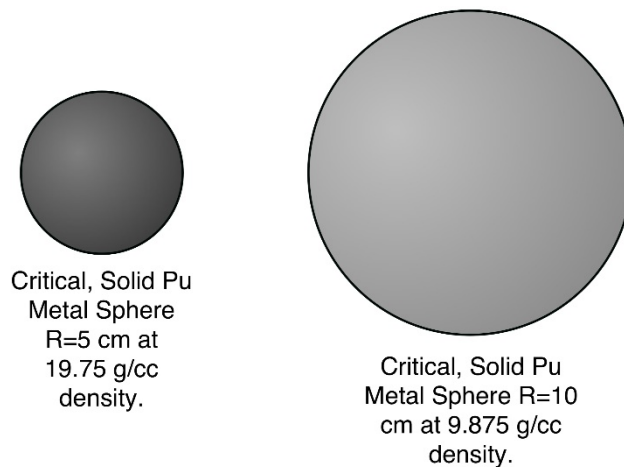
Figure 4-1. Illustration of Core Density Method Concept.

4.2.1 Theoretical Basis of Core Density Conversion

Extract from pg. 25, LA-3366 Rev, Reference 14: "If all dimensions of an assembly are scaled inversely as the density, any neutron path from one region to another scales in the same way, and the number and types of nuclei along this path remain unchanged, so there is no change in neutron processes. In other words, the relative number of neutrons producing fission, being captured, being scattered, and leaking from the system are not changed, so the assembly remains critical. Thus, critical dimensions are inversely proportional to the density, provided the density changes are uniform. For a reflected system in which the densities of core and reflector are changed by the same ratio, this implies that critical dimensions of both core and reflector scale inversely as the density. (If only the reflector density or only the core density changes, then the above relationship no longer applies to the core dimensions.)

When all densities are changed by the ratio r/r_o, it follows that any critical dimension, ℓ_c, is given by

$$\frac{\ell_c}{\ell_{co}} = \left(\frac{\rho}{\rho_o}\right)^{-1} \tag{76}$$

where ℓ_{co} applies to the initial density ρ_o. As core and reflector densities are seldom changed in the same proportion, this expression is most applied to unreflected fissile material."

For a bare sphere, the radius is inversely proportional to the density. Then the volume would be inversely proportional to the density cubed.

$$\frac{r}{r_o} = \left(\frac{\rho}{\rho_o}\right)^{-1}: \quad \frac{V}{V_o} = \left(\frac{r}{r_o}\right)^3 = \left(\frac{\rho}{\rho_o}\right)^{-3}$$

$$\frac{m}{m_o} = \frac{\rho V}{\rho_o V_o}: \quad \frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^1 \left(\frac{\rho}{\rho_o}\right)^{-3} = \left(\frac{\rho}{\rho_o}\right)^{-2} \tag{77}$$

Similarly, for a bare, infinite cylinder with initial density ρ_o, and initial critical radius r_{co}, the radius at any other density would be

$$\frac{r_c}{r_{co}} = \left(\frac{\rho}{\rho_o}\right)^{-1} \tag{78}$$

For an unreflected slab of critical thickness t_o, the thickness at any other density would be

$$\frac{t}{t_o} = \left(\frac{\rho}{\rho_o}\right)^{-1} \tag{79}$$

4.2.2 Core Density Conversion for Bare, Homogeneous Systems

Table 4-1 provides the useful relationships for bare, homogeneous systems. Additional information can be found in References 11, 12, and 14. The relationships for infinite cylinders and slabs are not as commonly used as the relationships for spheres.

Table 4-1. Core Density Conversion Relationships for Bare, Homogeneous Systems.

Geometry	Critical Radius Relationship	Critical Volume Relationship	Critical Mass Relationship
Sphere (Final radius, r, initial radius, r_0, etc.)	$\dfrac{r}{r_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-1}$	$\dfrac{V}{V_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-3}$	$\dfrac{m}{m_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-2}$
Infinite Cylinder (Final radius, r, initial radius, r_0, etc. V' is volume per unit length and m' is mass per unit length)	$\dfrac{r}{r_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-1}$	$\dfrac{V'}{V'_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-2}$	$\dfrac{m'}{m'_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-1}$
Infinite Slab (Final thickness, t, initial thickness, t_0, etc. V'' is volume per unit area and m'' is mass per unit area)	$\dfrac{t}{t_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-1}$	$\dfrac{V''}{V''_o} = \left(\dfrac{\rho}{\rho_o}\right)^{-1}$	$\dfrac{m''}{m''_o} = \left(\dfrac{\rho}{\rho_o}\right)^{0} = $ constant

4.2.3   Critical Data

Core density conversions are most applicable in systems with fissile metal or fissile powder and no moderation. A starting point would be critical data for bare metal spheres of various enrichments and assays. These data, along with pertinent densities, radii, and diluents, are listed in Table 4-2 from Reference 23.

Table 4-2. Critical Mass Data for Bare Fissile Metal Spheres.

Data from International Handbook of Evaluated Criticality Safety Benchmark Experiments						
Core Material	Density (g/cm³)	Radius (R_{exp}) (cm)	Total Mass (kg)	Diluent 1 Weight percent	Diluent 2 Weight percent	Diluent 3 Weight percent
U(93.8)	18.74	8.7407	52.420	U-238 5.27	U-234 1.02	N/A
Pu(95.5)	15.61	6.3915	17.073	Pu-240 4.454	Pu-241 0.297	Ga 1.02
^{233}U(98.1)	18.424	5.9838	16.535	U-234 1.24	U-235 0.03	U-238 0.60

For oxide materials, less information is available on critical masses. However, D.E. Cullen from LLNL (reference 24) has derived the proportionality constant for six oxide systems. This constant relates the mass of the material to the inverse of the square of its density. The systems and proportionality constants are given in Table 4-3. As with Table 4-2, the value given in parentheses is the weight percent of the dominant fissile isotope (e.g., Pu(95.5) represents 95.5 wt % Pu-239 with the rest of the materials as described in the diluent columns.)

Table 4-3. Critical Mass Data for Bare Fissile Oxide Spheres.

Core Material	Theoretical Density[14] (TD) (g/cm^3)	Proportionality Constant $(kg\text{-}g^2/cm^6)$	Total Mass at TD (kg)	Diluent 1 Weight percent	Diluent 2 Weight percent	Diluent 3 Weight percent
U(100)O$_2$	10.838	12295	104.7	U-234 0.0	U-238 0.0	N/A
U(92.94)O$_2$	10.845	13664	116.2	U-234 0.99	U-238 6.07	N/A
U(92.93)$_3$O$_8$	8.306	13030	188.9	U-234 0.99	U-238 6.08	N/A
Pu(100)O$_2$	11.460	3569	27.18	Pu-240 0.0	Pu-241 0.0	N/A
Pu(93.46)O$_2$	11.463	3729	28.38	Pu-240 6.02	Pu-241 0.52	N/A
Pu(62.87)O$_2$	11.483	4488	34.04	Pu-240 22.73	Pu-241 12.68	Pu-242 1.72

The information in Table 4-3 can be used with Eq. (77) to give the critical mass at any given density. For example, to determine the critical mass of Pu(93.46)O$_2$ at 6 g/cm^3,

$$\frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^{-2} \Rightarrow \frac{m}{28.38 \text{ kg}} = \left(\frac{6 \text{ g/cm}^3}{11.463 \text{ g/cm}^3}\right)^{-2} \quad m = 103.59 \text{ kg}$$

OR

using the proportionality constant $M = \dfrac{\text{const}}{\rho^2}$ \hfill (80)

$$M\,[kg] = \frac{3729 \left[\frac{\text{kg - g}^2}{\text{cm}^6}\right]}{(6 \text{ g/cm}^3)^2} = 103.58 \text{ kg}$$

The 0.01 kg difference is due to round-off.

Isotopic composition is important in the calculation of critical mass values. As shown in Table 4-3, the critical mass is strongly dependent on additional scatterers, as seen above for UO$_2$ versus U$_3$O$_8$, as well as how much neutron absorption is present. For uranium, those absorbers would include U-234, U-236, and U-238, whereas for plutonium, that would be Pu-240 and Pu-242. Increasing the neutron absorption will increase the critical mass. The limit of no absorber is represented by U(100)O$_2$ and Pu(100)O$_2$ in the table.

---

[14] The theoretical density for the isotope mixture is determined from the reference theoretical density for the compound divided by the molecular weight of the reference compound times the molecular weight of the isotope mixture compound. For example, the theoretical density of U(nat)$_3$O$_8$ is 8.39 g/cm^3 with a molecular weight of 842.0749 g/mole. For U(92.93)$_3$O$_8$, the molecular weight is 833.6397 g/mole. Thus, the theoretical density of U(92.93)$_3$O$_8$ is 8.306 g/cm^3.

The inclusion of neutron scatters such as oxygen has the effect of decreasing the theoretical density of the material, but it also decreases the critical mass for a given density. For example, to determine the critical masses of U(92.94)O_2 and U(92.93)$_3O_8$ at 6 g/cm^3,

$$U(92.94)O_2\text{:M } [kg] = \frac{13664 \left[\frac{\text{kg - g}^2}{\text{cm}^6}\right]}{(6 \text{ g/cm}^3)^2} = 379.56 \text{ kg}$$

While

$$U(92.94)_3O_8\text{:M } [kg] = \frac{13030 \left[\frac{\text{kg - g}^2}{\text{cm}^6}\right]}{(6 \text{ g/cm}^3)^2} = 361.94 \text{ kg}$$

(81)

which can also be seen by comparing the proportionality constants; the smaller the constant, the smaller the critical mass at a given density.

4.2.4   Core Density Conversion for Reflected, Homogeneous Systems

For reflected systems (see Figure 4-2) where the densities of core and reflector are changed by the same ratio, the relationships given in Table 4-1 are applicable. That is, the critical dimensions of both core and reflector scale inversely with the density. If only the reflector density or only the core density changes, then the relationships do not apply to the core dimensions. In fact, for the typical case where the reflector density is held constant and the core density changes, the core density conversion relationships cannot be stated in a simple exact form. The exponent varies with form of the core material (e.g., oxide versus metal), and with the reflector material (e.g., water versus natural uranium). There are a few historical studies that provide empirical correlations for the relationship between critical mass and density.
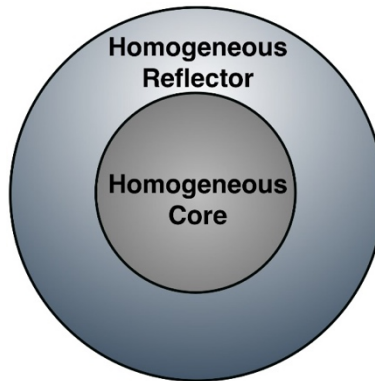
Figure 4-2. Illustration of a Reflected, Homogenous System.

One of the earliest documents providing an empirical relationship is LA-442, Part B written by E. Fermi. The empirical relationship "recommended by Oppenheimer (is)

$$\text{Critical Mass} \sim \rho^{-1.4}C^{-1.8}$$

(82)

where C is the fraction of 25[15] in the active material." (Reference 25, page 18). This relationship was applied to uranium-235 cores surrounded by uranium or tungsten carbide reflectors. A January 1955

---

[15] The term 25 refers to uranium-235. This is a shorthand for actinides where the first number (2) is the last digit of

report, LA-1958 (Reference 26, page 11), provides the following: "Critical masses of OY(93.5) spheres in thick normal uranium have been measured at various average densities of the oralloy. The resulting relation is of the form:

$$\text{Oy critical mass} \; \propto \; \rho^{-1.2"} \tag{83}$$

(Oy refers to oralloy or high-enriched uranium).

It appears that refinement of the experiments led to a change in the exponent from -1.4 to -1.2 for highly enriched uranium cores with natural (normal) uranium reflectors.

The Nuclear Criticality Safety Guide (Reference 27, page 75) indicates that for a highly enriched uranium metal core with an equivalent thick water reflector, the exponent is -1.4. This relationship applies to cores of highly enriched uranium and plutonium metal, as well as to UO_2, U_3O_8, UO_3, and PuO_2.

Cullen's work on mass and density relationships (Reference 24, page 4) provides exponents in the range of -1.46 to -1.51 for various uranium and plutonium oxides reflected by 10 cm of water. These relationships were derived using the TART computer program. Analyses of plutonium metal cores reflected by 30 cm water, and 20 cm of aluminum, titanium, and lead using the PARTISN code with Hansen–Roach cross sections provided exponent values between -1.36 and -1.46. Analysis of the same plutonium metal core reflected by natural uranium gives an exponent of -1.27.

Based on these analyses and reports, it appears that a reasonable estimate of critical mass based on density variation can be made using the relationships for water-reflected uranium and plutonium oxides:

$$\text{Critical Mass} \sim \rho^{-1.50} \tag{84}$$

while for water-reflected uranium and plutonium metal systems:

$$\text{Critical Mass} \sim \rho^{-1.45} \tag{85}$$

These relationships apply to all other reflectors except natural uranium and tungsten carbide. Systems with those reflectors seem to follow the relationship given in Eq. (83).

4.2.5   Variation of Critical Mass with uranium Enrichment

As indicated in Eq. (82), the critical mass of a uranium system reflected with either natural uranium or tungsten carbide varied with enrichment to the -1.8 power. Later work done at LANL in the 1950s indicates that the critical mass of uranium metal systems at a given density is proportional to the U-235 enrichment raised to the -1.7 power (Reference 25, pg. 11) and to the -1.71 power (Reference 28). This report shows the same relationship for unreflected and thick uranium–reflected uranium systems. "The critical mass of oralloy metal as a function of average U-235 concentration has been determined for nearly spherical oralloy in a reflector of thick normal uranium, and for a series of oralloy cylinders without reflector. After the data for the bare cylinders are corrected to apply to spheres, both sets of data are of the form Oy critical mass *is proportional to* (U-235 concentration) (-1.7). (Reference 25, pg.11). It

---

the atomic number of the element (= 9**2** for uranium), and the second number is the last digit of the atomic mass of the isotope (=23**5** for uranium-235). Thus, 49 would refer to plutonium-239 with an atomic number of 9**4** and an atomic mass of 23**9**.

should be noted that the relationship appears to break down for enrichments "in the neighborhood of 20%" (Reference 29, page 24).

PARTISN analyses for other reflectors indicate a variation with enrichment raised to the −1.5 power. Again, the exponent is dependent on the form of the core material and the type of reflector material. For unreflected systems, the exponent of −1.7 seems to apply. For example, using the critical mass of 51.6 kg total U for an unreflected U(93.8) metal core based on Godiva measurements (Reference 30, page 18), then the unreflected critical mass of U(37.7) would be:

$$\frac{m}{m_o} = \left(\frac{enrich}{enrich_o}\right)^{-1.7} \Rightarrow \frac{m}{51.6 \text{ kg}} = \left(\frac{37.7}{93.8}\right)^{-1.7} \quad m = 243.0 \text{ kg} \tag{86}$$

Calculating the critical U-235 mass in each enrichment gives 48.4 kg (=51.6 × 0.938) for U(93.8) and 91.6 kg (=243.0 × 0.377) for U(37.7). These results compare to about 49 kg and 91 kg, respectively, as read from Figure 4-3 (Figure 19, Reference 11). Note that enrichment can be entered into Eq. (85) either as a weight percent or a weight fraction if both values are consistent.
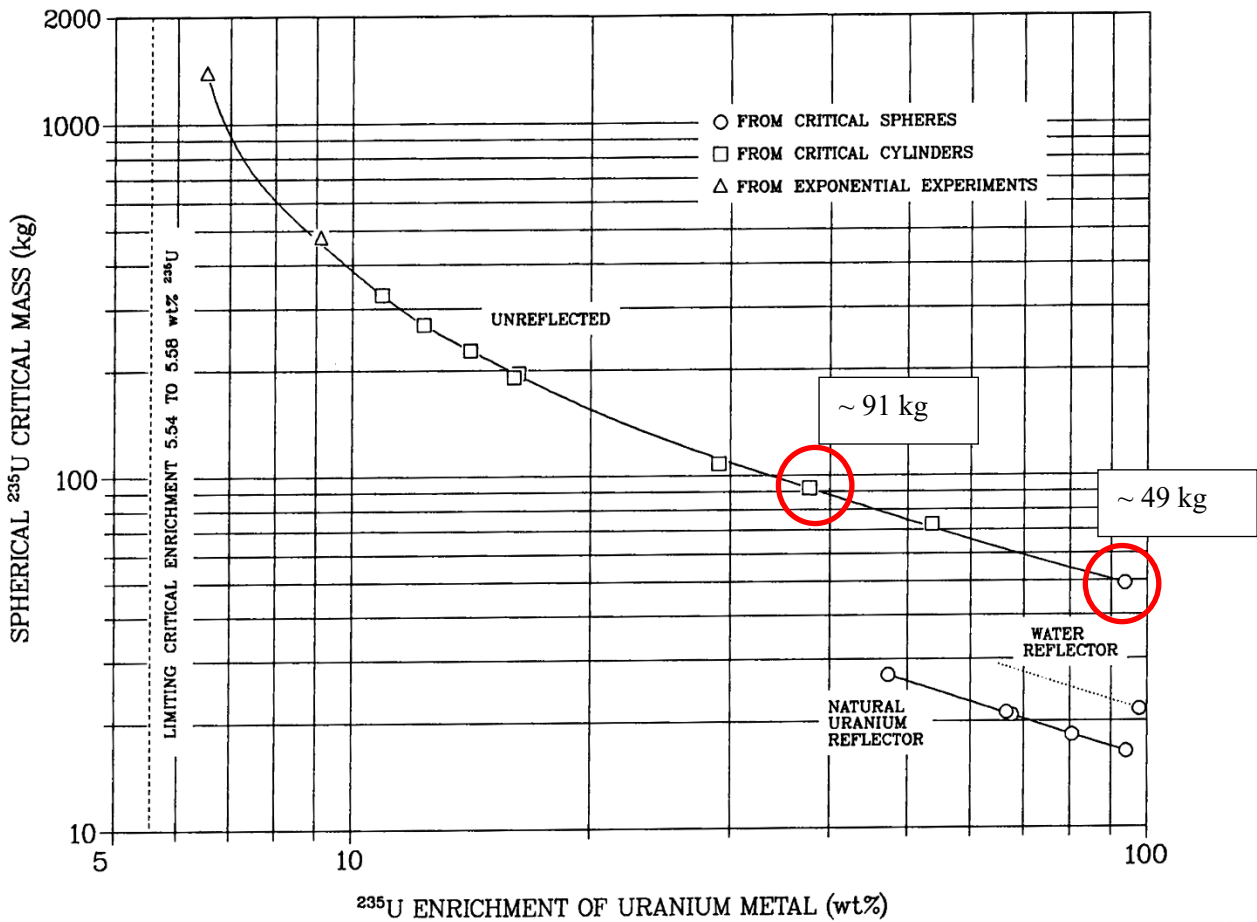
Figure 4-3. Critical Mass of U235 versus Enrichment of Uranium Metal. (Figure 19, page 43, LA-10860, reference 11.)

4.2.6   Critical Mass Data for Reflected Systems

Table 4-4 provides critical mass information for fissile metal spheres fully reflected by water. The data is extracted from Table 29 – page 97, Figure 43 – page 100, and Table 32 – page 101 in reference 11.

Table 4-4. Critical Mass Data for Fissile Metal Spheres Fully Reflected by Water.

Core Material	Density (g/cm³)	Radius (R_{exp}) (cm)	Fissile Mass (kg)	Total Mass (kg)
U(93.9)	18.5	6.83	U-235, 23.2	24.71
Pu(4.5)	15.61	5.05	Pu-239, 7.93	8.30
Pu(5.2)	19.74	4.20	Pu-239, 5.49	5.79
^{233}U(98.1)	18.42	4.66	U-233, 7.68	7.83

For oxide materials fully reflected by water, reference 24 is again used as the source of data. The systems are given in Table 4-3. As with Table 4-2, the value given in parentheses is the weight percent of the dominant fissile isotope (e.g., Pu[95.5] represents 95.5 wt. % Pu-239 with the rest of the materials as described in the diluent columns).

Table 4-5. Critical Mass Data for Fully Water Reflected Fissile Oxide Spheres.

	Data from Reference 24				
Core Material	Theoretical Density[16] (TD) (g/cm³)	Total Mass at TD (kg)	Diluent 1 Weight percent	Diluent 2 Weight percent	Diluent 3 Weight percent
U(92.94)O₂	10.845	41.68	U-234 0.99	U-238 6.07	N/A
U(92.93)₃O₈	8.306	72.39	U-234 0.99	U-238 6.08	N/A
Pu(93.46)O₂ *93.46% 239*	11.463	3.55	Pu-240 6.02	Pu-241 0.52	N/A
Pu(62.87)O₂ *62.87% 239*	11.483	4.70	Pu-240 22.73	Pu-241 12.68	Pu-242 1.72

4.3   USE OF CORE DENSITY CONVERSION

4.3.1   Application of the Core Density Conversion

The core density method is applicable for fissile material systems with the following characteristics and assumptions.

●   The system must have a uniform, homogeneous composition.

---

[16] The theoretical density for the isotope mixture is determined from the reference theoretical density for the compound divided by the molecular weight of the reference compound times the molecular weight of the isotope mixture compound. For example, the theoretical density of U(nat)₃O₈ is 8.39 g/cm³ with a molecular weight of 842.0749 g/mol. For U(92.93)₃O₈, the molecular weight is 833.6397 g/mol. Thus, the theoretical density of U(92.93)₃O₈ is 8.306 g/cm³.

- If the system is reflected, then the critical dimensions of both the core and reflector vary inversely with their density, assuming that the density of the core and reflector are changed by the same ratio.

- If the reflector density is held constant while the core density is changed, then the exponent in the relationship will be between −1.2 and −1.7 depending on the materials.

- For uranium systems with changes to the enrichment, the critical mass can be calculated based on the ratio of density changes and enrichment changes.

4.3.2   Limitations of the Core Density Conversion

The core density method has the following limitations to consider.

- The method cannot be used if the system contains heterogeneities such as lumps of fuel or fuel rods in a reactor.

- For reflected systems, if the reflector density changes, or if the core density changes are not uniform, then the relationships presented in this section cannot be used to derive new system dimensions.

4.4   CORE DENSITY EXAMPLE PROBLEMS

4.4.1   Core Density Example Problem 1

Calculate the critical mass for a spherical, unreflected Pu(4.5) metal system that is changed from delta phase (15.6 g/cm^3) to alpha phase with a density of 19.8 g/cm^3. Recall that Pu(4.5) is a system with 95.5 at. % Pu-239 and 4.5 at. % Pu-240. The core density conversion method can be used to calculate the bare critical mass for this system. The unreflected, spherical critical mass for a Pu(4.5) system with a density of approximately 15.6 g/cm^3 is approximately 16.8 kg (Reference 11, Table 32). Note that this is less than the critical mass of 17.07 kg given in Table 4-2. The difference is likely due to better experimental data and evaluation of uncertainties for the information in Table 4-2. This indicates that although the core density conversion process is exact, there can be significant variation in the values provided for critical masses. For this example, we will use both values and see what the range of results will be.

Using the spherical critical mass relationship in Table 12, the critical mass for this system can be calculated as follows:

$$\frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^{-2}$$

$$m = m_o\left(\frac{\rho}{\rho_o}\right)^{-2} = (16.8\text{kg}) \times \left(\frac{19.8\text{g/cm}^3}{15.6\text{g/cm}^3}\right)^{-2} = 10.43 \text{ kg}$$

$$m = m_o\left(\frac{\rho}{\rho_o}\right)^{-2} = (17.07\text{kg}) \times \left(\frac{19.8\text{g/cm}^3}{15.61\text{g/cm}^3}\right)^{-2} = 10.61 \text{ kg}$$

Thus, the initial difference of less than 2% creates a similar difference of less than 2% in the new critical masses. For hand calculations and most uses of these methods, the 2% variation will be acceptable for bounding and scoping calculations.

4.4.2 Core Density Example Problem 2

Calculate the critical radius for a spherical, unreflected U(93.5)-H_2O system with a density of 10.0 g/cm³, assuming that the initial density for this system was 18.9 g/cm³.

Recall that U(93.5) is a system with 93.5 at. % U-235 and 6.5 at. % diluent uranium. The core density conversion method can be used to calculate the bare critical mass for this system. Based on Figure III.B.9(93.5)-2 from Volume II, Reference 7, the unreflected volume at 18.9 g/cm³ is 2.15 L. We can also find the unreflected critical volume at 10.0 g/cm³ to be 4.8 L, which we will use to check our answer.

The critical radius for the system with density of 18.9 g/cm³ is as follows:

$$r = \left(\frac{3 \times V}{4\pi}\right)^{\frac{1}{3}} = \left(\frac{3 \times 2,150 cm^3}{4\pi}\right)^{\frac{1}{3}} = 8.01 cm$$

Then, using critical sphere radius relationship from Table 4-1, with the new density of 10.0 g/cm³,

$$\frac{r}{r_o} = \left(\frac{\rho}{\rho_o}\right)^{-1} r = r_o \left(\frac{\rho}{\rho_o}\right)^{-1} = 8.01 cm \left(\frac{10.0 g/cc}{18.9 g/cc}\right)^{-1} = 15.14 cm$$

compare the result against the value derived from Figure III.B.9(93.5)-2 from Volume II.

$$r = \left(\frac{3 \times V}{4\pi}\right)^{\frac{1}{3}} = \left(\frac{3 \times 4,850 cm^3}{4\pi}\right)^{\frac{1}{3}} = 10.46 cm$$

Note that the core density conversion gives a much larger radius than is actually the case. This indicates that core density conversion is not applicable to systems containing hydrogen (in this case, water) or those where the neutron spectrum is changed by the change in system density.

4.4.3 Core Density Example Problem 3

Repeat example problem 2 with systems containing U(92.94)O_2. Calculate the critical radius for a spherical, unreflected system with a density of 6 g/cm³, assuming that the initial density for this system was 10.845 g/cm³.

From Table 4-3, we find that the critical mass of U(92.94)O_2 at 10.845 g/cm³ is 116.2 kg. Using this, we can calculate the critical volume and critical radius at that density.

$$V = \frac{M_c}{\rho} = \frac{116.2 kg}{10.845 kg/liter} = 10.71 liters$$

$$r = \left(\frac{3 \times V}{4\pi}\right)^{\frac{1}{3}} = \left(\frac{3 \times 10,710 cm^3}{4\pi}\right)^{\frac{1}{3}} = 13.67 cm$$

Then, using critical sphere radius relationship from Table 4-1, with the new density of 5.0 g/cm³,

$$\frac{r}{r_o} = \left(\frac{\rho}{\rho_o}\right)^{-1} r = r_o\left(\frac{\rho}{\rho_o}\right)^{-1} = 13.67cm\left(\frac{5.0g/cc}{10.845g/cc}\right)^{-1} = 29.65cm$$

Checking these values against those from PARTISN, we find the critical radius at theoretical density (=10.845 g/cm³) is 13.65 cm, whereas the critical radius for the system with a density of 5.0 g/cm³ is 29.62 cm. The closeness of the values indicates that for uranium oxide systems, the core density conversion process is applicable and provides useful results.

4.4.4   Core Density Example Problem 4

Calculate the critical mass for a spherical, unreflected $^{239}PuO_2$ system with a density of 1, 3, 5, 7, and 9 g/cm³, assuming that the initial density for this system was 11.46 g/cm³ (i.e., theoretical density). Compare the results to the results calculated in Section 2.6.3 (Diffusion Theory Example Problem 3). The critical mass for an unmoderated $^{239}PuO_2$ system at theoretical density was calculated in Section 2.6.3, using diffusion theory,[17] as approximately 31 kg. Using the critical mass relationship from Table 4-1 for a spherical system, the critical mass for this unmoderated system can be calculated for the densities of interest. As an example of the process, we will calculate the critical mass for a density of 10 g/cm³:

$$\frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^{-2}$$

$$m = m_o\left(\frac{\rho}{\rho_o}\right)^{-2} = (31\text{kg}) \times \left(\frac{1.0\text{g/cm}^3}{11.46\text{g/cm}^3}\right)^{-2} = 4071 \text{ kg}$$

This calculation is repeated for the other densities of interest. The resulting critical mass estimates for the system are summarized in Table 4-6.

Table 4-6. Calculation Results for Core-Density Example Problem 4.

Density of Pu (g/cm³)	Critical Spherical Radius (cm)	Estimated Critical Mass of PuO₂ (kg) (One-Group Diffusion Theory)	Estimated Critical Mass of PuO₂ (kg) (Core-Density Method)
1.0	99.1	4,080	4,071
3.0	33.0	453	452
5.0	19.8	163	163
7.0	14.2	83	83
9.0	11.0	50	50

Notice that the results are essentially the same as the critical mass estimates from Section 2.6.3. If the initial critical mass is known with some confidence and the applicability of this technique is valid (Section 4.3), then the critical mass estimates at other densities can be estimated very accurately with the core density method. Note that the starting point being the critical mass determined from PARTISN calculations (27 kg) or from SCALE calculations (27.8 kg) leads to the same set of answers as provided in

---

[17] The diffusion theory value is used, as it is consistent with the diffusion theory critical mass values shown in Table 2-8 and those used for comparison in Table 4-6.

Table 2-8. That is, at 1.0 g/cm³ density, the critical mass from the core density conversion method is 3,546 kg from PARTISN, which is within round-off of the 3,540 kg in the table.

4.4.5   Core Density Example Problem 5

Calculate the water-reflected critical mass for a spherical U(93.5)O_2 system with a density of 5.0 g/cm³ if the oxide had an initial density of 10.85 g/cm³.

Using the information in Section 4.2.4, the critical mass of a water-reflected oxide systems should be related to density as expressed in Eq. (84). From a PARTISN run, the reflected critical mass of uranium oxide at theoretical density is 50.8 kg. Then the reflected critical mass at a density of 5.0 g/cm³ would be:

$$\frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^{-1.5}$$

$$m = m_o\left(\frac{\rho}{\rho_o}\right)^{-1.5} = (50.8\text{kg}) \times \left(\frac{5.0\text{g/cm}^3}{10.85\text{g/cm}^3}\right)^{-1.5} = 162.4 \text{ kg}$$

Calculations from PARTISN give a reflected critical mass of 162.4 kg at 5.0 g/cm³. This value matches quite well with that determined from the core density conversion. This is somewhat expected as the exponent in Eq. (84) was determined from parametric studies using PARTISN. This process of determining reflected critical mass is much less exact than many hand calculations, so it can be used for bounding of scoping calculations. In the case, the value calculated using Eq. (84) should provide a value within a few percent of that from the computer analysis.

4.4.6   Core Density Example Problem 6

Calculate the water-reflected critical mass for a spherical, Pu(5) metal systems with a density of 15.61 g/cm³ from a density of 19.8 g/cm³. Repeat problem for a density of 19.8 g/cm³ from a density of 15.61 g/cm³.

Another method of determining critical mass for reflected systems is given in Reference 11, page 19. This uses the same form of the core density conversion equation, with the exponent determined from the plot shown in **Figure 4-4**. The data are applicable to U(93.5) metal and δ-phase plutonium cores. The plot shows the variation of the exponent with the degree of reflection as characterized by the ratio of the reflected crtical radius to the unreflected critical radius.

$$\frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^{-n}$$

For this system, we need the reflected and unreflected critical mass of Pu(5) at any density. Most likely these values will be available for the theoretical density, but this is not always the case. Let's start with the 19.8 g/cm³ system and use that information to determine the critical mass for reflected plutonium metal at 15.61 g/cm³. The critical mass of a water reflected sphere of Pu(5) at 19.8 g/cm³ is 5.79 kg from Table 4-4. The unreflected critical mass of such a system was calculated in example problem 1 of this section (Section 4.4.1) and was determined to be 10.61 kg. Then, we need to calculate the ratio of the radii to determine the exponent from **Figure 4-4**.

$$\frac{r_{refl}}{r_{unrefl}} = \left(\frac{m_{refl}}{m_{unrefl}}\right)^{\frac{1}{3}} = \left(\frac{5.79 \text{ kg}}{10.61 \text{ kg}}\right)^{\frac{1}{3}} = 0.817$$

With an x-value of 0.817, the exponent read from **Figure 4-4** is 1.52. Using this, we can calculate the critical reflected mass at a density of 15.61 g/cm³.

$$\frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^{-1.52} \quad m = m_o\left(\frac{\rho}{\rho_o}\right)^{-1.52} \quad m = 5.79 \text{ kg} \left(\frac{15.61 \text{ g/cc}}{19.8 \text{ g/cc}}\right)^{-1.52} = 8.31 \text{ kg}$$

This value compares quite well with the 8.30 kg found in Table 4-4.

We will repeat the process for 15.61 g/cm³ data to determine the reflected critical radius of the system at a density of 19.8 g/cm³, The critical mass of a water reflected sphere of Pu(5)) at 15.61 g/cm³ is 8.30 kg from Table 4-4. The unreflected critical mass of such a system is given in Table 4-2 as 17.07 kg. Now we need to calculate the ratio of the radii to determine the exponent from **Figure 4-4**.

$$\frac{r_{refl}}{r_{unrefl}} = \left(\frac{m_{refl}}{m_{unrefl}}\right)^{\frac{1}{3}} = \left(\frac{8.30 \text{ kg}}{17.07 \text{ kg}}\right)^{\frac{1}{3}} = 0.786$$

With an x-value of 0.786, the exponent read from **Figure 4-4** is 1.45. Then, we can calculate the critical reflected mass at a density of 19.8 g/cm³.

$$\frac{m}{m_o} = \left(\frac{\rho}{\rho_o}\right)^{-1.45} \quad m = m_o\left(\frac{\rho}{\rho_o}\right)^{-1.45} \quad m = 8.30 \text{ kg} \left(\frac{19.8 \text{ g/cc}}{15.61 \text{ g/cc}}\right)^{-1.45} = 5.88 \text{ kg}$$

This value is a little bit higher than the 5.79 kg found in Table 4-4. This difference is partly due to variations in Pu-240 content among the various entries in Table 4-2 through Table 4-5. Also, variation of ±0.05 in the exponent leads to a variation of ±0.07 kg in critical mass. Notice that the value of the exponent from **Figure 4-4** matches that given in Eq. 85.

The results can be compared with SCALE 6.1.3 calculations for Pu(5) systems. For a density of 15.61 g/cm³, the total mass was 8.30 ± 0.04 kg, whereas for a density of 19.8 g/cm³, the total mass was 5.79 ± 0.03 kg.
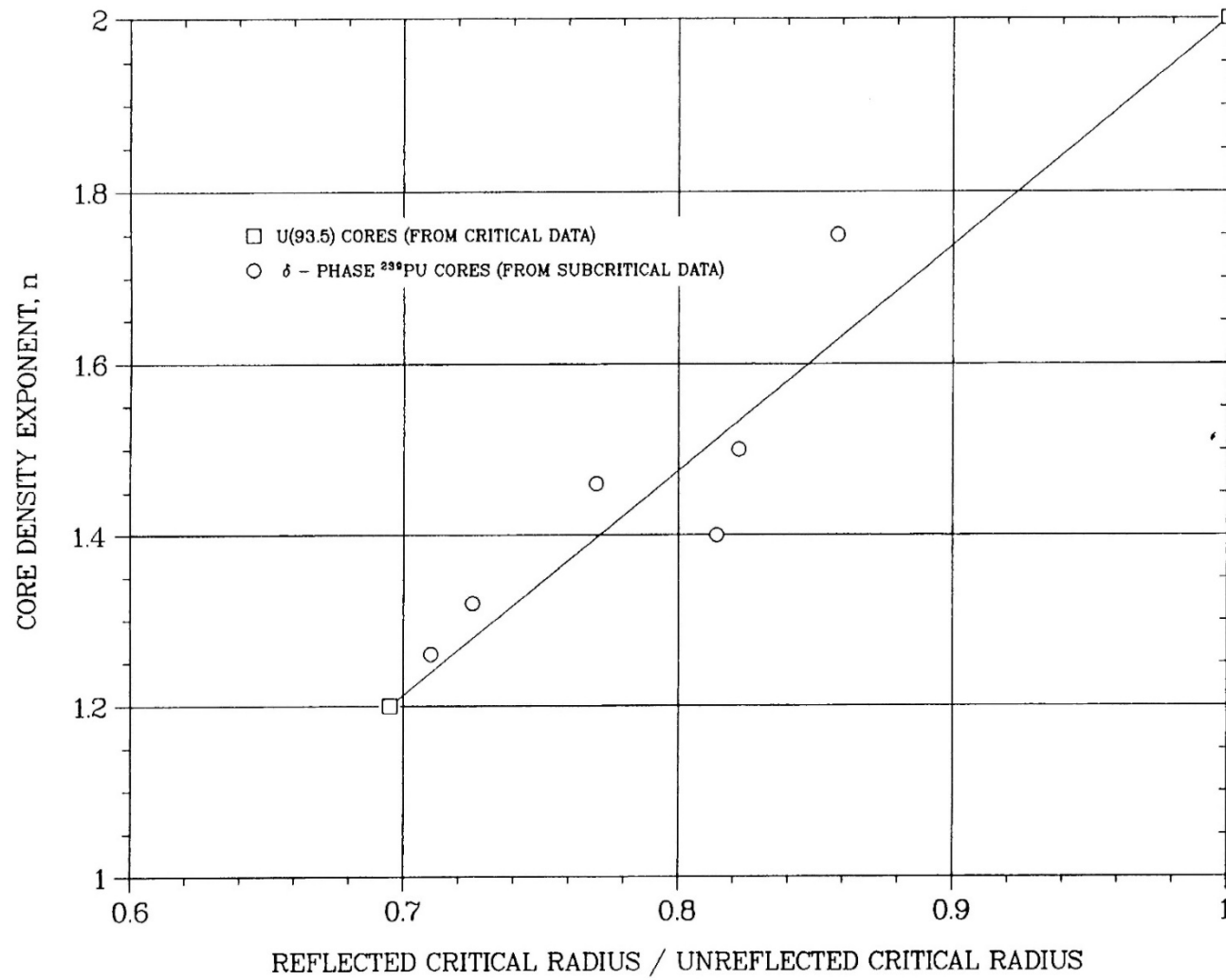
Figure 4-4. Density Exponents of Unmoderated Spherical Cores in Constant Density Reflectors. (Figure 8, page 20, Reference 11.)

5. ARRAY CRITICALITY CALCULATIONS

5.1 WHAT YOU WILL BE ABLE TO DO

- List the various hand calculation methods covered in this primer.
- Discuss the various hand calculation methods applicable to arrays of fissile materials.
- Identify the applicability, limitations, and data requirements needed for the various array methods.

5.2 OVERVIEW OF ARRAY CALCULATIONS

The best review of methods used to evaluate the criticality safety of arrays of fissile materials is provided by Hunt, 1976 (reference 31). He states,

The methods commonly used in this country to evaluate the criticality safety of fissile material arrays include density analog, NBN^2 surface density, equilateral hyperbola, albedo, and solid angle techniques. These can be divided into array unit interaction and semiempirical methods. The albedo and solid-angle techniques fall into the former class; the rest fall into the latter class.

A study reveals that interaction methods are useful in treating arrays of arbitrary mesh patterns (e.g., triangular or hexagonal) having only a few units, while the semiempirical techniques are more applicable to arrays with a large number of units. The density analog and surface density approaches are easy to apply but typically require more auxiliary calculations, while other methods are more difficult to use, but more broadly applicable.

None of the methods satisfactorily handle nonuniformly spaced arrays, arrays with arbitrary amounts of internal moderator, or "clumped" arrays, i.e., arrays of arrays. Most of the methods have some provision for treating mixed arrays, but these provisions often do not apply to arrays of arbitrarily arranged fast (e.g., metal) and slow (e.g., solution) units.

5.3 SUMMARY OF ARRAY CALCULATION METHODS COVERED IN THIS PRIMER

For what Hunt terms the *unit interaction methods*, this document covers only the solid angle technique. The solid angle method is applicable to the following:

- Small numbers of moderated fissile units.
- Each individual unit must have $k_{eff} \leq 0.8$, and a unit must be subcritical when subjected to full water reflection.
- If flooding is credible, then the separation between units must be ≥ 0.3 m (1 ft).
- Any reflector must not be more effective than a thick water reflector at the boundary of the array.
- The method is more practical and reliable for arrays consisting of a small number of units (for example, <64).

More detail provided in Section 6 – The Solid Angle Method.

For what Hunt terms the *semiempirical methods*, this document covers only the surface density, density analog, and limiting surface density (or NB_N^2) techniques.

The limiting surface density or NB_N^2 method is applicable to:

- Fissile arrays of any shape provided that the necessary array and fissile data are known (i.e., total number of units, mass of a unit, and the least number of units along an array edge).
- Must have at least 64 units in the array.
- Can have different fissile materials and different reflector materials.
- Method is comprehensive, so it can be more difficult than the other methods in its understanding and its application.

More detail is provided in Section 7 – The Limiting Surface Density or NB_N^2 method.

The surface density method is applicable to the following:

- Fissile array with one dimension limited (e.g., number of units high).
- Can handle units of irregular shapes (e.g., different pieces of equipment containing fissile material).
- Requires the dimensions of a water-reflected infinite slab of the same fissile material stored in the array.

More detail is provided in Section 8 – The Surface Density Method.

The density analog method is applicable to the following:

- Fissile arrays with no limitations on array arrangement but a finite number of units.
- Requires the dimensions of a water-reflected infinite slab of the same fissile material stored in the array.
- Requires the bare, spherical critical mass for the material stored in the array.

More detail is provided in Section 9 – The Density Analog Method.

Hunt's review for these models and methods leads to several general conclusions:

- Solid angle methods, including the ORGDP and albedo procedures, are more practical and reliable for arrays consisting of a small number of units (for example, <64). This is because these methods rely on interaction probabilities for two-unit interactions and do not adequately account for interposed units. For arrays with no interposed units, the methods are flexible and can often be used in determining the critical parameters of nonuniformly spaced, arbitrarily shaped arrays (e.g., an L-shaped or T-shaped planar array of cylinders with different unit spacing in different directions). These methods are most conservative for planar arrays of solution units and can be nonconservative for reflected three-dimensional arrays of compact metal units.
- Density analog and surface density methods are most applicable to arrays with many units. For density analog techniques, this is because of the analogy of "lumpy" arrays with single homogeneous solids, whereas for surface density methods, it occurs because of the assumption of mass nearly uniformly distributed over some specific area.
- The first two conclusions indicate that the two types of methods are complementary to each other, and that the user should be able to select one or the other depending on their need.
- There is currently no method that considers clumped arrays.
- No method offers a comprehensive treatment of internally moderated arrays.

- The albedo method involves the solution of a set of algebraic equations for application, whereas the ORGDP solid-angle method requires (a) calculation of the multiplication factor of a single array unit either bare or half-reflected, and (b) calculation of the total solid angle of interaction seen by the centermost unit of an array. In practice, the ORGDP method is easier to use but more approximate.
- The original Los Alamos Scientific Laboratory density analog work is easy to use but limited in applicability. The extension of this by Thomas as the NB_N^2 method is more flexible and comprehensive but harder to apply. In the NB_N^2 method, several factors, and array conversions based on these factors, must be calculated so that it is not a method that can be quickly and easily applied by a criticality engineer.
- The two surface density methods are readily applied by the nuclear safety specialist. The surface density method using unit shape factor, s/v version (Reference 32), has been more extensively developed and is preferred over the Paxton–Gutman version, since it considers more factors and is based on more reliable data.
- No method handles nonuniformly spaced arrays with many elements very well. The best attempt for large arrays is in the s/v method, where up to 15% nonuniformity in array unit spacing is permitted before the remainder of the model rules becomes invalid.
- The equilateral hyperbola formulation is useful and valid but needs more development before it is of much worth in solving a range of criticality problems.
- Most methods are based on weapons-related data that deal with high-enrichment material. The application of these methods to low-enrichment systems is usually possible if suitable input parameters are available. This point is discussed further and calculationally illustrated in Hunt and Dickinson (Reference 33).

6. SOLID ANGLE METHOD

6.1 WHAT YOU WILL BE ABLE TO DO

- Determine the total solid angle for a small number of moderated fissile units arranged in an array configuration.

- Based on solid angle restrictions for an array, calculate the minimum spacing that moderated fissile units can have in an array configuration.

6.2 SOLID ANGLE METHOD OVERVIEW

This technique has been around since the late 1940s. The basic idea behind this method is that the multiplication factor for fissile materials in an array configuration depends on the multiplication factor for a single, representative fissile unit in an array and the probability that a neutron will leak out of this fissile unit and interact with another unit. This interaction will increase the overall multiplication factor for the array system. The probability that a neutron leaks out of a fissile unit to intersect another is dependent upon the solid angle occupied at the most central unit by all the other units of the array. This method was developed as a quick, empirical means of evaluating interaction among small numbers of moderated fissile units (References 34 and 35). Application of the method, which is based on experiments with aqueous solutions, to small numbers of closely spaced units characterized by a fast neutron spectrum can result in nonconservative spacing. (Reference 36).

"Analytic representation of criticality in terms of the total solid angle subtended by the unit nearest the center of an array has permitted an evaluation of the margin of subcriticality implicit in an allowable total solid angle, Ω_A. It is shown that the method cannot have general applicability but is dependent upon the type of fissile material, the number and specific arrangement of the units in an array, and the array reflector conditions. The method is principally one of comparison. The relative difference between the allowed total solid angle and the total solid angle corresponding to criticality is a measure of the safety. This study demonstrates that the arbitrary application of an Ω_A to an array of fissile material without having established the magnitude of the margin of subcriticality is questionable. The method is usable provided the area of applicability is defined by a validated method" (Thomas, Reference 37).

This technique was developed by accumulating a great deal of experimental data in aqueous solutions and the development of a correlation that is dependent upon the reactivity of the individual units in the array and the maximum sold angle subtended at the central fissile unit by the other fissile units in the array. References 34 and 37 provide additional information about the development of this method for use in array calculations.

The solid angle method specifies a maximum allowable solid angle subtended at any unit, with a neutron multiplication factor k_{eff}, by all other units in the array. A given array is then judged to be subcritical if the actual solid angle is equal to or less than the allowed solid angle given by

$$\Omega_{allowable} = 9 - 10 \times k_{eff} \tag{87}$$

where: $\Omega_{allowable} =$ the allowable solid angle in steradians (sr) that may be subtended at the center of any fissile unit (the most reactive fissile unit) of the array by the remainder of the units in the array.

$k_{eff} =$ the effective multiplication factor for an unreflected fissile unit in the array.

This relationship has been shown to be acceptable for different array configurations and fissile materials. Figure 6-1 illustrates the allowable solid angle as a function of the multiplication factor for the array units under consideration. A certain configuration of array units is safe if the solid angle subtended by the units of the array falls to the left and below the curve in Figure 6-1.
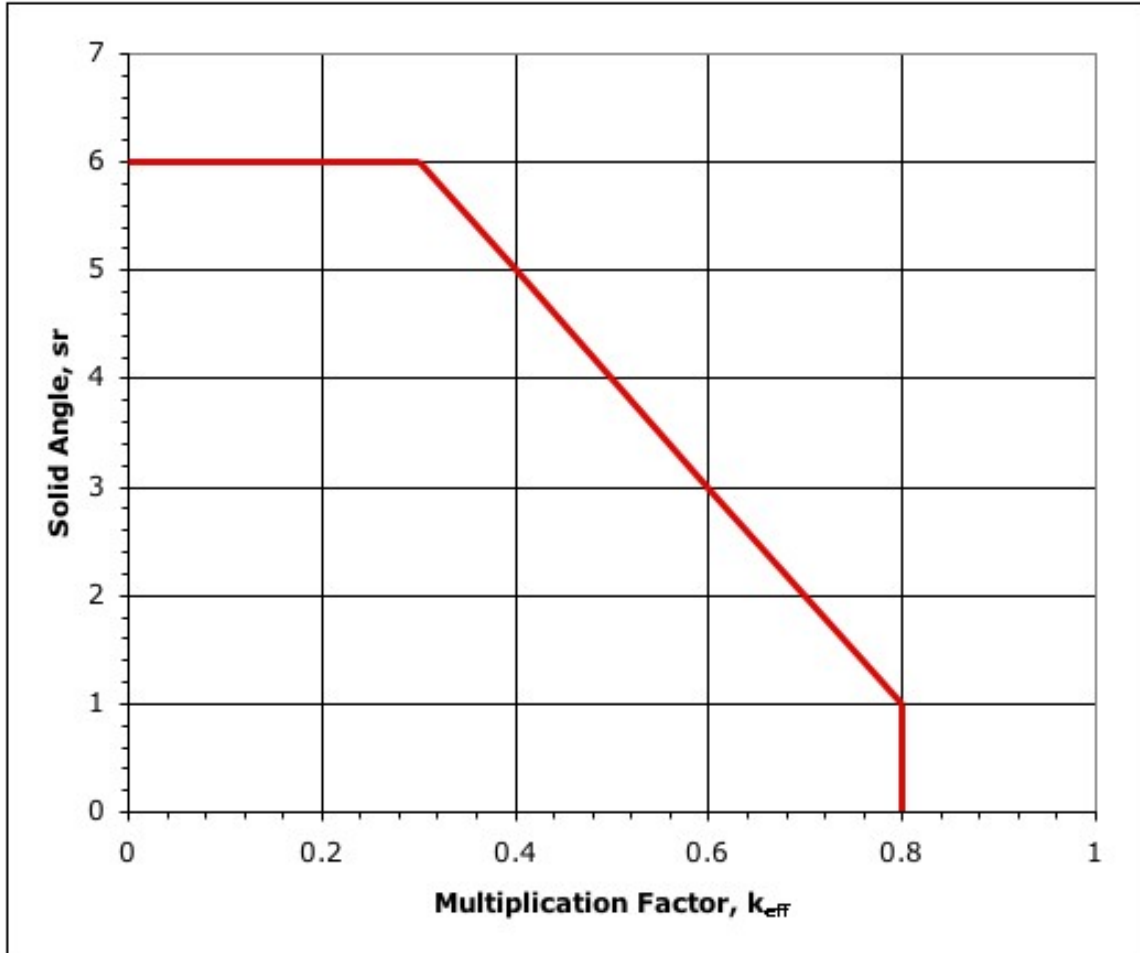
Figure 6-1. Allowable Solid Angle ($\Omega_{allowable} = 9\text{-}10k_{eff}$).
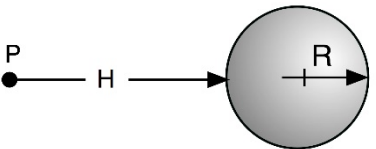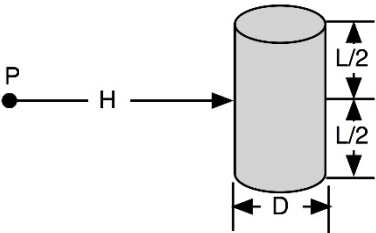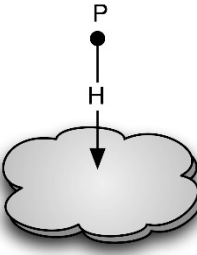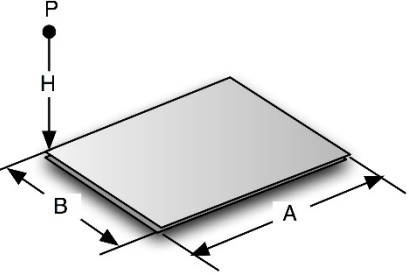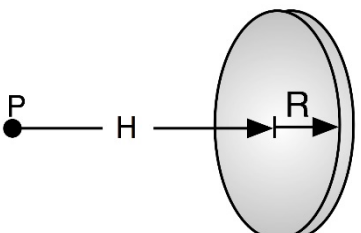
The solid angle between array units is calculated using the applicable method from Table 6-1. These methods consider the solid angle between a point and various shapes (e.g., arbitrary shape, disks, cylinders, spheres, planes, etc.). The point, P, in the figures is meant to represent the center-most unit of the array. Using these methods for each unit in the array, the total solid angle subtended at this center-most unit, P, is simply the sum of each of the solid angle contributions from the array units. Table 6-1 includes the most common formulae for use in this primer. More complicated situations such as determining the solid angle between the centermost array unit and an offset cylinder, plane or disk can be calculated using the guidance in Reference 35, (Figure 4-2, page 100) and will not be included here.

6.3   APPLICABILITY FOR THE SOLID ANGLE METHOD

There are some important points to consider when using this method. This method is applicable for the following situations and configurations.

- This technique is applicable to small numbers of moderated fissile units. The experimental data used to develop this technique considered aqueous solutions.

- Users wishing to apply this method to large arrays of metal or oxide systems with intermediate or fast neutron spectra should be cautioned that the results obtained from the solid angle method can be non-conservative (Reference 35).

- The multiplication factor, k_{eff}, of any unit should not exceed 0.80.

- Each unit considered should be subcritical with thick water reflection.

- The minimum separation distance between fissile units should be 0.3 m (1 ft).

- The allowed solid angle according to the method shall not exceed 6 steradians.

- The effectiveness of the reflector surrounding the array of fissile units should not be more effective than a thick water reflector located at the boundary of the array (Reference 35). The boundary location is no closer to the peripheral array units than about half of the edge-to-edge separation between fissile units. Concrete reflection on three sides of the array can be shown to meet the effectiveness criterion. For full reflection by concrete thicker than 12 cm, the allowable solid angle shall be reduced by 40% (Reference 35, page 101).

Table 6-1. Solid Angle Approximate Formulas (Reference 35).

Point-to-Sphere	Point-to-Cylinder	Point-to-Arbitrary Shape

Point-to-Sphere

$$\Omega = 2\pi \left(1 - \frac{1}{\sqrt{1 + \left(\frac{R}{H}\right)^2}} \right)$$

where:
R = radius of sphere
H = distance from the point to the surface of the sphere.

Point-to-Cylinder

$$\Omega = \frac{LD}{H \sqrt{\left(\frac{L}{2}\right)^2 + H^2}}$$

where:
L = length of cylinder
D = diameter of cylinder
H = distance from the point to the surface of the cylinder.

Point-to-Arbitrary Shape

$$\Omega = \frac{\text{Cross Sectional Area}}{H^2}$$

where:
H = distance from the point to the surface of the shape.

Point-to-Plane	Point-to-Disk

Point-to-Plane

$$\Omega = \sin^{-1}\left(\frac{AB}{\sqrt{A^2 + H^2} \times \sqrt{B^2 + H^2}} \right)$$

where:
A = length of one side of plane
B = length of other side of plane
H = perpendicular distance from the point to the corner of the plane.

If the point P is directly above the center of the plane with dimensions 2A × 2B, multiply W by 4 to obtain solid angle. This also works for cylinders with half height = A and radius = B.

Point-to-Disk

$$\Omega = 2\pi \left(1 - \frac{1}{\sqrt{1 + \left(\frac{R}{H}\right)^2}} \right) \leq \frac{\pi R^2}{H^2}$$

where:
R = radius of disk
H = distance from the point P to the surface of the disk.

6.4 SOLID ANGLE METHOD EXAMPLE PROBLEMS

6.4.1 Solid Angle Example Problem 1

Calculate the allowable solid angle for a 3×3×1 array of aluminum containers filled with a U(4.89)O$_2$F$_2$ and water mixture with a hydrogen to U-235 (H/X) ratio of 524. Figure 6-2 provides a sketch of the array looking down from the top. Each container has the following characteristics:

- Inside diameter of 15.24 cm (6 in.),
- Outside diameter of 15.56 cm (6.125 in.),
- Inside height of 100 cm (39.37 in.), and
- Outside height of 110 cm (43.31 in.).

Characteristics of Array (Figure 6-2):

- Separation (edge-to-edge, ETE) = 60.96 cm (24 in.)
- Pitch (center-to-center, CTC) = 76.52 cm (30.125 in.)
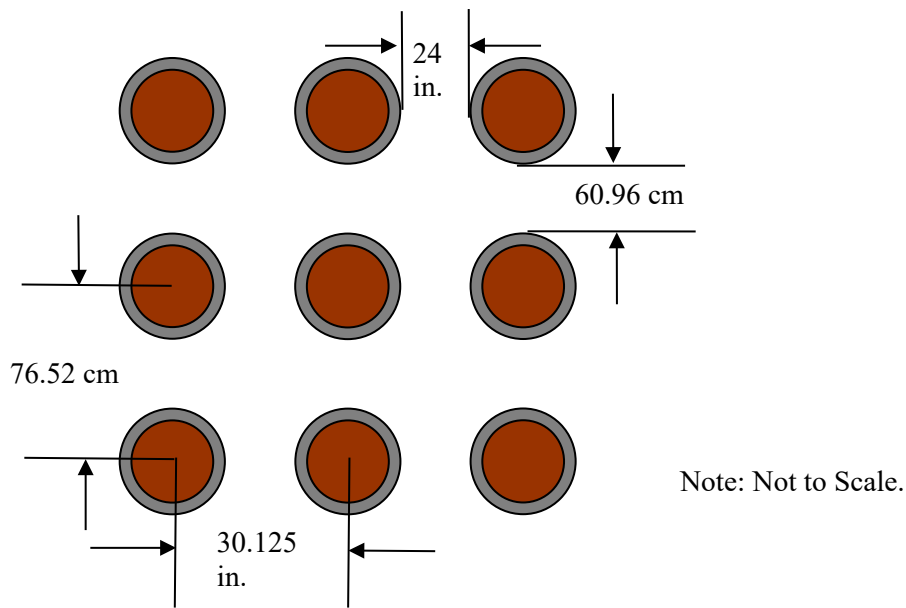
Figure 6-2. Illustration of the 3×3×1 Array for Solid Angle Example Problem 1.

There is a need to store the solution bottles in a 3×3×1 array as shown in Figure 6-3. A SCALE 6.1.3 calculation indicated the multiplication factor for an unreflected container of U(4.89)O$_2$F$_2$ solution is 0.378 ± 0.001. Therefore, each unit in this problem has a multiplication factor of less than 0.8 and meets the solid angle criteria. Also, the minimum separation distance between array units is 0.6 m, which is greater than the minimum solid-angle-method separation distance of 0.3 m.
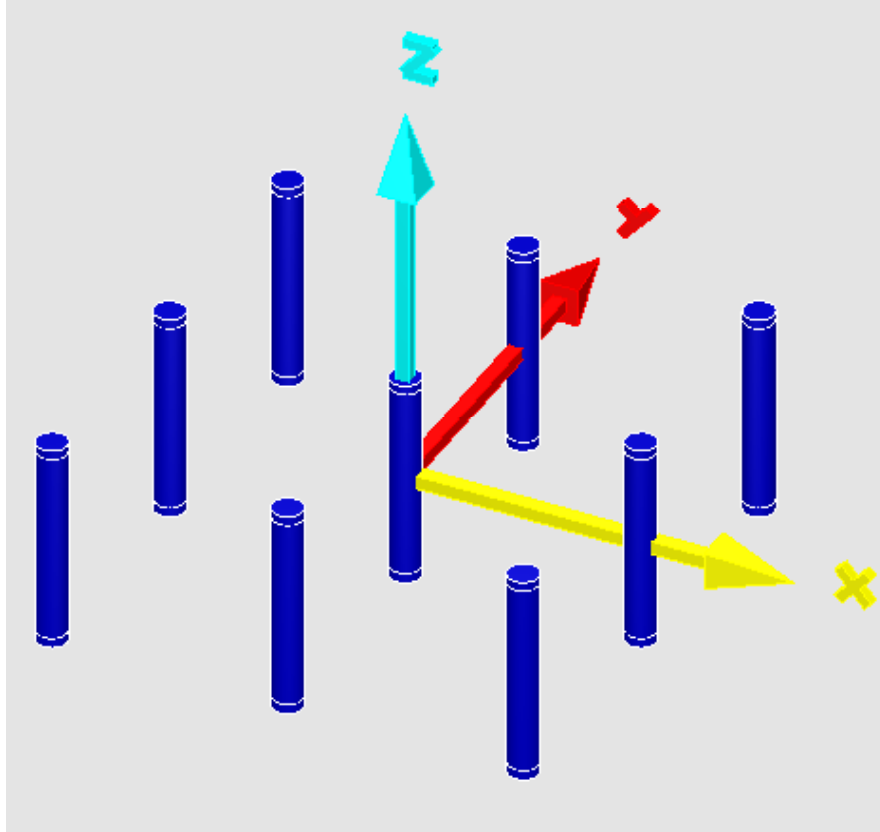
Figure 6-3. KENO3D Illustration of the Array for Solid Angle Example Problem 1.

In many cases, the analyst may not know the multiplication factor of an unreflected single unit before starting a solid angle problem; however, some approximations are presented in Appendix B, which can be used to perform the multiplication factor check. The array is not reflected externally by any materials such as water or concrete, so the solid angle analysis will provide conservative results because the method assumes that the array is externally reflected by water.

The "point-to-cylinder" solid angle formula from Table 6-1 may be used to calculate the solid angle for each unit in the array. The solid angle subtended by each unit in the array is then summed together to obtain the total solid angle, and the result is compared to the applicability plot in Figure 6-1.

$$\Omega = \frac{LD}{H\sqrt{\left(\frac{L}{2}\right)^2 + H^2}}$$

where, as indicated in Table 6-1,

L – length of each cylinder (cm)[18];
D – cylinder inside diameter (cm); and
H – distance from the point, P, and the cylindrical surface (cm).

---

[18] Although H is often used to indicate the height of a cylinder, the solid angle methodology uses L as the cylinder height or length and H is the point-to-surface distance used in the solid angle equations.

Note that H is the distance from the center point P of the "centermost" cylinder to the surface of another cylinder. This is equal to the pitch minus the cylinder radius. However, as the neutrons interact with the material inside the cylinder, this distance is usually calculated as the pitch minus the inside radius of the other cylinder.

Now, one can calculate the solid angle for each unit in the array. As shown in Figure 6-4, the four units identified as A have the same center-to-center distance with respect to the centermost unit, X. The value of *H* for these units would be 76.52 cm – (15.24 cm / 2) = 68.90 cm.
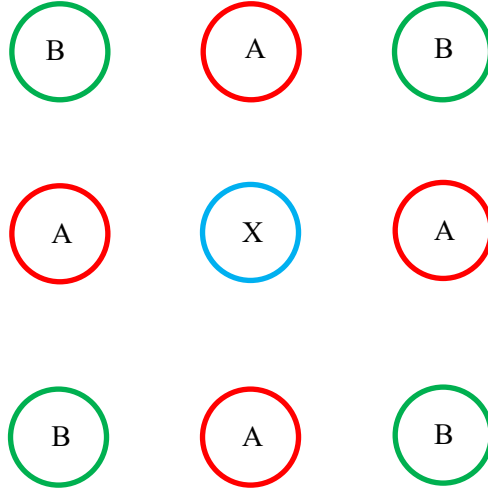
Figure 6-4. Units with Similar Distances from Centermost Unit, X.

Calculating the solid angle subtended by a cylinder of type A with respect to cylinder X,

$$\Omega_1 = \frac{LD}{H\sqrt{(\frac{L}{2})^2 + H^2}},$$

$$\Omega_1 = \frac{(100 \ cm)(15.24 \ cm)}{(68.90 \ cm) \times \sqrt{(100 \ cm/2)^2 + (68.90 \ cm)^2}},$$

$$\Omega_1 = 0.26 \ sr.$$

As there are four A units, the total solid angle from these units is:

$$\Omega_1 + \Omega_2 + \Omega_3 + \Omega_4 = 4 \times \Omega_1 = 4 \times 0.26 = 1.04 \ sr.$$

The solid angle from each of the remaining four units (B units at the four corners of the array) can now be calculated by using the same relationship as above with the appropriate value of H:

$$H_5 = Pitch \times \sqrt{2} - \frac{ID}{2} = 76.52cm \times \sqrt{2} - \frac{15.24cm}{2} = 100.6 \ cm$$

$$\Omega_5 = \frac{(100 \ cm)(15.24 \ cm)}{(100.60 \ cm) \times \sqrt{(100 \ cm/2)^2 + (100.60 \ cm)^2}},$$

$$\Omega_5 = 0.135 \ sr.$$

As before, the total solid angle for the B units is

$$\Omega_5 + \Omega_6 + \Omega_7 + \Omega_8 = 4 \times \Omega_5 = 4 \times 0.135 = 0.54 \ sr.$$

Therefore, the sum of the solid angles for all units is calculated as follows:

$$\Omega_1 + \Omega_2 + \Omega_3 + \Omega_4 + \Omega_5 + \Omega_6 + \Omega_7 + \Omega_8 = 1.04 + 0.54 = 1.58 \text{ sr.}$$

Comparing these results with Figure 6-1, for a multiplication factor of 0.378, the allowed solid angle is approximately 5.22 sr ($= 9 - 10 \times 0.378$). The calculated solid angle for all array units is 1.58 sr.; therefore, this storage array would be acceptable.

6.4.2 Solid Angle Example Problem 2

1. Reexamine the Solid Angle Example Problem 1 (Section 6.4.1) with array units spaced 30.48 cm (12 in.) edge-to-edge, instead of 60.96 cm (24 in.).
2. What minimum edge-to-edge spacing would be permitted using the solid angle method?

Part 1.

Because the multiplication factor is relatively low for a single unit (SCALE value $= 0.378 \pm 0.001$), spacing the units closer together could save valuable storage space in the process facility. Based on the applicability for the solid angle method, the units should be no closer than 0.3 m (30 cm) apart. This spacing meets the problem requirements, and the single unit multiplication factor is also below 0.8. The layout of the array is still as shown in Figure 6-4 with different distances for the A and B type cylinders.

The new value of H_1 would be: $30.48 + 15.56 - (15.24/2) = 38.42$ cm. Therefore, the solid angle for the side units of the array is determined from the following:

Calculating the solid angle subtended by a cylinder of type A with respect to cylinder X,

$$\Omega_1 = \frac{LD}{H\sqrt{(\frac{L}{2})^2 + H^2}},$$

$$\Omega_1 = \frac{(100 \text{ cm})(15.24 \text{ cm})}{(38.42 \text{ cm}) \times \sqrt{(100 \text{ cm}/2)^2 + (38.42 \text{ cm})^2}},$$

$$\Omega_1 = 0.629 \text{ sr.}$$

As there are four A units, the total solid angle from these units is:

$$\Omega_1 + \Omega_2 + \Omega_3 + \Omega_4 = 4 \times \Omega_1 = 4 \times 0.629 = 2.52 \; sr.$$

For the B unit, the solid angle can now be calculated by using the same relationship as above with the appropriate value of H:

$$H_5 = (ETE + OD) \times \sqrt{2} \; - \; \frac{ID}{2} = (30.48 \; cm \; + \; 15.56 cm) \times \sqrt{2} \; - \; \frac{15.24 cm}{2} = 57.49 \; cm$$

$$\Omega_5 = \frac{(100 \; cm)(15.24 \; cm)}{(57.49 \; cm) \times \sqrt{(100 \; cm/2)^2 + (57.49 \; cm)^2}},$$

$$\Omega_5 = 0.348 \; sr.$$

As before, the total solid angle for the B units is:

$$\Omega_5 + \Omega_6 + \Omega_7 + \Omega_8 = 4 \times \Omega_5 = 4 \times 0.348 = 1.39 \; sr.$$

Therefore, the sum of the solid angles for all units is calculated as follows:

$$\Omega_1 + \Omega_2 + \Omega_3 + \Omega_4 + \Omega_5 + \Omega_6 + \Omega_7 + \Omega_8 = 2.52 + 1.39 = 3.91 \; sr.$$

Comparing these results with Figure 6-1, for a multiplication factor of 0.378, the allowed solid angle is approximately 5.22 sr (= 9 – 10 x 0.378). The calculated solid angle for all array units is 3.91 sr.; therefore, this storage array would be acceptable.

The total solid angle for the array units spaced 30.48 cm apart is well below the allowed 5.22 steradians as calculated in the previous example problem. Therefore, this array will remain subcritical for normal spacing conditions. As indicated from a SCALE calculation for a fully reflected 3×3×1 array with 30.48 cm ETE, the k_{eff} is 0.646 ± 0.001, so it is still safely subcritical.

For the allowable solid angle to be 3.9 sr, the individual-array-unit multiplication factor must be greater than 0.51. Thus, 30 cm spacing is subcritical for units with a maximum $k_{eff} < 0.51$.

Part 2.

Using a spreadsheet, for example, it is not difficult to iterate on the surface-to-surface spacing between array units, using the methodology discussed in Part A, to determine where the solid angle reached the limiting value from Figure 6-1 (5.22 sr.). The results are shown in Table 6-2. The spacing that gives the maximum allowed solid angle would be 23.1 cm; however, use of the solid angle method requires a minimum 30 cm spacing. Reducing the spacing below 30 cm requires that another analysis method be used to evaluate the safety of such a configuration.

The minimum 30 cm spacing was imposed to provide for thick water reflection. It also turns out that spacing closer than 30 cm impacts the assumptions made to derive the solid angle equation. For this 3×3 array, it was determined that a spacing of 0.0 cm produced a k_{eff} of 0.996 + 0.001 when water was present in the interstitial spaces.

Table 6-2. Solid Angle versus Edge-to-Edge (ETE) Spacing for Example Problem 2.

Edge-to-Edge (cm)	Solid Angle (steradians)
15.0	7.62
20.0	5.99
23.1	*5.22*
25.0	4.83
30.0	3.98
30.5	3.91
40.0	2.83
50.0	2.10
60.0	1.62
61.0	1.58
75.0	1.15
100.0	0.71
125.0	0.48
150.0	0.35
200.0	0.21
250.0	0.13
300.0	0.09

Notice that as the surface-to-surface spacing between array units is increased from the 0.3 m (30 cm) applicability limit for the solid angle method, the total array solid angle exponentially drops asymptotically to zero (Figure 6-5). These results clearly show the effect of neutron interaction between array units; the effects of interaction are greatest when the array units are close together and quickly decrease as a function of distance.
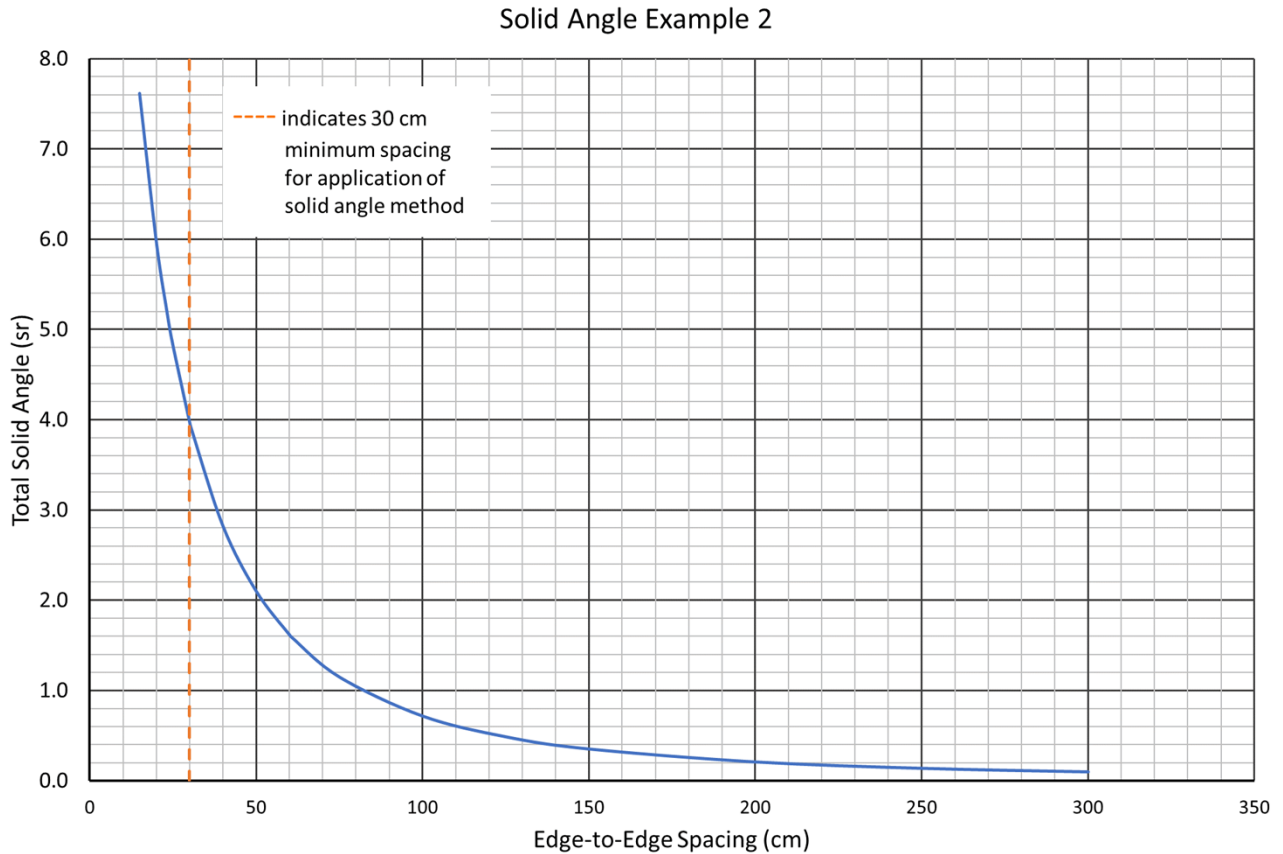
Figure 6-5. Solid Angle Method Example Problem 2 Spacing Parametric Results.

6.4.3 Solid Angle Example Problem 3

A plutonium processing facility needs to store plutonium solution $(Pu(4)O_2)$ in a $3\times3\times1$ unreflected planar array of 4 L spherical bottles. The plutonium in the solution contains 4 at. % Pu-240. The array is assumed to be only one unit high (i.e., the containers are not stacked). The bottles are spaced 1 ft apart under normal conditions in fixed storage locations. The plutonium solution concentration can vary significantly over the range 20 gPu/L to 200 gPu/L. Will this storage arrangement be safe over this concentration range?

Characteristics of array (Figure 6-6):

- Separation (edge-to-edge, ETE) = 30.48 cm (12 in.)
- Pitch (center-to-center, CTC) = 50.80 cm (20 in.)

146
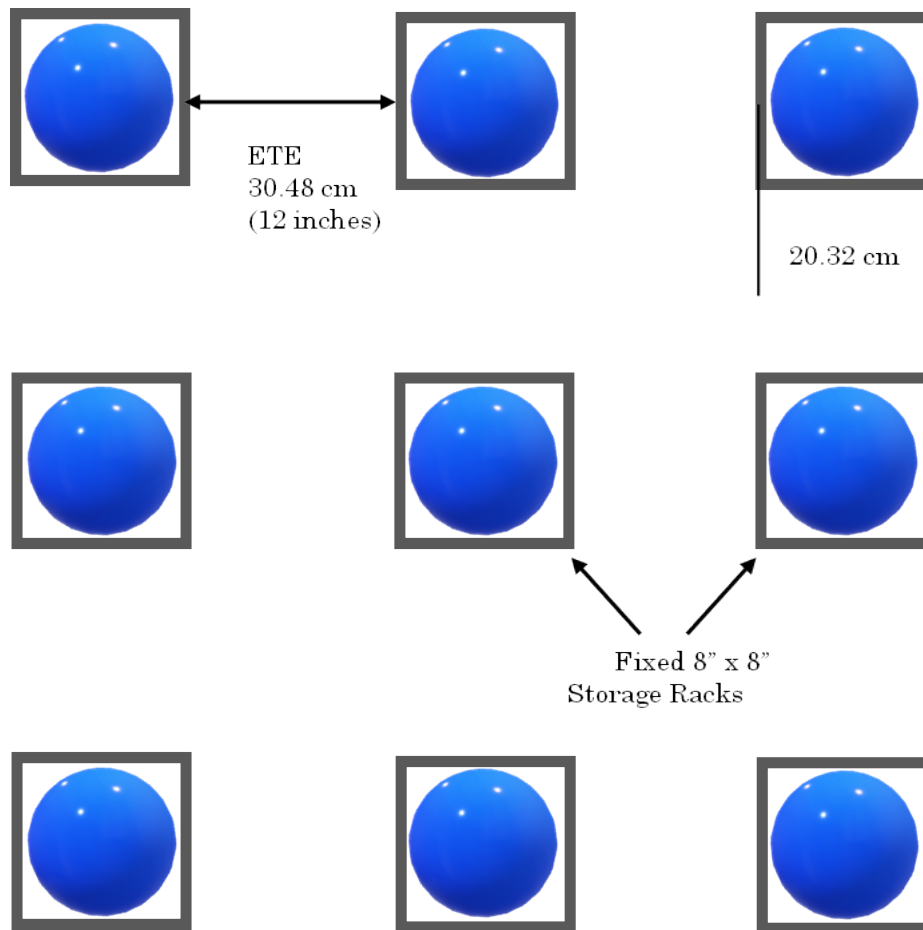
Figure 6-6. Illustration of Problem Geometry for Solid Angle Example Problem 3.

The multiplication factor of a single, unreflected unit in the array can be approximated using the figures and Tables in Appendix B. Figure B-4 provides the multiplication factor as a function of the fraction of critical mass. Pu concentration. The critical masses are from Table B-2 for 4 wt % plutonium solutions. The estimated values of k_{eff} are read from Figure B-4 with the appropriate fraction critical. The multiplication factor plots in Appendix B for Pu solutions assume Pu with 4 at. % Pu-240.

Table 6-3 shows that the array units, regardless of concentration, meet the solid angle criteria that no unreflected, individual array unit has a multiplication factor of greater than 0.8. Estimates of k_{eff} are read from Figure B-3. Empirical equations in Appendix B for k_{eff} as a function of k_∞ are valid for fraction critical values of 0.3 or greater, which does not apply to the conditions for this example.

Table 6-3. Multiplication Factor Estimation for Solid Angle Example Problem 3.

Pu Conc. (g Pu/liter)	Bare Pu Critical Mass (g)	Pu Mass (kg)	Fraction of Critical Mass	[19]Est. k_{eff}
20	1090	$20\frac{\text{g - Pu}}{\text{liter}} \times 4 \text{ liters} = 80 \text{ g - Pu}$	$\frac{80 \text{ g - Pu}}{1090 \text{ g - Pu}} = 0.073$	0.37
30	1060	$30\frac{\text{g - Pu}}{\text{liter}} \times 4 \text{ liters} = 120 \text{ g - Pu}$	$\frac{120 \text{ g - Pu}}{1060 \text{ g - Pu}} = 0.113$	0.42
50	1290	$50\frac{\text{g - Pu}}{\text{liter}} \times 4 \text{ liters} = 200 \text{ g - Pu}$	$\frac{200 \text{ g - Pu}}{1290 \text{ g - Pu}} = 0.155$	0.47
200	4030	$200\frac{\text{g - Pu}}{\text{liter}} \times 4 \text{ liters} = 800 \text{ g - Pu}$	$\frac{800 \text{ g - Pu}}{4030 \text{ g - Pu}} = 0.199$	0.54

The results in Table 6-3 show that the maximum multiplication factor for an unreflected, spherical single unit would be about 0.54, which is within the solid angle method applicability of 0.8. Thus, the 4 L Pu spheres would be acceptable for the solid angle method.

The first step is to determine whether the arrangement, shown in Figure 6-6, meets the applicability criteria for the solid angle method:

- The distance between units is 1 ft (30.48 cm) apart, which is greater than the minimum separation distance of 30 cm.

- The array considered is a bare system that has no external neutron reflectors present.

- Table 6-3 shows that the maximum multiplication factor for an unreflected, spherical single unit would be about 0.54. Thus, regardless of concentration, the 4 L Pu spheres meet the solid angle criteria that no unreflected, individual array unit has a multiplication factor of greater than 0.8.

The first part of the problem is to determine the radius of a sphere with 4 L volume.

$$V_{sphere} = \frac{4}{3}\pi r^3 \quad \text{Solve this for r:}$$

$$r = \sqrt[3]{\frac{3 \times V_{sphere}}{4 \times \pi}} = \sqrt[3]{\frac{3 \times 4 \text{ liters} \times \frac{1000 \text{ cm}^3}{\text{liter}}}{4 \times \pi}} = 9.847 \text{ cm} \quad \text{(inside radius)}$$

As before, there are two "types" of units in the array: A and B. The center to surface distance for each is calculated as follows:

---

[19] Calculated k_{eff} values from PARTISN with 16 group Hansen-Roach cross sections give 0.372, 0.426, 0.479, and 0.544 for the different concentrations.

$$pitch = ETE + storage\ width$$

$$pitch = 30.48\ cm + 20.32\ cm = 50.80\ cm$$

$$H_A = pitch - inside radius$$

$$H_A = 50.80\ cm - 9.847\ cm = 40.95\ cm$$

$$H_B = pitch \times \sqrt{2} - inside radius$$

$$H_B = 50.80\ cm \times \sqrt{2} - 9.847\ cm = 62.00\ cm$$

The "point-to-sphere" solid angle formula from Table 6-1 may be used to calculate the solid angle for each unit in the array. As in Solid Angle Example problems 1 and 2, the solid angle subtended by each unit in the array is then summed together to obtain the total solid angle, and the result is compared to the applicability plot in Figure 6-1. The "point-to-sphere" solid angle formula from Table 16 can be used as follows:

$$\Omega = 2\pi \left(1 - \frac{1}{\sqrt{1 + \left(\frac{R}{H}\right)^2}} \right)$$

Starting with the A units:

$$\Omega_A = 2\pi \left(1 - \frac{1}{\sqrt{1 + \left(\frac{9.847\ cm}{40.95\ cm}\right)^2}} \right) = 0.174\ \text{sr}$$

$$\text{Total A solid angle} = 4 \times \Omega_A = 0.696\ \text{sr}$$

Then for the B units (those on the diagonals),

$$\Omega_B = 2\pi \left(1 - \frac{1}{\sqrt{1 + \left(\frac{9.847\ cm}{62.00\ cm}\right)^2}} \right) = 0.078\ \text{sr}$$

$$\text{Total B solid angle} = 4 \times \Omega_B = 0.312\ \text{sr}$$

The total solid angle for 4 L spherical bottles of Pu(4)O$_2$ solution in a $3 \times 3 \times 1$ array is 1.01 sr = 0.696 sr + 0.312 sr. Based on the maximum k_{eff} of 0.54 at 200 g-Pu/L, Figure 6-1 shows a maximum allowable solid angle of 3.6 sr. So, the array configuration with the given spacing and fissile material will be subcritical. A SCALE calculation of a reflected $3 \times 3 \times 1$ array of Pu(4)O$_2$ solution at 0.200 g Pu/cm^3 gives a $k_{eff} = 0.818 \pm 0.001$.

6.4.4   Solid Angle Example Problem 4

It is desired to establish the safe spacing for a 10-unit array of 10 in. diameter cylinders (schedule 20 pipe) each 6 feet long on a square lattice pattern in two rows of five. The cylinders are to contain 4.98% enriched uranyl fluoride of maximum 3.2 g U/cm^3 concentration. From ORNL data[20] (Reference 38), a bare stainless steel cylinder of U(4.98)O$_2$F$_2$ solution was critical with a radius of 19.55 cm and a height of 101.7 cm. Use the solid angle criterion to estimate a safe spacing for this configuration.
To apply the solid angle method to this problem, the multiplication factor, k$_{eff}$, of the solution cylinder must be found. We can use the following equation to estimate k$_{eff}$:

$$k_{eff} = \frac{1 + B_m^2 M^2}{1 + B_g^2 M^2} = \frac{k_\infty}{1 + B_g^2 M^2}$$

For nuclear criticality safety purposes, the two usual ways of maintaining safety in these situations is either through a mass limit or through fixed geometry. For this situation, the geometry is fixed, and the concentration can vary (i.e., the mass varies by concentration) up to a maximum of 3.2 g U/cm^3 or a U-235 concentration of 0.1594 g U-235/cm^3. Because there is a wide range of concentrations possible for these units, a review of the critical geometry information in Figure 6-7, shows the minimum critical diameter of a water-reflected infinite cylinder is 28.5 cm (11.22 in.). So, the 10 in. diameter cylinders should always be subcritical as individual units regardless of the concentration of solution and reflection conditions.

---

[20] The experiment had an H/X of 496, a U-235 concentration of 0.04487 g 235/ cm^3, a uranium concentration of 0.901 g U/ cm^3, and a solution density of 2.020 g/ cm^3.
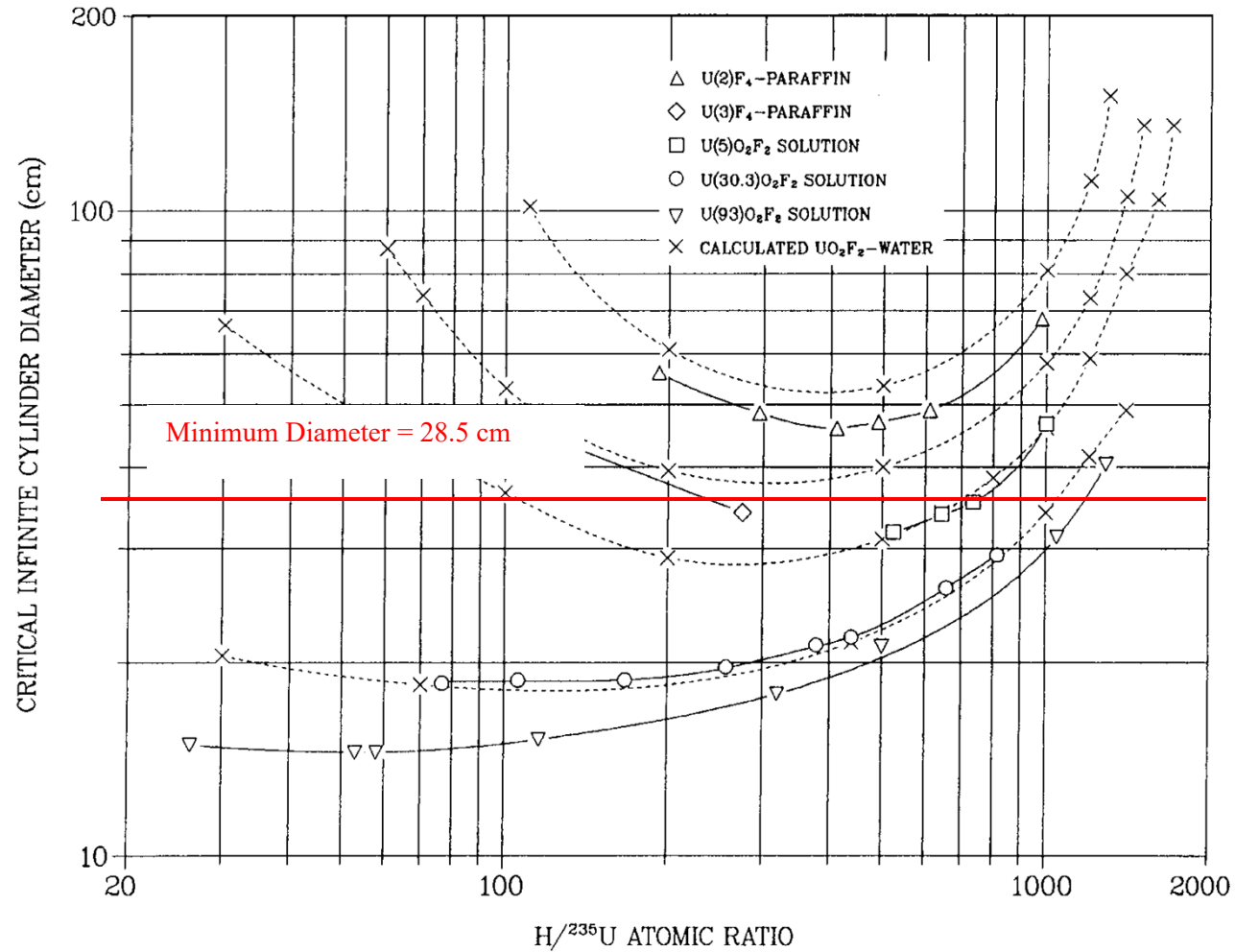
Fig. 16. Estimated critical diameters of infinitely long water-reflected cylinders of hydrogen-moderated U(93), U(30.3), U(5.00), U(3.00) and U(2.00).

Figure 6-7. Critical Diameters of Infinite Cylinders for Various Enrichments of Uranium. (Reference 11, Figure 16.)
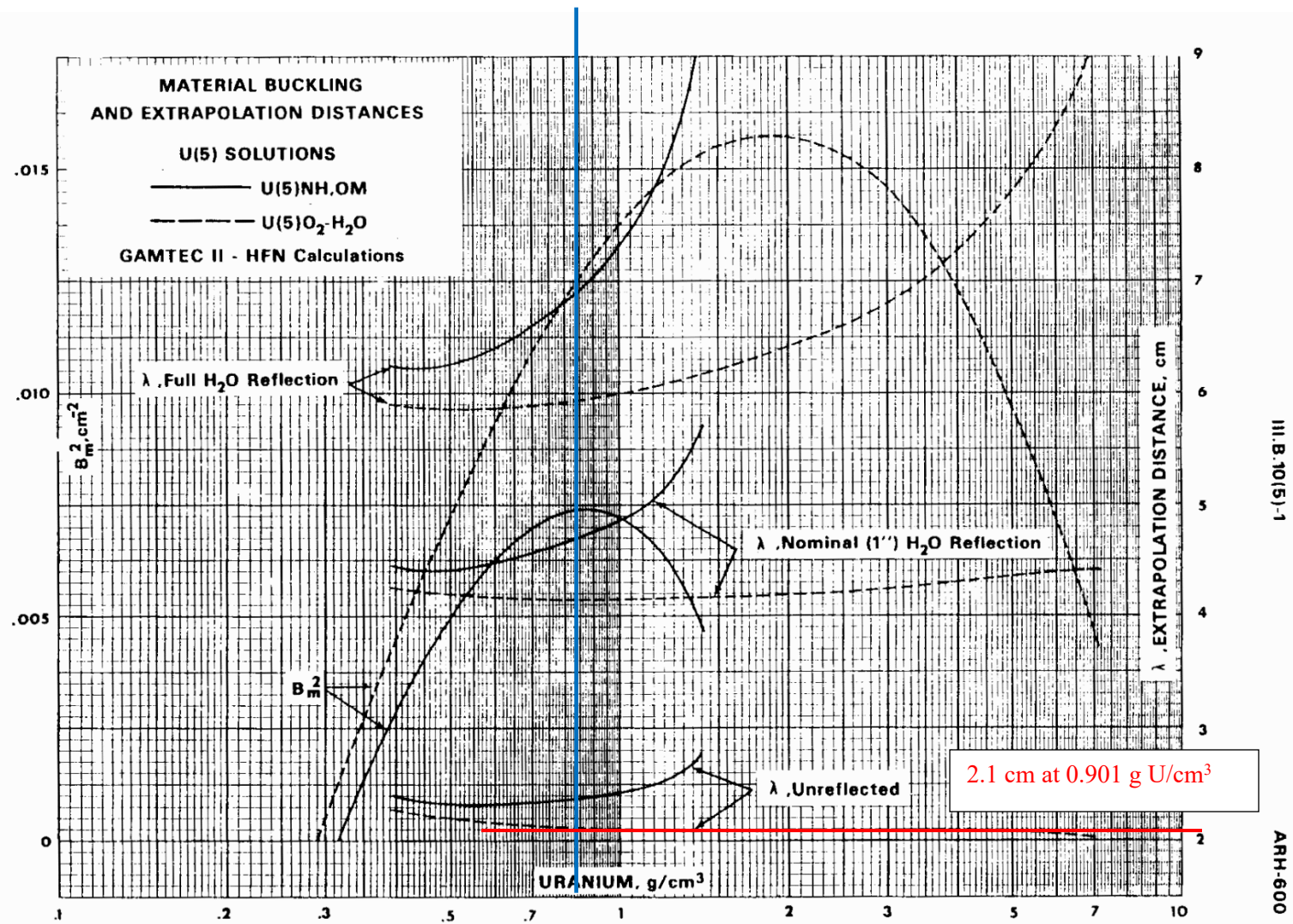
Figure 6-8. Extrapolation Distance Data for U(5)O$_2$-H$_2$O System. (Reference 7, Figure III.B.10(5)-1.)

152
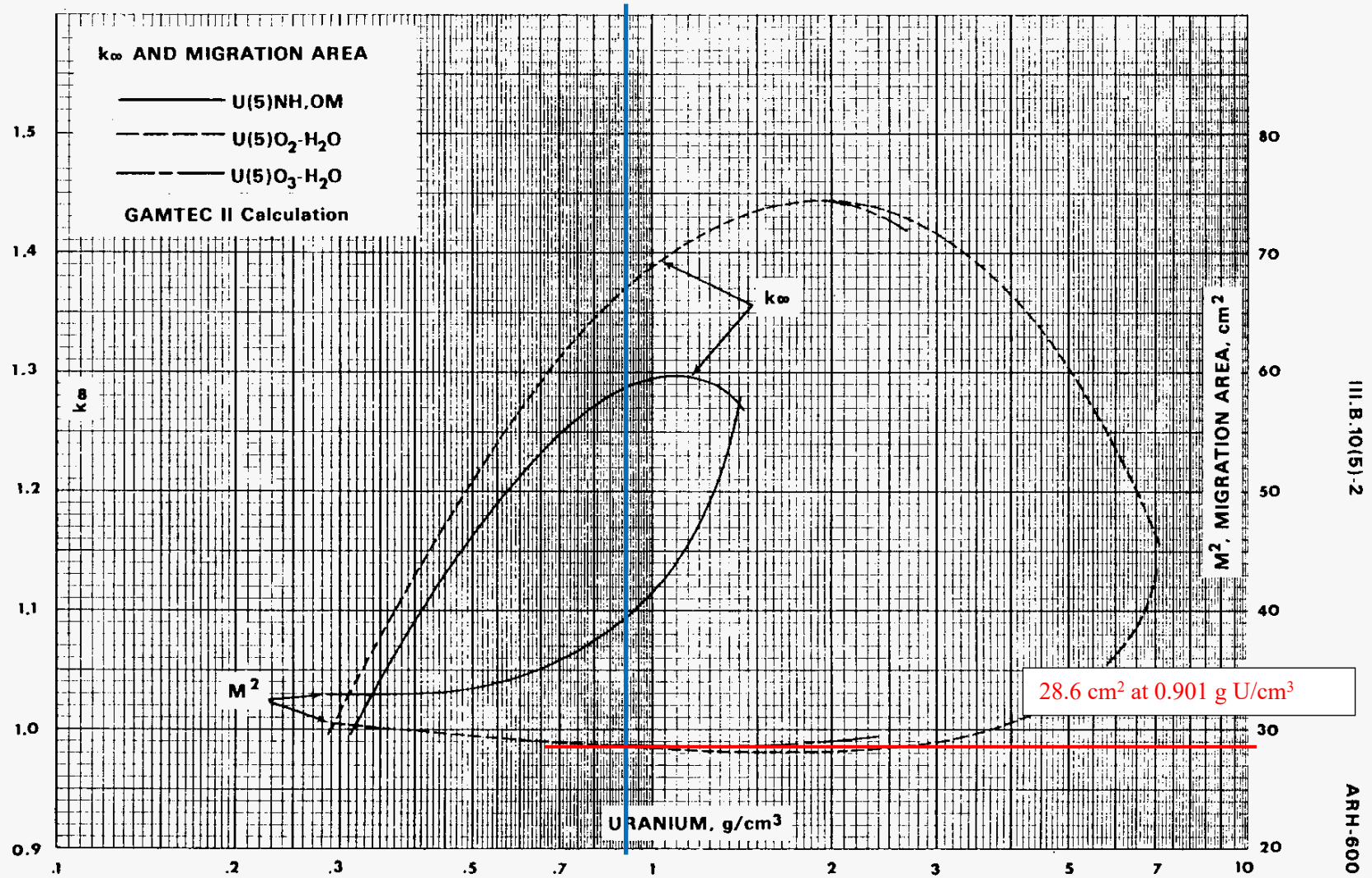
Figure 6-9. Migration Area Data for U(5)O₂-H₂O System. (Reference 9, Figure III.B.10(5)-2.)

153

Now to calculate the material buckling from the experimental information and use an extrapolation distance, d, of 2.1 cm from Figure 6-8, the buckling at critical (i.e., material buckling) is

$$B_g^2 = \left(\frac{2.405}{r+d}\right)^2 + \left(\frac{\pi}{L+2d}\right)^2,$$

$$B_g^2 = \left(\frac{2.405}{19.55\ cm + 2.1\ cm}\right)^2 + \left(\frac{\pi}{101.7\ cm + 2 \times 2.1\ cm}\right)^2 = 0.01322\ cm^{-2}.$$

For 10 in. diameter, schedule 20 pipe, the inside diameter is 10.25 in. and the wall thickness is 0.25 in., which gives an outside diameter of 10.75 in. Then, the solution cylinder dimensions are

$$r = \frac{10.25\ inches}{2} \times \frac{2.54\ cm}{inch} = 13.0175\ cm$$

$$L = 6\ ft \times \frac{12\ inches}{ft} \times \frac{2.54\ cm}{inch} = 182.88\ cm$$

Substitute these values into the geometric buckling relationship for a finite cylinder using the same extrapolation distance of 2.1 cm from Figure 6-8:

$$B_g^2 = \left(\frac{2.405}{r+d}\right)^2 + \left(\frac{\pi}{L+2d}\right)^2,$$

$$B_g^2 = \left(\frac{2.405}{13.0175\ cm + 2.1\ cm}\right)^2 + \left(\frac{\pi}{182.88\ cm + 2 \times 2.1\ cm}\right)^2 = 0.02559\ cm^{-2}.$$

For migration areas, we refer to Figure 6-9, and find $M^2 = 28.6$ cm^2 at 0.901 g U/cm^3. Then we can use the diffusion theory approximation (Eq. 75) to estimate the k_{eff}:

$$k_{eff} = \frac{1 + B_m^2 M^2}{1 + B_g^2 M^2} = \frac{k_\infty}{1 + B_g^2 M^2}$$

$$k_{eff} = \frac{1 + 0.01322 cm^{-2} \times 28.6\ cm^2}{1 + 0.02559 cm^{-2} \times 28.6\ cm^2} = \frac{1.37803}{1.73179} = 0.796$$

This k_{eff} is just below the upper limit for use of the solid angle method.[21] This is the maximum k_{eff} expected for the range of concentrations that could be stored in the unit.

For U(4.89)O$_2$F$_2$, Figure 6-7 shows that a minimum diameter of 28.5 cm is required to make a reflected solution critical. Thus, the unit cylinder's diameter of 26.035 cm should be subcritical for concentrations of interest. Furthermore, no reflectors better than water are expected in this facility. Thus, this problem meets two of the three criteria for applicability for the solid angle method (i.e., unit k_{eff} less than 0.8 and fully water-reflected unit subcritical). Now, the safe spacing can be determined for the proposed array.

---

[21] A PARTISN analysis of U(4.98)O2F2 at H/X = 496 gives a k_{eff} of 0.7565. As was indicated in the chapter on buckling conversion equation 3.16 over predicts the actual k_{eff}. KENO gives a k_{eff} of 0.7558 ±0.0012 for the cylinder without stainless steel and 0.7841 ± 0.0012 for the unit with the stainless steel.

The solid angle criterion for this problem, based on the calculated k_{eff} for this unit cylinder is:

$$\Omega_{allowed} = 9 - 10k_{eff} = 9 - 10 \times 0.796 = 1.04 \; steradians$$

This is consistent with the solid angle criterion shown in Figure 6-1.

The total solid angle, Ω_{total}, is the sum of the solid angles subtended by the visible surrounding individual units. Figure 6-10 illustrates the parameters used to calculate the solid angle due to the height of the cylinders above the center point of the central array unit. For this configuration, the most central unit is chosen for the calculation of the solid angle. Figure 6-10 illustrates the array configuration with the central unit center identified as point P.
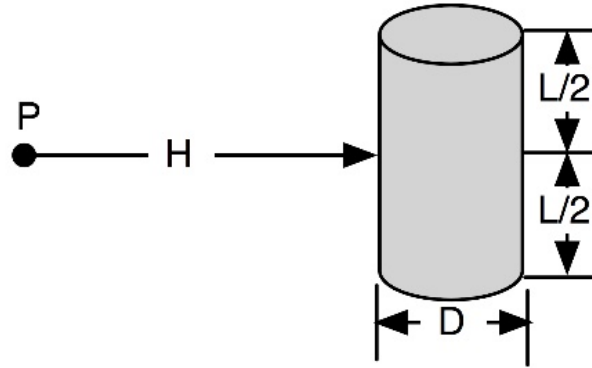
Figure 6-10. Parameters for Determination of Solid Angle for Unit Cylinders.

In Figure 6-10, L is the total height of the cylinder, D is the diameter of the cylinder and H is the point-to-surface distance = Pitch – ID/2 (note: H is measured from point P to surface of fissile material so inside diameter is used). The solid angle calculations will be based on determining the value of the point-to-surface distance for the three unit types that gives the allowable solid angle. For a square array, the separation distance, S, can be determined from the pitch minus the outside diameter (S = Pitch - OD).

The point-to-cylinder formula from Table 6-1 that matches Figure 6-10 is

$$\Omega_i = \frac{L \times ID}{H_i \sqrt{(\frac{L}{2})^2 + H_i^2}}$$

155

3

1 2

$S_1 = H - \dfrac{D}{2}$

P $\quad S_1 = H - \dfrac{D}{2} \rightarrow$ 1

$S_1 = H - \dfrac{D}{2}$

1 2

Not Visible to P 3

Not Visible to P 3

1 2

$S_2 = \sqrt{2}H - \dfrac{D}{2}$

P 1

$S_2 = \sqrt{2}H - \dfrac{D}{2}$

1 2

Not Visible to P 3

Not Visible to P 3

1 $S_3 = \sqrt{5}H - \dfrac{D}{2}$ 2

P 1

1 $S_3 = \sqrt{5}H - \dfrac{D}{2}$ 2

Not Visible to P 3
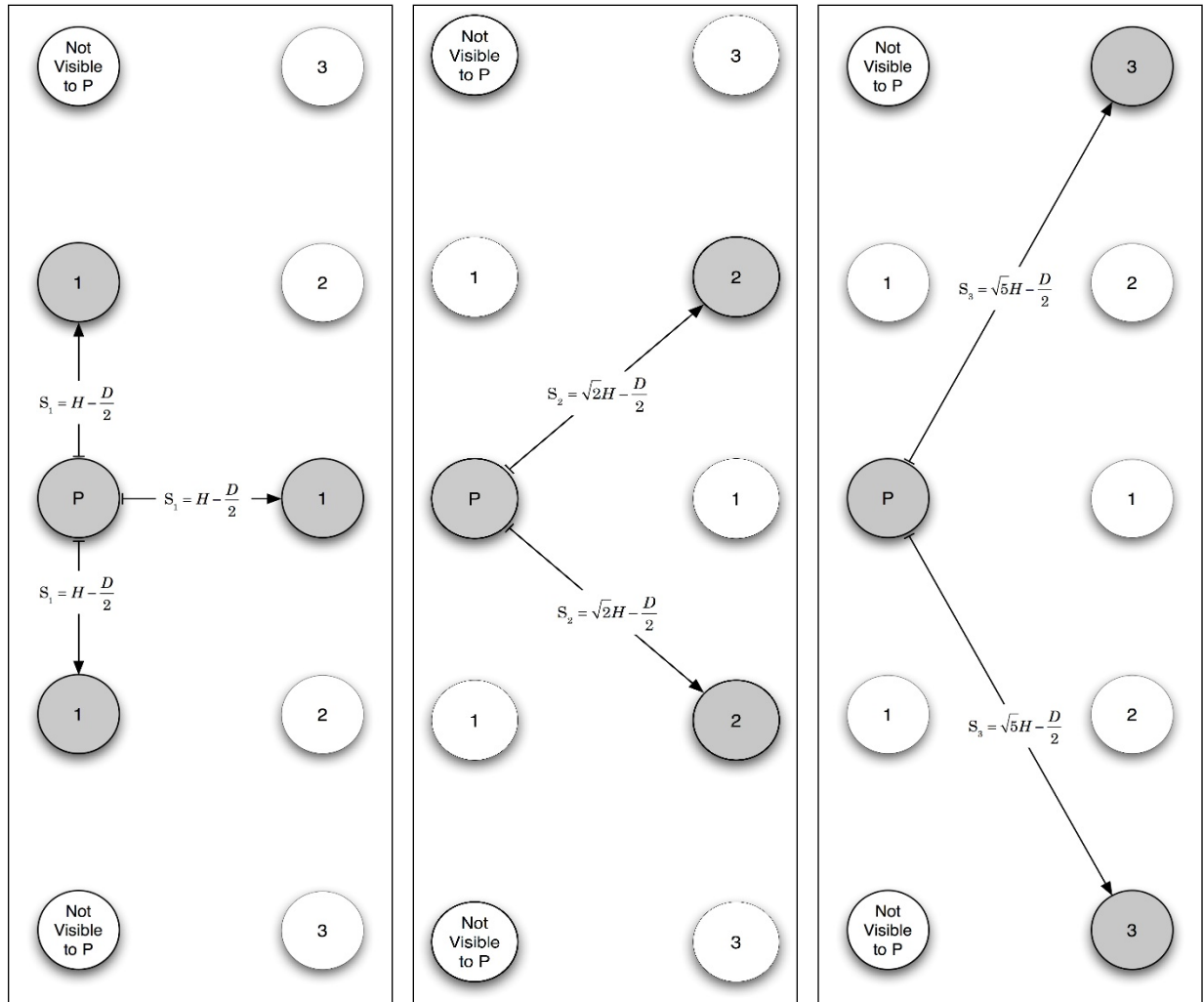
Figure 6-11. Illustrations of 10-unit Array for Solid Angle Example Problem 4.

Because of symmetry, the units can be separated into 4 types; each type identified by distance from the central unit: Unit 1 is one pitch away, Unit 2 is √2 × pitch distant, Unit 3 is √5 × pitch distant, and Units 4 are in the corners and fully shadowed by Unit 1 in the vertical direction. So, three solid angle calculations have to be performed to determine the total solid angle.

Based on the information illustrated in Figure 6-11, the total solid angle can be represented as follows:

$$\Omega_{\text{total}} = 3 \times \Omega_1 + 2 \times \Omega_2 + 2 \times \Omega_3.$$

Using H_i to represent the point-to-surface distance of Unit i, Figure 6-11 gives the following equations:

$$H_1 = Pitch - \frac{ID}{2}$$

$$H_2 = \sqrt{2}Pitch - \frac{ID}{2}$$

$$H_3 = \sqrt{5}Pitch - \frac{ID}{2}$$

With these equations and cylinder dimensions ($D = 2 \times 13.0175$ cm and $L = 182.88$ cm), the solid angle for each unit can be determined:

$$\Omega_1 = \frac{LD}{H_1\sqrt{\frac{L}{(2)^2} + H_1^2}} = \frac{182.88 \text{ cm} \times 26.035 \text{ cm}}{(Pitch - 13.0175)\sqrt{\frac{182.88 \text{ cm}}{(2)^2 + (Pitch - 13.0175)^2}}}$$

$$\Omega_2 = \frac{LD}{H_2\sqrt{\frac{L}{(2)^2} + H_2^2}} = \frac{182.88 \text{ cm} \times 26.035 \text{ cm}}{(Pitch \times \sqrt{2} - 13.0175)\sqrt{\frac{182.88 \text{ cm}}{(2)^2 + (Pitch \times \sqrt{2} - 13.0175)^2}}}$$

$$\Omega_3 = \frac{LD}{H_3\sqrt{\frac{L}{(2)^2} + H_3^2}} = \frac{182.88 \text{ cm} \times 26.035 \text{ cm}}{(Pitch \times \sqrt{5} - 13.0175)\sqrt{\frac{182.88 \text{ cm}}{(2)^2 + (Pitch \times \sqrt{5} - 13.0175)^2}}}$$

A spreadsheet can be used to set up these equations to determine the safe spacing between array units. Table 6-4 provides the results of the iterative search on the array unit spacing. The pitch has is varied searching for the value where the total solid angle equals the limiting solid angle value of 1.04 sr.

Table 6-4. Solid Angle Method Example Problem 4 Safe Spacing Results.

Pitch (in.)	Pitch (cm)	H_1 (cm)	Ω_1 (sr)	H_2 (cm)	Ω_2 (sr)	H_3 (cm)	Ω_3 (sr)	Ω_{total} (sr)
62	157.5	144.5	0.193	209.7	0.099	339.1	0.040	0.857
60	152.4	139.4	0.205	202.5	0.106	327.8	0.043	0.912
58	147.3	134.3	0.218	195.3	0.113	316.4	0.046	0.972
56	142.2	129.2	0.233	188.1	0.121	305.0	0.049	1.038
54	137.2	124.1	0.249	181.0	0.130	293.7	0.053	1.111
52	132.1	119.1	0.266	173.8	0.140	282.3	0.057	1.192
50	127.0	114.0	0.286	166.6	0.150	271.0	0.061	1.281
48	121.9	108.9	0.307	159.4	0.163	259.6	0.067	1.381
47.25	120.0	107.0	0.316	156.7	0.167	255.3	0.069	1.421
47	119.4	106.4	0.319	155.8	0.169	253.9	0.069	1.435
46	116.8	103.8	0.331	152.2	0.176	248.2	0.072	1.492

Based on these results, the minimum pitch that will result in a safe configuration is 56 in. (142.24 cm). However, pitch is difficult to measure in situ, so we need the edge-to-edge separation distance, which is the pitch minus the outside diameter. From the problem statement, the outside diameter is 10.75 inches (27.305 cm), so the minimum edge-to-edge distance is 56 – 10.75 = 45.25 in. (=142.24 – 27.31 = 114.93

cm) or 45.25 ni., a little less than 4 ft. The results also show that, as expected, it is the closest units that provide the largest solid angle or the most interaction, and the interaction between array units decreases rapidly as the spacing between units is increased.

Notice that a change of two in. in spacing, from 56 to 54 in., has an effect of about 0.07 sr on the allowable angle. This translates to a variation of 0.007 in the k_{eff} of the unit, which is the difference between the diffusion calculated k_{eff} and the KENO value for the unit with a SS container. Thus, use of Eq. (75) gives a first approximation to spacing.

6.4.5 Solid Angle Example Problem 5

1. Use the Solid Angle Method to determine if an array of 4,500 g alpha-phase (α) Pu(4.5) metal ingots ($L/D = 1$) spaced 30 cm apart in a 3×3×1 array would be acceptable.
2. What if the ingots have an $L/D = 7$; how does that affect the spacing?

Part 1.

The layout of this 3×3×1 array is approximated in Figure 6-2 (plan view) and Figure 6-3 (elevation view, but with $L/D^{22} = 1$ rather than $L/D = 7.07$). Because the multiplication factor is relatively low for a single unit, spacing the units closer together could save valuable storage space in the process facility. Based on the applicability for the solid angle method, the units should be no closer than 0.3 m (30 cm) apart. This spacing meets the problem requirements. The applicability criteria for the single unit multiplication factor can be determined using the following methodology based on fraction critical relationships (See Appendix B).

The fraction of critical mass, F, can be calculated based on the information in Appendix B. Table B-1 gives the critical mass of an unreflected α-Pu(4.5) sphere as 10.6 kg or 10,600 g.

$$F = \frac{4,500 \ grams}{10,600 \ grams} = 0.425$$

For an Pu metal system, the multiplication factor for a system can be approximated using equation B.1 from Appendix B:

$$k_{eff} = F^{0.3}. \quad \text{For } F = 0.425, \ k_{eff} = (0.425)^{0.3} = 0.774.$$

Thus, the application criterion of $k_{eff} \leq 0.8$, as described in Section 6.3, is met.

We should also check that a fully water-reflected unit is subcritical. Again, referring to Table B-1, the critical mass of a water-reflected αPu(4.5) sphere is 5.9 kg or 5,900 grams. Then the fraction critical for a fully water-reflected unit is

$$F = \frac{4,500 \ grams}{5,900 \ grams} = 0.763$$

For an Pu metal system, the multiplication factor for a system can be approximated again using equation B.1 (applies to both bare and reflected plutonium metal systems):

---

[22] For the solid angle example problems, the height (or length) of a cylinder will be denoted by L to avoid confusion with the point-to-surface parameter, H.

$$k_{eff} = F^{0.3}. \quad \text{For } F = 0.763, \ k_{eff} = (0.763)^{0.3} = 0.922.$$

Thus, the application criterion of a water-reflected unit being subcritical, as described in Section 6.3, is met.

Some of the criteria for application of solid angle are not met. First, these ingots are not moderated systems, and second, being ingots, it is likely that they may be stored in concrete reflected arrays. As the thickness of concrete is unknown, we will reduce the allowable solid angle by 40%.

Using the point-to-cylinder solid angle formula from Table 6-1, the solid angle for each unit in the array may now be calculated. The solid angle subtended by each unit in the array is then summed to obtain the total solid angle. The result will then be compared to 40% of the value determined from Figure 6-1. Based on the bare unit k_{eff}, the allowable solid angle is:

$$\Omega_{allowable} = 9 - 10k_{eff} = 9 - 10 \times 0.774 = 1.26 * 0.4 = 0.504$$

To determine the dimensions of each ingot, we use the density of 19.6 g/cm³ (from Appendix B) and calculate the volume:

$$V_{ingot} = \frac{4,500 \text{grams}}{19.6 \text{grams/cm}^3} = 229.6 \text{cm}^3$$

$$V_{ingot} = \pi \frac{D^2}{4} L \quad \text{For L/D} = 1, \text{solve this for D:}$$

$$V_{ingot} = \pi \frac{D^3}{4} = 229.6 \text{cm}^3 D = \sqrt[3]{\frac{4 \times 229.6 \text{cm}^3}{\pi}} = 6.637 \text{ cm}$$

Ingot dimensions: $D = 6.637$ cm, $r = 3.3185$ cm, $L = 6.637$ cm,

The point-to-cylinder formula from Table 6-1 is:

$$\Omega_i = \frac{LD}{H_i \sqrt{(\frac{L}{2})^2 + H_i^2}}$$

Where L is the total height of the cylinder (6.637 cm), D is the diameter of the cylinder (6.637 cm) and H is the point-to-surface distance, which depends on the Pitch. The Pitch = edge-to-edge + 2 × radius (3.3185 cm).

Using S = 30 cm as the minimum spacing, then Pitch = 30 cm + 2 × 3.3185 cm = 36.637 cm.

The point-to-surface distance depends on unit location. For the A type units, H_A = Pitch – radius, whereas for B type units, H_B = Pitch x √2 – radius. So H_A = 36.637 cm - 3.3185 cm = 33.3185 cm, and H_B = 36.637 cm x √2 – 3.3185 cm = 48.494 cm.

Based on the information illustrated in Figure 6-4, the total solid angle can be represented as follows:

$$\Omega_{total} = 4 \times \Omega_A + 4 \times \Omega_B.$$

For the units of type A (see Figure 6-4), the solid angle will be

$$\Omega_A = \frac{LD}{H\sqrt{(\frac{L}{2})^2 + H^2}},$$

$$\Omega_A = \frac{(6.637\ cm)(6.637\ cm)}{(33.3185\ cm) \times \sqrt{(6.637\ cm/2)^2 + (33.3185\ cm)^2}},$$

$$\Omega_A = 0.0395\ sr.$$

For the units of type B (see Figure 6-4), the solid angle will be:

$$\Omega_B = \frac{LD}{H\sqrt{(\frac{L}{2})^2 + H^2}},$$

$$\Omega_B = \frac{(6.637\ cm)(6.637\ cm)}{(48.494\ cm) \times \sqrt{(6.637\ cm/2)^2 + (48.494\ cm)^2}},$$

$$\Omega_B = 0.0187\ sr.$$

The total solid angle is then:

$$\Omega_{total} = 4 \times \Omega_A + 4 \times \Omega_B \quad = 4 \times 0.0395 + 4 \times 0.0187 = 0.2328\ sr$$

As 40% of the maximum allowed solid angle is 0.504, and the calculated solid angle with 30 cm separation is 0.233, this storage array would be acceptable. It is important to note that larger arrays, particularly with unmoderated materials, are not amenable to evaluation by the solid angle method. However, in most cases, this is not an issue, as solid angle evaluation of arrays with more than 50 units is tedious; so solid angle evaluation likely would not be the first choice for an analysis method.

Part 2.

What if the ingots have an $L/D = 7$; this presents more surface area, so the solid angle should increase. From the previous calculation, we know the volume is 229.6 cm³, so we need the dimensions with $L/D = 7$.

$$V_{ingot} = \pi \frac{D^2}{4} L \quad \text{For L/D} = 7, \text{solve this for D:}$$

$$V_{ingot} = \pi \frac{7 \times D^3}{4} = 229.6\text{cm}^3 D = \sqrt[3]{\frac{4 \times 229.6\text{cm}^3}{7 \times \pi}} = 3.469\ \text{cm}$$

Ingot dimensions: D = 3.469 cm, r = 1.7345 cm, L = 24.283 cm

The point-to-cylinder formula from Table 6-1 is:

$$\Omega_i = \frac{LD}{H_i \sqrt{(\frac{L}{2})^2 + H_i^2}}$$

Where L is the total height of the cylinder (24.283 cm), D is the diameter of the cylinder (3.469 cm) and H is the point-to-surface distance, which depends on the pitch. The pitch = edge-to-edge + 2 × radius (1.7345 cm).

Using $S = 30$ cm as the minimum spacing, then Pitch = 30 cm + 2 × 1.7345 cm = 33.469 cm.

The point-to-surface distance depends on unit location. For the A type units, H_A = Pitch – radius while for B type units, H_B = Pitch × √2 – radius. So, H_A = 33.469 cm – 1.7345 cm = 31.7345 cm, and H_B = 33.469 cm × √2 – 1.7345 cm = 45.598 cm.

Based on the information illustrated in Figure 6-4, the total solid angle can be represented as follows:

$$\Omega_{total} = 4 \times \Omega_A + 4 \times \Omega_B.$$

For the units of type A (see Figure 6-4), the solid angle will be

$$\Omega_A = \frac{LD}{H \sqrt{(\frac{L}{2})^2 + H^2}},$$

$$\Omega_A = \frac{(24.283\ cm)(3.469\ cm)}{(31.7345\ cm) \times \sqrt{(24.283\ cm/2)^2 + (31.7345\ cm)^2}},$$

$$\Omega_A = 0.0781\ sr.$$

For the units of type B (see Figure 6-4), the solid angle will be:

$$\Omega_B = \frac{LD}{H \sqrt{(\frac{L}{2})^2 + H^2}},$$

$$\Omega_B = \frac{(24.283\ cm)(3.469\ cm)}{(45.598\ cm) \times \sqrt{(24.283\ cm/2)^2 + (45.598\ cm)^2}},$$

$$\Omega_B = 0.0392\ sr.$$

The total solid angle is then:

$$\Omega_{total} = 4 \times \Omega_A + 4 \times \Omega_B \quad = 4 \times 0.0781 + 4 \times 0.0392 = 0.469\ sr$$

As 40% of the maximum allowed solid angle is 0.504, and the calculated solid angle for h/d = 7 with 30 cm separation is 0.469, this storage array would still be acceptable. Note that increasing the L/D from 1 to 7 doubled the solid angle. If the shape of a unit is not known, then bounding calculations are necessary to confirm that the proposed array with a given spacing is acceptable.

Also note that although the solid angle doubled, this does not mean that the array with L/D=7 units has a higher k_{eff} than the array with L/D=1 units. The L/D=7 unit does have a greater solid angle, but it also has much greater leakage. In fact, the k_{eff} of a L/D=7 unit is about 0.54 versus the k_{eff} of the L/D=1 unit of 0.76. This indicates that an increase in solid angle is not always indicative of an increase in k_{eff} of an array.

6.4.6   Solid Angle Example Problem 6

The 10 units of 10 in. diameter cylinders (schedule 20 pipe) each 6 feet long **U(4.98)O$_2$F$_2$ solution** cylinders from Example Problem 4) are to be placed vertically along the corner walls of a room as shown in Figure 6-12. Use the solid angle criterion to estimate a safe spacing for this configuration.
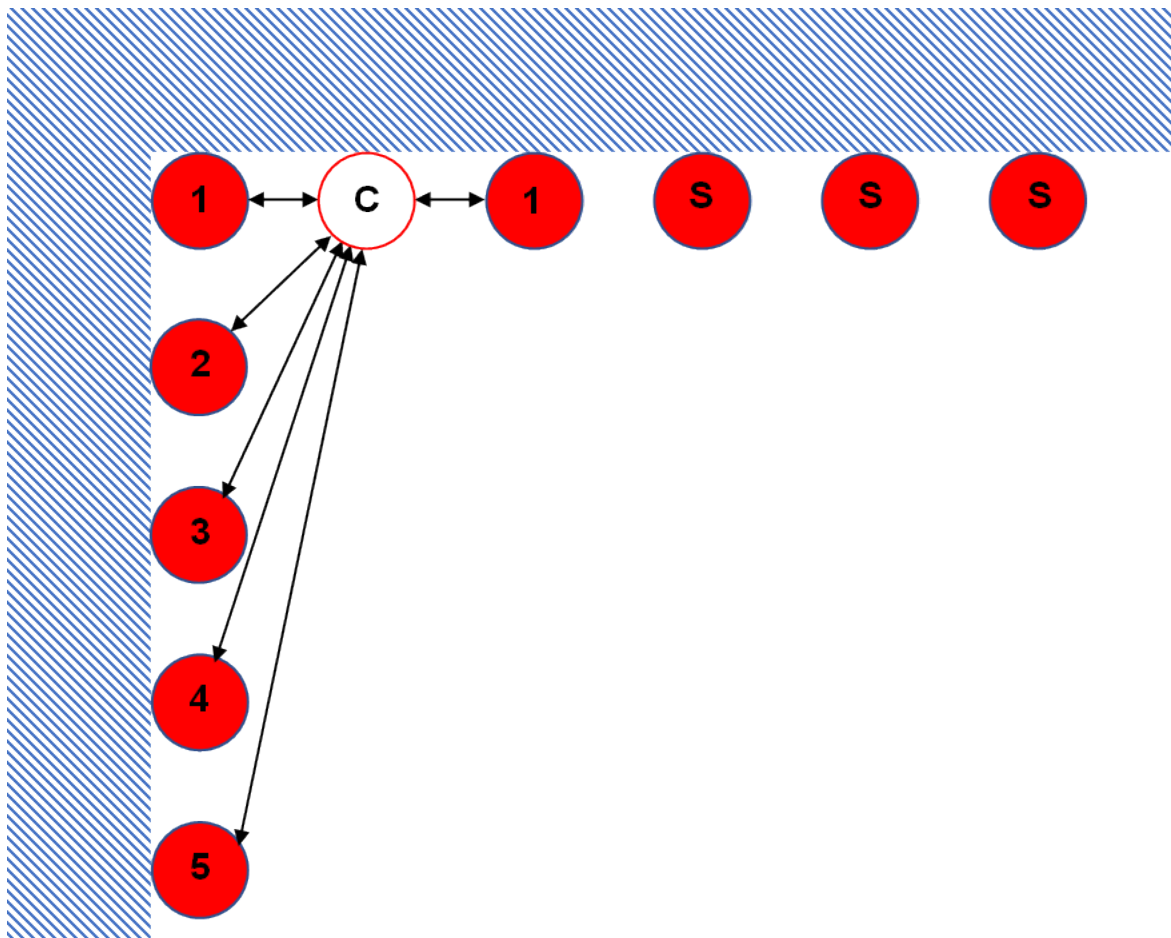
Figure 6-12. Layout of 10-unit Array for Solid Angle Example Problem 6.

The cylinder arrangement as shown in Figure 6-12 has three cylinders along the top that are shadowed from the "center" unit by a cylinder of type 1. For solid angle analyses, these shadowed units are ignored in the calculations. Although the shadowed cylinders have no direct impact or neutron connection with the center unit, they will provide some additional neutrons to the rightmost unit 1. After using the solid angle method to analyze the spacing in this problem, SCALE will be used to analyze the impact of the shadowed units.

Using H_i to represent the point-to-surface distance of Unit i, Figure 6-12 gives the following equations:

$$H_1 = Pitch - \frac{ID}{2}$$

$$H_2 = \sqrt{2}Pitch - \frac{ID}{2}$$

$$H_3 = \sqrt{5}Pitch - \frac{ID}{2}$$

$$H_4 = \sqrt{10}Pitch - \frac{ID}{2}$$

$$H_5 = \sqrt{17}Pitch - \frac{ID}{2}$$

With these equations and cylinder dimensions ($D = 2\text{x}13.0175$ cm and $L = 182.88$ cm), the solid angle for each unit can be determined:

$$\Omega_1 = \frac{LD}{H_1\sqrt{(\frac{L}{2})^2 + H_1^2}} = \frac{182.88\ cm \times 26.035\ cm}{(Pitch - 13.0175)\sqrt{(\frac{182.88\ cm}{2})^2 + (Pitch - 13.0175)^2}}$$

$$\Omega_2 = \frac{LD}{H_2\sqrt{(\frac{L}{2})^2 + H_2^2}} = \frac{182.88\ cm \times 26.035\ cm}{(Pitch \times \sqrt{2} - 13.0175)\sqrt{(\frac{182.88\ cm}{2})^2 + (Pitch \times \sqrt{2} - 13.0175)^2}}$$

$$\Omega_3 = \frac{LD}{H_3\sqrt{(\frac{L}{2})^2 + H_3^2}} = \frac{182.88\ cm \times 26.035\ cm}{(Pitch \times \sqrt{5} - 13.0175)\sqrt{(\frac{182.88\ cm}{2})^2 + (Pitch \times \sqrt{5} - 13.0175)^2}}$$

$$\Omega_4 = \frac{LD}{H_4\sqrt{(\frac{L}{2})^2 + H_4^2}} = \frac{182.88\ cm \times 26.035\ cm}{(Pitch \times \sqrt{10} - 13.0175)\sqrt{(\frac{182.88\ cm}{2})^2 + (Pitch \times \sqrt{10} - 13.0175)^2}}$$

$$\Omega_5 = \frac{LD}{H_5\sqrt{(\frac{L}{2})^2 + H_5^2}} = \frac{182.88\ cm \times 26.035\ cm}{(Pitch \times \sqrt{17} - 13.0175)\sqrt{(\frac{182.88\ cm}{2})^2 + (Pitch \times \sqrt{17} - 13.0175)^2}}$$

Again, the use of a spreadsheet allows one to iterate on spacing. The total solid angle is

$$\Omega_{total} = 2 \times \Omega_1 + 1 \times \Omega_2 + 1 \times \Omega_3 + 1 \times \Omega_4 + 1 \times \Omega_5.$$

For this system, a total solid angle of 1.04 (based on $k_{eff} = 0.796$) is found with a pitch of 44.25 inches (112.4 cm). This pitch gives an edge-to-edge spacing of 33.5 in. (85.1 cm). If the KENO calculated k_{eff} of 0.756 (air gap in place of the steel can), the allowable solid angle becomes 1.44 sr. This is found to be a pitch of 36.75 in. (93.35 cm) and an edge-to-edge spacing of 26 in. (66 cm). Thus, the use of diffusion

163

theory to calculate k_{eff} results in a very conservative spacing—one that is 7.5 in. (19.05 cm) wider than that from a computer calculation. Analysis of the array with SCALE indicated that the k_{eff} at 30 cm edge-to-edge separation was 0.8879 ± 0.0012; so, indeed, the method is quite conservative for these well-moderated units.

Using a pitch of 44.25 in. (112.4 cm) in the solid angle equations gives the following results:

$$\Omega_1 = \frac{182.88 \ cm \ \times 26.035 \ cm}{(112.4 \ cm - 13.0175)\sqrt{(\frac{182.88 \ cm}{2})^2 + (112.4 \ cm - 13.0175)^2}} = 0.3548 \ \text{sr}$$

$$\Omega_2 = \frac{182.88 \ cm \ \times 26.035 \ cm}{(112.4 \ cm \times \sqrt{2} - 13.0175)\sqrt{(\frac{182.88 \ cm}{2})^2 + (112.4 \ cm \times \sqrt{2} - 13.0175)^2}} = 0.1894 \ \text{sr}$$

$$\Omega_3 = \frac{182.88 \ cm \ \times 26.035 \ cm}{(112.4 \ cm \times \sqrt{5} - 13.0175)\sqrt{(\frac{182.88 \ cm}{2})^2 + (112.4 \ cm \times \sqrt{5} - 13.0175)^2}} = 0.0783 \ \text{sr}$$

$$\Omega_4 = \frac{182.88 \ cm \ \times 26.035 \ cm}{(112.4 \ cm \times \sqrt{10} - 13.0175)\sqrt{(\frac{182.88 \ cm}{2})^2 + (112.4 \ cm \times \sqrt{10} - 13.0175)^2}} = 0.0392 \ \text{sr}$$

$$\Omega_5 = \frac{182.88 \ cm \ \times 26.035 \ cm}{(112.4 \ cm \times \sqrt{17} - 13.0175)\sqrt{(\frac{182.88 \ cm}{2})^2 + (112.4 \ cm \times \sqrt{17} - 13.0175)^2}} = 0.0230 \ \text{sr}$$

The total solid angle is

$$\Omega_{total} = 2 \times 0.3548 \ \text{sr} + 1 \times 0.1894 \ \text{sr} + 1 \times 0.0783 \ \text{sr} + 1 \times 0.0392 \text{sr} + 1 \times 0.0230 \ \text{sr}$$

$$\Omega_{total} = 1.0395 \ \text{sr.}$$

This verifies the result from the spreadsheet.

6.4.6.1 Effect of Shadowed Units

As discussed in the beginning of this example problem, fully shadowed units are ignored in the calculation of an array solid angle. For this problem, some KENO analyses were performed to determine the impact of ignoring the shadowed units to the left of the type 1 unit. For the units with a SS container, ignoring the three units created a k_{eff} within one sigma of the k_{eff} for the array analysis. This was true for both a 60 cm unit spacing and a 30 cm unit spacing. So, there appears to be no statistically significant impact on k_{eff} from the shadowed units in this example.

The analysis was continued to determine the effects of the units down the left side of the array. Removal of the type 2 unit reduced the k_{eff} by 0.0095 ± 0.0017; removal of type 3 did not create a statistically significant change in k_{eff} as was also true for removal of type 4 and removal of type 5. As can be seen in

Figure 6-12, type 3, type 4, and type 5 are a significant distance from the "center" unit and have small solid angles due to that distance. Type 3 contributes about 7.5% to the total solid angle, while types 4 and 5 contribute about 3.8% and 2.2%, respectively for a total of 13.5% from the three units. In addition, type 4 and type 5 are somewhat shadowed (type 4 about 25% by type 3 and type 5 about 50% by type 4). Thus, the combination of distance and partial shadowing reduced the impact of the more distant units. If it is assumed that only the type 1 and type 2 units contribute to the neutron exchange, then the edge-to-edge spacing calculated for an allowed solid angle of 1.04 sr would be 30.75 in. (76.2 cm); a reduction of 2.25 in. from the value determined with all five types.

6.4.6.2 Interesting Observations from KENO Runs

Several runs were made with H/X = 525 (optimum moderation). These demonstrate that the addition of a SS container (thickness = 0.5 in. or 1.27 cm) to the model increases the k_{eff} by 0.0283 ±0.0017 (from 0.7558 ± 0.0012 to 0.7841 ± 0.0012) over the model assuming an air gap. However, for a fully reflected unit, the unit without stainless steel had a k_{eff} = 0.9141 ± 0.0012. The addition of the SS container to the model decreases the k_{eff} by 0.0371 ± 0.0017 to 0.8770 ± 0.0012. The increase for the bare system is due to the SS container reflecting some of the neutrons back into the fissile solution. When reflected, the SS container absorbs the more thermal neutrons being reflected by the water so the k_{eff} is reduced.

As discussed in Example Problem 4, a small variation in the k_{eff} of a unit can lead to differences of a few inches in spacing. As shown above, the variation in bare unit k_{eff} from diffusion theory (0.796) to that calculated by transport theory (0.756), leads to a difference of 7.5 in. in spacing for a variation of 0.04 in k_{eff}. Because the diffusion theory estimates of k_{eff} are usually greater than those determined from transport theory for water-moderated systems, the application of the solid angle technique to these systems will result in conservative spacing guidelines.

7. LIMITING SURFACE DENSITY METHOD

7.1 WHAT YOU WILL BE ABLE TO DO

- Determine the critical mass and critical unit spacing between fissile units in the array for arrays of any shape provided that the necessary array and fissile material data are known.

- Determine spacing between fissile array units for individual units of any shape or density.

- Calculate spacing between fissile array units with different fissile materials in the array or different reflectors (i.e., water vs. concrete).

- Calculate the multiplication factor for various array configurations.

7.2 LIMITING SURFACE DENSITY METHOD OVERVIEW

The limiting surface density or NB_N^2 method combines the density analog method and diffusion theory into a thorough method for performing array criticality calculations. Reference 39 states that the NB_N^2 method for calculating critical parameters of reflected cubic arrays is used to define a surface density parameter that permits the interpretation of many practices with and perturbations to arrays of fissile material. The geometric buckling for a single unit is expanded analogously for a water-reflected cubic array, which can then be expanded to arrays of various shapes, such as rectangular and planar arrays, and other reflection conditions, such as concrete. The concept of the NB_N^2 method is that units in each vertical column of the array are projected downward to smear the fissile material from the column onto a sheet that uniformly covers one face of a unit cell. Thomas (Reference 39) describes the surface density of a critical array as follows assuming the product of the number of units in a stacked column, n, and the array unit mass, m, divided by dimension of a cubic array cell, $2a_n$:

$$\sigma(m) = \frac{nm}{(2a_n)^2} \tag{88}$$

This method assumes that if this projected fissile slab is subcritical, then the projected surface density of the array will also be subcritical (Reference 40). As the number of units in the array, N (equal to n^3 for a cubic array) approaches infinity, the limiting surface density approaches the value $\sigma(a_n)$ (Reference 31). Figure 7-1 illustrates this concept.
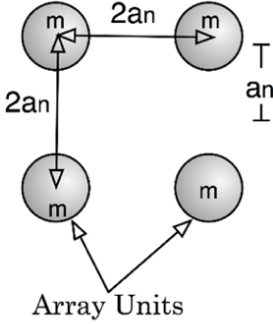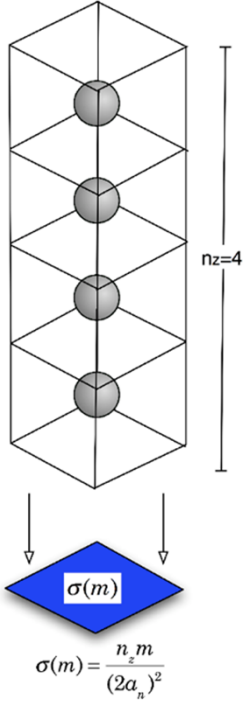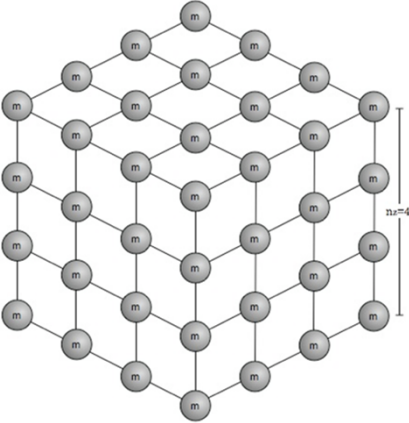
| Illustration of the Center-to-Center Spacing between Array Units | Surface Density of a 64 Unit Array with $n_z = 4$. The surface density is equal to the total mass of fissile material in the stack divided by the area of one array unit. | Illustration of a 64 unit Cubic Array. For the cubic array illustrated above N=64 and is equal to the number of units present in the array (4×4×4) |

Figure 7-1. Concept of Surface Density for Cubic Arrays of Fissile Material.

7.2.1   Geometrical Array Characteristics

The Thomas representation of the NB_N^2 method is used to determine critical spacing of array units of a given mass. The limiting surface density, σ(m), for a cubic array for identical, air-spaced, spherical units with a thick water reflector at the outside the cubic array boundary is defined by the following relationship that define the geometrical configuration of the cubic array:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2$$

or

$$\sigma(m) = \left\{\frac{n_z}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2\right\}m$$

(89)

Where:

n – the least number of units along an array edge, equal to $\sqrt[3]{N}$ for a cubic array (n_z is the number of units high in the z-direction),

m – the mass of an array unit (kg),

a_n – half of the center-to-center spacing between units in the array (cm) as illustrated in Figure 7-1,

c – an empirically determined constant equal to 0.55 ± 0.18 (Reference 39), and

N – the total number of fissile units in the array.

The term $\frac{nm}{(2a_n)^2}$ represents the surface density (g/cm²) of a stack of n units with mass m and a center-to-center spacing $2a_n$ as illustrated in Figure 7-1.

7.2.2 Material Characteristics of the Array

Another relationship can be defined that is dependent on the material properties of the array units based on experimental observations:

$$\sigma(m) = c_2(m_0 - m)$$

or

$$\sigma(m) = c_2 m\left(\frac{m_0}{m} - 1\right)$$

(90)

where

c_2 is a constant that depends on all material properties of the array except for the mass, m, and is also equal to the slope of the "material-line" discussed later (cm⁻²) (Table 7-1 provides values for this constant for various fissile systems);

m_0 is the critical mass (kg) of an unreflected, single fissile unit in the array (Figure 7-1); and

m is the mass (kg) of a fissile unit in the array (Figure 7-1).

Both expressions for $\sigma(m)$ are linear relationships with the independent variable being fissile unit mass, m, and the dependent variable, the surface density, $\sigma(m)$. If this method is applied to array units that are not air-spaced, e.g., fissile materials in containers, fissile solutions, or interstitial materials between array units, the m, $\sigma(m)$ relationship may be non-linear and the Thomas derivation of the NB_N^2 method will not be applicable (Reference 34).

Equations (89) and (90) can be combined into a relationship that includes both the geometrical and material properties of the array for a single picture of the criticality of an array:

$$\sigma(m) = \left\{\frac{n_z}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2\right\} m = c_2(m_0 - m)$$

(91)

This relationship can be used to solve for the fissile material mass, m^1, or array unit center-to-center spacing, d_0, required for the array to achieve a critical state. These relationships are defined below.

Solving Eq. (91) for the array unit mass[23], $m = m^1$, provides the mass required to create a critical array.

---

[23] In equation 91, m is the mass of a unit in the array. When solving for the intersection of the material line and the geometry line, we are finding the mass of a unit that makes the array critical. We identify this mass as m^1, or the mass where k_{eff} of the array = 1.

$$m^1 = \frac{m_0}{1 + \frac{n_z}{c_2(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2} \qquad (92)$$

Equation (92) provides the unit mass, m^1, necessary for a critical array of N units on a center-to-center spacing of $2a_n = d_0$.

Solving this equation for the array unit center-to-center spacing, $2a_n = d_0$, allows one to estimate the critical array unit spacing for units of mass m^1.

$$d_0 = \sqrt{\frac{n_z}{c_2\left(\frac{m_0}{m^1} - 1\right)}\left(1 - \frac{c}{\sqrt{N}}\right)^2} \qquad (93)$$

As can be seen in Eqs. (92) and (93), m^1 and d_0 are related – m^1 is the critical mass associated with the spacing d_0 while d_0 is the critical spacing associated with the mass m^1. You can choose one of the two, but the other is then determined from Eq. (92) or Eq. (93) as appropriate. Because the geometrical (equation 89) and material (equation 90) expressions for the limiting surface density, $\sigma(m)$, (i.e., the dependent variable), are linear relationships and are set equal, the critical point of an array can be determined by plotting these relationships to determine where the two expressions intersect. Figure 7-2 illustrates that the m is the independent variable and $\sigma(m)$ is the dependent variable. The slope of the material line is $-c_2$, and its intercept is $c_2 m_0$, which is the surface density for m_0, $\sigma(m_0)$.
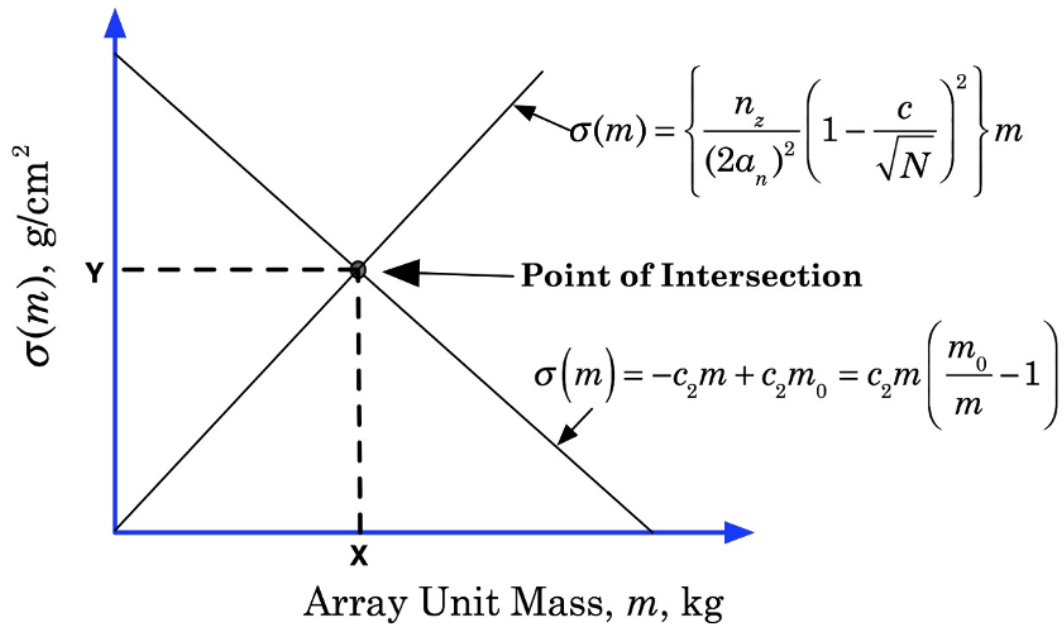
Figure 7-2. Illustration of the Limiting Surface Method.

169

7.3 APPLICABILITY OF THE LIMITING SURFACE DENSITY METHOD

The base NB_N^2 technique is valid for cubic array configurations of spherical or cylindrical (H/D ratio between 0.3 and 3), air-spaced array units. At least 64 units (4×4×4 cubic array) is required, although the method works well for some smaller arrays, such as 3×3×3 cubic arrays with 27 units. The neutron reflection considered in the method are 20 cm slabs of water reflection (or equivalent reflector thickness for another material) outside the array boundaries. With fewer than 64 units, the spherical shape of an array unit may not be the most limiting shape for the array, and the calculation results may not be conservative. Material data to support the method is available for some dry and moderated (Hydrogen-to-fissile or H/X ratio of 20 or less) fissile units and the unreflected critical mass for the fissile array units must be known to apply to the calculation. The method can be adapted for rectangular or planar arrays, non-spherical array unit shapes, or external concrete reflection (Reference 41). However, it is the most comprehensive and flexible of the array methods presented here.

The limiting surface density method is easily adapted to a spreadsheet or computer code, where quick parametric studies on the factors affecting criticality safety can be performed. The NB_N^2 method can be adapted for other configurations to include planar, that is, non-cubic arrays, non-spherical array units, and reflector materials other than water. This method has been adapted for arrays of type 9975 fissile material packages that resulted in a non-linear adaptation of the method for a very specific application (Reference 42). Additional derivations and variations of the method are described in more detail elsewhere (References 39, 41-46) and in Appendix B (method derivation from References 39 and 42).

The limiting surface density method is a versatile and comprehensive method to perform array studies for a variety of fissile materials and array configurations. This method is applicable for the following situations.

- This method was developed for cubic arrays (air-spaced units) reflected by water at least 200 mm thick. Guidance for applying this method with arrays located next to concrete reflectors can be found in Reference 41.
- Arrays of units of any shape can be treated provided the data for c_2 and m_o are available (Reference 47).
- The array units should have an H/D ratio between 0.3 and 3.
- To achieve a limiting value for the surface density, the use of the method is limited to cubic arrays with at least 64 fissile units (some of the example problems apply the method to arrays with fewer units, but do not achieve a limiting surface density value).
- This method does not specifically account for non-uniform moderation within the arrays; however, the data in Table 7-1 consider moderated units with an H/X ratio of up to 20. Thus, this technique can be used for slightly moderated units but not for solutions.
- References 31 and 45 state that if a cubic array has less than 64 units, then a sphere may not be the most limiting fissile array unit.
- If the method is to be used for various array units with different fissile material compositions, care should be exercised when mixing units with significantly different levels of moderation.
- A disadvantage of this method is that, for some problems, scaling one array type to another to ultimately yield the configuration of interest may involve a significant number of calculations (see example problems for the limiting surface density method in Reference 16), which can introduce opportunities for error.

Table 7-1. Bare Spherical Critical Masses and Characteristic Constants for Some Fissile Materials in Water Reflected Cubic Arrays. (Reference 41, Table III)

No.	Material	H/X	Spherical Unit Unreflected Critical Mass, m_o (kg)	Characteristic Constant, c_2, for Criticality of Water-Reflected Arrays (10^{-3} cm^{-2})	
				c_2	$\pm$
1	Metal, U(100)[24]	0	45.68	1.806	0.036
2	Metal, U(93.2)	0	52.10	1.762	0.017
3	Oxide, U(93.2)O_2	0.4	90.24	0.854	0.007
4	Oxide, U(93.2)O_2	3	63.59	0.758	0.008
5	Oxide, U(93.2)O_2	10	31.43	0.778	0.007
6	Oxide, U(93.2)O_2	20	17.34	0.805	0.004
7	Metal, U(80)	0	69.89	1.359	0.012
8	Oxide, U(80)O_2	0.4	111.36	0.780	0.006
9	Oxide, U(80)O_2	3	74.08	0.713	0.006
10	Oxide, U(80)O_2	10	36.16	0.725	0.006
11	Oxide, U(80)O_2	20	18.67	0.779	0.005
12	Metal, U(70)	0	89.16	1.192	0.018
13	Oxide, U(70)O_2	0.4	133.39	0.723	0.006
14	Oxide, U(70)O_2	3	83.44	0.686	0.006
15	Oxide, U(70)O_2	10	36.89	0.735	0.004
16	Oxide, U(70)O_2	20	19.30	0.793	0.004
17	Metal, U(50)	0	159.60	0.901	0.008
18	Oxide, U(50)O_2	0.4	207.73	0.589	0.005

---

[24] U(X) denotes uranium enriched to X weight percent in U-235 (i.e., U[100] denotes isotopically pure U-235 with no U-238 present and U(93.2) indicates uranium enriched to 93.2 weight percent U-235 with the remainder U-238).

Table 7-1. Bare Spherical Critical Masses and Characteristic Constants for Some Fissile Materials in Water Reflected Cubic Arrays (continued). (Reference 41.)

No.	Material	H/X	Spherical Unit Unreflected Critical Mass, m_o (kg)	Characteristic Constant, c_2, for Criticality of Water-Reflected Arrays (10^{-3} cm^{-2})	
				c_2	$\pm$
19	Oxide, U(50)O$_2$	3	112.82	0.594	0.004
20	Oxide, U(50)O$_2$	10	55.14	0.520	0.006
21	Oxide, U(50)O$_2$	20	21.48	0.777	0.005
22	Metal, U(40)	0	228.06	0.787	0.016
23	Metal, U(30)	0	379.70	0.589	0.007
24	Oxide, U(30)O$_2$	0.4	409.60	0.450	0.003
25	Oxide, U(30)O$_2$	3	150.01	0.603	0.005
26	Oxide, U(30)O$_2$	10	54.01	0.636	0.004
27	Oxide, U(30)O$_2$	20	25.15	0.744	0.005
28	Metal, Pu(0)[25]	0	9.95	4.356	0.112
29	Oxide, Pu(0)O$_2$	0.4	26.66	1.542	0.015
30	Oxide, Pu(0)O$_2$	3	28.65	1.113	0.010
31	Oxide, Pu(0)O$_2$	10	20.21	0.965	0.007
32	Oxide, Pu(0)O$_2$	20	14.05	0.885	0.008
33	Metal, Pu(5.2)	0	10.34	4.138	0.091
34	Oxide, Pu(5.2)O$_2$	0.4	27.93	1.561	0.013
35	Oxide, Pu(5.2)O$_2$	3	32.78	1.097	0.011
36	Oxide, Pu(5.2)O$_2$	10	28.74	0.817	0.007
37	Metal, Pu(20)	0	11.69	4.261	0.099
38	Oxide, Pu(20)O$_2$	0.4	32.14	1.529	0.023
39	Oxide, Pu(20)O$_2$	3	42.43	1.022	0.013
40	Oxide, Pu(20)O$_2$	10	47.81	0.679	0.005
41	Metal, U-233	0	15.75	2.751	0.022
42	Oxide, U-233O$_2$	0.4	34.46	1.199	0.008
43	Oxide, U-233O$_2$	3	31.69	0.939	0.008
44	Oxide, U-233O$_2$	10	17.64	0.907	0.010
45	Oxide, U-233O$_2$	20	10.28	0.947	0.009
46	Metal, U(93.2)-10 wt. % Mo	0	73.06	1.305	0.009

7.3.1   Calculating the Multiplication Factor of an Array

A useful relationship developed by Thomas (Reference 39) for calculating the effective multiplication factor, k_{eff}, for a cubic array configuration. This expression is a function of m^k, which is the mass of a spherical fissile unit in an array with a given k_{eff}, and m^1, the mass of a spherical fissile unit in a critical array ($k_{eff} = 1$).

By substituting the expression for the fissile material density, this equation can be rearranged to be a function of only the radius of each unit. Recall that the volume of a sphere is equal to $V = \frac{4}{3}\pi r^3$, and the density is the mass divided by the volume:

---

[25] Pu(Y) denotes plutonium with Y atom percent Pu-240 (i.e., Pu[5.2] denotes plutonium with 5.2 atom percent Pu-240 and the remainder Pu-239).

$$\rho = \frac{\text{mass}}{\text{volume}} = \frac{m}{V} = \frac{m}{\frac{4}{3}\pi r^3} \tag{94}$$

Solve for m = mass in sphere with density, ρ.

$$m = \frac{4}{3}\pi r^3 \rho \tag{95}$$

Now substitute into Eq. (94) for the multiplication factor (note that the spacing between array units remains constant, and the material density, ρ, does not change as it is the same fissile material for both units):

$$k_{eff} = \left(\frac{m^k}{m^1}\right)^{\frac{1}{3}} = \left(\frac{\frac{4}{3}\pi(r^k)^3\rho}{\frac{4}{3}\pi(r_0)^3\rho}\right)^{\frac{1}{3}} = \frac{r^k}{r_0} \tag{96}$$

The k_{eff} for an array is simply the ratio of the subcritical spherical radius, r^k, of an array unit to the spherical radius, r_0, of a unit that makes the array critical. This relationship holds well for fast systems; however, the linear relationship may not hold well for thermal systems (see Appendix B on k_{eff} vs. critical mass). The use of this relationship will be illustrated in the example problems to follow. Also, this expression for the k_{eff} of an array can be used to derive relationships for the center-to-center spacing, d, between array units, and the k_{eff} as a function of d.

7.3.2 Limiting Surface Density Relationships for Subcritical Arrays

Unlike the surface density and density analog methods, the limiting surface density relationships derived in Section 7.2 are valid for critical array configurations. Using these relationships and the k_{eff} relationship in Section 7.3.1, expressions for the unit mass, m^k, to get an array k_{eff}, and the center-to-center spacing, $d=2a_n$, can be derived as a function of the desired k_{eff} for a particular array configuration.

Begin the derivation with Eq. (96) for the k_{eff} for an array as defined in Section 7.3.1.

$$k_{eff} = \left(\frac{m^k}{m^1}\right)^{\frac{1}{3}}$$

Recall that the mass m^1 in a critical array with spacing, d_0, is given by Eq. (93) or as rearranged:

$$m^1 = m_0 \times \left(\left[\frac{n_z\left(1-\frac{c}{\sqrt{N}}\right)^2}{c_2 d_0^2}\right] + 1\right)^{-1} \quad \text{OR} \quad \left(\frac{m_0}{m^1}\right) = \left(\left[\frac{n_z\left(1-\frac{c}{\sqrt{N}}\right)^2}{c_2 d_0^2}\right] + 1\right) \tag{97}$$

Now from Eq. (94) for the k-effective, whenever we have m^1 / m_0, we can substitute $m^k / m_0 * 1 / k_{eff}^3$ or for m_0 / m^1, we can substitute $m_0 / m^k * k_{eff}^3$. Substituting into Eq. (98):

$$\left(\frac{m_0}{m^1}\right) = \left(\left[\frac{\left|n_z\left(1-\frac{c}{\sqrt{N}}\right)^2\right|}{c_2 d_0^2}\right] + 1\right) \quad \Rightarrow \left(\frac{m_0}{m^k}\right) \times k_{eff}^3 = \left(\left[\frac{\left|n_z\left(1-\frac{c}{\sqrt{N}}\right)^2\right|}{c_2 d_0^2}\right] + 1\right)$$

(98)

Then solving Eq. (98) for the k_{eff} associated with a given mass, m^k, and a given unit spacing, d_0, we find

$$k_{eff}^3 = \left(\left[\frac{\left|n_z\left(1-\frac{c}{\sqrt{N}}\right)^2\right|}{c_2 d_0^2}\right] + 1\right) \times \left(\frac{m^k}{m_0}\right)$$

OR

(99)

$$k_{eff} = \left\{\left(\left[\frac{\left|n_z\left(1-\frac{c}{\sqrt{N}}\right)^2\right|}{c_2 d_0^2}\right] + 1\right) \times \left(\frac{m^k}{m_0}\right)\right\}^{\frac{1}{3}}$$

Notice that there are three interrelated parameters: k_{eff}, m_k, and d_0. We can choose any two of them and then solve for the related value of the third. So, if we want to determine the mass, m^k, associated with a given spacing, d_0, and a given, k_{eff}:

$$m^k = m_0 \frac{k_{eff}^3}{\left(\left[\frac{\left|n_z\left(1-\frac{c}{\sqrt{N}}\right)^2\right|}{c_2 d_0^2}\right] + 1\right)}$$

(100)

where d_0 is the center-to-center spacing for a critical array, c_2 is the constant for the fissile material and m_0 is the unreflected spherical critical mass for the fissile material—both found in Table 7-1—$c = 0.55$, n_z is the least number of units in any direction, N is the total number of units in the array, and m^k is the mass of a unit that gives an array the desired k_{eff}.

Now we can determine the center-to-center spacing, d_k, that gives a particular k_{eff} in an array composed of units with mass, m^k.

$$d_k = \sqrt{\frac{n_z\left(1-\frac{c}{\sqrt{N}}\right)^2}{c_2\left(k_{eff}^3 \frac{m_0}{m^k} - 1\right)}}$$

(101)

The following equation gives the ratio of the unreflected critical mass of an array unit to the array unit mass in a critical array $= m_0 / m^1$. Noting that the right-hand sides of Eq. (98) and (99) are the same, we can write the following equation for the left-hand sides:

$$\frac{m_0}{m^1} = \frac{m_0}{m^k} \times k_{eff}^3$$

(102)

Note that Eq. (103) makes sense as $m^k = m^l$ when $k_{eff} = 1$.

Substituting $k_{eff} = 1$ and m^l in Eq. (102), we can determine the critical center-to-center spacing, d_0, for a critical array with mass, m^l.

$$d_0 = \sqrt{\frac{n_z\left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2\left(\frac{m_0}{m^1} - 1\right)}} \tag{103}$$

Replacing m^l with m^k ($m^k < m^l$) and retaining the spacing, d_0, will produce an array with a $k_{eff} < 1$ as shown in Eq. (100) (repeated below).

$$k_{eff} = \left\{\left(\left[\frac{n_z\left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2 d_0^2}\right] + 1\right) \times \left(\frac{m^k}{m_0}\right)\right\}^{\frac{1}{3}} \tag{104}$$

7.3.3 Summary of the Fundamental Limiting Surface Density Relationships

This section summarizes the fundamental limiting surface density relationships defined up to this point of Section 7. Other relationships are defined to consider changes in array unit density, for example, and will be considered in subsequent sections. For these equations, there are three interrelated parameters, k_{eff} – the k_{eff} of the array, m^k – the mass in an array with a given k_{eff}, and d_k – the center-to-center spacing for an array with a particular k_{eff}. We can choose any two of them and then solve for the related value of the third. For a critical array, $d_k = d_0$, $m^k = m^l$, and $k_{eff} = 1$.

Array k_{eff} as a function of array unit mass, m^k and center-to-center spacing, d_k – Eq. (105):

$$k_{eff} = \left\{\left(\left[\frac{n_z\left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2 d_k^2}\right] + 1\right) \times \left(\frac{m^k}{m_0}\right)\right\}^{\frac{1}{3}} \tag{105}$$

Array unit mass, m^k, required for a desired array k_{eff} and center-to-center spacing, d_k – Eq. (106):

$$m^k = m_0 \frac{k_{eff}^3}{\left(\left[\frac{n_z\left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2 d_k^2}\right] + 1\right)} \tag{106}$$

Array unit center-to-center spacing, d_k, as a function of the mass, m^k, and array k_{eff} – Eq. (107):

$$d_k = \sqrt{\frac{n_z \left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2 \left(k_{eff}^3 \frac{m_0}{m^k} - 1\right)}}$$

(107)

7.4 EXAMPLE PROBLEMS FOR LIMITING SURFACE DENSITY

Using the graphical technique, as illustrated in Figure 7-3, can be helpful to visualize changes to the critical points of an array during a parametric study. This concept will be shown in some of the example problems that follow. Table 7-1 provides values of the unreflected spherical critical mass and characteristic constants for a variety of materials for use in the example problem solutions. The example problem solutions and a comparison to a computer code (SCALE or MCNP) are provided in Chapter 10.
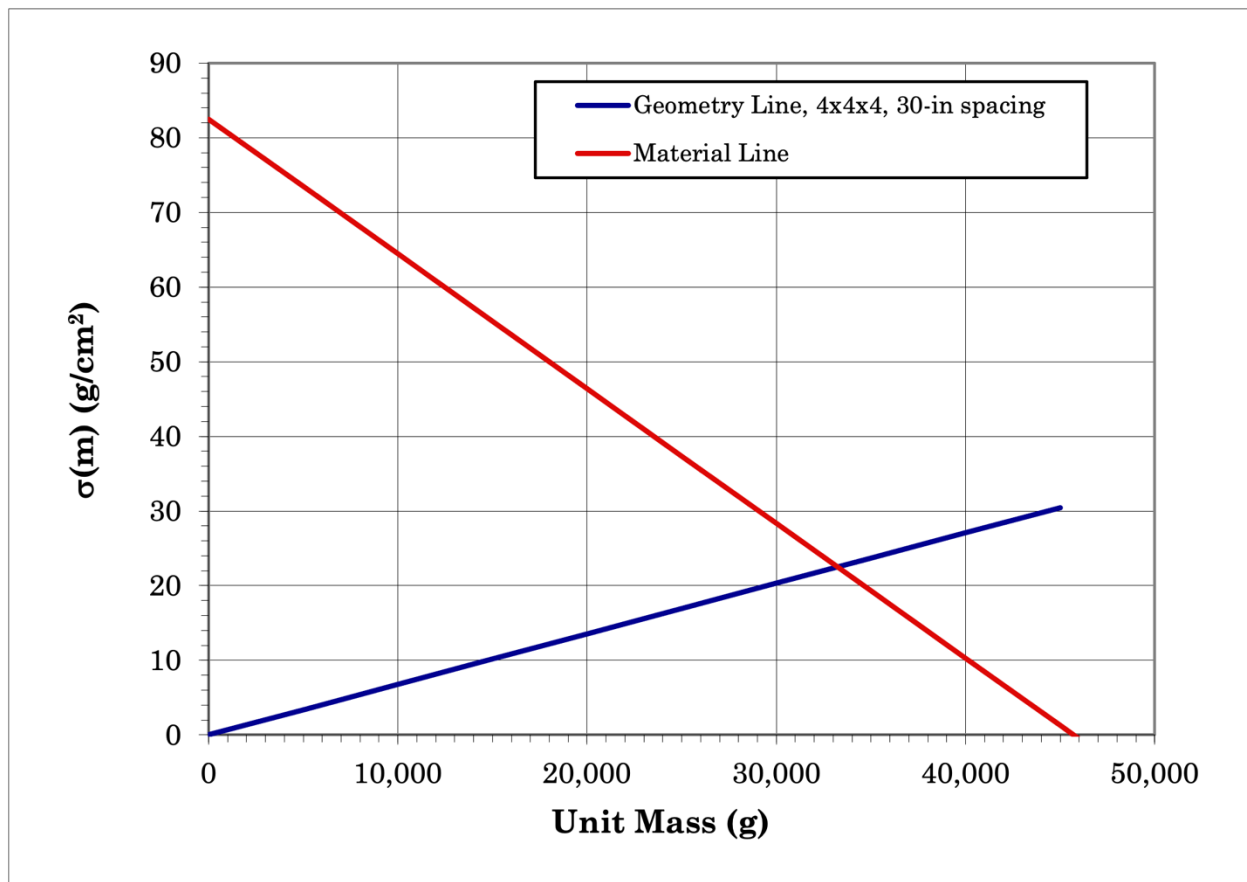
Figure 7-3. U(100) Metal Critical Array Solution for 4×4×4 Array (30 in. spacing).

7.4.1 Limiting Surface Density Example Problem 1

For 2×2×2, 4x4x4, 10×10×10, and 100×100×100 arrays, what is the minimum center-to-center spacing of plutonium oxide ($^{239}PuO_2$) containers loaded with 4,500 g of Pu per container? Assume that the Pu oxide density is 11.48 g/cm³, which is the theoretical density for PuO_2, and the Pu is pure Pu-239
The limiting surface density relationships were developed from array configurations with 64 or more units. Thus, this method should not be used for the 2×2×2 array; however, the other cubic arrays, the

176

4x4x4, 10×10×10, and 100×100×100 configurations, can be evaluated using this method. From Section 7.1, the center-to-center spacing between array units can be calculated as follows.

$$d_0 = \sqrt{\frac{n_z\left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2\left(\frac{m_0}{m^1} - 1\right)}}$$

where:

m_o	–	26.66 kg for ^{239}PuO$_2$ oxide with an H/X = 0.4 (Table 7-1);
m^1	–	4.5 kg from *the* problem description[26];
n_z	–	4, 10 and *100* from the problem description;
c_2	–	0.001542 *cm*$^{-2}$ (Table 7-1) – note that the values in Table 7-1 are multiplied by 1000;
N	–	equal to n^3=64, 1,000, and 1,000,000; and
c	–	0.55, *defined* previously.

Note that there is a small quantity of moisture (H/X = 0.4) in the critical mass and c_2 data listed in Table 7-1. This fact should not affect the result significantly because a small quantity of moisture tends to reduce only the density of the Pu oxide instead of providing significant moderation. Substituting the values for each variable into the array critical mass relationship provides the following center-to-center unit spacing results.

The $4 \times 4 \times 4$ cubic array center-to-center spacing is given by

$$d_0 = \sqrt{\frac{4\left(1 - \frac{0.55}{\sqrt{64}}\right)^2}{0.001542 \text{ cm}^{-2}\left(\frac{26.66 \text{ kg}}{4.5 \text{ kg}} - 1\right)}} \approx 21.4 \text{ cm} \approx 8.5 \text{ inches}$$

This center-to-center spacing of PuO$_2$ units would make the 4×4×4 cubic array critical. The edge-to-edge spacing would be 21.4 cm—the diameter of the 4.5 kg sphere. From the footnote on the previous page, the diameter is 9.468 cm, so the spheres would be spaced 11.9 cm (or about 4.75 in.) apart to create a critical 4×4×4 array.

The $10 \times 10 \times 10$ cubic array center-to-center spacing is given by

$$d_0 = \sqrt{\frac{10\left(1 - \frac{0.55}{\sqrt{1000}}\right)^2}{0.001542 \text{ cm}^{-2}\left(\frac{26.66 \text{ kg}}{4.5 \text{ kg}} - 1\right)}} \approx 35.7 \text{ cm} \approx 14 \text{ inches}$$

This spacing of PuO$_2$ units would make the 10×10×10 cubic array critical.

---

[26] The 4.5 kg of Pu is in the form of PuO$_2$, so multiplying by 271.05 g PuO$_2$ / mole and dividing by 239.05 g Pu/mole gives 5.1 kg for the weight of the PuO$_2$. At a density of 11.48 g/cm^3, this gives a volume of 444.46 cm^3. This volume in spherical form would have a radius of 4.734 cm and a diameter of 9.468 cm.

For a 100×100×100 array, one would expect that the critical, center-to-center spacing would be much larger than that for the 10×10×10 array—just as the spacing for the 10×10×10 array was larger than that for the 4×4×4 array. The 100×100×100 cubic array center-to-center spacing is given by:

$$d_0 = \sqrt{\frac{100\left(1 - \frac{0.55}{\sqrt{1,000,000}}\right)^2}{0.001542 \ cm^{-2}\left[\frac{26.66 \ kg}{4.5 \ kg} - 1\right]}}$$

$$d_0 = (2a_n) = 114.7 \ cm \ (\sim 45.0 \ in.)$$

This is significantly more spacing between units than for the 10×10×10 case. Although the 100×100×100 array is unrealistic, it was used here to show the trend in spacing as one moves towards an infinite array.

Note that the surface density of the arrays given by $\frac{n \times m}{d^2}$ approaches a limiting value, as n gets larger. For the 4×4×4 array, the surface density is

$$\frac{n \times m}{d^2} = \frac{4 \times 4,500 \ g}{(21.4 \ cm)^2} = 39.3 \ \frac{g}{cm^2}, \text{ whereas the surface density for the 10×10×10 array is}$$

$$\frac{n \times m}{d^2} = \frac{10 \times 4,500 \ g}{(35.7 \ cm)^2} = 35.3 \ \frac{g}{cm^2}, \text{ and the surface density for the 100×100×100 array is}$$

$$\frac{n \times m}{d^2} = \frac{100 \times 4,500 \ g}{(114.7 \ cm)^2} = 34.2 \ \frac{g}{cm^2}.$$

A quick calculation with a spreadsheet shows that the limiting value for the surface density for this example problem is about 34.2 g/cm² as the array size increases toward an infinite number of units. A simpler way to determine the limiting value for the surface density is to calculate it using the definition for the surface density as given in Eq. (90), which is dependent upon the material properties of the array:

$$\sigma(m) = c_2(m_0 - m) \text{ , where } c_2, m_0, \text{ and } m \text{ are previously defined.}$$

Substituting these values into this relationship results in the same limiting surface density value as calculated above:

$$\sigma(m) = 1.542 x 10^{-3} \ cm^{-2}(26.68 \ kg - 4.5 \ kg)\left[\frac{10^3 \ grams}{kg}\right] = 34.2 \ \frac{grams}{cm^2}$$

7.4.2 Limiting Surface Density Example Problem 2

1. Using the limiting surface density method, determine the minimum center-to-center spacing for 4×4×4 and 10×10×10 arrays of 4,500 g Pu(5) metal ingots.
2. Calculate the center-to-center spacing that would give a $k_{eff} = 0.8$ for a 10×10×10 array of the 4,500 g Pu(5) metal ingots.

$$d_0 = \sqrt{\frac{n_z\left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2\left(\frac{m_0}{m^1} - 1\right)}}$$

where:

m_o — 10.34 kg for Pu(5.2) metal (Table 7-1)

m — 4.5 kg from the problem description

nz — 4 and 10 from the problem description

c2 — 0.004138 cm² (Table 7-1)

N — equal to $n^3 = 64$ and 1,000

c — 0.55, defined previously.

Note that the data from Table 7-1 for Pu metal is for Pu(5.2), which contains 5.2 wt % Pu-240 rather than 5 wt % as in the problem statement. This should not significantly affect the results. Substituting the values for each variable into the array critical mass relationship provides the following center-to-center unit spacing result for the 4×4×4 array.

$$d_0 = \sqrt{\frac{4\left(1 - \frac{0.55}{\sqrt{64}}\right)^2}{0.004138 \text{ cm}^{-2}\left(\frac{10.34 \text{ kg}}{4.5 \text{ kg}} - 1\right)}} \approx 25.4 \text{ cm} \approx 10.0 \text{ inches}$$

This is the center-to-center spacing of 4.5 kg Pu(5.2) metal units required to make the 4×4×4 cubic array critical.

For a 10×10×10 array, one would expect that the critical, center-to-center spacing would be much larger than that of the 4×4×4 array. The 10×10×10 cubic array center-to-center spacing is given by:

$$d_0 = \sqrt{\frac{10\left(1 - \frac{0.55}{\sqrt{1000}}\right)^2}{0.004138 \text{ cm}^{-2}\left(\frac{10.34 \text{ kg}}{4.5 \text{ kg}} - 1\right)}} \approx 42.4 \text{ cm} \approx 16.75 \text{ inches}$$

This is a greater spacing between units than that for the 4×4×4 case, as expected.

PART 2 – A relationship was derived for this Primer to consider the array unit center-to-center spacing as a function of the array k_{eff} (Eq. 102, Section 7.3.2). Thus, if a criticality safety engineer wanted a center-to-center spacing, d_k, result that resulted in an array k_{eff} of 0.8, the following calculation could be done.

For a subcritical array, Eq. (102) gives the center-to-center spacing between array units for a given k_{eff}:

$$d_k = \sqrt{\frac{n_z\left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_2\left(k_{eff}^3 \frac{m_0}{m^k} - 1\right)}}$$

For a 10×10×10 array, the spacing for units of 4.5 kg and $k_{eff} = 0.8$:

$$d_k = \sqrt{\frac{10\left(1 - \frac{0.55}{\sqrt{1,000}}\right)^2}{0.004138 \ \mathrm{cm}^{-2}\left((0.8)^3 \frac{10.34 \ \mathrm{kg}}{4.5 \ \mathrm{kg}} - 1\right)}} \approx 115.0 \ \mathrm{cm} \approx 45.25 \ \mathrm{inches}$$

Thus, to maintain a subcritical configuration for this large array size, it makes sense that the array units should be spaced much farther apart than for the critical array (i.e., 45.25 in. for $k_{\mathrm{eff}} = 0.8$ versus 16.75 in. for critical).

7.4.3 Limiting Surface Density Example Problem 3

1. Using the limiting surface density method, calculate the critical mass for each array unit required for a water-reflected cubic array of fully enriched U(100) metal for a 4×4×4 array with a center-to-center spacing of 30 in. (76.2 cm).
2. After the critical mass is calculated, determine the multiplication factor for storing 20 kg of U(100) units in the 4×4×4 array.

<u>Non-graphical solution</u>

PART 1 – For a 4×4×4 cubic array with the given spacing

$$n = n_x = n_y = n_z = 4$$

$$a_n = a_x = a_y = a_z = 30/2 = 15 \ \mathrm{in.} \ (38.1 \ \mathrm{cm})$$

the following relationship (Eq. 101 with $k_{\mathrm{eff}} = 1$) for a cubic array can be used to determine the critical mass per unit to maintain the array in a critical condition for U(100) metal units.

$$m^1 = m_0 \frac{1}{\left(\left[\frac{\left(n_z\left(1 - \frac{c}{\sqrt{N}}\right)\right)^2}{c_2 d_0^2}\right] + 1\right)}$$

where

m_o	–	45.68 kg from Table 7-1
n_z	–	4 from the problem statement above
d_0	–	center-to-center spacing (ctc) = 30 in. (76.2 cm) from the problem statement
c_2	–	0.001806 cm^{-2} from Table 7-1
N	–	equal to $n^3 = 64$
c	–	0.55, defined previously.

Substituting the values for each variable into the array critical mass relationship provides the following result:

$$m^1 = 45.68 \ \mathrm{kg} \ \frac{1}{\left(\left[\frac{4\left(1 - \frac{0.55}{\sqrt{64}}\right)^2}{0.001806 \ \mathrm{cm}^{-2}(76.2 \ \mathrm{cm})^2}\right] + 1\right)} = 34.3 \ \mathrm{kg}$$

180

This is the mass of U(100) metal required in each array unit to make the 4×4×4 cubic array critical.

PART 2 – Now, the multiplication factor can be calculated if one is interested in storing 20 kg U(100) metal units in each array location. The resulting multiplication factor is calculated using Eq. (95), where m^k is the desired unit mass to be stored (20 kg) and m^1 is the calculated critical mass in the array as calculated above:

$$k_{eff} = \left(\frac{m^k}{m^1}\right)^{\frac{1}{3}} = \left(\frac{20 \text{ kg}}{34.3 \text{ kg}}\right)^{\frac{1}{3}} = 0.835$$

With the specified 30 in. (76.2 cm) spacing between units of 20 kg each, this array configuration will remain subcritical.

Graphical solution

Referring to Figure 7-3, we see that the characteristics of a geometry line are

$$\text{slope:} \quad = \left(\frac{\sqrt[3]{N}}{(2a_n)^2}\right)\left(1 - \frac{0.55}{\sqrt{N}}\right)^2$$
$$\text{y - intercept:} \quad = 0$$
$$\text{equation:} \quad \sigma(m) = \text{slope} \times m + 0$$

And then the characteristics of a material line are

$$\text{slope:} \quad = -c_2$$
$$\text{y - intercept:} \quad = c_2 \times m_0$$
$$\text{equation:} \quad \sigma(m) = \text{slope} \times m + c_2 \times m_0$$

The mass at the intersection of the geometry and material lines is calculated as

$$m = \frac{m_0}{\left(\frac{\text{geom line slope}}{c_2} + 1\right)} \quad \text{or} \quad \frac{m_o}{\left(\frac{\left(\frac{\sqrt[3]{N}}{(2a_n)^2}\right)\left(1 - \frac{0.55}{\sqrt{N}}\right)^2}{c_2} + 1\right)}$$

Then, for the example,

Geometry Line:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{4m}{(76.2 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{64}}\right)^2$$

$$\sigma(m) = 5.974x10^{-4} \times m[cm]^{-2} \text{or} \quad \frac{\sigma(m)}{m[\text{grams}]} = 5.974x10^{-4}[cm]^{-2}$$

181

Material line for U(100): $\sigma(m) = c_2(m_0 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right]$ Note that the intercept is:: $c_2\, m_0 = 1.806 \times 10^{-3}$ * $45,680 = 82.5$ g/cm^2, which is $s(m_0)$.

$$\sigma(m) = 1.806x10^{-3}(45,680 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right] \quad \text{or} \quad \frac{\sigma(m)}{m} = 1.806x10^{-3}\left(\frac{45,680}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

Equating the geometrical and material line relationships,

$$\frac{\sigma(m)}{m[\text{grams}]} = 5.974x10^{-4}[cm]^{-2} = 1.806x10^{-3}\left(\frac{45,680}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

$$m[\text{grams}] = 34,326 \text{ grams}$$

Or calculating the mass from the intersection point as,

$$m = \frac{m_0}{\left(\frac{\text{geom line slope}}{c_2} + 1\right)} \quad \text{or} \quad \frac{45.68\text{kg}}{\left(\frac{5.974x10^{-4}\text{cm}^{-2}}{1.806x10^{-3}\text{cm}^{-2}} + 1\right)} = 34.326 \text{ kg}$$

Note that the graphical solution (Figure 7-4) indicates the array critical unit mass is approximately 34,300 grams for this 64-unit array, which corresponds to a limiting surface density of about 20.5 g/cm^2.

PART II – Using the graphical method, what would be the effect on critical array unit mass if the U(100) metal was adjusted to a more realistic material such as highly enriched uranium, U(93.2)?

The change of material can be made simply by finding the value of c_2 and m_o for U(93.2) metal in Table 7-1 (m_o= 52.1 kg or 52,100 grams and c_2 = 0.0001762 cm^{-2}) and replacing the U(100) value in the material line as follows:

Material line: $\sigma(m) = c_2(m_0 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right]$

$$\frac{\sigma(m)}{m} = 1.762x10^{-3}\left(\frac{52,100}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

The geometry line equation is unchanged: $\frac{\sigma(m)}{m[\text{grams}]} = 5.974x10^{-4}[cm]^{-2}$

Setting the geometry line equal to the material line results in the following:

$$\frac{\sigma(m)}{m[\text{grams}]} = 5.974x10^{-4}[cm]^{-2} = 1.762x10^{-3}\left(\frac{52,100}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

$$m[\text{grams}] = 38,908 \text{ grams}$$
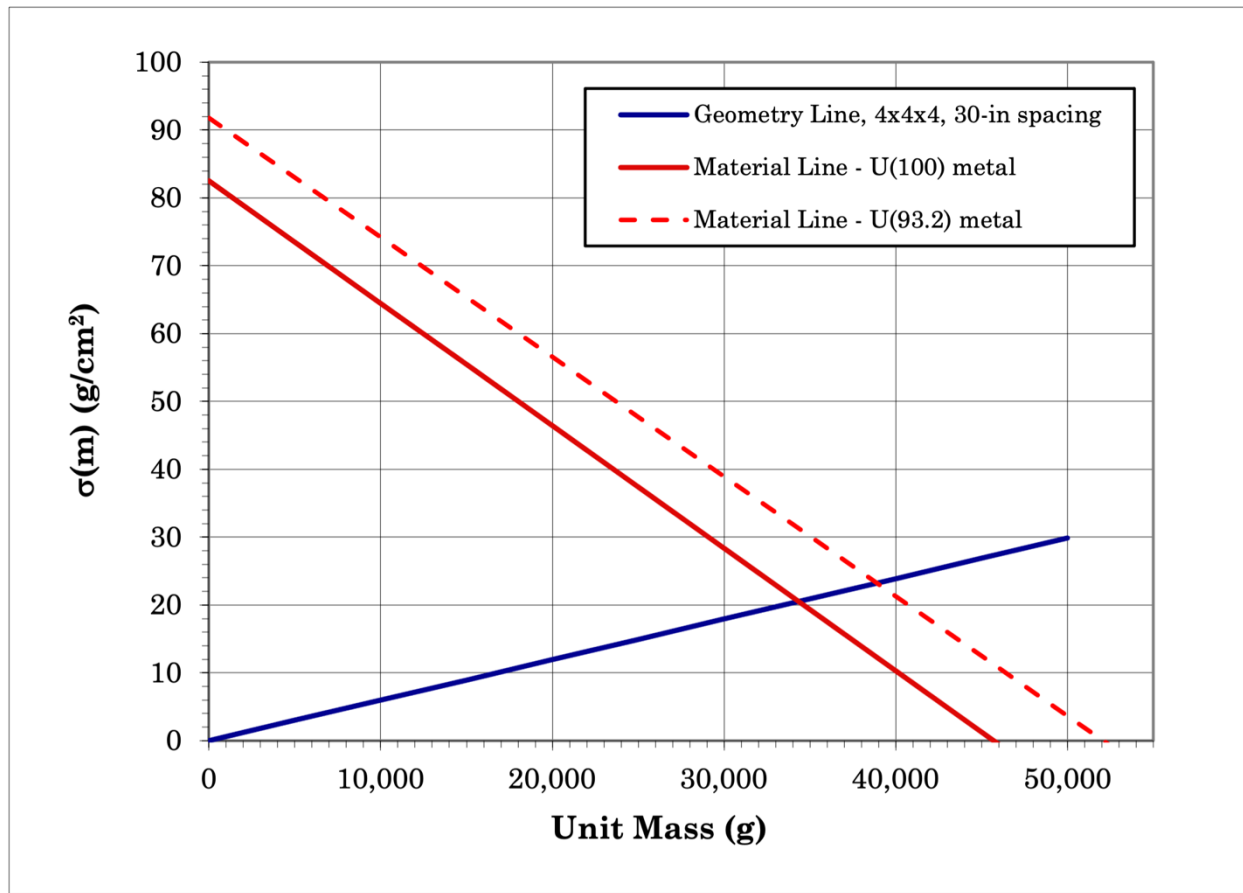
Figure 7-4. U(93.2) Metal Critical Array Solution 4x4x4 Array (30" spacing).

Figure 7-5 shows the new material line for U(93.2) next to the U(100) material line. The decrease in U-235 enrichment for the uranium metal units results in an increase in the array unit mass necessary for criticality from 34,374 g to 38,964 g (increase 4,590 g of uranium mass). This calculation estimates the level of conservatism associated with the use of U(100) metal to bound the storage of HEU metal in a process facility.

The k_{eff} for 20 kg U(93.2) metal units in each array location can be calculated and compared to the U(100) k_{eff}.

$$k_{eff} = \left(\frac{m^k}{m^1}\right)^{\frac{1}{3}} = \left(\frac{20 \text{ kg}}{38.964 \text{ kg}}\right)^{\frac{1}{3}} = 0.801$$

With the 20 kg units spaced 30 in., center-to-center, changing from U(100) to U(93.2) reduces the k_{eff} from 0.835 to 0.801.
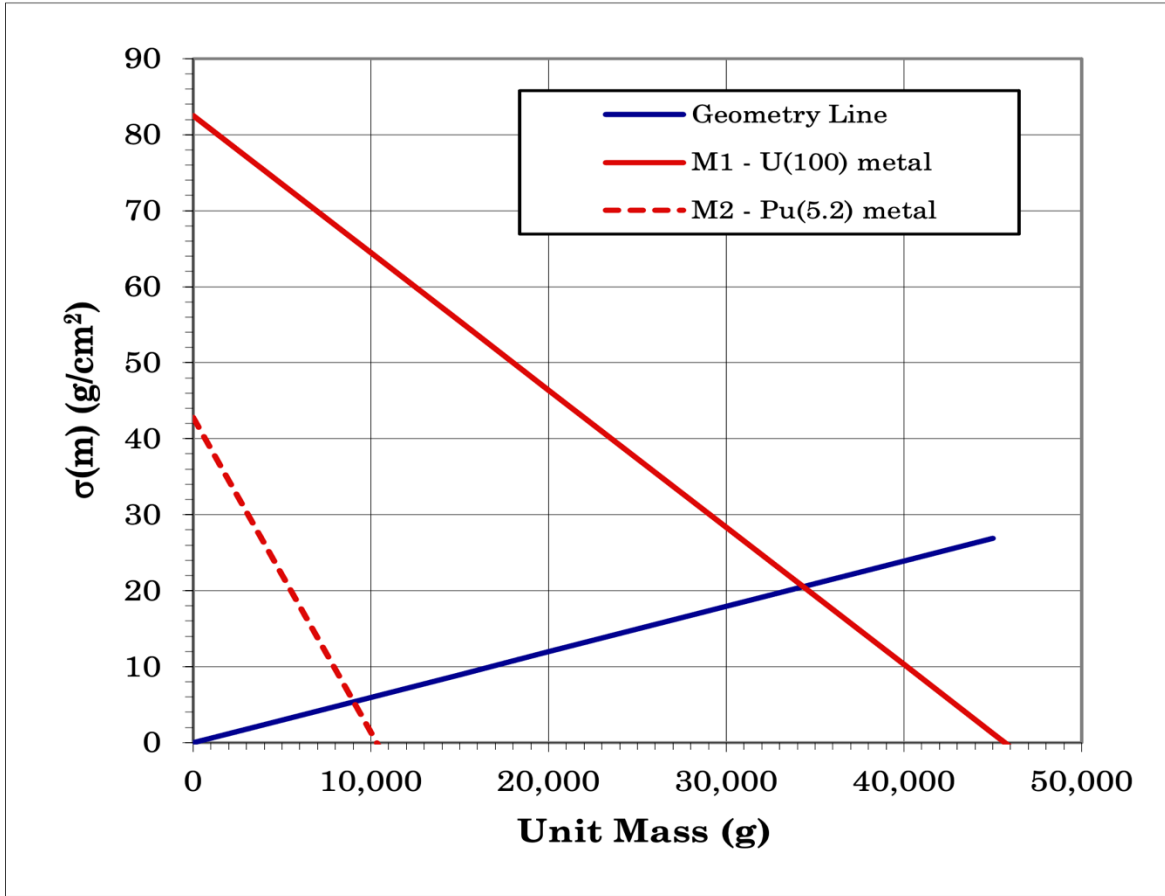
Figure 7-5. Solution for Limiting Surface Density Example Problem 4.

7.4.4   Limiting Surface Density Example Problem 4

1. Using the limiting surface density method, calculate the critical mass for each array unit required for a water-reflected cubic array of 5 kg Pu(5.2) metal units in a 4×4×4 array with a center-to-center spacing of 30 in. (76.2 cm).
2. After the critical mass is calculated, determine the multiplication factor for storing 5 kg of Pu(5.2) units in the 4×4×4 array.

Non-graphical solution:

$$m^1 = m_0 \frac{1}{\left(\left[\dfrac{\left[n_z\left(1 - \dfrac{c}{\sqrt{N}}\right)\right]^2}{c_2 d_0^2} \right] + 1 \right)}$$

where

m_o	–	10.34 kg (Table 7-1)
n_z	–	4 from the problem statement above
d_0	–	center-to-center spacing (ctc) = 30 in. (76.2 cm) from the problem statement
;;c_2	–	0.004138 cm^{-2} (Table 7-1)

N –   equal to $n^3 = 64$

c –   0.55, defined previously

Substituting the values for each variable into the array critical mass relationship provides the following result:

$$m^1 = 10.34 \text{ kg } \frac{1}{\left(\left[\frac{4}{0.004138 \text{ cm}^{-2}(76.2 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{64}}\right)^2\right] + 1\right)} = 9.035 \text{ kg}$$

This is the mass of Pu(5.2) metal required in each array unit to keep the 4×4×4 cubic array critical at a center-to-center spacing of 30 in. (76.2 cm). Note that this critical mass is significantly lower than the 34.3 kg required for U(100) metal in the same configuration.

Now, the k_{eff} can be calculated if one is interested in storing 5 kg Pu(5.2) metal units in each array location. The resulting k_{eff} is calculated below where m is the desired unit to be stored (5 kg) and m' is the calculated critical mass in the array as calculated above:

$$k_{eff} = \left(\frac{m^k}{m^1}\right)^{\frac{1}{3}} = \left(\frac{5 \text{ kg}}{9.04 \text{ kg}}\right)^{\frac{1}{3}} = 0.821$$

Storing 5 kg Pu(5.2) metal units in a 4×4×4 array with about 30 in. (76.2 cm) spacing between array units is subcritical under normal conditions.

Graphical Solution

Notice that the array geometry is unchanged from the previous example problem. For comparison purposes, the final plot will include the data from the last example problem to illustrate the change to the system when the array units are Pu(5.2) metal instead of U(100) metal while keeping the array geometrical configuration constant.

Geometry Line:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{4m}{(76.2 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{64}}\right)^2$$

$$\sigma(m) = 5.97x10^{-4} \times m[cm]^{-2} \text{ or } \frac{\sigma(m)}{m[\text{grams}]} = 5.97x10^{-4}[cm]^{-2}$$

Material line for Pu(5.2): $\sigma(m) = c_2(m_0 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right]$ Note that the intercept is: $c_2 m_0 = 4.138 \times 10^{-3}$ * $10336 = 42.8 \text{ g/cm}^2$, which is $s(m_0)$ for Pu(5.2).

$$\frac{\sigma(m)}{m} = 4.138x10^{-3}\left(\frac{10,336}{m[\text{grams}]} - 1\right)[cm^{-2}]$$

Equating the geometrical and material line relationships,

$$\frac{\sigma(m)}{m[\text{grams}]} = 5.974x10^{-4}[cm]^{-2} = 4.138x10^{-3}\left(\frac{10,336}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

$$m[\text{grams}] = 9,032 \text{ grams}$$

Note that the graphical solution (Figure 7-6) illustrates a solution for the array critical unit mass at about 9 kg (illustrated by the M2 line in the plot), which corresponds to a limiting surface density of about 5.4 g/cm². This plot clearly shows how much more reactive Pu(5.2) metal is as compared to U(100) metal. The higher infinite multiplication factor of Pu(5.2) requires a much lower array unit mass than does U(100) metal for the same k_{eff}, keeping the array geometry constant.
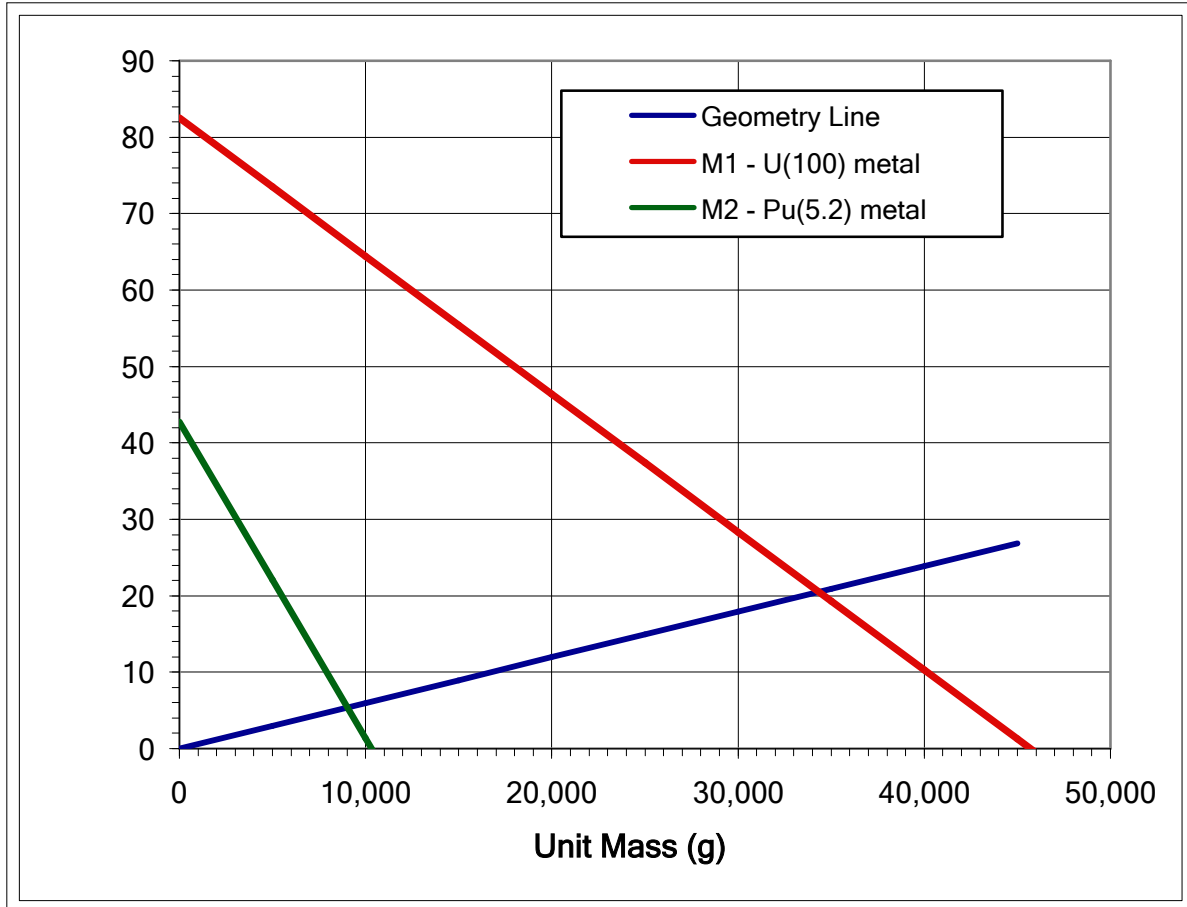
Figure 7-6. Demonstration of Mass Equivalence.

7.4.5   Limiting Surface Density Example Problem 5

Based on the results of the previous example problem in Section 7.4.4 (Limiting Surface Density Example Problem 4), calculate the required array unit mass that results in a multiplication factor of 0.9 using the same limiting surface density relationships.

The first step for this problem is to calculate the mass required for this array to have a multiplication factor of 0.9 by rearranging Eq. (94).

$$k_{eff} = \left(\frac{m^k}{m^1}\right)^{\frac{1}{3}} \Rightarrow \frac{m^k}{m^1} = k_{eff}^3 \Rightarrow m^k = m^1 \times k_{eff}^3$$

Note that m^1 is the critical array mass calculated in the last problem: 9,035 g.

$$m^k = m^1 \times k_{eff}^3 = 9{,}032 \text{ grams} \times (0.9)^3 = 6{,}584 \text{ grams}$$

The array unit mass necessary for a k_{eff} of 0.9 reduces the array unit mass by 2,448 g.

7.5   THE EQUIVALENCE OF DIFFERENT FISSILE UNITS IN WATER-REFLECTED ARRAYS

Units of different fissile material or of different reactivity may be defined as equivalent when a substitution of units in a reflected array does not produce a change in the array multiplication factor (Reference 39). This array condition will be true if the following is true.

$$\frac{\sigma(m)}{m} = \frac{\sigma(m')}{m'} \tag{108}$$

In this relationship, the variables m and m' represent the different masses of different materials in the same array configuration (i.e., a_n, N and n_z do not change as these represent the geometrical configuration of the array). (Note: the prime superscript will be used to denote a different fissile material). One can derive an equivalence relationship for this situation as follows.

The ratio of the geometry and material lines for the two different array fissile materials can be used to derive a relationship for the "equivalent" mass of a different fissile material to maintain array criticality.

Geometry line:

$$\frac{\sigma(m)}{m} = \frac{n_z}{(d)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 \tag{109}$$

Material line:

$$\frac{\sigma(m)}{m} = c_2\left(\frac{m_0}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}] \tag{110}$$

Equating the geometry and material lines results in the following equivalence relationship:

$$\frac{n_z}{(d)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = c_2\left(\frac{m_0}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}] \tag{111}$$

For two different types of fissile materials, masses m and m' have unreflected critical masses m_0 and m_0', respectively. The equivalence relationship modified for the substituted material and noting that the geometrical properties of the array do not change can be written as follows:

$$\frac{n_z}{(d)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = c_2'\left(\frac{m_0'}{m'[\text{grams}]} - 1\right)[\text{cm}^{-2}] \tag{112}$$

Taking the ratio of the equivalence relationship for each material,

$$\frac{\frac{n_z}{(d)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2}{\frac{n_z}{(d)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2} = \frac{c_2\left(\frac{m_0}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]}{c_2'\left(\frac{m_0'}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]} = 1 \tag{113}$$

Simplify this relationship and then solve for the mass of the substituted unit, m':

$$c_2'\left(\frac{m_0'}{m'[\text{grams}]} - 1\right)[\text{cm}^{-2}] = c_2\left(\frac{m_0}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}] \tag{114}$$

Then,

$$m'^1 = \frac{m_0'}{\left[\frac{c_2}{c_2'}\left(\frac{m_0}{m^1} - 1\right) + 1\right]}$$

Notice that the grams units have been removed. If the masses in the ratios have the same units, then it does not matter whether these are expressed as grams or as kilograms.

Thus, this relationship can be used to consider an "equivalent" mass, m', of a different fissile material to maintain criticality of the array.

Calculation of Equivalent Mass for given k_{eff}

The "equivalent" mass, $m^{k'}$, of a different fissile material for a given k_{eff}, d, n_z, and N is

$$m'^k = m'^1 \times k_{\text{eff}}^3 \text{ or}$$

$$m'^k = \frac{m_0' \times k_{\text{eff}}^3}{\left[\frac{c_2}{c_2'}\left(\frac{m_0}{m^1} - 1\right) + 1\right]} \tag{115}$$

And similarly, k_{eff} can be calculated as

$$k_{\text{eff}} = \left(\frac{m'^k}{m'^1}\right)^{\frac{1}{3}} \text{ or}$$

$$k_{\text{eff}} = \left\{\frac{m'^k}{m_0'}\left[\frac{c_2}{c_2'}\left(\frac{m_0}{m^1} - 1\right) + 1\right]\right\}^{\frac{1}{3}} \tag{116}$$

Where: $m^{1'}$ is the "equivalent" mass to produce a critical array, m^1 is the mass of the first nuclide that creates a critical array, and m_0 is the critical mass of a single unit sphere of the first nuclide.

7.5.1 Limiting Surface Density Example Problem 6

Use the equivalence relationship derived in Section 7.5 to confirm the results of the example problem 4 from Section 7.4.4 for Pu(5.2) metal units in a 4×4×4 array.

The values for the characteristic constants, c_2 and c_2' and the bare, spherical critical masses can be found in Table 7-1.

$$
\begin{array}{lll}
m_o' & - & \text{10.34 kg for Pu(5.2) metal} \\
c_2' & - & \text{4.138×10}^{-3} \text{ cm}^{-2} \text{ for Pu(5.2) metal} \\
m^1 & - & \text{34.30 kg for U(100) metal (result from example problem in Section 7.4.3)} \\
m_o & - & \text{45.68 kg for U(100) metal} \\
c_2 & - & \text{1.806×10}^{-3} \text{ cm}^{-2} \text{ for U(100) metal}
\end{array}
$$

The equivalence relationship, Eq. (111) from Section 7.5 can be used to find the equivalent mass of Pu(5.2) in the critical 4×4×4 array of U(100) metal units:

$$
m'^1 = \frac{m_0'}{\left[\frac{c_2}{c_2'} \left(\frac{m_0}{m^1} - 1 \right) + 1 \right]}
$$

$$
m'^1 = \frac{10.34 \text{ kg}}{\left[\frac{1.806x10^{-3}\text{cm}^{-2}}{4.138x10^{-3}\text{cm}^{-2}} \left(\frac{45.68 \text{ kg}}{34.30 \text{ kg}} - 1 \right) + 1 \right]} = 9.032 \text{ kg}
$$

$$
m' = 9.03 \; kg
$$

Within roundoff, this is the same critical mass as calculated in Section 7.4.4 (9.035 kg), which represents the mass of Pu(5.2) metal units that would be required to maintain criticality of the 4×4×4 array. Equation (111) provides a technique to examine the effect of array unit fissile material substitutions for situations where the array geometry, such as array size and array unit dimensions, is unchanged.

Looking at Figure 7-7 shows how the mass equivalence works graphically. The geometry line is the same for both U(100) metal units and Pu(5.2) metal units as the array is the same. The intersection of a material line with the geometry line gives the unit mass that result in k_{eff} = 1.0 for the given array. For U(100) metal units, the mass is about 34,000 g, whereas for Pu(5.2) metal units, the mass is about 9,000 g. If other units were to be placed in the same array, that equivalent mass would be determined from the intersection of its material line with the geometry line. For example, if we want to add U-233 metal units, Table 7-1 gives m_o = 15,750 grams and c_2 = 0.002751 cm^{-2}. Then the material line for U-233 would be

Material line: $\sigma(m) = 0.002752 \, \text{cm}^{-2} \times (15,750 - m)\text{grams}$

Then plotting this against the geometry line shows a mass of 12,940 grams for the U-233 metal unit to be critical in the specified array (see Figure 7-8).
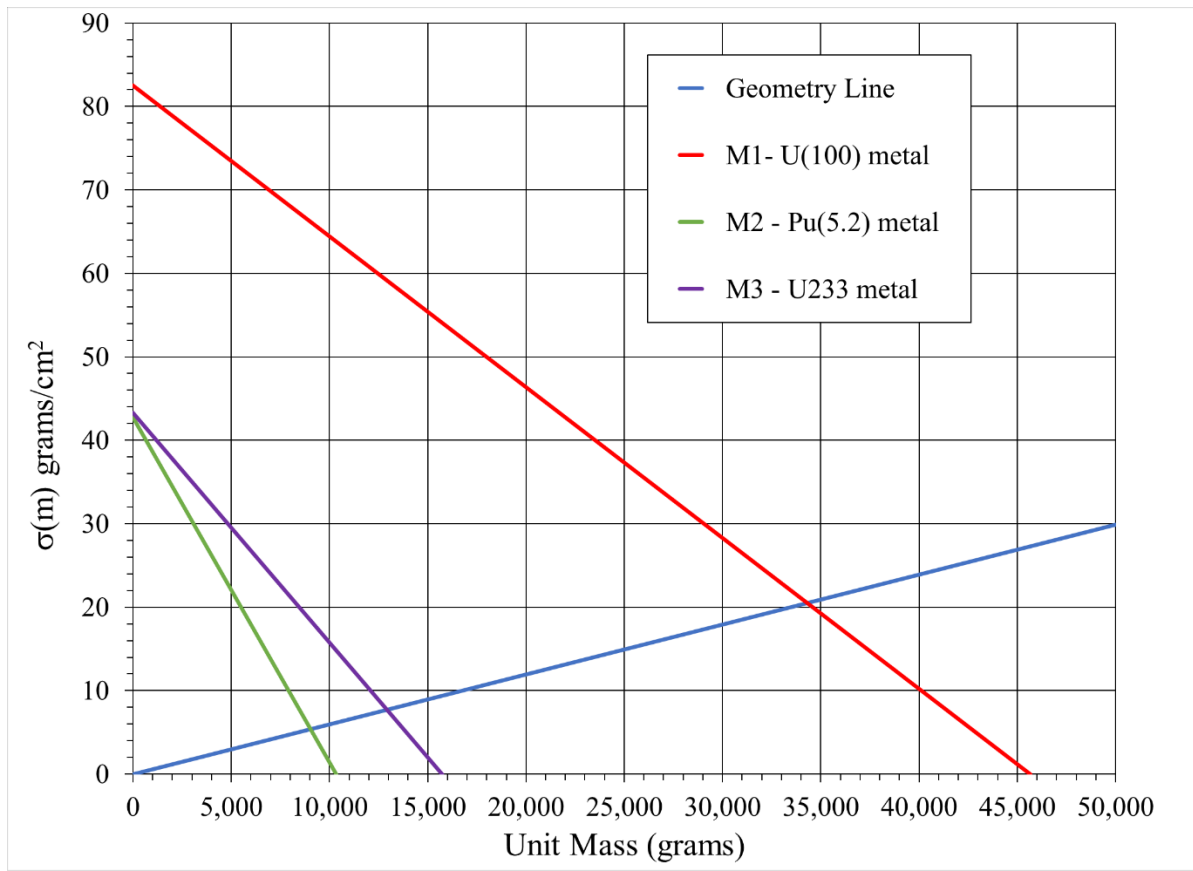
Figure 7-7. Use of Plots to Demonstrate Mass Equivalence.

Figure 7-8 shows that the U-233 metal unit mass of 12,940 g is equivalent to a Pu(5.2) metal unit of 9,032 g or a U(100) metal unit of 34,326 g.

4x4x4 Array

8x4x2 Array
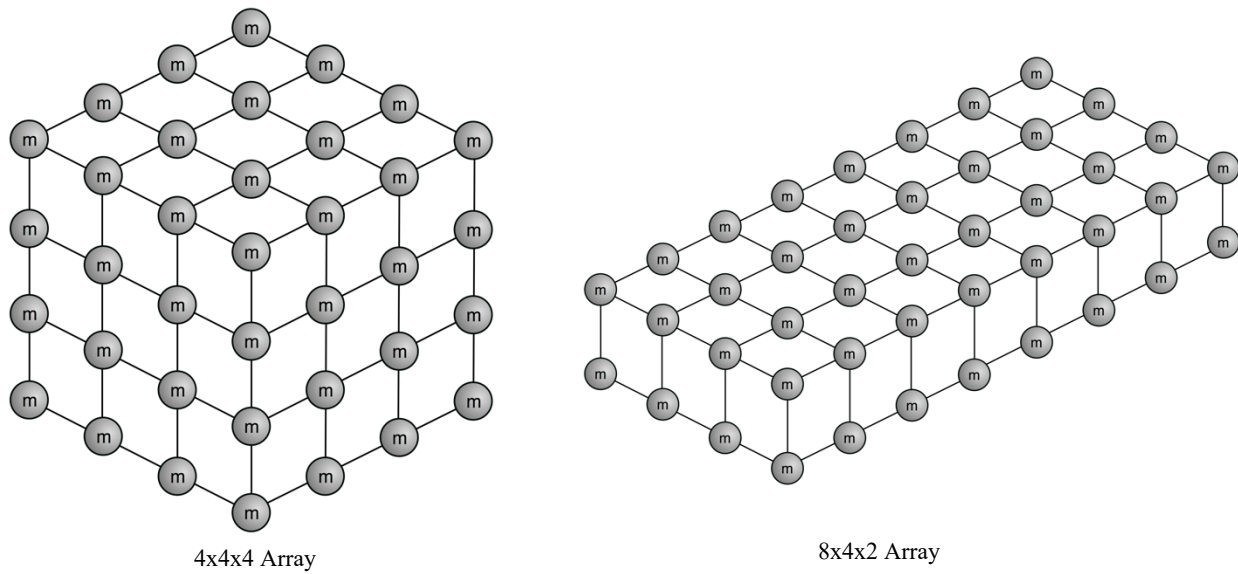
Figure 7-8. Illustration of Two Different 64 Unit Arrays.

7.6   THE EFFECT OF ARRAY SHAPE (NON-CUBIC ARRAYS) ON ARRAY CRITICALITY

So far, the discussions about the limiting surface density method have focused on cubic arrays that have at least 64 units, corresponding to at least a 4×4×4 array. This method can also be used for arrays that may be cuboidal in shape instead of cubic. In other words, the 4×4×4 array can be transformed to allow the analyst to determine the characteristics of a critical array with the same number of units that has a different shape or layout such as a 16×2×2 or an 8×4×2 array (Figure 7-9). It is somewhat intuitive that a cubic array with a certain number of units will be more reactive than a non-cubic or cuboidal array with the same number of fissile units. The non-cubic array is less reactive than the cubic array because the neutron leakage increases. To maintain criticality, the unit mass must increase, the distance between units be reduced, or the number of units in the array be increased.
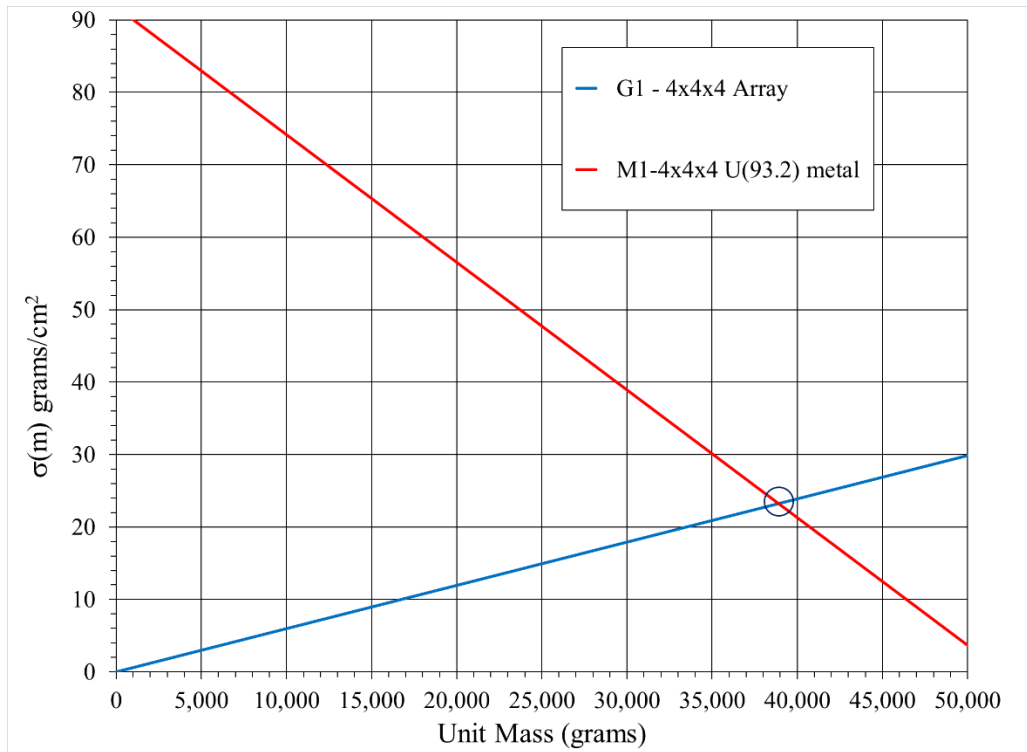
Figure 7-9. Solution for the U(93.2) metal 4×4×4 Array

The limiting surface density method can be applied to non-cubic arrays (cuboidal) simply by using a shape factor to adjust the slope of the material line, $-c_2$, to account for the neutron leakage characteristics of the transformed array. Once the array is adjusted for a new configuration, a 4×4×4 array to an 8×4×2 array, for example (Figure 7-9), the new array parameters can be adjusted to determine the characteristics for a critical array of this new size. The approach provided here, as defined in Reference 39, can be used to adjust the array shape.

In most facilities with fissile material operations, it is much more common to experience storage arrays that are not cubic but non-cubic in shape as illustrated in Figure 7-9. Furthermore, in a process facility, arrays are usually made up of drums of fissile material stored on the floor or on pallets in arrays, for example, and not of ideal, compact arrangements such as those shown in this section. However, ideally, to account for an array change of shape from a cubic to non-cubic arrangement, the ratio of the surface to volume ratio for the array shape change can be calculated to determine a shape factor, R. The shape factor

is then used in subsequent calculations to determine the new characteristics that the units in the new array must have to remain in a critical configuration. The shape factor, R, can be derived as follows.

The surface area for a noncubic array, S_{nc}, can be calculated by the following where n_x, n_y and n_z represent the number of array units/cells in the x, y, and z directions, respectively. Also, recall the center-to-center spacing is denoted by $2a_n$.

$$S_{nc} = (2a_n)^2 [n_x n_y + n_x n_z + n_y n_z] \tag{117}$$

The volume of the cubic storage cells, V_{nc}, in the noncubic array can be expressed as follows:

$$V_{nc} = (2a_n)^3 [n_x n_y n_z] \tag{118}$$

Now, the suface area-to-volume ratio for the noncubic array can be determined by calculating the ratio S_{nc} to V_{nc} as follows:

$$\frac{S_{nc}}{V_{nc}} = \frac{1}{2a_n}\left[\frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z}\right] \tag{119}$$

For a cubic array, the surface area-to-volume ratio, n is equal for each side of the array, $n = n_x = n_y = n_z$. Recall that $N = n^3$ or $n = \sqrt[3]{N}$:

$$\frac{S_c}{V_c} = \frac{1}{2a_n}\left[\frac{1}{n} + \frac{1}{n} + \frac{1}{n}\right] = \frac{1}{2a_n}\left[\frac{3}{n}\right] = \frac{1}{2a_n}\left[\frac{3}{\sqrt[3]{N}}\right] \tag{120}$$

Now, the shape factor, R, can be calculated by dividing the ratio S_{nc}/V_{nc} for noncubic arrays by the ratio S_c/V_c for cubic arrays:

$$R = \frac{\left(\frac{S_{nc}}{V_{nc}}\right)}{\left(\frac{S_c}{V_c}\right)} = \frac{\sqrt[3]{N}}{3}\left[\frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z}\right] \tag{121}$$

It should be noted that N is independent of the array shape and does not have to be an integer value. According to Reference 41, the maximum value that R can have is 5.34. Computationally, if R exceeds this value, then it should be assigned a value of 5.34. This limitation is required to avoid criticality with a single unit of the array.

Now that the new shape of the array has been accounted for, c_2' c_2^{nc} can be calculated, which considers the increased neutron leakage for the non-cubic array. The following relationship was developed by Thomas (Reference 39) to account for the new leakage characteristics for the modified, non-cubic array that is valid for U(93.2) metal units, each having a mass of 10.42 kg.

$$c_2^{nc} = \frac{4n_z^{nc}}{n_z}\left(\frac{c_2}{5R^{-0.672} - 1}\right) \tag{122}$$

where n_z^{nc} is the least number of units along an array edge, which is equal to $\sqrt[3]{N}$ or n_z in the cubic array configuration, R is the shape factor (not to exceed 5.34), and c_2 is previously defined. This relationship was developed for 10.4 kg, U(93.2) metal units in a 512-unit array (Reference 41) and can be used in conjunction with the equivalence relationship derived in Section 7.5 to convert from one type of fissile material to another after determining the appropriate values of R and c_2^{nc}. The following equation can be used to determine the unit mass required to make a non-cubic array critical.

$$m^{1nc} = \frac{m_0}{\left[\frac{c_2}{c_2^{nc}} \frac{n_z^{nc}}{n_z}\left(\frac{m_0}{m^1} - 1\right) + 1\right]} = \frac{m_0}{\left[\frac{(5R^{-0.672} - 1)}{4}\left(\frac{m_0}{m^1} - 1\right) + 1\right]} \tag{123}$$

7.6.1 Limiting Surface Density Example Problem 7

Using the methodology presented in Section 7.6 and the results from Example Problem 3-II, calculate the critical mass for each array unit required for a water-reflected cubic array of fully enriched U(100) metal units in a 8×4×2 array.

Because the noncubic technique is referenced to U(93.2) units, the characteristics of a noncubic array with those units must be determined first. As discussed in Section 7.6, the first step is to calculate the critical array unit mass for U(93.2) metal units arranged in a cubic arrangement. After this is done, the shape factor, R, can be calculated to determine the critical array unit mass for the 8×4×2 array for the U(93.2) metal units. The last step will involve using the equivalence relationship from Section 7.5 to determine the critical array unit mass for U(100) metal units. A calculation of this type must be done in these steps because the shape factor for limiting surface density was developed based on experiments involving arrays of U(93.2) metal units. This solution will involve the graphical solution discussed previously.

Step 1

Assume a 4×4×4 cubic array,

$$n = n_x = n_y = n_z = 4$$

$$a_n = a_x = a_y = a_z = 15 \text{ in. } (38.1 \text{ cm}).$$

The following relationship for a cubic array can be used to determine the critical mass per unit to maintain the array in a critical condition for U(93.2) metal units. Array information for U(93.2) metal and other relevant data are as follows:

m_o –   52.1 kg from Table 7-1
c_2 –   0.001762 cm^{-2} from Table 7-1
N –   equal to $n^3 = 64$
c –   0.55

Geometry line equation:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{4m}{(2 \times 38.1 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{64}}\right)^2$$

$$\sigma(m) = 5.974x10^{-4} \times m[cm]^{-2} \text{ or } \frac{\sigma(m)}{m[grams]} = 5.974x10^{-4}[cm]^{-2}$$

Material line: $\sigma(m) = c_2(m_0 - m)\left[\frac{grams}{cm^2}\right]$

$$\frac{\sigma(m)}{m} = 1.762x10^{-3}\left(\frac{52,100}{m[grams]} - 1\right)[cm^{-2}]$$

Setting the geometry line equal to the material line results in the following:

$$\frac{\sigma(m)}{m[grams]} = 5.974x10^{-4}[cm]^{-2} = 1.762x10^{-3}\left(\frac{52,100}{m[grams]} - 1\right)[cm^{-2}]$$

$$m[grams] = 38,908 \text{ grams}$$

Note that the graphical solution (indicated by the circle on Figure 7-10) illustrates a solution for the array critical unit mass at about 38,900 g, which corresponds to a limiting surface density of about 23 g/cm² (i.e., s(m) = 23 g/cm² for m = 38,900 g).
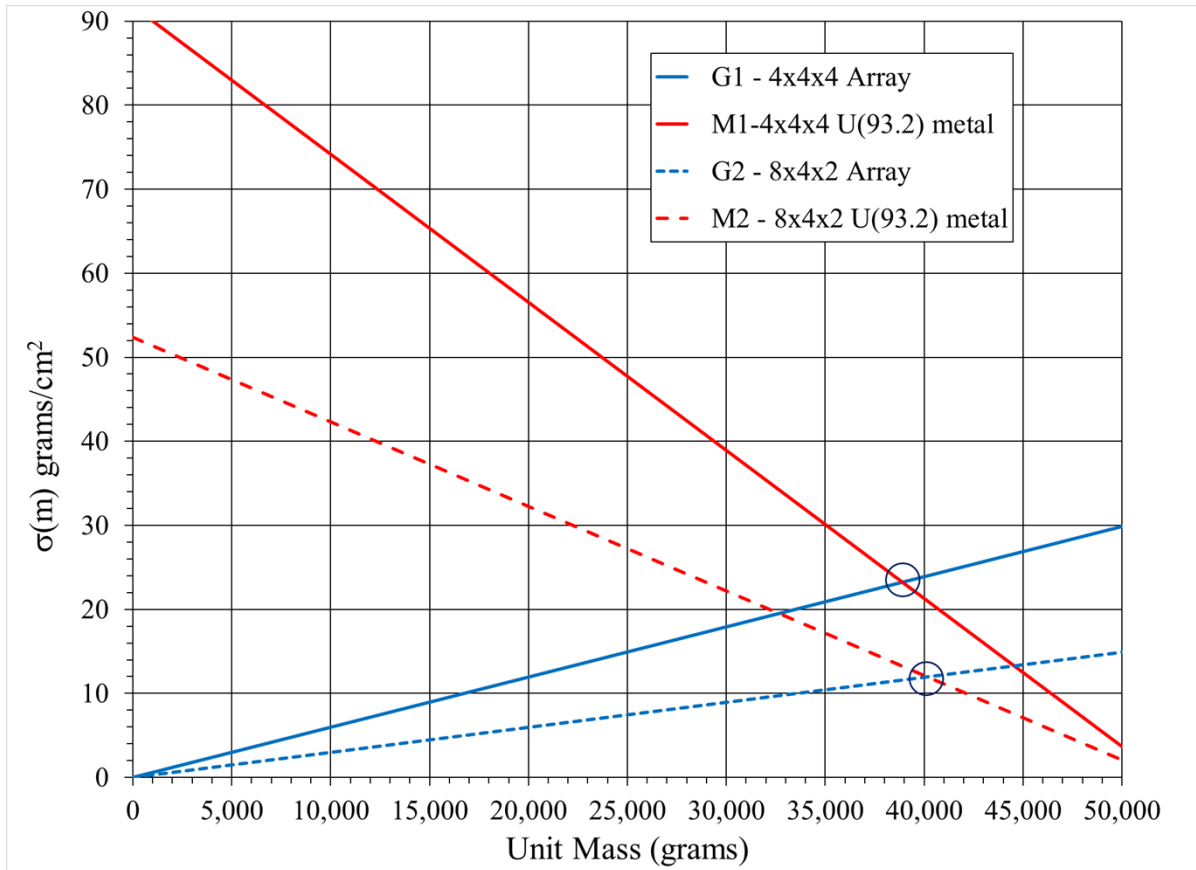
Figure 7-10. Transformation of a U(93.2) Metal 4×4×4 Array to an 8×4×2 Array

<u>Step 2</u>

The next step is to compute the shape factor from Eq. (118) and determine c_2^{nc} that considers the increased leakage due to changing the shape of the array from a cubic (4×4×4) to non-cubic in shape (8×4×2).

$$R = \frac{\left(\frac{S_{nc}}{V_{nc}}\right)}{\left(\frac{S_c}{V_c}\right)} = \frac{\sqrt[3]{N}}{3}\left[\frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z}\right]$$

$$R = \frac{\sqrt[3]{64}}{3}\left[\frac{1}{8} + \frac{1}{4} + \frac{1}{2}\right] = 1.167$$

With R calculated, the new characteristic constant c_2^{nc} for the modified array can be calculated from Eq. (119) from Section 7.6.

$$c_2^{nc} = \frac{4n_z^{nc}}{n_z}\left(\frac{c_2}{5R^{-0.672} - 1}\right)$$

$$c_2^{nc} = \frac{4 \times 2}{4}\left(\frac{1.762x10^{-3}[\text{cm}^{-2}]}{5 \times (1.167)^{-0.672} - 1}\right) = 1.005x10^{-3}[\text{cm}^{-2}]$$

Changing the array shape changes the geometry line. The new geometry line is

$$\sigma(m) = \frac{n_z m}{(d)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{2m}{(2 \times 38.1 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{64}}\right)^2$$

$$\sigma(m) = 2.987x10^{-4} \times m[cm]^{-2} \text{or} \quad \frac{\sigma(m)}{m[\text{grams}]} = 2.987x10^{-4}[cm]^{-2}$$

Because the geometric characteristics of the array have changed, the new array unit critical mass, m^{Inc},) can be calculated from Eq. (120).

$$m^{1nc} = \frac{m_0}{\left[\frac{c_2}{c_2^{nc}}\frac{n_z^{nc}}{n_z}\left(\frac{m_0}{m^1} - 1\right) + 1\right]} = \frac{m_0}{\left[\frac{(5R^{-0.672} - 1)}{4}\left(\frac{m_0}{m^1} - 1\right) + 1\right]}$$

$$m^{1nc} = \frac{52.1 \text{ kg}}{\left[\frac{1.762x10^{-3}[\text{cm}^{-2}]}{1.005x10^{-3}[\text{cm}^{-2}]} \times \frac{2}{4} \times \left(\frac{52.1 \text{ kg}}{38.9 \text{ kg}} - 1\right) + 1\right]} = 40.16 \text{ kg}$$

$$m^{1nc} = \frac{52.1 \text{ kg}}{\left[\frac{5 \times (1.167)^{-0.672} - 1}{4}\left(\frac{52.1 \text{ kg}}{38.9 \text{ kg}} - 1\right) + 1\right]} = 40.16 \text{ kg}$$

This corresponds to the mass of U(93.2) metal units required to keep the 8×4×2 array in a critical state after the array was transformed from a 4×4×4 array (Figure 7-11).
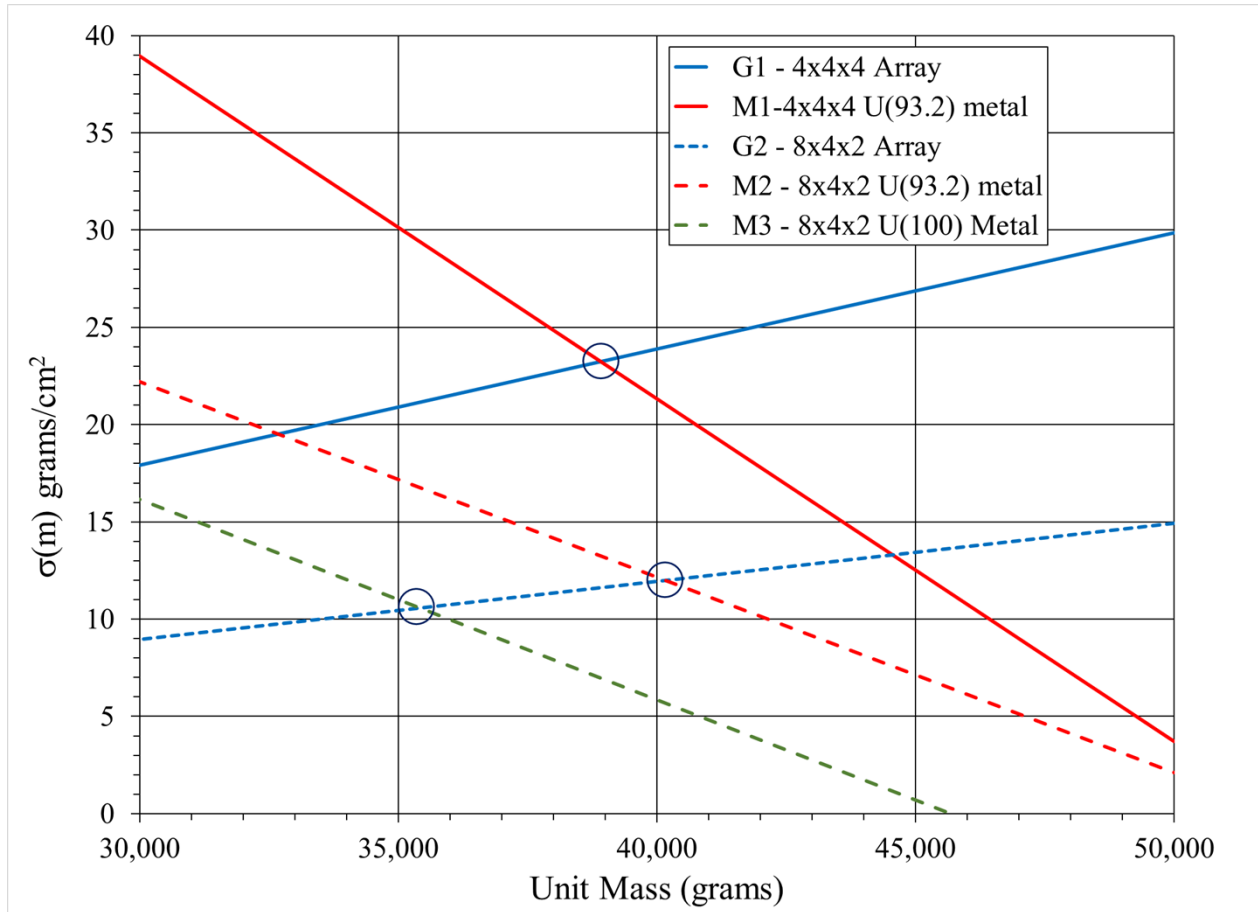
Figure 7-11. Graphical Solution for an 8×4×2 Array with U(100) Metal Units.

The new material line is

Material line:
$$\sigma(m) = c_2^{nc}(m_0 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right]$$

$$\frac{\sigma(m)}{m} = 1.005x10^{-3}\left(\frac{52{,}100}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

Note that the change in array shape to 2 layers high instead of 4 layers high reduced the slope of the geometry line by ½ and decreased the limiting surface density from 91.8 grams/cm2 to 52.36 grams/cm2. This increased the mass of a U(93.2) unit from 38.9 kg to 40.2 kg as indicated by the bottom circle on Figure 7-11.

Now the equivalence relationship derived in Section 7.5 can be used to determine the unit mass for U(100) metal units to maintain the 8×4×2 array in a critical state based on the results for a U(93.2) metal system. First, the c_2^{nc} value for U(100) metal needs to be calculated because the data from Table 7-2 apply to cubic arrays, not a cuboidal, 8×4×2, array. The following approach can be taken to calculate c_2^{nc} for the 8×4×2 array of U(100) metal units.

The ratio of the limiting surface density relationships can be calculated as follows. Note that the variables a_n, m_0, n_z, c, and N do not change. The unit spacing, fissile material type and number of units in the array are the same before and after the transformation from a 4×4×4 array to an 8×4×2 array.

For the U(93.2) array:

$$\left(c_2^{nc}\right)_{\substack{8x4x2 \\ U(93.2)}} = \frac{4n_z^{nc}}{n_z}\left(\frac{\left(c_2^{c}\right)_{\substack{4x4x4 \\ U(93.2)}}}{5R^{-0.672}-1}\right)$$

For the U(100) array:

$$\left(c'^{nc}_2\right)_{\substack{8x4x2 \\ U(100)}} = \frac{4n_z^{nc}}{n_z}\left(\frac{\left(c'^{c}_2\right)_{\substack{4x4x4 \\ U(100)}}}{5R^{-0.672}-1}\right)$$

Calculate the ratio:

$$\frac{\left(c'^{nc}_2\right)_{\substack{8x4x2 \\ U(100)}}}{\left(c_2^{nc}\right)_{\substack{8x4x2 \\ U(93.2)}}} = \frac{\frac{4n_z^{nc}}{n_z}\left(\frac{\left(c'^{c}_2\right)_{\substack{4x4x4 \\ U(100)}}}{5R^{-0.672}-1}\right)}{\frac{4n_z^{nc}}{n_z}\left(\frac{\left(c_2^{c}\right)_{\substack{4x4x4 \\ U(93.2)}}}{5R^{-0.672}-1}\right)}$$

Because the geometric properties of the array will not change for the fissile material transformation from U(93.2) to U(100) metal units (i.e., $n_z^{nc} = n_z'^{nc}$), the previous relationship can be simplified to the following ratio of c_2 values.

$$\frac{\left(c'^{nc}_2\right)_{\substack{8x4x2 \\ U(100)}}}{\left(c_2^{nc}\right)_{\substack{8x4x2 \\ U(93.2)}}} = \frac{\left(c'^{c}_2\right)_{\substack{4x4x4 \\ U(100)}}}{\left(c_2^{c}\right)_{\substack{4x4x4 \\ U(93.2)}}}$$

Rearranging the ratio provides the following result that can be used to calculate the c_2^{nc} value for the U(100) 8×4×2 array:

$$\left(c'^{nc}_2\right)_{\substack{8x4x2 \\ U(100)}} = \left(c_2^{nc}\right)_{\substack{8x4x2 \\ U(93.2)}} \times \frac{\left(c'^{c}_2\right)_{\substack{4x4x4 \\ U(100)}}}{\left(c_2^{c}\right)_{\substack{4x4x4 \\ U(93.2)}}}$$

$$\left(c'^{nc}_2\right)_{\substack{8x4x2 \\ U(100)}} = 1.005x10^{-3}[\text{cm}^{-2}] \times \frac{1.806x10^{-3}[\text{cm}^{-2}]}{1.762x10^{-3}[\text{cm}^{-2}]} = 1.030x10^{-3}[\text{cm}^{-2}]$$

The mass required to maintain criticality of the 8×4×2 array with U(100) metal units can now be determined using Eq. (111) and equating the surface densities of the noncubic arrays for the U(93.2) material and the replacement fissile material.

$$m'^{1nc} = \frac{m'_0}{\left[\frac{c_2^{nc}}{c'^{nc}_2}\left(\frac{m_0}{m^{1nc}} - 1\right) + 1\right]}$$

This is the mass required to maintain array criticality in an 8×4×2 configuration with U(100) metal units. Note the primed parameters refer to U(100) while the parameters without primes refer to U(93.2) and m^{1nc} is the mass of U(93.2) in the noncubic critical array configuration.

Substitute the relevant variable values:

m_0' = 45.68 kg for U(100) metal with H/U = 0 (Table 7-1),
$c_2'^{nc}$ = 1.030×10^{-3} cm^{-2} for U(100) metal with H/U=0 for the 8×4×2 array calculated above,
m^{1nc} = 40.16 kg corresponding to the critical unit mass for U(93.2) metal units in the 8×4×2 array calculated previously,
c_2^{nc} = 1.005×10^{-3} cm^{-2} for U(93.2) metal for the 8×4×2 array calculated above, and
m_0 = 52.1 kg for U(93.2) metal from Table 7-1.

The final result is

$$m'^{1nc} = \frac{45.68 \text{ kg}}{\left[\frac{1.005x10^{-3}[\text{cm}^{-2}]}{1.030x10^{-3}[\text{cm}^{-2}]}\left(\frac{52.1 \text{ kg}}{40.16 \text{ kg}} - 1\right) + 1\right]} = 35.41 \text{ kg}$$

The graphical solution is illustrated in Figure 7-12.

As the array shape is still 8×4×2, the G2 geometry line applies to both U(93.2) and U(100) units. To zoom in on the intersection points, the x-axis has been expanded on this figure to show mass values from 30 kg to 50 kg. The dashed green line on Figure 7-12 shows the material line for U(100) units in an 8×4×2 array, and the leftmost circle indicates the mass of 35.4 kg required to maintain a critical 8×4×2 array with the center-to-center spacing of 76.2 cm.
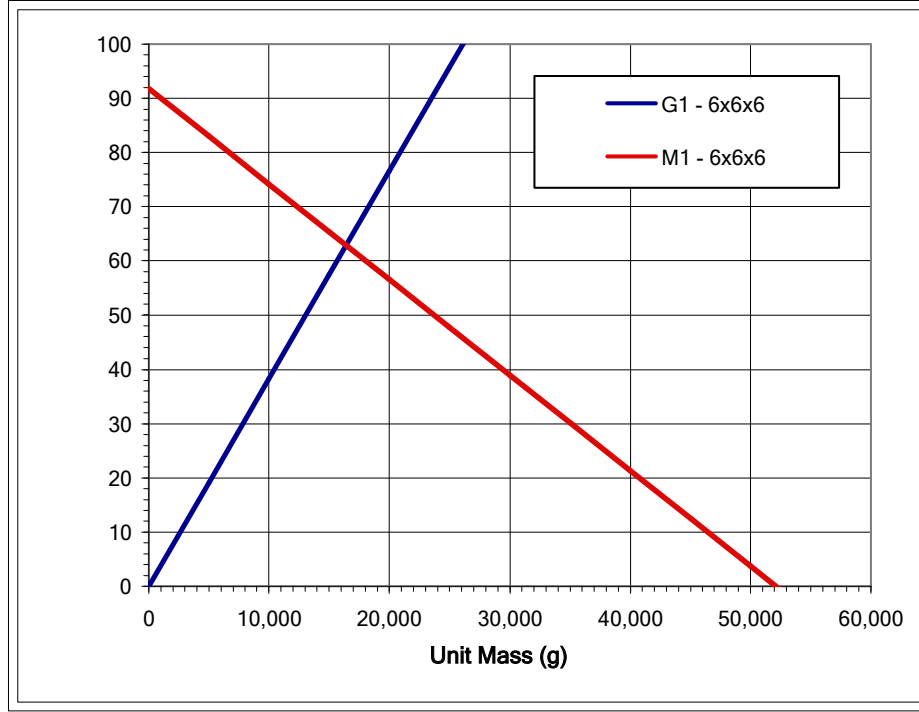
Figure 7-12. Solution for Limiting Surface Density Example Problem 8

7.6.2 Limiting Surface Density Example Problem 8

This problem will be done in parts to demonstrate the strength of the method for array analyses.
Part 1. Using the limiting surface density method, calculate the spherical critical mass of U(93.2) metal required for criticality in a 216-unit water-reflected cubic array (6×6×6). The center-to-center spacing $(2a_n)$ of the array units is 38.1 cm.

Geometry line equation:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{6m}{(38.1 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{216}}\right)^2$$

$$\sigma(m) = 3.830x10^{-3} \times m[cm]^{-2} \text{or} \quad \frac{\sigma(m)}{m[\text{grams}]} = 3.830x10^{-3}[cm]^{-2}$$

Material line: $$\sigma(m) = c_2(m_0 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right]$$

$$\frac{\sigma(m)}{m} = 1.762x10^{-3}\left(\frac{52{,}100}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

Setting the geometry line equal to the material line results in the following:

$$\frac{\sigma(m)}{m[\text{grams}]} = 3.830x10^{-3}[cm]^{-2} = 1.762x10^{-3}\left(\frac{52{,}100}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

$$m[\text{grams}] = 16{,}416 \text{ grams}$$

199

See Figure 7-13 for plot of material and geometry lines intersecting at m ≈16,400 g and a surface density of s(m) ≈ 64 g/cm².
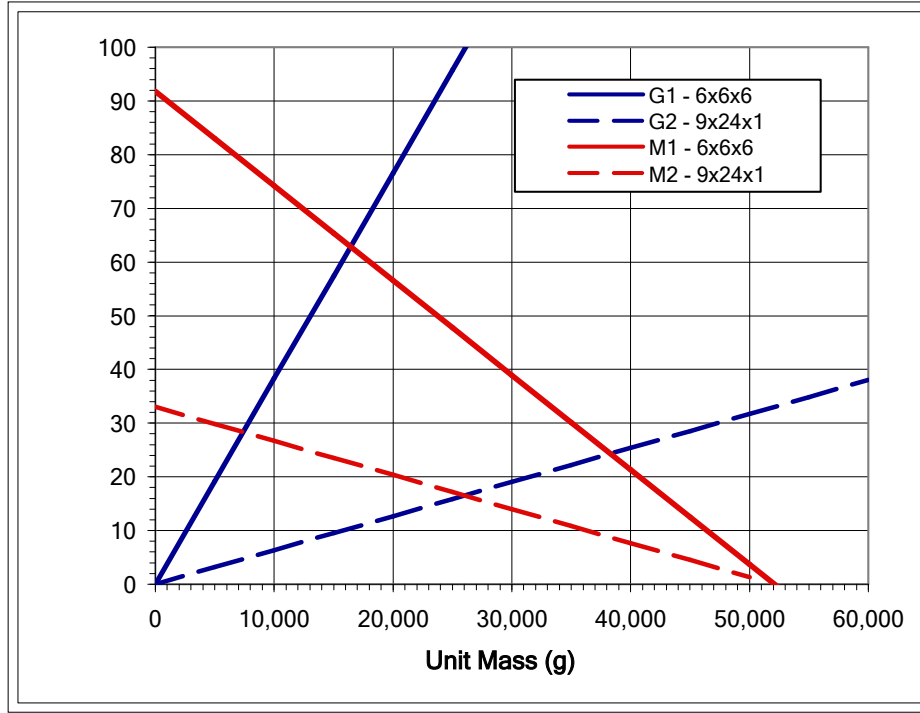
Figure 7-13. Solution for the Change from a 6×6×6 Array to a 9×24×1 Array

Part 2. What would be the multiplication factor of this array if the units were rearranged into a water-reflected 9×24×1 cuboidal array?

The first step is to compute the shape factor and determine $c^{nc}{}_2$ and new value for $\sigma(m^{nc})/m^{nc}$ that considers the increased neutron leakage due to changing the shape of the array from a cubic (6×6×6) to non-cubic in shape (24×9×1). Using the methodology from Section 7.6 and the example problem in Section 7.6.1, the multiplication factor can be calculated.

The shape factor, R, can be calculated as follows:

$$R = \frac{\sqrt[3]{N}}{3}\left[\frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z}\right]$$

$$R = \frac{\sqrt[3]{216}}{3}\left[\frac{1}{24} + \frac{1}{9} + \frac{1}{1}\right] = 2.306$$

With R calculated, $c^{nc}{}_2$ can be calculated from this relationship from Section 7.6:

$$c_2^{nc} = \frac{4n_z^{nc}}{n_z}\left(\frac{c_2}{5R^{-0.672} - 1}\right)$$

$$c_2^{nc} = \frac{4 \times 1}{6}\left(\frac{1.762x10^{-3}[cm]^{-2}}{5 \times (2.306)^{-0.672} - 1}\right) = 6.343x10^{-4}[cm]^{-2}$$

200

Now, calculate the value for $\sigma'(m)/m$ (the new geometry line) so that the new array unit critical mass, m', can be calculated, which can be related to the multiplication factor relationships defined in Section 7.3.1.

$$\frac{\sigma(m^{nc})}{m^{nc}} = \frac{n_z^{nc}}{n_z}\frac{\sigma(m)}{m}$$

$$\frac{\sigma(m^{nc})}{m^{nc}} = \frac{1}{6}(3.830x10^{-3}[\text{cm}^{-2}]) = 6.383x10^{-4}[\text{cm}^{-2}]$$

Thus, the slope of the noncubic array geometry line is 1/6 the slope of the cubic array geometry line. Substitute this value into the limiting surface density material line expression:

$$\frac{\sigma(m^{nc})}{m^{nc}} = c_2^{nc}\left(\frac{m_0}{m^{nc}} - 1\right) = 6.383x10^{-4}[\text{cm}^{-2}]$$

The type of fissile material in the array has not changed. Therefore, $m_0 = 52.1$ kg. Next, solve for m^{nc}:

$$c_2^{nc}\left(\frac{\textbf{52.1 kg}}{\textbf{\textit{m}}^{\textbf{\textit{nc}}}} - \textbf{1}\right) = \textbf{6.383}\textit{x}\textbf{10}^{-\textbf{4}}[\text{cm}^{-2}]$$

$$\textbf{\textit{m}}^{\textbf{\textit{nc}}} = \left(\frac{\textbf{6.343}\textit{x}\textbf{10}^{-\textbf{4}}[\text{cm}^{-2}] \times \textbf{52.1 kg}}{\textbf{6.383}\textit{x}\textbf{10}^{-\textbf{4}}[\text{cm}^{-2}] + \textbf{6.343}\textit{x}\textbf{10}^{-\textbf{4}}[\text{cm}^{-2}]}\right) = \textbf{25.968} \text{ kg}$$

This result is consistent with the graphical solution shown in Figure 7-14.

The multiplication factor can now be calculated using the relationships in Section 7.3.1.

$$k_{eff} = \left(\frac{m^{cubic}}{m^{noncubic}}\right)^{\frac{1}{3}} = \left(\frac{16.4 \text{ kg}}{26.0 \text{ kg}}\right)^{\frac{1}{3}} = 0.858$$

Part 3. What ^{239}Pu metal (Pu[0]) mass will result in an array multiplication factor of 0.9 for the 6×6×6 and 9×24×1 arrays?

This part involves a different type of fissile material than in the last two parts of the problem, a pure ^{239}Pu metal system, so one can therefore proceed as in Part 1 for each array type. For the 6×6×6 array, the critical array unit mass can be calculated as before, using the data from Table 14 for Pu(0) metal.
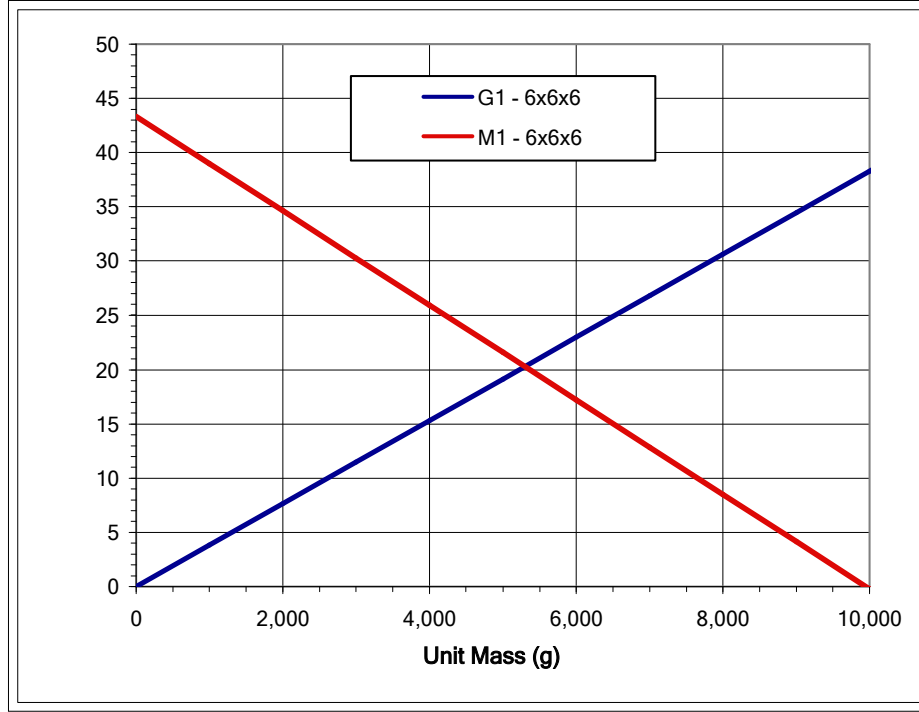
Figure 7-14. Solution for Pu(0) metal 6x6x6 Critical Array

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{6m}{(38.1 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{216}}\right)^2$$

$$\sigma(m) = 3.830x10^{-3} \times m[cm]^{-2} \text{ or } \frac{\sigma(m)}{m[\text{grams}]} = 3.830x10^{-3}[cm]^{-2}$$

$$\sigma(m) = c_2(m_0 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right]$$

Material line:
$$\frac{\sigma(m)}{m} = 4.356x10^{-3}\left(\frac{9,950}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

For this case, the geometry line is unchanged. The material line changes due to the change of fissile material.

Equating the geometrical and material line relationships,

$$\frac{\sigma(m)}{m[\text{grams}]} = 3.830x10^{-3}[cm]^{-2} = 4.356x10^{-3}\left(\frac{9,950}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

$$m[\text{grams}] = 5,295 \text{ grams}$$

Thus, an array unit of 5,295 g of Pu-239 metal creates a critical system in a 6×6×6 array. (see Figure 7-15.)

202
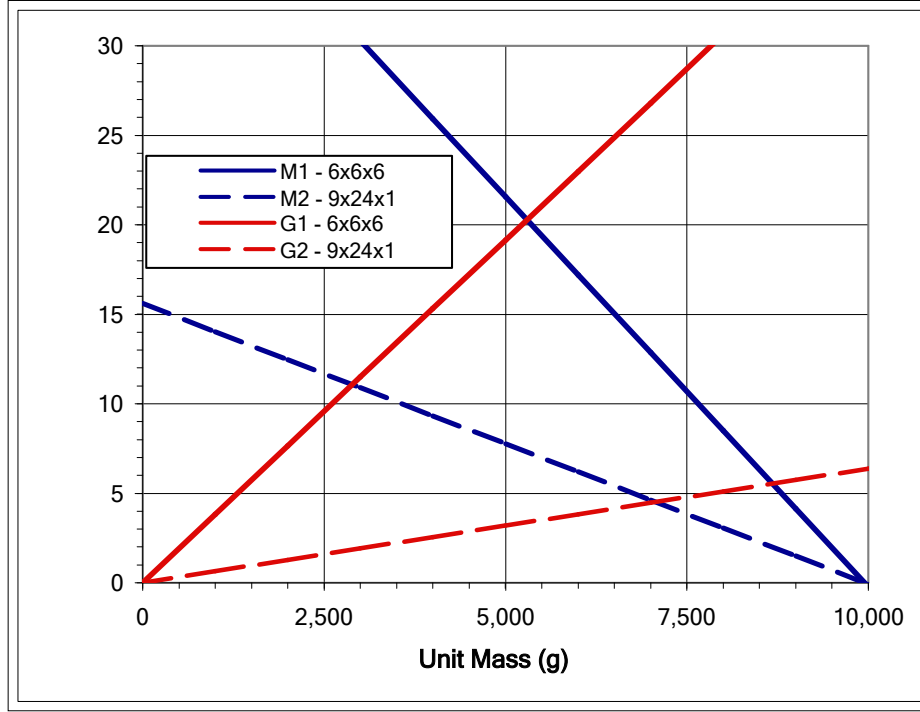
Figure 7-15. Solution for a Pu(0) Metal 9×24×1 Critical Array

The unit array mass needed to result in a k_{eff} of 0.9 can be calculated as follows.

$$k_{eff} = \left(\frac{m_{kcubic}}{m_{critcubic}}\right)^{\frac{1}{3}} \Rightarrow m_{kcubic} = k_{eff}^3 m_{critcubic} = (0.9)^3 5{,}295g = 3{,}860g$$

Solving for m_{kcubic} (recall that $m_{critcubic}$ is the mass of a spherical unit in the critical array while m^k_{cubic} is the mass of a spherical unit in a subcritical array with a given k_{eff}) gives a mass of 3,860 g.

Thus, for the 6×6×6 array, units of 3.86 kg Pu(0) metal array units will result in a k_{eff} of 0.9.

For the 9×24×1 array, the calculations in Part 2 can be used in this problem to calculate a new value of c_2 for this Pu(0) system by using a similar equivalence methodology presented in Section 7.5. The calculation in Part 2 involved the calculation of the shape factor R and calculation of the critical array unit mass change from a 6×6×6 array to a 9×24×1 array. Thus, using the same approach discussed in Section 7.6, a relationship can be derived to determine a new $c_2'^{nc}$ for the 9×24×1 array for a Pu(0) metal system.

For the U(93.2) array:

$$(c_2^{nc})_{\substack{9x24x1 \\ U(93.2)}} = \frac{4n_z^{nc}}{n_z}\left(\frac{(c_2^c)_{\substack{6x6x6 \\ U(93.2)}}}{5R^{-0.672} - 1}\right)$$

For the Pu(0) array

$$\left(c_2'^{nc}\right)_{\substack{9x24x1 \\ Pu(0)}} = \frac{4n_z^{nc}}{n_z}\left(\frac{\left(c_2'^{C}\right)_{\substack{6x6x6 \\ Pu(0)}}}{5R^{-0.672}-1}\right)$$

Calculate the ratio of $\left(c_2'\right)_{\substack{9\times24\times1 \\ U(93.2)}}$ to $\left(c_2'\right)_{\substack{9\times24\times1 \\ Pu(0)}}$

$$\frac{\left(c_2'^{nc}\right)_{\substack{9x24x1 \\ Pu(0)}}}{\left(c_2'^{nc}\right)_{\substack{9x24x1 \\ U(93.2)}}} = \frac{\frac{4n_z^{nc}}{n_z}\left(\frac{\left(c_2'^{C}\right)_{\substack{6x6x6 \\ Pu(0)}}}{5R^{-0.672}-1}\right)}{\frac{4n_z^{nc}}{n_z}\left(\frac{\left(c_2^{C}\right)_{\substack{6x6x6 \\ U(93.2)}}}{5R^{-0.672}-1}\right)}$$

Rearranging the ratio provides the following result that can be used to calculate the $c_2'^{nc}$ value for the Pu(0) 9×24×1 array:

$$\left(c_2'^{nc}\right)_{\substack{9x24x1 \\ Pu(0)}} = \left(c_2^{nc}\right)_{\substack{9x24x1 \\ U(93.2)}} \times \frac{\left(c_2'^{C}\right)_{\substack{6x6x6 \\ Pu(0)}}}{\left(c_2^{C}\right)_{\substack{6x6x6 \\ U(93.2)}}}$$

$$\left(c_2'^{nc}\right)_{\substack{8x4x2 \\ U(100)}} = 6.343x10^{-4}[\text{cm}^{-2}] \times \frac{4.356x10^{-3}[\text{cm}^{-2}]}{1.762x10^{-3}[\text{cm}^{-2}]} = 1.568x10^{-3}[\text{cm}^{-2}]$$

Based on the fact that the value for $\sigma(m)/m$ is constant for the 9×24×1 array calculation in Part 2, the new c_2' value can be used to calculate the critical array mass (Figure 7-16) for the 9×24×1 array for the Pu(0) metal system:
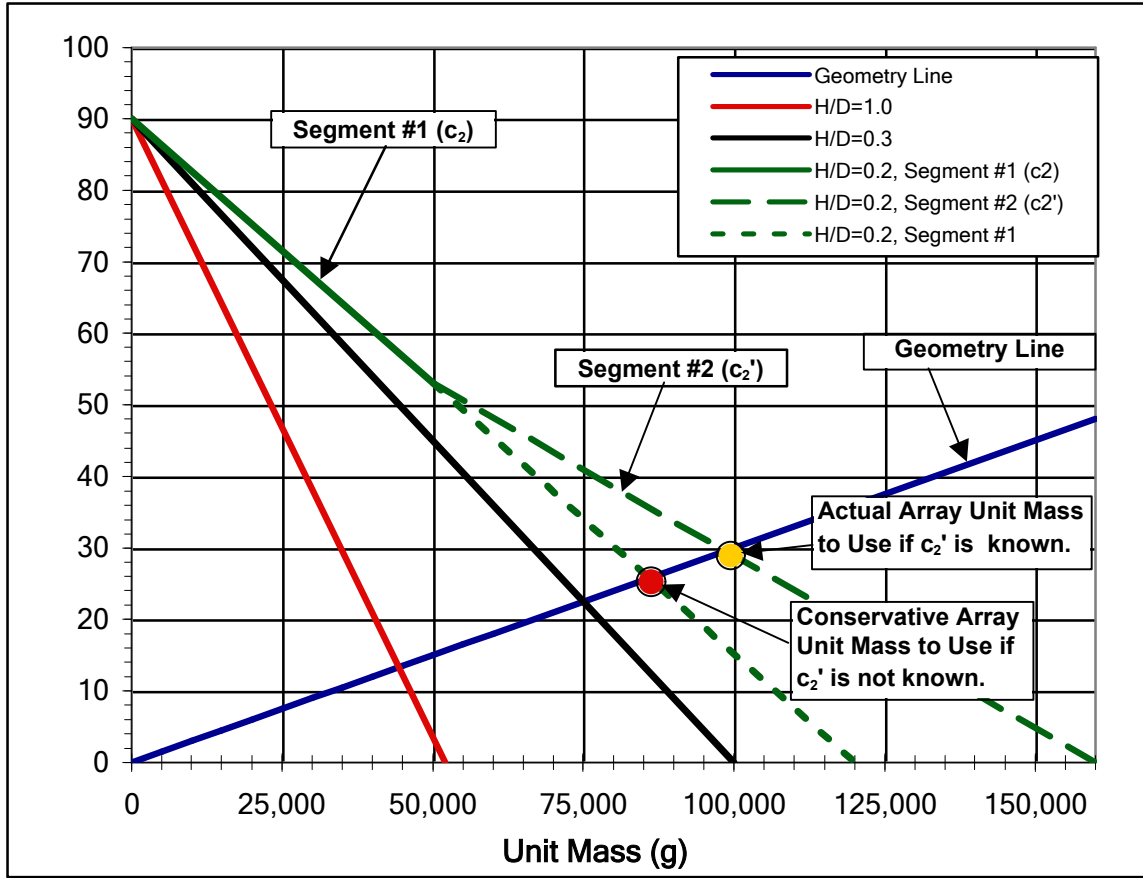
Figure 7-16. Critical Water-Reflected Cubic Arrays of U(93.2) Metal Cylinders with Various Height-to-Diameter Ratios

The material line can be written as:

$$\frac{\sigma(m'^{nc})}{m'^{nc}} = (c_2')_{\substack{9x24x1 \\ Pu(0)}}\left(\frac{m_0'}{m'^{nc}} - 1\right)\left[\frac{1}{cm^2}\right]$$

$$\frac{\sigma(m'^{nc})}{m'^{nc}} = 1.568x10^{-3}\left(\frac{9,950 \text{ g}}{m'^{nc} \text{ g}} - 1\right)\left[\frac{1}{cm^2}\right]$$

The geometry line for a 9×24×1 array is $\quad \dfrac{\sigma(m'^{nc})}{m'^{nc}} = 6.383x10^{-4}\left[\dfrac{1}{cm^2}\right]$

Equating the material and geometry lines and solving for m':

$$c_2^{nc}\left(\frac{9.95 \text{ kg}}{m^{nc}} - 1\right) = 6.383x10^{-4}[cm^{-2}]$$

$$m^{nc} = \left(\frac{1.568x10^{-3}[cm^{-2}] \times 9.95 \text{ kg}}{6.383x10^{-4}[cm^{-2}] + 1.568x10^{-3}[cm^{-2}]}\right) = 7.071 \text{ kg}$$

205

This mass corresponds to the array unit Pu(0) metal mass required to maintain the 9×24×1 array in a critical state. The mass necessary to result in a keff of 0.9 can now be calculated:

$$k_{eff} = \left(\frac{m'_{knoncubic}}{m'_{critnoncubic}}\right)^{\frac{1}{3}} \Rightarrow m'_{knoncubic} = k^3_{eff} m'_{critnoncubic} = (0.9)^3 7{,}071g = 5{,}155g$$

Table 7-2. Summary of Limiting Surface Density Example Problem 8

Pu-239		
Array Shape	m_{crit}	$m_{k=0.9}$
6 x 6 x 6	5.295 kg	3.856 kg
24 x 9 x 1	7.071 kg	5.155 kg

Notice that an array of **24×9×1** with 5.155 kg units has a $k_{eff} = 0.9$, while rearranging those same units in a **6×6×6** array would result in a $k_{eff} = 0.991$.

7.7   THE EFFECT OF UNIT SHAPE ON ARRAY CRITICALITY

The limiting surface density method was derived for cubic arrays of U(93.2) metal spheres. If the shape of the fissile units in the cubic array were changed to a cylindrical geometry, as the height-to-diameter (*H/D*) ratio changes, then the value for m_o or the unreflected critical mass for the fissile material changes due to an increase or decrease in neutron leakage. However, over a very well-defined *H/D* range, $0.3 \le H/D \le 3$, the limiting surface density method will still apply. Outside of this *H/D* range, more than one line segment may be necessary to describe the limiting surface density over a wide range of unit masses. In other words, more than one value for the characteristic constant, c_2, is necessary to provide an accurate representation of the array unit mass or limiting surface density. In this case, data for c_2 representing the array unit shapes, outside of the previously specified range, may not be available and may need to be calculated using the relationship $\sigma(m) = c_2(m_o-m)$, as discussed in Reference 39. However, as Figure 7-17 shows, a conservative estimate of the critical or subcritical unit mass can be made by assuming that the material line is straight from $\sigma(0)$ to the intercept of the x-axis, which corresponds to the green, dashed line in the figure.

For example, for an *H/D* ratio of 1.0, which falls in the range of applicability of the limiting surface density method as discussed above, the method provides an estimate for the critical unit array mass at approximately 44 kg of U(93.2) metal. This critical unit array mass increases to about 75 kg to maintain the array at a critical state for cylindrical units with an *H/D* of 0.3 (also within range of applicability). The large increase in mass is due to the significant increase in the neutron leakage for H/D shape in the array.

Outside the range of applicability, an array of U(93.2) metal cylinders with an *H/D* of 0.2 does not result in a linear relationship between the unit mass and the limiting surface density. As Figure 7-17 shows, two material lines are needed to describe this system with each line having its own characteristic constant (slope), c_2, value. Unless the c_2 value (noted in Figure 7-17 as c_2') for segment #2 for the *H/D* of 0.2, is calculated via the Thomas methodology (Reference 39), the analyst may be stuck. However, because the experimental data slopes upward to the ordinate for the *H/D = 0.2* case, a line can be extended from segment #1 to the abscissa (green dashed line corresponding to segment #1), and the intersection of this material line "extension" with the geometry line can be used as a conservative value of the array unit mass for a subcritical array. For the U(93.2) metal cylinders shown in Figure 7-17, the conservative array unit mass, indicated by the "red dot," is about 87 kg. If c_2' were known, the actual intersection of the

material (segment #2) and geometry lines would result in a critical array unit mass of about 98 kg, as shown by the yellow dot.
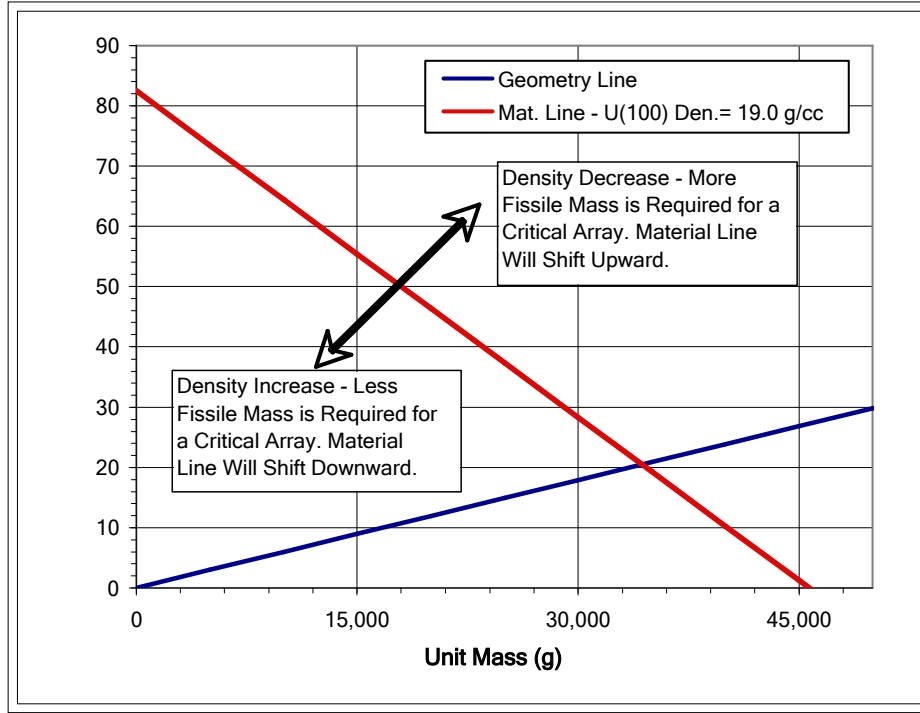
Figure 7-17. Density Change in a Critical 4×4×4 Array with U(100) Metal Units.

7.8   EFFECT OF A FISSILE UNIT DENSITY CHANGE

The effect of a density change of array units can be determined by a simple calculation to determine a new value of the characteristic constant, c_2, corresponding to the array unit density change. For example, the limiting surface density method can be used to determine the critical array characteristics for a storage array of alpha-phase plutonium ingots (ρ = 19.75 g/cm³) that were replaced with delta-phase plutonium ingots (ρ = 15.75 g/cm³). The core density conversion from Chapter 4 can be used to determine the new value for c_2 due to the change in density of a fissile material:

$$\frac{m_0^{\rho_0}}{m_0^{\rho_1}} = \left(\frac{\rho_1}{\rho_0}\right)^2 \tag{124}$$

where $m_0^{\rho_1}$ and ρ_1 represent the unreflected critical mass and density, respectively, for the new fissile material shape, and $m_0^{\rho_0}$ and r_0 represent the unreflected critical mass and density for the original, spherical unit.

The limiting surface density where $m = 0$, $\sigma(0)$ is equal for both cases:

$$\sigma(0) = \sigma(0)^\rho = c_2 m_0^{\rho_0} = c_2^{\rho_1} m_0^{\rho_1}$$

Solving for the new characteristic constant, c_2':

$$\frac{c_2^{\rho_1}}{c_2} = \left(\frac{m_0^{\rho_0}}{m_0^{\rho_1}}\right) = \left(\frac{\rho_1}{\rho_0}\right)^2 \quad \text{OR} \quad c_2^{\rho_1} = c_2\left(\frac{\rho_1}{\rho_0}\right)^2 \tag{125}$$

A simple change in unit density does not result in any other change to the array as long as the unit cell volume remains constant. That is, the geometry line for the array is invariant, whereas the material line changes along with the density change. The effect of a change in the characteristic constant, c_2 to $c_2^{\rho_1}$, will result in a corresponding shift in the array unit mass required to maintain a critical array. For a reduction in the density of the fissile material, common sense concludes that the array unit fissile mass must increase for the array to maintain a critical state. Likewise, if the density of the fissile material increases, then the array unit mass is shifted lower to maintain criticality of the array.

To determine the new fissile array unit mass needed to obtain a critical array configuration at a lower fissile density, the "equivalence relationship" from Section 7.5 can be used to compare the NB_n^2 parameters for two critical arrays. The ratio of the limiting surface density relationships can be calculated as follows. Note that the variables a_n, m_o and N do not change. The unit spacing, fissile material type and number of units in the array are the same before and after the transformation from array units with density ρ_0 to ρ_1.

This relationship shows that the mass required to maintain a critical array increases for a reduction in the fissile material density and decreases when the density is increased. These trends are illustrated in Figure 7-18. The following equation describes the effect of a change in array units of the same fissile material but with a different density.
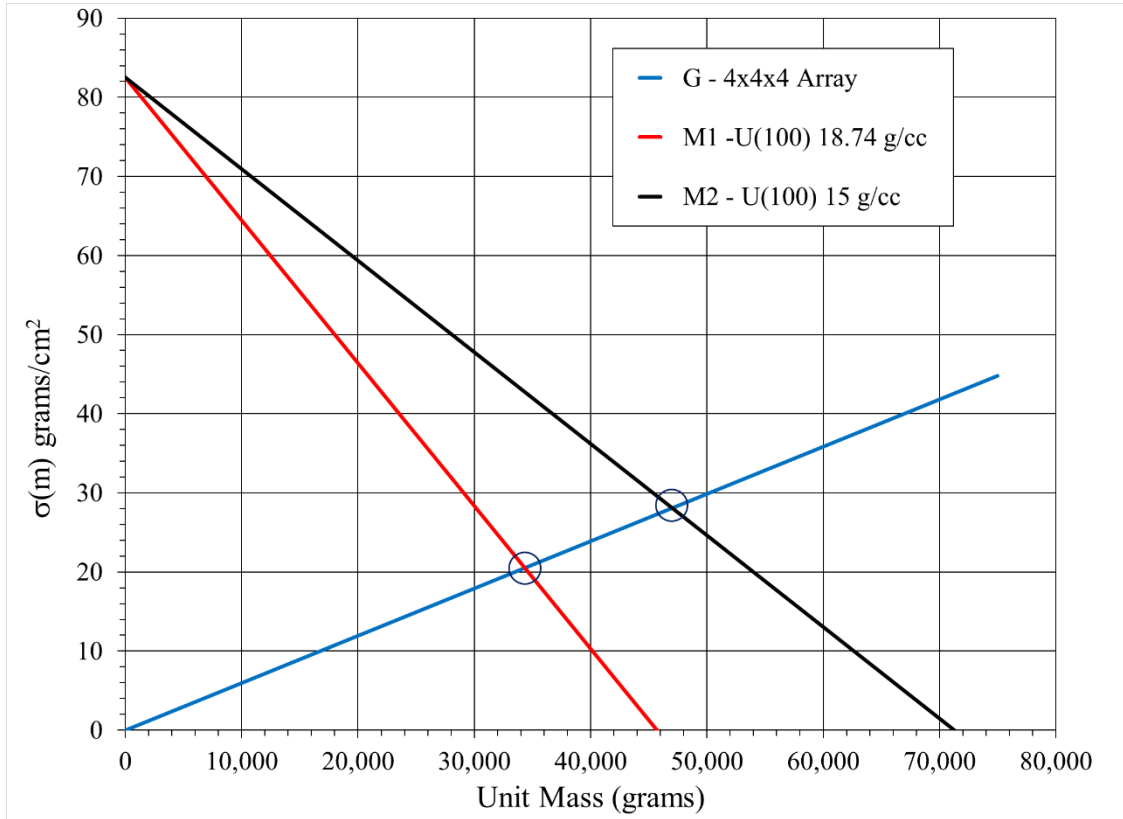
Figure 7-18. Solution for Limiting Surface Density Example Problem 9.

$$m^{\rho_1} = \frac{m^{\rho_0}}{\left[\frac{m^{\rho_0}}{m_0^{\rho_0}}\left(\frac{\rho_1}{\rho_0}\right)^2 + \left(1 - \frac{m^{\rho_0}}{m_0^{\rho_0}}\right)\right]}$$

(126)

Reference 39 provides additional information about fissile material density changes in array configurations.

7.8.1 Limiting Surface Density Example Problem 9

Using the limiting surface density method, calculate the critical mass for each array unit required for a water-reflected cubic array of fully enriched U(100) metal for a 4×4×4 array with a center-to-center spacing of 30 in. (76.2 cm) due to a change in array density change from 18.74 g/cm³ (limiting surface density example problem 3) to 15 g/cm³.

Non-graphical solution from Section 7.4.3:

For a 4×4×4 cubic array with the given spacing:

- $n = n_x = n_y = n_z = 4$
- $a_n = a_x = a_y = a_z = 30/2 = 15$ in. (38.1 cm)

The following relationship for a cubic array can be used to determine the critical mass per unit, m^1, to maintain the array in a critical condition for U(100) metal units.

$$m^1 = m_0 \frac{1}{\left(\left[\frac{n_z}{c_2(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2\right] + 1\right)}$$

where

m_o	–	45.68 kg from Table 14
n_z	–	4 from the assumptions specified above
a_n	–	15 in. (38.1 cm) from the assumptions specified above
c_2	–	0.001806 cm⁻² from Table 7-1
N	–	equal to $n^3 = 64$
c	–	0.55, defined previously

Substituting the values for each variable into the array critical mass relationship provides the following result:

$$m^1 = 45.68 \text{ kg} \frac{1}{\left(\left[\frac{4}{0.001806 \text{ cm}^{-2}(2 \times 38.1 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{64}}\right)^2\right] + 1\right)}$$

$$m^1 = 34.325 \text{ kg}$$

Equation (124) is used to calculate the how the array unit critical mass is affected via density change.

$$m^{\rho_1} = \frac{m^{\rho_0}}{\left[\frac{m^{\rho_0}}{m_0^{\rho_0}}\left(\frac{\rho_1}{\rho_0}\right)^2 + \left(1 - \frac{m^{\rho_0}}{m_0^{\rho_0}}\right)\right]}$$

For this problem, the original fissile unit density was assumed to be 18.74 g/cm³, which is the density of U(93.5) metal as indicated in Appendix B.[27] Assume for these problems, the fissile units were swapped out with the same material at a reduced density (15 g/cm³).

ρ^I — 15.0 g/cm³
ρ^0 — 18.74 g/cm³

The other variables in the problem stay the same; the geometrical characteristics of the array (n_z, N, a_n) are unchanged for this problem.

$$m^{\rho_1} = \frac{34.325 \text{ kg}}{\left[\frac{34.325 \text{ kg}}{45.68 \text{ kg}}\left(\frac{15.0 \frac{g}{cm^3}}{18.74 \frac{g}{cm^3}}\right)^2 + \left(1 - \frac{34.325 \text{ kg}}{45.68 \text{ kg}}\right)\right]}$$

$$m^{\rho_1} = 47.020 \text{ kg}$$

The new critical mass of an unreflected sphere of U(100) at a density of 15 g/cm³ can be determined from Eq. (122):

$$\frac{m_0^{\rho_0}}{m_0^{\rho_1}} = \left(\frac{\rho_1}{\rho_0}\right)^2 \Rightarrow m_0^{\rho_1} = m_0^{\rho_0}\left(\frac{\rho_0}{\rho_1}\right)^2 = 45.68 \text{ kg}\left(\frac{18.74 \text{ g/cm}^3}{15 \text{ g/cm}^3}\right)^2 = 71.30 \text{ kg}$$

The new value of the characteristic constant, c_2' found using Eq. (123), is

$$c_2^{\rho_1} = c_2\left(\frac{\rho_1}{\rho_0}\right)^2 = 0.001806 \text{ cm}^{-2}\left(\frac{15 \frac{g}{cm^3}}{18.745 \frac{g}{cm^3}}\right)^2 = 0.001157 \text{ cm}^{-2}$$

These values allow us to plot the new material line that represents 15 g/cm³.

$$\frac{\sigma(m^{\rho_1})}{m^{\rho_1}} = 1.157x10^{-3}\left(\frac{71,300 \text{ g}}{m^{\rho_1} \text{ g}} - 1\right)\left[\frac{1}{cm^2}\right]$$

The geometry line for a **4×4×4** array is $\frac{\sigma(m)}{m} = 5.974x10^{-4}\left[\frac{1}{cm^2}\right]$ as calculated in Section 7.4.3.

7.9   CONCRETE REFLECTED ARRAYS

The limiting surface density method was developed for water-reflected arrays of U(93.2) metal units. For various situations, such as one involving a concrete storage vault, it may be more appropriate to consider concrete reflection. Depending upon the thickness of concrete considered in the analysis, this may result in a reduction or in an increase in the array unit mass required to maintain the array in a critical state. The

---

[27] Varying the uranium density from 18.74 g/cm³ to 18.9 g/cm³ only affects the critical unit density by about 1%, changing from 47.0 kg to 47.5 kg.

magnitude of the increase or decrease in the reactivity of an array with respect to changing the assumed reflector from water to concrete depends upon the overall shape of the array and the type of fissile material present in the array. Thomas (Reference 39) has calculated the characteristic constant, c_2, for various thicknesses of concrete based on Monte Carlo calculations with a 216 unit array of 9 kg U(93.2) metal units with a center-to-center spacing of 12.835 cm. Thomas replaced the water reflector with concrete of various thicknesses and documented the results in Reference 39, Table 7. This table also provides the characteristic constant, c_2, for each thickness of concrete. Using the value of c_2 for the water reflected U(93.2) metal units (1.762×10^{-3} cm^{-2} from Table 7-1), the ratio of c_2 for concrete and water can be calculated for each concrete thickness. These ratios are listed in

Table 7-3.

Table 7-3 also provides a c_2 value from Reference 39 for an array of Pu(94.8) metal units with concrete reflection.

Table 7-3. Comparison of U(93.2) Metal Arrays with Water and Concrete Reflectors

Concrete Thickness (cm)	c_2 for the 216-unit U(93.2) Metal Units Reflected by This Thickness of Concrete ($\times 10^{-3}$ cm^{-2})	c_2 for the 216-unit U(93.2) Metal Units Reflected by Water ($\times 10^{-3}$ cm^{-2})	Ratio of c_2 for Concrete and Water, $\dfrac{c_2(\text{concrete})}{c_2(\text{water})}$
10.16	2.007		1.139
12.70	1.694		0.961
15.24	1.432		0.813
20.32	1.240	1.762	0.704
25.40	1.156		0.656
30.48	1.128		0.640
30.48 for Pu(94.8)	3.050		1.333
40.64	1.085		0.616

Using the relationships defined in Section 7.5, the characteristic constant for other fissile materials can be calculated. The neutronic characteristics for concrete can vary a great deal (Reference 48) based, primarily, on the water content of the concrete. Thomas (Reference 39) used Oak Ridge concrete for the calculations to determine the c_2 values listed in

Table 7-3. Oak Ridge concrete has a water content of about 5.53 wt %, whereas the water content ranges from 2.97 for Magnuson concrete to 10.99 wt % for Hanford concrete (Reference 48). If the water content of the various types on concrete is known, this information should be considered before the

Table 7-3 data are used in a calculation.

7.9.1   Limiting Surface Density Example Problem 10

1. Using the limiting surface density method, calculate the critical mass for each array unit required for a concrete-reflected cubic array of fully enriched U(100) metal for a 4×4×4 array with a center-to-center spacing of 30 in. (76.2 cm). Assume that the concrete is the Oak Ridge mixture and that there is 30.48 cm (12 in.) of concrete reflection instead of the minimum 20 cm (7.87 in.) present in the calculations for example problem 3 (Section 7.4.3).

2. After the critical mass is calculated, determine the multiplication factor for storing 20 kg of U(100) units in the 4×4×4 array.

Part 1. The limiting surface density method assumes a 200 mm (20 cm) thick water-reflected array (Section 7.3). For this concrete-reflected array (30.48 cm thick), the change from a water (minimum 20 cm thick) to a concrete-reflected array results in a change in the array unit mass required to maintain array criticality.

<u>Non-graphical solution</u>

Assume a 4×4×4 cubic array:

$n = n_x = n_y = n_z = 4$
$a_n = a_x = a_y = a_z = 15$ in. (38.1 cm)

The following variables were defined in Section 7.4.3; however, the value for c_2 will have to be adjusted for a reflector change from water to concrete:

m_o	–	45.686 kg from Table 7-1
n_z	–	4 from the problem description
a_n	–	15 in. (38.1 cm) from the problem description
c_2	–	1.806×10^{-3} cm^{-2} from Table 7-1 for U(100) metal for a 12 in. thick water reflector
N	–	equal to $n^3 = 64$
c	–	0.55, defined previously

Before the mass is calculated, determine c_2^{conc} corresponding to the concrete reflected array. From

Table 7-3, the c_2 concrete-to-water ratio for 30 cm (12 in.) of Oak Ridge Concrete reflection is 0.640:

$$\frac{c_2^{conc}}{c_2^{h2o}} = 0.640$$

Rearrange the equation to solve for the c_2 of concrete:

$$c_2^{conc} = 0.640 \times c_2^{h2o} = 0.640 \times 1.806x10^{-3} \text{cm}^{-2} = 1.156x10^{-3} \text{cm}^{-2}$$

Substituting the values for each variable into the array critical mass relationship provides the following result:

$$m^{1conc} = m_0 \frac{1}{\left(\left[\frac{n_z}{c_2^{conc}(2a_n)^2}\left(1-\frac{c}{\sqrt{N}}\right)^2\right]+1\right)}$$

$$m^{1conc} = 45.68 \text{ kg} \frac{1}{\left(\left[\frac{4}{0.001156 \text{ cm}^{-2}(2 \times 38.1 \text{ cm})^2}\left(1-\frac{0.55}{\sqrt{64}}\right)^2\right]+1\right)}$$

$$m^{1conc} = 30.116 \text{ kg}$$

This is the mass of U(100) metal required in each array unit to keep the 4×4×4 cubic array critical, which is about 4.2 kg less U(100) metal per array unit because of the change from a 30 cm (12 in.) water reflector to a 30 cm (12 in.) concrete reflector.

Part 2. Now, the multiplication factor can be calculated if one is interested in storing 20 kg U(100) metal units in each array location. The resulting k_{eff} is calculated below, where m is the desired unit to be stored (20 kg) and m' (30.116 kg) is the calculated critical mass in the array as calculated above:

$$k_{eff} = \left(\frac{m^{kconc}}{m^{1conc}}\right)^{\frac{1}{3}} = \left(\frac{20 \text{ kg}}{30.116 \text{ kg}}\right)^{\frac{1}{3}} = 0.872$$

With 30 cm (12 in.) spacing between units, this array configuration will remain subcritical, although the multiplication is about 3% higher for a concrete reflected system than for the same array with water reflection.

Graphical Solution

Geometry line is unchanged by substitution of reflector material:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{4m}{(2 \times 38.1 \text{ cm})^2}\left(1 - \frac{0.55}{\sqrt{64}}\right)^2$$

$$\sigma(m) = 5.974x10^{-4} \times m[cm]^{-2} \text{ or } \frac{\sigma(m)}{m[\text{grams}]} = 5.974x10^{-4}[cm]^{-2}$$

Material line:

$$\sigma(m) = c_2(m_0 - m)\left[\frac{\text{grams}}{\text{cm}^2}\right]$$

$$\frac{\sigma(m)}{m} = 1.156x10^{-3}\left(\frac{45,680}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

Equating the geometrical and material line relationships:

$$\frac{\sigma(m)}{m[\text{grams}]} = 5.974x10^{-4}[cm]^{-2} = 1.156x10^{-3}\left(\frac{45,680}{m[\text{grams}]} - 1\right)[\text{cm}^{-2}]$$

$$m[\text{grams}] = 30,116 \text{ grams}$$

Figure 7-19 shows the critical array unit mass changed from 34.3 kg to about 30.1 kg, which is a reduction of about 4.2 kg due to concrete being a better neutron reflector than water. Note that the graphical solution (Figure 7-19) illustrates a solution for the array critical unit mass at about 30 kg, which corresponds to a limiting surface density of about 18 g/cm^2.

Figure 7-19 illustrates this solution.
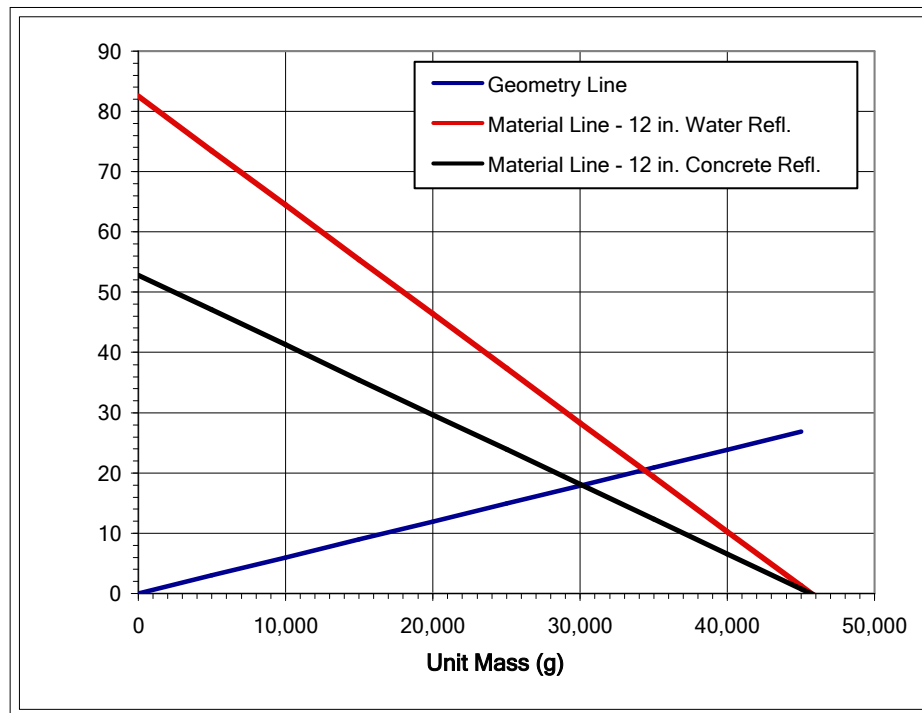
Figure 7-19. Solution for Limiting Surface Density Example Problem 10

8.   SURFACE DENSITY METHOD

8.1   WHAT YOU WILL BE ABLE TO DO

- Determine the center-to-center spacing between fissile units in an array configuration where the array dimension in one direction is limited.

- Estimate the required spacing between array units that have irregular shapes, such as equipment items with fissile material present, stored on a process floor.

- Perform comprehensive parametric studies on various array parameters (fissile mass, spacing, array size, etc.).

8.2   SURFACE DENSITY METHOD OVERVIEW

This method can be used to estimate the required spacing between fissile material units stored in a large configuration where the array size in one direction is limited or controlled administratively. For example, the surface density method would be valid for a planar array that is limited to stacking the fissile materials no more than two units high. This limitation would be controlled at the facility via an engineered or administrative control. Information beyond that covered in this section can be found in References 35, 41, 49, 47, and 50.

As described by Paxton (Reference 14), "A surface-density "rule of thumb" is convenient for distinguishing clearly subcritical arrays of fissionable material from others that may require closer examination. This rule is easily applicable to many process arrangements in which each unit is substantially subcritical."

Consider a planar array of fissionable units. The surface density of fissionable material is the mass of the units divided by the array of the array based on the unit cells. If that surface density does not exceed a reference value for the given fissionable material and unit configuration, then the array will be subcritical. Reference surface density values and corresponding unit size limits for selected fissionable materials are given in Table 8-1.

As an illustration, consider 10 kg units of highly enriched uranium metal U(93) in a square array with 36 cm center-to-center spacing. Review of Table 8-1 shows that the 10 kg unit is less than the maximum unit size of 15 kg, so the reference surface density is 13 g/cm^2 or 12 kg/ft^2. The surface density of the array is then:

$$\sigma = \frac{\text{mass of unit}}{\text{area of unit cell}} = \frac{10 \text{ kg}}{(36 \text{ cm})^2} \times \frac{1000 \text{ g}}{1 \text{ kg}} = 7.7 \frac{g}{cm^2}$$

So the array surface density of 7.7 g/cm^2 is less than the reference value of 13 g/cm^2. This indicates the array is acceptably subcritical in the given configuration and no further evaluation is necessary.

Table 8-1. (from Table VII, pg. 32, Reference 14)

Composition	Maximum Unit Size	Reference Surface Density	
Reference Surface Densities for Selected Fissile Materials			
U(93) solution	5.0-inch OD cylinder	1.6 ml/cm^2	(1.5 liter/ft^2)
	5.5-inch OD cylinder	1.4 ml/cm^2	(1.2 liter/ft^2)
	6.0-inch OD cylinder	1.2 ml/cm^2	(1.1 liter/ft^2)
U(93) solution $\leq$ 50 g U/liter	6.5-inch OD cylinder	3.6 ml/cm^2	(3.4 liter/ft^2)
U(5) solution	8.0-inch OD cylinder	9.6 ml/cm^2	(9.0 liter/ft^2)
Stable Pu(NO$_3$)$_4$ solution	4.7-inch OD cylinder	1.4 ml/cm^2	(1.3 liter/ft^2)
^{233}U solution	4.5-inch OD cylinder	1.3 ml/cm^2	(1.2 liter/ft^2)
U(93) metal	15 kg U [a]	13 g/cm^2	(12 kg/ft^2)
U(93)O$_2$	27 kg U [a]	12.5 g/cm^2	(11.5 kg/ft^2)
U(93)F$_4$	50 kg U [a]	11.5 g/cm^2	(10.5 kg/ft^2)
U(93)F$_6$ +0.1 HF	50 kg U [a]	7.5 g/cm^2	(7 kg/ft^2)
α-phase Pu	3 kg U [a]	5.5 g/cm^2	(5.2 kg/ft^2)
δ-phase Pu, or ^{233}U metal	4.5 kg U [a]	5.5 g/cm^2	(5.2 kg/ft^2)

[a]Reduced 5% for container effects

Extension beyond the "rule of thumb" was done by deriving equations based on the limiting surface density method, experimental and calculated critical data. The surface density method depends on knowing the critical dimensions for a water- reflected infinite slab for the fissile material stored in the array. This method projects the fissile material mass of the array units onto an area of a plane (Reference 35) and compares the resulting surface density to that of the critical surface density for the infinite water-reflected critical slab for the fissile material in question to determine if the array configuration is safe from a criticality safety perspective. Figure 8-1 illustrates this concept.

The average surface density, $\bar{\sigma}$, is the average when all fissile material is projected onto the largest face. This basically means projecting onto a surface, w, where the number of units, n_w, is the minimum of (n_x, n_y, n_z) with n$_x$ being the number of units in the x-direction, etc.

Again, this formulation of the surface density method (Reference 35) was derived from limiting surface density relationships (Reference 38, 44, and 45). Section 7 provides a more comprehensive description of the limiting surface density method. The surface density method was developed to determine a center- to-center spacing that would provide a subcritical configuration. The method applies to individual units having a maximum effective multiplication factor, k$_{eff}$, of 0.9, that corresponds to a fraction critical mass of 0.73 for unreflected spherical array units. A simplified derivation from Reference 40 for the surface density method is shown below.

There are two units in the direction of the projection and the fissile material mass in each unit is m (grams).
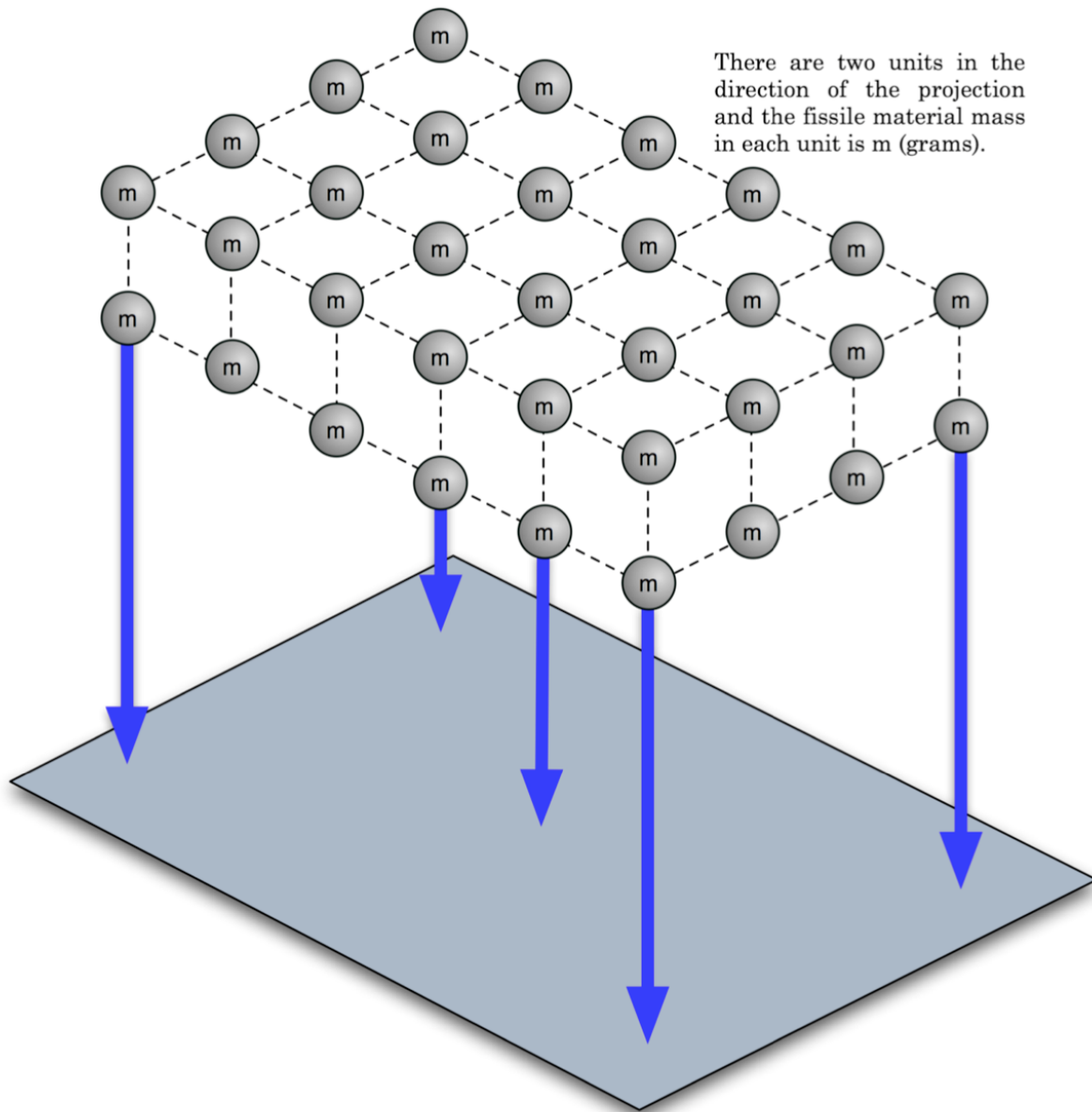
Fissile material projection in direction of limited array dimension to compare to the critical surface density for an infinite water-reflected, critical slab. The width of the slab is equal to the width of the units in the array.

Figure 8-1. Illustration of the Surface Density Method

Begin with the limiting surface density relationship for the array **material** characteristics:

$$\sigma(m) = c_2 m_0 \left[1 - \frac{m}{m_0}\right] \tag{127}$$

The limiting surface density relationship for the array **geometric** characteristics can be written as follows:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 \tag{128}$$

The surface density method assumes an infinite planar array that is of finite height (i.e., n units high). Thus, the limiting surface density relationships can be modified to reflect this type of array.

For an infinite planar array (large number of units, N), the relationship that describes the geometric characteristics of the array can be modified as follows:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{\infty}}\right)^2 = \frac{nm}{(2a_n)^2}(1-0)^2 = \frac{nm}{(2a_n)^2} \tag{129}$$

This relationship can be simplified more by knowing that the quantity $2a_n$ is the center-to-center spacing between array units, d.

$$\sigma(m) = \frac{nm}{d^2} \tag{130}$$

Solving Eq. (130) for d results in a relationship for the center-to-center spacing as a function of the number of units in the finite direction, n, the array unit mass, m, and the limiting value of the surface density for the array, σ, which is dependent upon the material characteristics of the array:

$$d^2 = \frac{nm}{\sigma(m)} \quad \Rightarrow \quad d = \sqrt{\frac{nm}{\sigma(m)}} \tag{131}$$

The next step in the derivation is to calculate the allowed surface density for an infinite planar array. Recall that the array material characteristics are described with Eq. (129) from the limiting surface density method. The expression is also known as the allowed surface density:

$$\sigma(m) = c_2 m\left(\frac{m_0}{m} - 1\right) \tag{132}$$

The fraction of a critical mass, f, present at each location in the array is m/m_0. The surface density method requires that the fraction critical, f, not exceed a value of 0.73. Using the definition of fraction critical, the effective multiplication factor, k_{eff}, is defined as follows.

$$k_{eff} = \left(\frac{m}{m_0}\right)^{\frac{1}{3}} = (f)^{\frac{1}{3}} \tag{133}$$

For $f = 0.73$, the k_{eff} is:

$$k_{eff} = \left(\frac{m}{m_0}\right)^{\frac{1}{3}} = (0.73)^{\frac{1}{3}} = 0.9.$$

Thus, each unit in the array must be less than this k_{eff} value. This safety margin can be incorporated into the allowed surface density for the array (Note the $1/0.73 = 1.37$ so $1.37 * m < m_0$). Rearranging Eq. (132) and incorporating the safety margin gives

$$\sigma(m) = c_2 m_0 \left(1 - \frac{m}{m_0}\right) = c_2 m_0 (1 - f)$$

adding the safety margin: $\sigma(m) = c_2 m_0 (1 - 1.37f)$

(134)

Equation (134) ensures that the fraction critical be less than 0.73. If f were equal to 0.73, the allowed surface density for that array would be zero:

$$\sigma(m) = c_2 m_0 (1 - 1.37(0.73)) = c_2 m_0 (1 - 1) = 0$$

This means that the surface density method cannot be used to define a safe spacing for this array because the multiplication factor for each unit in the array is too high. This method would provide an infinite calculational result for the required distance between array units.

The previous expressions for the allowed surface density can now be modified using experimental and calculational data for various infinite planar array configurations.

Examine the geometrical relationship for the allowed surface density. When $m = 0$, the allowed surface density is that of an infinite water reflected slab. When $m = 0$:

$$\sigma(m) = c_2 m_0 \left(1 - 1.37 \frac{0}{m_0}\right) = c_2 m_0.$$

The allowed surface density when the array unit mass is zero, $\sigma(0)$, is also denoted σ_0.

Now, the expression in Reference 35, Eq. 4.5, defines the allowed surface density, with a coefficient that limits the allowed surface density to 54% of the allowed surface density, σ_0:

$$\sigma(m) = 0.54\sigma_0 \left(1 - 1.37 \frac{m}{m_0}\right) = 0.54\sigma_0 (1 - 1.37f).$$

(135)

This coefficient of 0.54 is the product of two factors; one is for the shape of the array, and the second is for the reflector material surrounding the array. In Eq. (135), the product $0.54\,\sigma_0$ is the term that precludes the array containing small array units from achieving criticality, and the product $1.37f$ precludes the array from achieving criticality for large array units. These two products in the relationship for the allowed surface density ensure that the resultant center-to-center spacing results will provide an array that is subcritical (Reference 40). The center-to-center spacing between array units for the surface density method was defined in Eq. (131) as:

$$d = \sqrt{\frac{nm}{\sigma(m)}}$$

Substitute the expression for the allowed surface density from Eq. (135) to obtain[28] the following expression for d:

---

[28] The 1.37 in front of the square root sign is the rounded value of the square root of 1/0.536. The 0.54 value in

$$d = \sqrt{\frac{nm}{0.54\sigma_0(1 - 1.37f)}} = 1.37\sqrt{\frac{nm}{\sigma_0(1 - 1.37f)}} \qquad (136)$$

Each of the variables for d is defined below for Thomas' representation of the surface density method (Reference 35):

σ_0 — the surface density of the water-reflected infinite slab (g/cm^2);

f — the ratio of the mass of a unit in the array to the critical mass of the unreflected sphere of the same fissile material (**must not exceed 0.73 for this method to be applicable**);

n — the number of fissile material units in the direction of the projection onto a wall or the floor of the storage location; and

m — the fissile material mass per array unit (g).

8.3 APPLICABILITY OF THE SURFACE DENSITY METHOD

The surface density method can be used for a variety of fissile materials and array configurations. The surface density method is applicable for the following situations:

- This method, as described above, is applicable to infinite planar arrays reflected by water at least 155 mm thick (6.1 in.) or its nuclear equivalent (Reference 35, page 96). The reflector cannot be located closer to the units in the array than the boundaries of the cells associated with the units. Guidance for applying this method with arrays located next to concrete reflectors can be found in Reference 39, page 29, and Reference 40, page 8.

- This method can be used in situations where the fissile units have irregular geometries such as where equipment that contains fissile materials are stored on a process floor, for example (Reference 16, page 78). This method is useful for this situation because the surface density of an infinite, water-reflected slab bounds the mass of each fissile unit in the array.

- Perturbations in the reflector materials, array unit shape, and array shape are discussed in greater detail in References 35 and 39. The example problems consider arrays with water reflection only. Reference 40 provides information about effects of concrete compared to water for the surface density method.

- An engineered or administrative control would be required to limit the number units in one direction. For example, an array of fissile units can be stored infinitely on the floor of a facility; however, the units can only be stacked in a limited fashion (i.e., finite). If units need to be stored in an unlimited fashion, the density analog method may be a better method to use for that situation.

---

equation 8.9 appears to be the rounded value of the 0.536.

8.4 SURFACE DENSITY METHOD EXAMPLE PROBLEMS

8.4.1 Surface Density Example Problem 1

Calculate the minimum spacing for a planar array of 2-liter bottles of Pu, with 5-wt. % [240]Pu, solution, assuming a maximum concentration of 400 gPu/l? The array is assumed to be only one unit high (i.e., no stacking).

The first step in the solution for this problem is to calculate the surface density of a water-reflected infinite slab, σ_o, and the value of f, the ratio of the mass of a unit in the array to the critical mass of an unreflected sphere of the same material.

The value of s_0 can be determined by taking the product of the slab height of an infinite, water-reflected slab and the Pu concentration. The water-reflected, infinite slab thickness for a Pu(5)-H$_2$O solution system (400 g Pu/L) can be estimated from Figure 8-2 as 2.75 in. or 6.99 cm.

$$\sigma_0 = 6.99 \text{ cm} \times 400 \frac{\text{g Pu}}{L} \times 0.001 \frac{L}{\text{cm}^3} = 2.80 \frac{\text{g Pu}}{\text{cm}^2}$$

The mass of Pu in each bottle of solution is:

$$M_{\text{2L bottle}} = \frac{2 \text{ L}}{\text{bottle}} \times 400 \frac{\text{g Pu}}{L} = 800 \frac{\text{g Pu}}{\text{bottle}}$$

The critical mass of an unreflected sphere of a mixture of Pu metal and water can be found by multiplying the Pu concentration by the spherical critical volume at the maximum concentration (23 L from Figure 8-3):

$$m_0 = 400 \frac{\text{g Pu}}{L} \times 23.0 \text{ L} = 9,200 \text{ g Pu}$$

This is equal to the Pu critical mass for a system with 5wt.% [240]Pu from Figure 8-4 for this concentration). Next, f needs to be calculated based on the critical mass (9,200 g Pu) of an unreflected sphere of a mixture of Pu metal and water with 5 wt. % [240]Pu:

$$f = \frac{\text{mass of Pu in 2 L bottle}}{\text{critical mass, unrefl. Pu (5) - H2O mixture}}$$

$$f = \frac{800 \text{ g Pu}}{9,200 \text{ g Pu}} = 0.087$$
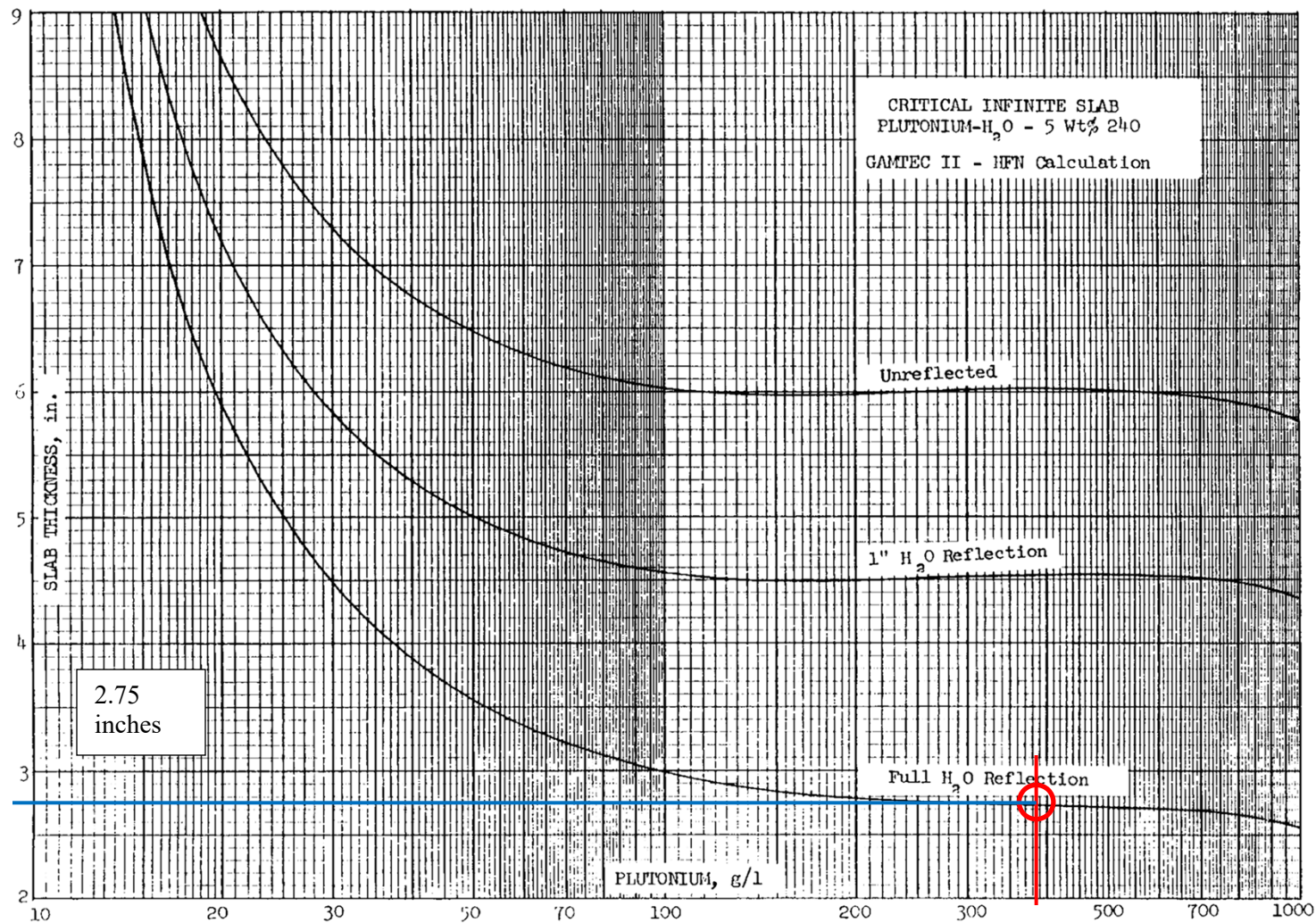
Figure 8-2. Critical Infinite Slab Thickness of a Mixture of Plutonium and Water. (Reference 7, Figure III.A.5.95-3).
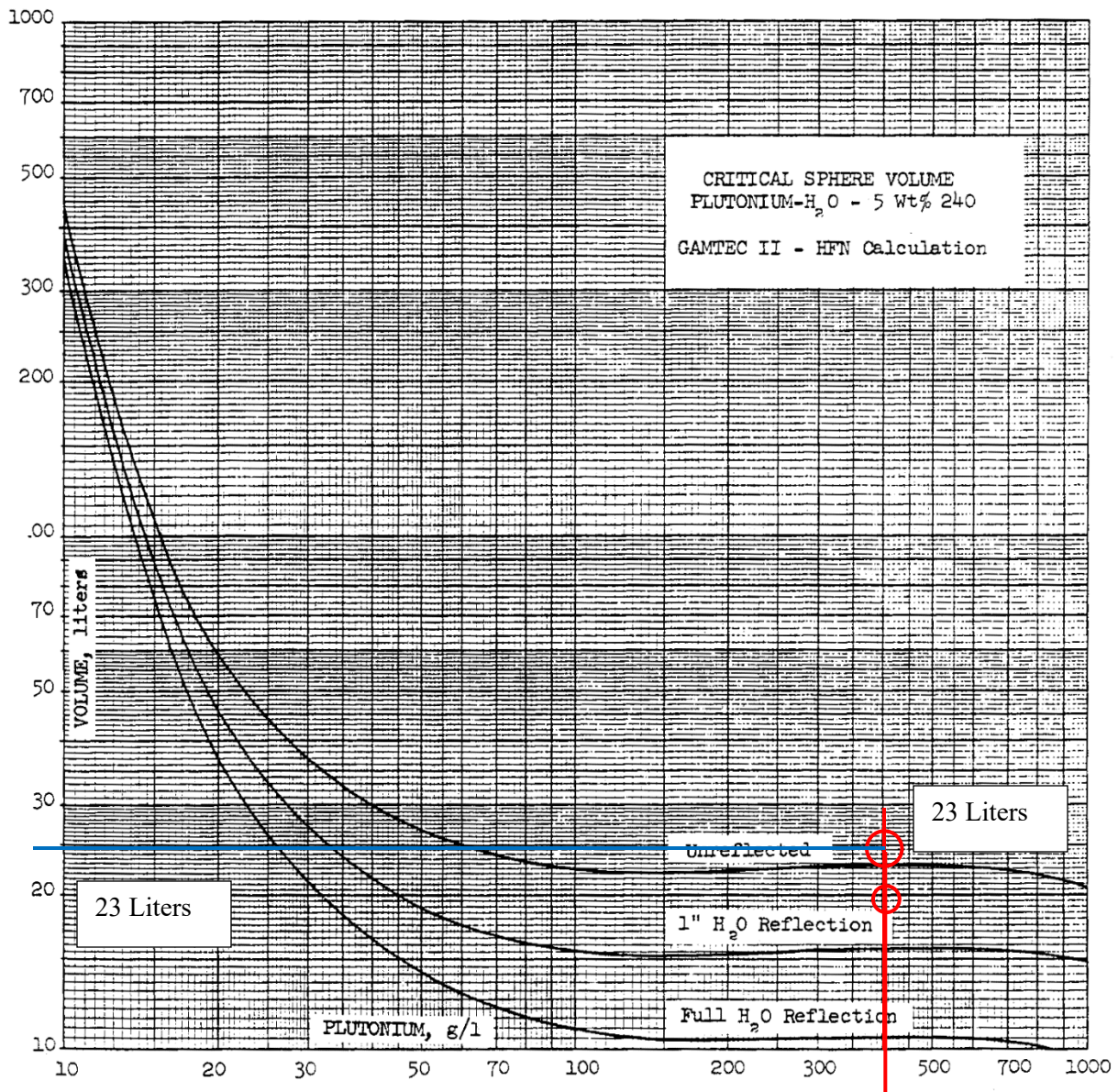
Figure 8-3. Critical Infinite Slab Thickness of a Mixture of Plutonium and Water. (Reference 7, Figure III.A.9.95-3)
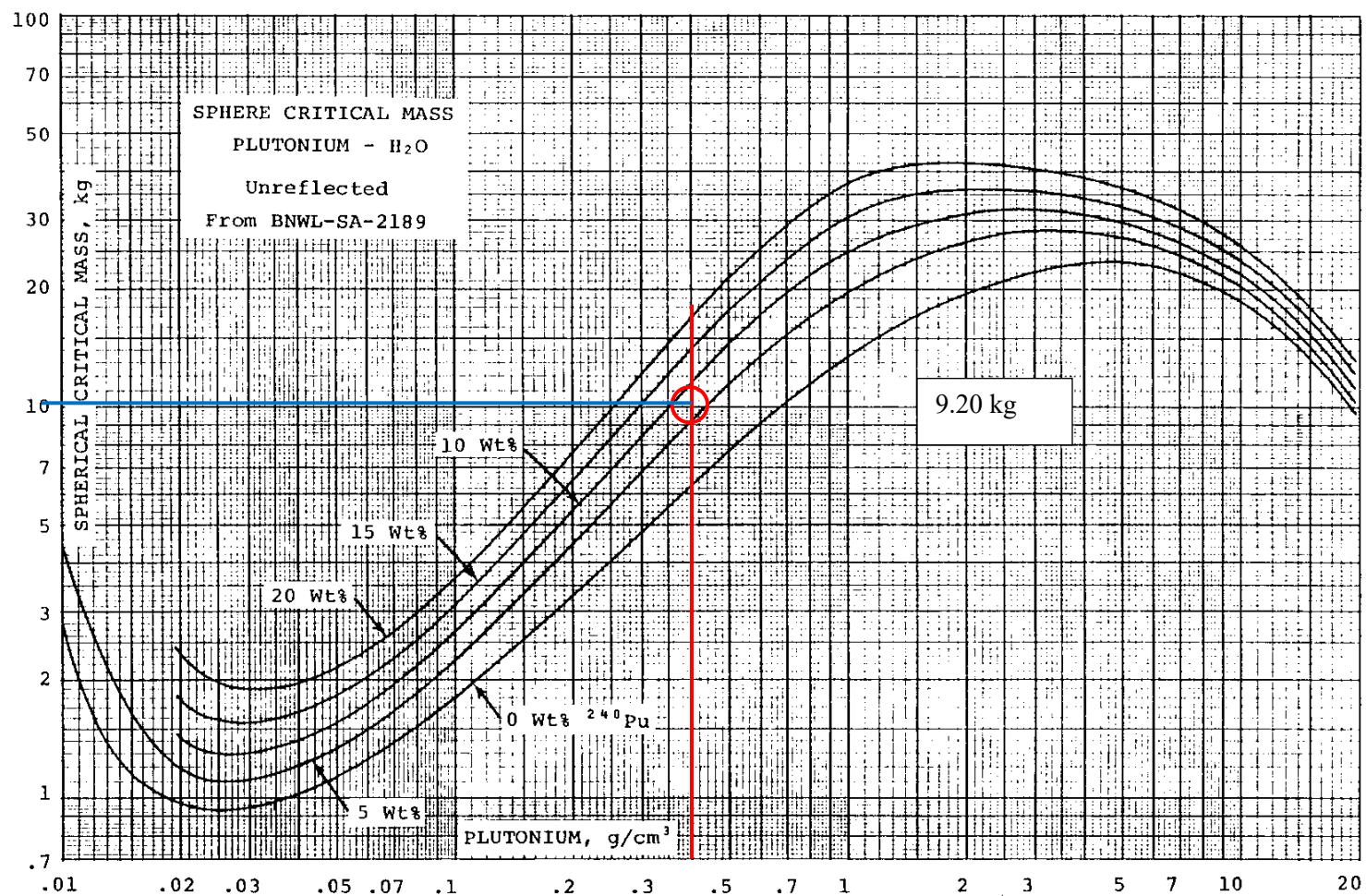
Figure 8-4. Spherical Critical Mass of an Unreflected Mixture of Plutonium and Water. (Reference 7, Figure III.A.6-2).

Knowing σ_o and f, equation 8.10 can be used to determine the center-to-center spacing for an infinite array stacked one unit high ($n = 1$):

$$d = 1.37 \sqrt{\frac{nm}{\sigma_0(1 - 1.37f)}}$$

$$d = 1.37 \sqrt{\frac{1 \times 800 \text{ g Pu}}{2.8 \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37(0.087))}} = 24.7 \text{ cm } (9.7 \text{ inches})$$

Therefore, as a limit, the center-to-center spacing for this one-unit-high, infinite array of Pu solution bottles containing 5 wt. % ^{240}Pu should not be less than 25.4 cm (10 in.) where we have rounded up for conservatism.

To summarize, values are for the unreflected critical spherical mass and the mass of a unit in the array. These are used to calculate the fraction critical. Then the surface density calculated from the reflected critical slab thickness and fissile atom density/concentration is used to calculate the minimum center-to-center spacing to keep the array subcritical.

8.4.2 Surface Density Example Problem 2

What is the minimum center-to-center spacing for an infinite planar array of plutonium oxide (^{239}PuO$_2$) containers loaded with 4,500 grams of Pu per container? Assume that the Pu oxide density is 11.48 g/cm³, which is the theoretical density for PuO$_2$, that the Pu is pure ^{239}Pu, and the array is assumed to be only one unit high (i.e., no stacking).
This case can be solved using the same procedure as used in the last example problem. Recall that the first step in the surface density method is to calculate the surface density of a water-reflected infinite slab, σ_o, and then f, the ratio of the mass of a unit in the array to the critical mass of an unreflected sphere of the same material

The value of s_0 can be determined by taking the product of the slab height of an infinite, water-reflected slab and the density of the fissile material (in this case, the Pu). The water-reflected, infinite slab thickness for a ^{239}PuO$_2$ system can be determined via Reference 11, Table 16, page 70 that shows 1.60 cm for pure 239 PuO$_2$ at a density of 9.96 g Pu/cc. In this example, the Pu density is 10.13 g Pu/cc so the critical slab thickness should apply.

$$\sigma_0 = 1.60 \text{ cm} \times 11.48 \frac{\text{g PuO}_2}{\text{cm}^3} = 18.37 \frac{\text{g PuO}_2}{\text{cm}^2}$$

Next, f needs to be calculated based on the critical mass of an unreflected sphere of ^{239}PuO$_2$. From Reference 49, the critical, unreflected spherical mass of ^{239}PuO$_2$ at 11.48 gPuO$_2$/cm³ is about 26,700 g.

$$f = \frac{\text{mass of PuO}_2}{\text{critical mass, unrefl. Pu O}_2 \text{ at theoretical density}}$$

$$f = \frac{4,500 \text{ g Pu}}{26,700 \text{ g Pu}} \times \frac{271.05 \text{ g PuO}_2}{239.05 \text{ g Pu}} = 0.191$$

Knowing σ_o and f, equation 8.10 is used to calculate the center-to-center spacing for an infinite array stacked one unit high ($n = 1$):

$$d = 1.37 \sqrt{\frac{1 \times 5{,}102 \text{ g Pu}O_2}{18.37 \frac{\text{g Pu}O_2}{\text{cm}^2}(1 - 1.37(0.191))}} = 26.6 \text{ cm (10.5 inches)}$$

Therefore, as a limit, the center-to-center spacing for this one-unit-high, infinite array of ^{239}PuO$_2$ containers is about 26.6 cm (10.5 in.). If the array were 2 units high ($n = 2$) and infinite in extent in the lateral directions, the center-to-center spacing between containers would increase to about 37.6 cm (14.8 in.), which is somewhat intuitive because of the presence of additional fissile material in the array.

The full water reflection makes the limited dimension have zero leakage, making it effectively infinite (Figure 8-5).
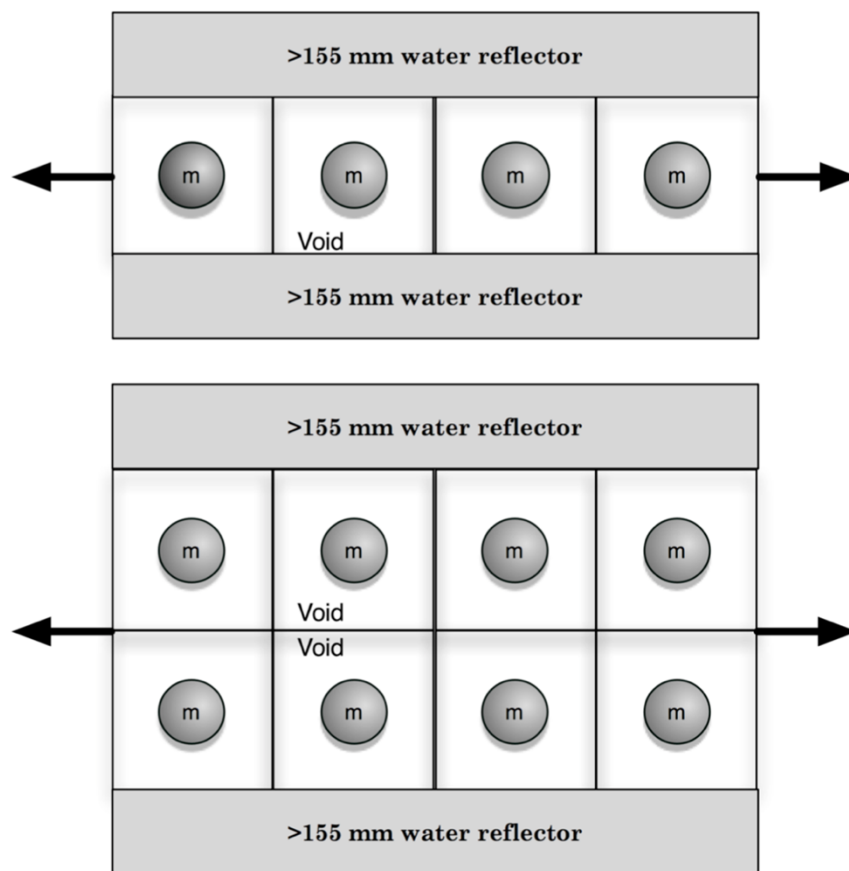
Figure 8-5. Illustration of the Surface Density Water Reflection Assumptions.

8.4.3   Surface Density Example Problem 3

What is the minimum center-to-center spacing of an infinite planar array of 4,500 g Pu(5) metal ingots. For this problem, assume that the density of the Pu(5) metal ingots is the same as alpha-phase Pu, 19.75 g/cm³, and that the array is assumed to be only one unit high (i.e., no stacking).

This case is very similar to the last two example problems. As before, the surface density depends on the slab height of an infinite, water-reflected slab. The water-reflected, infinite slab thickness for an alpha-phase Pu(5) metal system can be determined via Reference 11, Figure 34, as 0.82 cm (0.32 in.). Note that the slab thickness is for Pu(3.1) and not Pu(5). Assuming a lower ^{240}Pu content for this case results in more of the fissile ^{239}Pu isotope being present; thus, the slab thickness used will be conservative. Now, calculate the surface density for the water-reflected, infinite slab.

$$\sigma_0 = 0.82 \text{ cm} \times 19.75 \ \frac{\text{g Pu}(5)}{\text{cm}^3} = 16.20 \ \frac{\text{g Pu}(5)}{\text{cm}^2}$$

Next, f needs to be calculated based on the critical mass of an unreflected sphere of Pu(5) metal. From Figure 8-6, the critical, unreflected spherical mass of Pu metal with 5 wt. % ^{240}Pu at 19.75 gPu/cm^3 is about 10,300 g.

$$f = \frac{\text{mass of Pu}(5)}{\text{critical mass, unrefl. Pu}(5) \text{ at } 19.75 \text{ g/cm}^3}$$

$$f = \frac{4{,}500 \text{ g Pu}}{10{,}300 \text{ g Pu}} = 0.437$$

Knowing σ_o and f, the center-to-center spacing can be determined for an infinite array stacked one unit high ($n = 1$):

$$d = 1.37 \sqrt{\frac{1 \times 4{,}500 \text{ g Pu}(5)}{16.20 \ \frac{\text{g Pu}(5)}{\text{cm}^2}(1 - 1.37(0.437))}} = 36.0 \text{ cm } (14.2 \text{ inches})$$

Therefore, as a limit, the center-to-center spacing for this one-unit-high, infinite array of Pu(5) metal ingot containers is a little more than 36.0 cm (14.2 in.). If the array were 2 units high ($n = 2$) and infinite in extent in the lateral directions, the required center-to-center spacing between containers would increase to about 51 cm (20.1 in.).
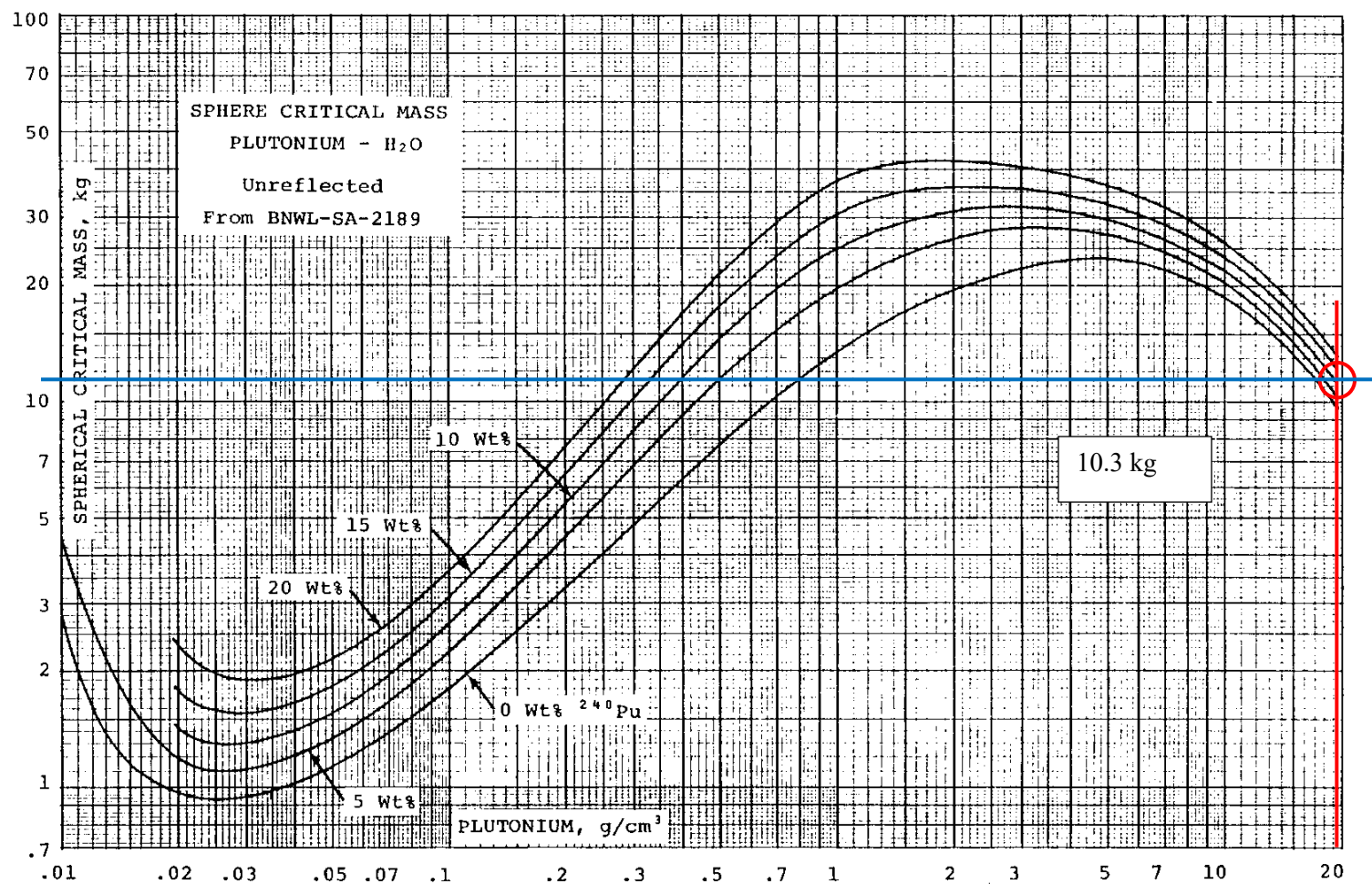
Figure 8-6. Spherical Critical Mass of an Unreflected Mixture of Plutonium and Water. (Reference 7, Figure III.A.6-2).

228

8.4.4 Surface Density Example Problem 4

1. Repeat the previous problem with delta-phase Pu, 15.6 g/cm³. What is the minimum center-to-center spacing of an infinite planar array of 4,500 g Pu(5) delta-phase metal ingots in a one unit high array?
2. Then calculate the maximum delta ingot mass if the center-to-center spacing is 20 cm (7.87 in.).

This problem involves a change of density from the 19.75 g/cm³ used in the last example to 15.6 g/cm³ in this example. Because we are using the same material, but changing the density, we can use the Core Density Conversion ratios from Table 4-1.

The critical water-reflected slab thickness from Example Problem 3 was 0.82 cm (0.32 in.). The critical water-reflected slab thickness for the new density is calculated as:

$$\frac{t}{t_0} = \left(\frac{\rho}{\rho_0}\right)^{-1} = \left(\frac{\rho_0}{\rho}\right) t = t_0 \times \left(\frac{\rho_0}{\rho}\right) = 0.82 \text{ cm} \times \left(\frac{19.75 \text{ g/cc}}{15.6 \text{ g/cc}}\right) = 1.04 \text{ cm}$$

Now, calculate the surface density for the water-reflected, infinite slab.

$$\sigma_0 = 1.04 \text{ cm} \times 15.6 \frac{\text{g Pu(5)}}{\text{cm}^3} = 16.20 \frac{\text{g Pu(5)}}{\text{cm}^2}$$

Note that the surface density remains unchanged as it is the product of the thickness and the material density, and the thickness is inversely proportional to the material density.

Next, f needs to be calculated. Again, we can use the relationship from Table 4-1 to determine the critical mass of an unreflected sphere of Pu(5) metal at the new density.

$$\frac{m}{m_0} = \left(\frac{\rho}{\rho_0}\right)^{-2} = \left(\frac{\rho_0}{\rho}\right)^2 m = m_0 \times \left(\frac{\rho_0}{\rho}\right)^2 = 10,300 \text{ gm} \times \left(\frac{19.75 \text{ g/cc}}{15.6 \text{ g/cc}}\right)^2 = 16,500 \text{ gm}$$

$$f = \frac{\text{mass of Pu(5)}}{\text{critical mass, unrefl. Pu (5) at 15.6 g/cm}^3}$$

$$f = \frac{4,500 \text{ g Pu}}{16,500 \text{ g Pu}} = 0.273$$

Knowing σ_o and f, the center-to-center spacing can be determined for an infinite array stacked one unit high ($n = 1$):

$$d = 1.37 \sqrt{\frac{1 \times 4,500 \text{ g Pu(5)}}{16.20 \frac{\text{g Pu(5)}}{\text{cm}^2}(1 - 1.37(0.273))}} = 28.9 \text{ cm (11.4 inches)}$$

Therefore, as a limit, the center-to-center spacing for this one-unit-high, infinite array of Pu(5) delta metal ingot containers is a little more than 28.9 cm (11.4 in.). The smaller spacing makes sense as there is less fissile material per unit volume.

Then calculate the maximum delta ingot mass if the center-to-center spacing is 20 cm (7.87 in.).

We need to rearrange equation 8.10 to solve for mass. After some algebra, we find:

$$m = \frac{d^2\sigma_0}{(1.37)^2 n + 1.37\left(\frac{d^2\sigma_0}{m_0}\right)}$$

Using the values for m0, n, and s$_0$ as before and changing the center-to-center spacing to 20 cm, we get a mass of:

$$m = \frac{(20 \text{ cm})^2 \times 16.20 \text{ gPu}(5)/\text{cm}^2}{(1.37)^2 \times 1 + 1.37\left(\frac{(20 \text{ cm})^2 \times 16.20 \text{ gPu}(5)/\text{cm}^2}{16,500 \text{ gPu}(5)}\right)} = 2,680 \text{ gPu}(5)$$

In this case, a reduction of 0.692 in spacing requires a reduction of 0.596 in mass. This is not too surprising as the mass is related to the square of the spacing. So, if mass is directly proportional to spacing squared, then the mass should be reduced by $(0.692)^2 = 0.479$. However, because of the constant $(1.37)^2$ in the denominator, the reduction in mass is somewhat less than expected in relation to the square of the spacing.

8.4.5   Surface Density Example Problem 5

Paxton (Reference 51) also describes a smeared density approach to determining acceptable spacing for smaller arrays. The smeared thickness is defined as:

expression for *d*:

$$\text{Smeared Thickness} = \frac{\text{Volume of Fissionable Material in Array}}{\text{Area of Array}} \tag{137}$$

The criteria for safe spacing is:

expression for *d* :

$$t_{safe} \leq 0.5 \times t_c, \tag{138}$$

where: t_{safe} = center-to-center spacing of units in array; and
t_c = critical thickness for a fully reflected infinite slab of the appropriate fissionable material.

Apply this approach to the situation given in Section 6.4.4. That is, calculate the safe spacing for a 10-unit array of 10-inch diameter cylinders (schedule 20 pipe) each 6 feet long on a square lattice pattern in two rows of five. The cylinders are to contain 4.98% enriched uranyl fluoride of maximum 3.2 g U/cm^3 concentration. The volume of each cylinder is 97.36 liters.

So the smeared thickness is: $\text{Smeared Thickness} = \frac{97.36 \frac{\text{liters}}{\text{cyl}} \times 10 \text{ cyl}}{10 \text{ cyl} \times d^2}$. The critical water reflected slab thickness for U(5) solution is 5 inches as shown in Figure 8-7. Substituting these into equation 8.12, we get:

230

$$\frac{97.36\ \frac{liters}{cyl}\ \times\ 10\ cyl}{10\ cyl\ \times\ d^2} \ \ £0.5\ \times\ 5\ inches\,, \quad OR$$

$$d^2 \geq \frac{97.36\ liters\ \times\ 10^3\frac{cm^3}{liter}}{2.5\ inches\ \times\ 2.54\ \frac{cm}{inch}} = 15{,}332\ cm^2$$

$$d \geq 123.8\ cm \ \ or\ 48.7\ inches$$
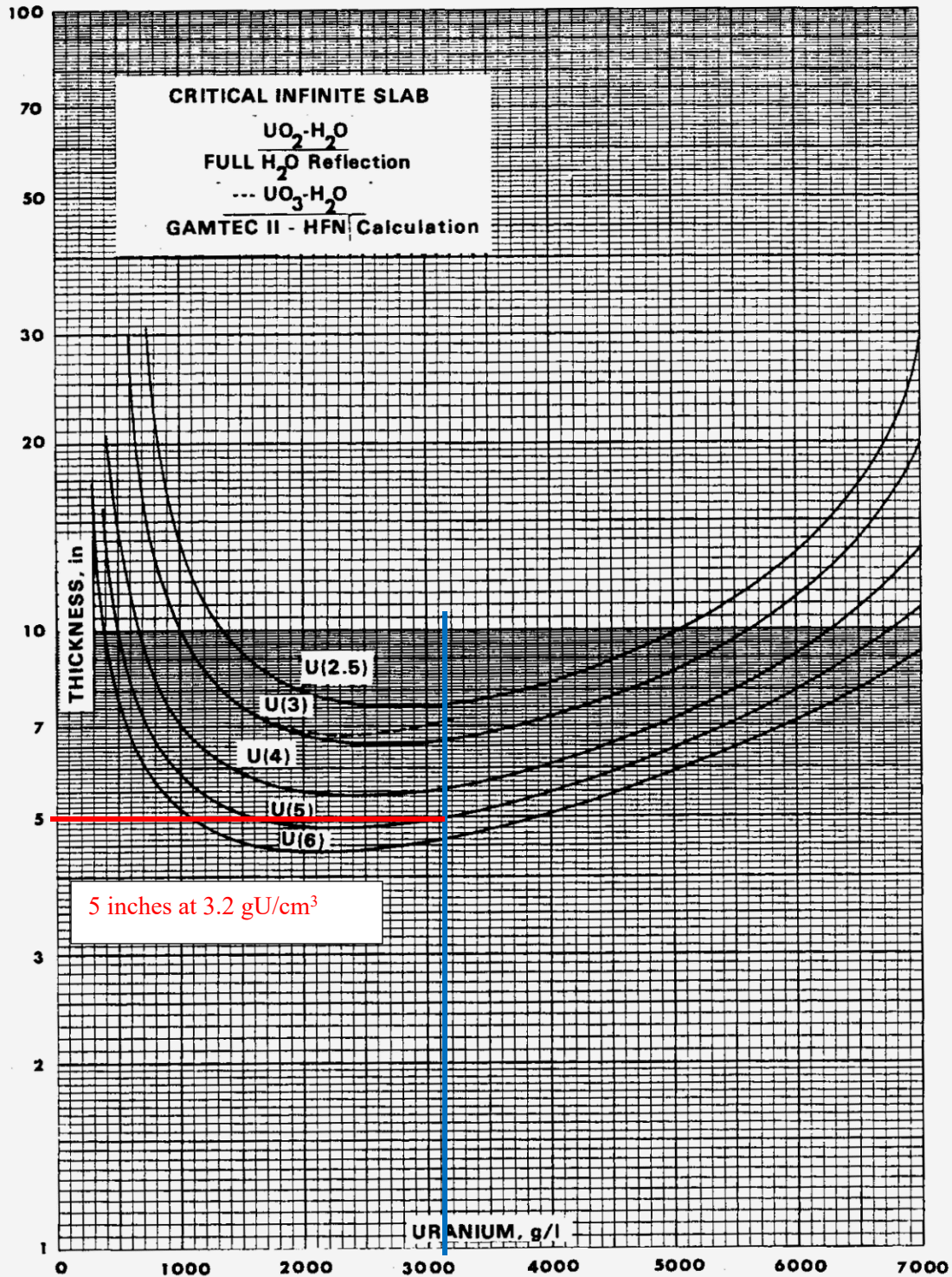
Figure 8-7. Critical Slab Thickness for U(5)O₂-H₂O System. (Reference 7, Figure III.B.5-6).

This spacing of 123.8 cm or 48.7 inches compares with 142.2 cm (56 inches) as calculated from the solid angle method in Section 6.4.4. In that calculation the k_{eff} of 0.796 was used as determined from buckling calculations. If the computer calculated k_{eff} value of 0.757 is used, then the spacing 120.0 cm (47.25 inches).

For this situation with a small array of solution cylinders, the smeared density approach appears to give reasonable results.

9. DENSITY ANALOG METHODS

9.1 WHAT YOU WILL BE ABLE TO DO

- Determine the center-to-center spacing between fissile array units stored in array configurations, independent of the actual storage arrangement.

- Estimate the required spacing between array units that have irregular shapes, such as equipment items with fissile material present stored on a process floor. This method will result in a more conservative (cubic arrays only) but efficient required subcritical spacing.

- Perform comprehensive parametric studies on various array parameters (fissile mass, spacing, array size, etc.).

9.2 DENSITY ANALOG METHOD OVERVIEW

This method is useful for addressing criticality limits for fissile materials stored or staged in array configurations regardless of the actual storage arrangement. Information beyond that covered in this section can be found in References 35, 41, and 47. Like the surface density method, this method was derived from experimental and calculated critical data and depicts the number of fissile units or total mass of all the fissile units in a critical, reflected array as a function of the average fissile material density in the array (Reference 41). This method was developed in the 1940s to consider the storage of weapon capsules in various array configurations (Reference 50). This method was modified and improved over the years because of inconsistencies between the subcritical measurements (used to derive relationships between the various array parameters) and critical array experiments performed in the 1960s.

This formulation of the density analog method is also like the surface density method because it, too, depends on knowing the critical dimensions for a water-reflected infinite slab and the bare, spherical critical mass for the fissile material stored in the array. While the surface density method does limit the array dimension in one direction, there is no such limitation in the density analog method. The density analog method provides a fissile array unit spacing that results in a subcritical arrangement without any limitations to the size or shape of the array. In addition to critical conditions for a water-reflected infinite slab and the bare, spherical critical mass of the fissile material being stored in the array, the mass of the individual units, the number of units in the array, and their unit-to-unit spacing are the key parameters needed to apply the method.

As was the case for the surface density method, the Thomas formulation of the density analog method (Reference 35) was derived from limiting surface density relationships (Reference 39, 44, and 45). The method applies to individual units having a maximum effective multiplication factor, *keff*, of 0.9, which corresponds to a fraction critical mass of 0.73 for unreflected spherical array units (Section 7.3.1).

Up to and including equation 8.8, the derivation is the same as given in Chapter 8 for the Surface Density Method. Equation 8.8 is repeated here as the beginning of the rest of the derivation of the Density Analog Method.

$$\sigma(m) = c_2 m_0 (1 - 1.37f). \tag{139}$$

As before, the factor of 1.37 precludes the array from achieving criticality for large array units (i.e., unit $k_{eff} \leq 0.9$).

Now $c_2 m_0$ is determined as the product of two factors: one is for the shape of the array, and the second is for the reflector material surrounding the array. For density Analog, the coefficient is 2.1 σ_0 rather than 0.54 σ_0 as found in the Surface Density Method. The difference being that for surface density, the array is a limited series of "infinite" planar arrays while the shape can be anything form cubic to single planar for density analog. The 2.1 σ_0

$$\sigma(m) = 2.1\sigma_0(1 - 1.37f). \tag{140}$$

From equation 8.5, *d* as the center-to-center spacing is given as a function of the number of units in the finite direction, *n*, the array unit mass, *m*, and the limiting value of the surface density for the array, σ, which is dependent upon the material characteristics of the array:

$$d = \sqrt{\frac{nm}{\sigma(m)}} \tag{141}$$

For Density Analog, $n = N^{1/3}$ as the cubic array is the most reactive configuration. Inserting the definition of $\sigma(m)$ from equation 9.2 into equation 9.3 gives;

$$d = \sqrt{\frac{\sqrt[3]{N}m}{2.1\sigma_0(1 - 1.37f)}} \tag{142}$$

Equation 9.4 is like equation 4.8 in Reference 35. Each of the variables for *d* is defined below for Thomas' representation of the density analog method (Reference 35):

σ_0 – the surface density of the water-reflected infinite slab (g/cm^2);
f – the ratio of the mass of a unit in the array to the critical mass of the unreflected sphere of the same fissile material (**must not exceed 0.73 for this method to be applicable**);
N – the total number of fissile material units in the array; and
m – the fissile material mass per array unit (g).

This equation can be used to determine the subcritical limits for array configurations for any shape reflected by at least 20 cm-thick water. (Reference 35). A relationship for the number of units as a function of unit cell array volume is derived as follows. Starting with equation 9.4 and raising both sides of the equation to the 3rd power.

$$(d^2)^3 = \left[\frac{nm}{\sigma_0(1 - 1.37f)}\right]^3. \tag{143}$$

Substitute the definitions for the array unit volume, $V = d^3$, and the number of units in the array, N:

$$V^2 = N\left[\frac{m}{\sigma_0(1 - 1.37f)}\right]^3. \tag{144}$$

Solving equation 9.6 for N:

$$N = \left[\frac{\sigma_0(1 - 1.37f)}{m}\right]^3 V^2. \tag{145}$$

This is like equation 4.7 in Reference 35.

9.3   APPLICABILITY OF THE DENSITY ANALOG METHOD

The density analog method can be used for a variety of fissile materials and array configurations. This method is applicable for the following situations:

- infinite planar arrays reflected by water at least 200 mm thick or its nuclear equivalent (Reference 35). Guidance for applying this method with arrays located next to concrete reflectors can be found in Reference 41;

- situations where the fissile units have irregular geometries such as when equipment that contains fissile materials is stored on a process floor, for example (Reference 14). This method is useful for this situation, because the surface density of an infinite, water-reflected slab bounds the mass of each fissile unit in the array;

- Perturbations in the reflector materials, array unit shape and array shape are discussed in greater detail in References 35 and 41. The example problems consider arrays with water reflection only; and.

- While the surface density method can be used for square or cubic arrays, the density analog method can be used for arrays that have any shape.

9.4   DENSITY ANALOG METHOD EXAMPLE PROBLEMS

The following example problems illustrate the use of the density analog method. The first three example problems used to demonstrate the use of the surface density method are also used to demonstrate the use of the density analog method. This will allow a direct comparison of both methods.

9.4.1   Density Analog Example Problem 1

Using the density analog method, repeat the example problem in Section 8.4.1 for 2×2×2, 4×4×4, 10×10×10, and 100×100×100 arrays and compare the results. Recall that each unit of the array contains a 2-liter bottle of Pu(5) solution with a maximum concentration of 400 gPu/l.
From the example problem in Section 8.4.1, the values of σ_o and f are the same, because the system has not changed; the only change is in the method used to calculate the center-to-center spacing between units. So, the values of σ_o and f are summarized below.

$$\sigma_0 = 2.80 \frac{gPu}{cm^2}$$

$$f = 0.087$$

Knowing σ_o and f, the center-to-center spacing using the density analog method can be determined as follows.

Analysis of all four array configurations starts with equation 9.4:

$$d = \sqrt{\frac{\sqrt[3]{N}m}{2.1\sigma_0(1 - 1.37f)}}$$

For the smallest array, $2 \times 2 \times 2$ (8 units):

$$d = \sqrt{\frac{\sqrt[3]{8} \times\ 800 \text{ g Pu}}{2.1 \times 2.80\ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.087)}} = 17.6 \text{ cm (6.9 in.)}$$

For the next array, $4 \times 4 \times 4$ (64 units):

$$d = \sqrt{\frac{\sqrt[3]{64} \times\ 800 \text{ g Pu}}{2.1 \times 2.80\ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.087)}} = 24.9 \text{ cm (9.8 in.)}$$

For the middle-size array, $10 \times 10 \times 10$ (1,000 units):

$$d = \sqrt{\frac{\sqrt[3]{1000} \times\ 800 \text{ g Pu}}{2.1 \times 2.80\ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.087)}} = 39.3 \text{ cm (15.5 in.)}$$

For the largest array, $100 \times 100 \times 100$ (1,000,000 units):

$$d = \sqrt{\frac{\sqrt[3]{1,000,000} \times\ 800 \text{ g Pu}}{2.1 \times 2.80\ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.087)}} = 124.3 \text{ cm (48.9 in.)}$$

In Section 8.4.1, the surface density method provides a center-to-center spacing between fissile units of about 25 cm (9.8 in.). This is for an infinite number of Pu solution bottles in a planar array that is limited one unit high with no stacking. In contrast, the density analog results for the $2 \times 2 \times 2$, $4 \times 4 \times 4$, $10 \times 10 \times 10$, and $100 \times 100 \times 100$ arrays demonstrate that, as one would expect, the center-to-center spacing would increase as the array got taller indicating the array is more reactive as the number of units in the z-direction increases. The density analog method is more applicable to finite arrays that contain stacked fissile units. The array calculations above bound 8, 1,000 and 1,000,000 units for the $2 \times 2 \times 2$, $4 \times 4 \times 4$, $10 \times 10 \times 10$, and $100 \times 100 \times 100$ arrays respectively. For any number of units in the z-direction less than the number in a cubic array, the density analog calculated spacing for the cubic array will be adequate. If, for example, there were 500 solution bottles stacked in a $10 \times 10 \times 5$ array configuration, the calculated spacing, 39.8 cm (15.7 in.) for the $10 \times 10 \times 10$ array would provide adequate spacing for the units in the array.

9.4.2   Density Analog Example Problem 2

Using the density analog method, repeat example problem in Section 8.4.2 for $2 \times 2 \times 2$, $4 \times 4 \times 4$, $10 \times 10 \times 10$, and $100 \times 100 \times 100$ arrays. Recall that each container in the array contains Plutonium Oxide ($^{239}\text{PuO}_2$) loaded with up to 4,500 grams of Pu.

From the example problem in Section 8.4.2, the values of σ_o and f are the same, because the system has not changed; only the method used to calculate the center-to-center spacing between units has changed. So, the values of σ_o and f are summarized below:

$$\sigma_0 = 18.37 \frac{gPu}{cm^2}$$

$$f = 0.191.$$

Knowing σ_o and f, the center-to-center spacing using the density analog method can be determined as follows. Again, start with the density analog relationship equation 9.4:

$$d = \sqrt{\frac{\sqrt[3]{N}m}{2.1\sigma_0(1 - 1.37f)}}$$

For the $2 \times 2 \times 2$ array:

$$d = \sqrt{\frac{\sqrt[3]{8} \times 4,500 \text{ g Pu}}{2.1 \times 18.37 \frac{\text{g Pu}}{cm^2}(1 - 1.37 \times 0.191)}} = 17.8 \text{ cm (7.0 in.)}$$

For the $4 \times 4 \times 4$, array:

$$d = \sqrt{\frac{\sqrt[3]{64} \times 4,500 \text{ g Pu}}{2.1 \times 18.37 \frac{\text{g Pu}}{cm^2}(1 - 1.37 \times 0.191)}} = 25.1 \text{ cm (9.9 in.)}$$

For the $10 \times 10 \times 10$ array:

$$d = \sqrt{\frac{\sqrt[3]{1,000} \times 4,500 \text{ g Pu}}{2.1 \times 18.37 \frac{\text{g Pu}}{cm^2}(1 - 1.37 \times 0.191)}} = 39.7 \text{ cm (15.6 in.)}$$

For the $100 \times 100 \times 100$ array:

$$d = \sqrt{\frac{\sqrt[3]{1,000,000} \times 4,500 \text{ g Pu}}{2.1 \times 18.37 \frac{\text{g Pu}}{cm^2}(1 - 1.37 \times 0.191)}} = 125.7 \text{ cm (49.5 in.)}$$

Consider a situation in a fissile material storage area where 1,000 Pu oxide containers are stored in a 50 × 20 × 1 array. The density analog method for this example recommends a spacing of 39.7 cm (~15.6 in.) for 1,000 units arranged in a 10 × 10 × 10 array. This result would bound the 50 × 20 × 1 array because 1,000 units in a cubic array (10 × 10 × 10) is the most reactive array configuration. Spreading the 1,000 units out in any other configuration is less reactive than the 10 × 10 × 10 configuration. Therefore, the recommended spacing as calculated by the density analog method would be sufficient to maintain a subcritical arrangement under normal operating conditions.

The surface density method for the same problem results in a center-to-center spacing of 26.6 cm (10.5 in.) for an ∞ × ∞ × 1 array. If an administrative or engineered control is put into place to prevent the stacking of containers, then this method allows a much closer spacing (about 13 cm {5 in.} closer) than the density analog recommended spacing. The following conditions could affect which method to consider:

- Available spacing in the facility, and
- Issues related to implementing a control on the stack height permitted in the storage array.

9.4.3 Density Analog Example Problem 3

Using the density analog method, repeat the example problem in Section 8.4.3 (Surface Density Example Problem 3) for $2 \times 2 \times 2$, $4 \times 4 \times 4$, $10 \times 10 \times 10$, and $100 \times 100 \times 100$ arrays. Recall that each fissile unit in the array is a 4,500 g alpha-phase Pu(5) metal ingot.

From the example problem in Section 8.4.3, the values of σ_o and f are the same, because the system has not changed; only the method used to calculate the center-to-center spacing between units has changed. So, the values of σ_o and f are summarized below:

$$\sigma_0 = 16.20 \ \frac{gPu}{cm^2}$$

$$f = 0.437.$$

Knowing σ_o and f, the center-to-center spacing using the density analog method can be determined as follows. Again, start with the density analog relationship equation 9.4:

$$d = \sqrt{\frac{\sqrt[3]{Nm}}{2.1\sigma_0(1 - 1.37f)}}$$

For the $2 \times 2 \times 2$ array:

$$d = \sqrt{\frac{\sqrt[3]{8} \times 4{,}500 \text{ g Pu}}{2.1 \times 16.20 \ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.437)}} = 25.7 \text{ cm (10.1 in.)}$$

For the $4 \times 4 \times 4$, array:

$$d = \sqrt{\frac{\sqrt[3]{64} \times 4{,}500 \text{ g Pu}}{2.1 \times 16.20 \ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.437)}} = 36.3 \text{ cm (14.3 in.)}$$

For the $10 \times 10 \times 10$ array:

$$d = \sqrt{\frac{\sqrt[3]{1{,}000} \times 4{,}500 \text{ g Pu}}{2.1 \times 16.20 \ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.437)}} = 57.4 \text{ cm (22.6 in.)}$$

For the $100 \times 100 \times 100$ array:

$$d = \sqrt{\frac{\sqrt[3]{1{,}000{,}000} \times 4{,}500 \text{ g Pu}}{2.1 \times 16.20 \ \frac{\text{g Pu}}{\text{cm}^2}(1 - 1.37 \times 0.437)}} = 181.6 \text{ cm (71.5 in.)}$$

The results from Section 6.4.3 for a 100 × 100 × 100 subcritical array is 182 cm (~72 in.). Because of the safety margin that is incorporated into the method, the density analog method will provide a larger center-to-center spacing between array units than the limiting surface density method. A critical array unit spacing result from the limiting surface density method is not the most practical guidance to implement. However, the k_{eff} relationships in Section 7.3.1 can be used to determine the array unit mass for a desired multiplication factor.

As one would expect, the Pu metal ingots require more spacing (i.e., 57.4 cm (~22.6 in.) for a 10x10x10 array) than the Pu solution bottles in Section 9.4.1 (i.e., 39.3 cm (~15.5 in. for a 10x10x10 array) or the Pu oxide containers in Section 9.4.2 spacing (i.e., 39.7 cm (~15.6 in. for a 10x10x10 array) because of the higher fissile mass that is present.

Also, the surface density method for the same problem (Section 8.4.3) results in a center-to-center spacing of 36.0 cm (14.2 in.) for an $(\infty \times \infty \times 1)$ array. If an administrative or engineered control is put into place to prevent the stacking of containers, then the surface density method allows a much closer spacing, more than 21.4 cm (8.4 in.) closer, than the density analog recommended spacing for a $10 \times 10 \times 10$ array. Again, the array hand calculation method to use for a particular problem depends upon the situation. If you can limit the stacking for a given array, then the Surface Density Method will provide a closer spacing than the Density Analog Method. However, if you have a limited number of containers or a limited floor space, then the Density Analog Method will likely be more applicable.

9.4.4 Density Analog Example Problem 4

Using the Density Analog Method, analyze the situation given in Section 6.4.4. That is, calculate the safe spacing for a 10-unit array of 10-inch diameter cylinders (schedule 20 pipe) each 6 feet long on a square lattice pattern in two rows of five. The cylinders are to contain 4.98% enriched uranyl fluoride of maximum 3.2 g U/cm³ concentration. From ORNL data[29] (Reference 38), a bare stainless steel cylinder of U(4.98)O$_2$F$_2$ solution was critical with a radius of 19.55 cm and a height of 101.7 cm.
The first step in the solution for this problem is to calculate the value of f, the ratio of the mass of a unit in the array to the critical mass of an unreflected sphere of the same material, and the surface density of a water-reflected infinite slab, σ_o.

Because the units to be stored are cylinders with an h/d = 7.2, and the critical information is given for cylinders with an h/d = 2.6, we need to do buckling conversions to convert each cylinder to an equivalent spherical geometry.

Recall that the geometric buckling for a cylinder is:

$$B_g^2 = \left[\frac{2.405}{R_{cyl} + d}\right]^2 + \left[\frac{\pi}{H + 2d}\right]^2.$$

Now to calculate the material buckling from the experimental information and use an extrapolation distance, d, of 2.1 cm from Figure 9-1, the buckling at critical (i.e., material buckling) is:

---

[29] The experiment had an H/X of 496, a U-235 concentration of 0.04487 g 235/ cm³, a uranium concentration of 0.901 g U/ cm³, and a solution density of 2.020 g/cm³.

$$B_g^2 = \left(\frac{2.405}{r+d}\right)^2 + \left(\frac{\pi}{L+2d}\right)^2,$$

$$B_g^2 = \left(\frac{2.405}{19.55\ cm + 2.1\ cm}\right)^2 + \left(\frac{\pi}{101.7\ cm + 2 \times 2.1\ cm}\right)^2 = 0.01322\ cm^{-2}.$$
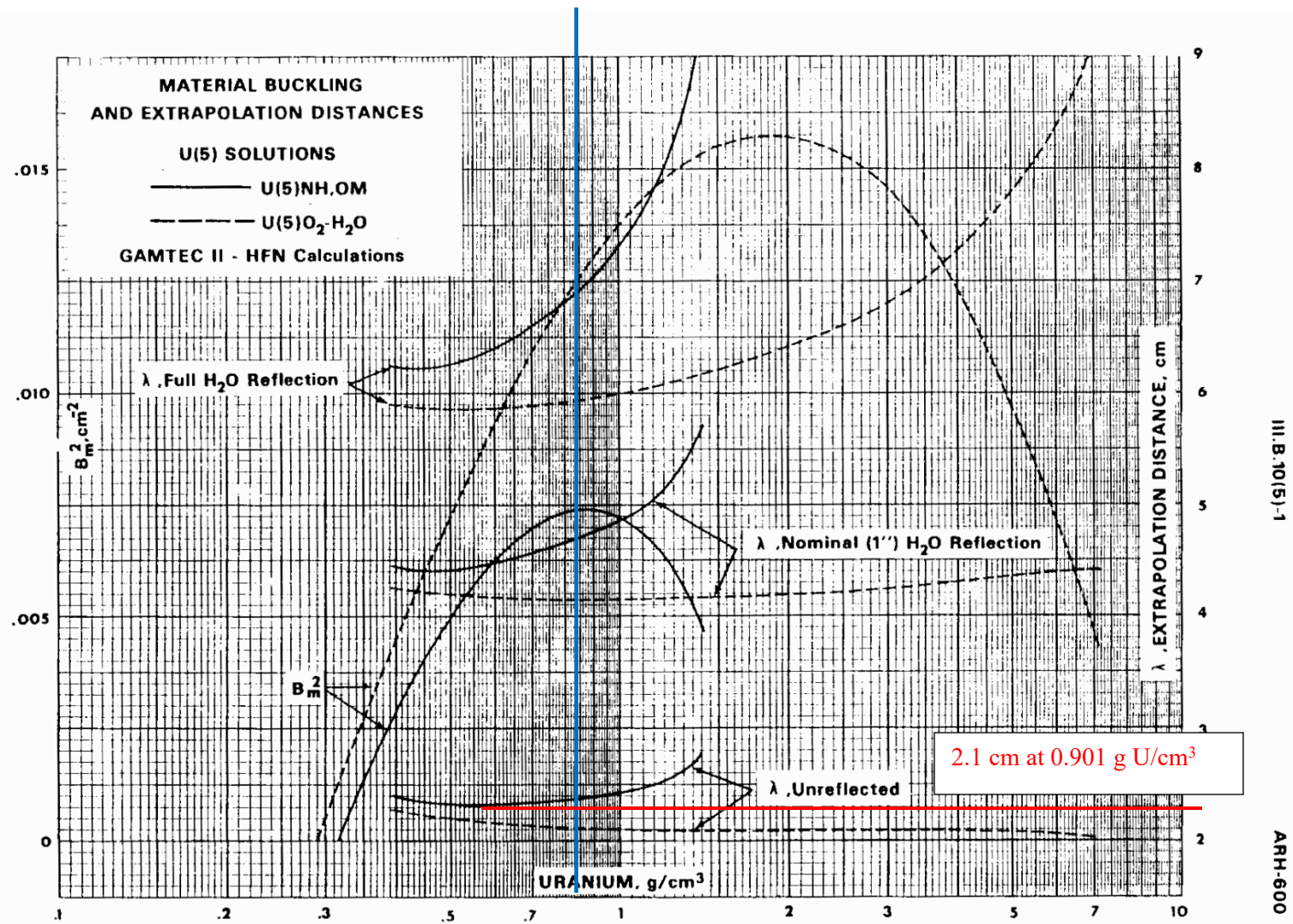
Figure 9-1. Extrapolation Distance Data for U(5)O₂-H₂O System. (Reference 7, Figure III.B.10(5)-1).

Now calculate the radius of a sphere with the same buckling.

$$\left[\frac{\pi}{R_{sph}+d}\right]^2 = \left[\frac{2.405}{R_{cyl}+d}\right]^2 + \left[\frac{\pi}{H+2d}\right]^2 = 0.01322 \text{ cm}^{-2}$$

Solving the equation for R_{sph}:

$$\left[\frac{\pi}{R_{sph}+2.1 \text{ cm}}\right]^2 = 0.01322 \text{ cm}^{-2} \Rightarrow R_{sph} = 25.22 \text{ cm}$$

For 10-inch diameter, schedule 20 pipe, the inside diameter is 10.25 inches and the wall thickness is 0.25 inch, which gives an outside diameter of 10.75 inches. Then, the solution cylinder dimensions are:

$$r = \frac{10.25 \text{ } inches}{2} \times \frac{2.54 \text{ } cm}{inch} = 13.0175 \text{ } cm$$

$$L = 6 \text{ } ft \times \frac{12 \text{ } inches}{ft} \times \frac{2.54 \text{ } cm}{inch} = 182.88 \text{ } cm$$

Substitute these values into the geometric buckling relationship for a finite cylinder and using the same extrapolation distance of 2.1 cm from Figure 9-1:

$$B_g^2 = \left(\frac{2.405}{r+d}\right)^2 + \left(\frac{\pi}{L+2d}\right)^2,$$

$$B_g^2 = \left(\frac{2.405}{13.0175 \text{ } cm + 2.1 \text{ } cm}\right)^2 + \left(\frac{\pi}{182.88 \text{ } cm + 2 \times 2.1 \text{ } cm}\right)^2 = 0.02559 \text{ } cm^{-2}.$$

Now calculate the radius of a sphere with the same buckling.

$$\left[\frac{\pi}{R_{sph}+d}\right]^2 = \left[\frac{2.405}{R_{cyl}+d}\right]^2 + \left[\frac{\pi}{H+2d}\right]^2 = 0.02559 \text{ cm}^{-2}$$

Solving the equation for R_{sph}:

$$\left[\frac{\pi}{R_{sph}+2.1 \text{ cm}}\right]^2 = 0.02559 \text{ cm}^{-2} \Rightarrow R_{sph} = 17.54 \text{ cm}$$

To compute fraction critical, we can take the ratios of the equivalent spherical volumes.

$$V_{sphere} = \frac{4}{3}\pi r^3 \quad \text{for r } = 17.54 \text{ cm}, \text{V } = 22.604 \text{ liters}$$

$$\text{for r}_{crit} = 25.22 \text{ cm}, \text{V}_{crit} = 67.193 \text{ liters}.$$

$$\text{So } f = \frac{V}{V_{crit}} = \frac{22.604 \text{ liters}}{67.193 \text{ liters}} = 0.3364$$

The value of s_0 can be determined by taking the product of the slab height of an infinite, water-reflected slab and the ^{235}U concentration. The water-reflected, infinite slab thickness for a U(5)O$_2$F$_2$ solution system (3.2 g U/cm^3 = 0.16 g U235/ cm^3) can be estimated from Figure 9-2 as 5 in. or 12.7 cm.

$$\sigma_0 = 12.7 \text{ cm} \times 0.16 \frac{\text{g U235}}{\text{cm}^3} = 2.032 \frac{\text{g U235}}{\text{cm}^2}$$

The volume of each solution cylinder is:

$$V_{cyl} = \pi r_{cyl} h_{cyl} = \pi \times (13.0175 \text{ cm})^2 \times 182.88 \text{ cm} = 97.36 \text{ liters}$$

The mass of ^{235}U in each bottle of solution is:

$$m_{cyl} = \frac{97.36 \text{ L}}{\text{cyl}} \times 0.16 \frac{\text{g U235}}{\text{cm}^3} \times \frac{1000 \text{ cm}^3}{L} = 15,577 \frac{\text{g U235}}{\text{cyl}}$$

So, the values of f, σ_o, and m are summarized below:

$$f = 0.3364$$

$$\sigma_0 = 2.032 \frac{\text{g U235}}{\text{cm}^2}$$

$$m = 15,577 \frac{\text{g U235}}{\text{cyl}}$$
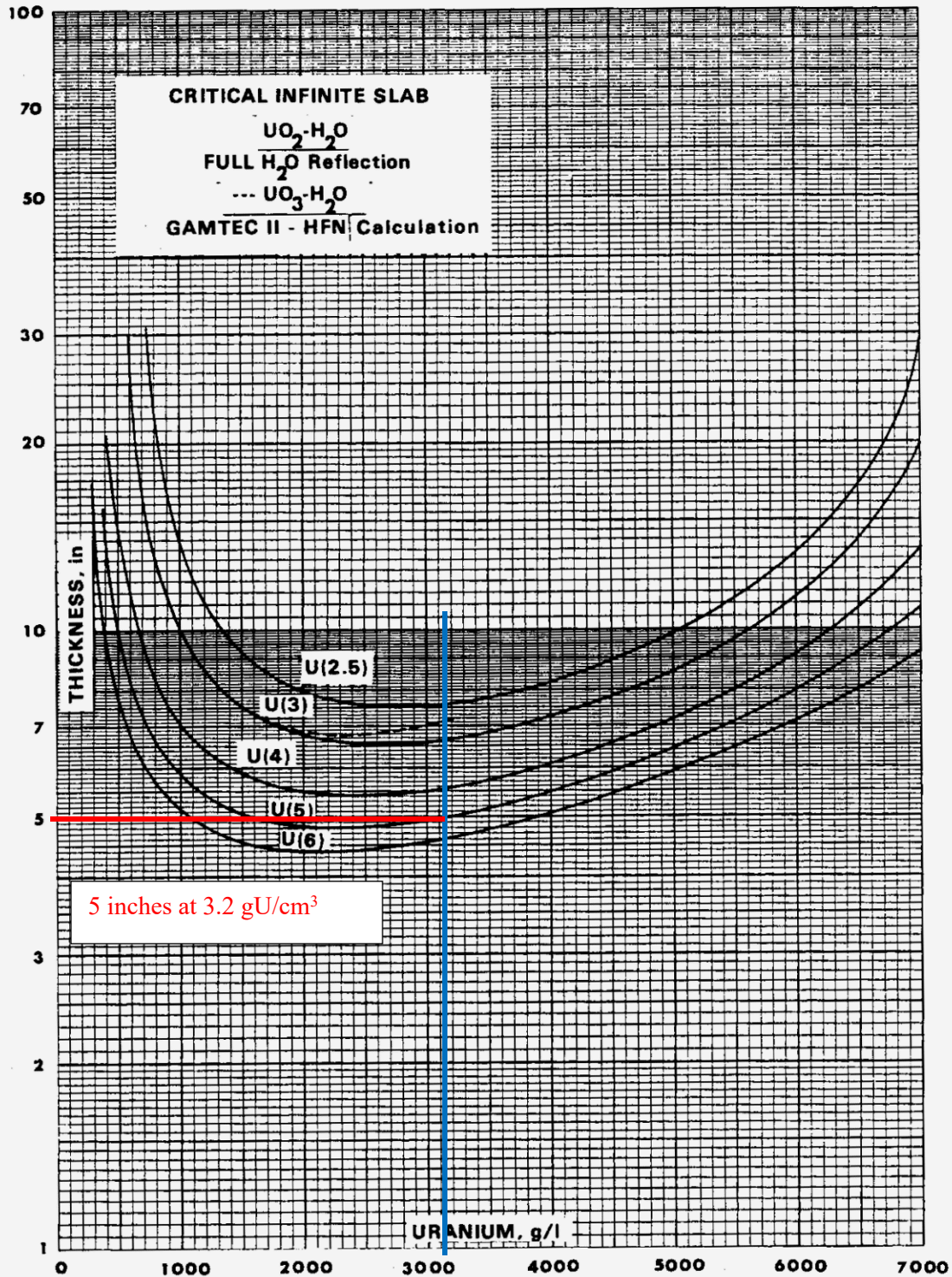
Figure 9-2. Critical Slab Thickness for U(5)O₂-H₂O System. (Reference 7, Figure III.B.5-6)

Knowing N, m, σ_o, and f, the center-to-center spacing using the density analog method can be determined using the density analog relationship equation 9.4:

$$d = \sqrt{\frac{\sqrt[3]{Nm}}{2.1\sigma_0(1 - 1.37f)}}$$

$$d = \sqrt{\frac{\sqrt[3]{10} \times 15{,}577 \text{ g U235}}{2.1 \times 2.032 \frac{\text{g U235}}{\text{cm}^2}(1 - 1.37 \times 0.3364)}} = 120.8 \text{ cm (47.6 in.)}$$

As this is the same situation as for Solid Angle Example Problem 4 (6.4.4) and Surface Density Example Problem 5 (8.4.5), we can compare the results for the three methods.

A review of Table 9-1 indicates that all three methods produce very similar values for this problem.

Table 9-1. Comparison of Results from Three Different Methods,

Method	Assumptions	Center-to Center Spacing (cm)
Solid Angle	$k_{eff} = 0.796$	142.2 cm (56 in.)
	$k_{eff} = 0.757$	120.0 cm (47.25 in.)
Smeared Thickness	$t_{safe} \leq 0.5 \times t_c$	123.8 cm (48.7 in.)
Density Analog	$f = 0.3364$	120.8 cm (47.6 in.)

10. ESTABLISHING CONFIDENCE IN HAND CALCULATIONAL METHODS

10.1 SUMMARY OF HAND CALCULATIONAL RESULTS

This section summarizes the results of each of the preceding example problems and compare them with experimental data, actual dimensions, MCNP or KENO calculations, or a criticality safety handbook. The following sections break out the results and comparisons for each single unit and array method. This information can also be useful in some cases for the analyst to determine which method may be applicable to support criticality safety analyses for fissile material operations.

10.2 CONFIDENCE IN SINGLE UNIT HAND CALCULATIONS

The example problem results presented in Sections 2 through 4 along with the corresponding comparison results are summarized in Table 10-1, Table 10-2, and Table 10-3.

Table 10-1. One-Group and Modified One-Group Diffusion Theory Confidence Comparison.

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
2.6.1	Godiva U(93.5) metal, (ρ = 18.74 g/cm³) unreflected system. One-group diffusion theory, estimate the spherical critical radius.	8.44 cm	8.6 cm (actual) 8.87 cm PARTISN 8.79 cm SCALE 6.1.3
2.6.2	Jezebel delta-phase plutonium, (ρ = 15.61 g/cm³) unreflected system. One-group diffusion theory, estimate the spherical critical radius. Spherical Critical Radius with pure Pu-239 Spherical Critical Radius with Pu(4.5) and Ga and collapsed cross sections	6.93 cm 6.64 cm	6.385 cm (actual) 6.391 cm PARTISN 6.39 cm SCALE 6.1.3
2.6.3	²³⁹PuO₂ with a density of 1, 3, 5, 7, 9, and 11.46 g/cm³. One-group diffusion theory, critical, bare, spherical mass.	11.46 g/cm³ – 31 kg	11.46 g/cm³ – 27.0 kg PARTISN 11.46 g/cm³ – 27.8 kg SCALE Hand calc values about 12% greater than computer in all cases.
2.6.4	Slab tank ²³⁹Pu - H₂O at 0.1 g Pu239/cm³ Modified one-group diffusion theory, estimate the critical slab thickness.	13.12 cm	5.6 in (14.2 cm) Ref. 7 Figure III.A.5.2 14.1 cm PARTISN 13.8 cm SCALE 6.1.3
2.6.5	Fully enriched uranyl sulfate (UO₂SO₄) with a concentration of 30 g ²³⁵U/l (0.03 g/cm³). Modified one-group diffusion theory, estimate the critical infinite cylindrical tank radius. Repeat for U(14.7)O₂SO₄ at 0.03 gU235/cm³.	17.36 cm 19.16 cm	17.60 cm, PARTISN 17.52 cm SCALE 19.61 cm PARTISN 19.55 cm SCALE

Table 10-1. One-Group and Modified One-Group Diffusion Theory Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
2.6.6	U(5)O2 – H2O at 0.05 g U235 / cm3. Modified one-group diffusion theory, estimate critical spherical radius for bare system. Repeat for a system reflected with 30 cm of water.	24.4 cm 21.55 cm Based on reflector savings	24.77 cm, Ref. 7 ARH-600, Fig. III.B.3-4 24.30 cm, PARTISN 24.39 cm SCALE 21.56 cm, Ref. 11 LA-10860, Fig. 15 20.44 cm, PARTISN 20.57 cm SCALE

Conclusions from Comparisons in Table 10-1.

Based on the results shown in Table 10-1, one-group diffusion theory works well in calculations for fissile metal systems or dry (H/X < 20) fissile oxide systems. The accuracy of the calculations is quite dependent on the cross sections used. Those tabulated in Section 2 work quite well for uranium systems, but they tended to overpredict absorption in plutonium systems. A collapsed set of plutonium cross sections is provided in Table 2-6 and used in Example Problem 2. These reduced the difference between the hand calculated value and the actual Jezebel radius.

For systems with moderators, typically solutions, it was demonstrated that one-group diffusion theory was insufficient and not applicable. The application of modified one-group theory provided results sufficient for scoping or bounding studies of bare and reflected systems. Although one-group and modified one-group diffusion theory calculations take significant time, it is suggested this be done for new systems due to the significant physical insight that is gained from these analyses.

Table 10-2. Buckling Conversion Confidence Comparison.

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
3.5.1	ICPP Process Accident 1978, volume of 315.5 liters uranyl nitrate solution {U(82)O$_2$(NO$_3$)$_2$} in bare cylinder with *H/D*=1.75 and a mass of 6.08 kg U-235. Use buckling conversion to determine the equivalent spherical mass involved in the accident	4.41 kg	4.34 kg, Table 9, pg. 58. Reference 6. 4.38 kg PARTISN 4.39 kg SCALE

Table 10-2. Buckling Conversion Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
3.5.2	Pu(5) metal – water mixture at 20 g Pu(5) / liter: 1. Buckling conversion for water-reflected, critical radius for a cylindrical tank with height = 20 cm.	r_{crit} = 31.1 cm	28.1 cm PARTISN 28.8 cm SCALE
	2. Buckling Conversion for water-reflected, infinite cylinder radius	r_∞ = 14.24 cm	13.79 cm PARTISN 14.02 cm SCALE
	3. Fractional Leakage bare cylinder, r=42.9 cm, H=25 cm.	radial = 0.20 axial = 0.80	Radial = 0.204 Axial = 0.796 (From PARTISN)
	4. Water-reflected, critical height for a cylindrical tank with radius = 15 cm.	h_{crit} = 38.3 cm	34.2 cm PARTISN 34.8 cm SCALE
	5. Water-reflected, critical height for a cylindrical tank with a 15 cm diameter cylinder.	subcritical	subcritical
3.5.3	Unreflected, deep well of Pu(5) metal-water solution with concentration of 200 gPu/l .	17.38 cm	16.99 cm PARTISN 17.29 cm SCALE
	Buckling conversion for critical spherical radius	18.32 cm	17.69 cm PARTISN 18.25 cm SCALE
	Buckling conversion for critical solution height in deep well, 129.54 cm in length, 35.56 cm in width..		
3.5.4	Two cylindrical, unfavorable geometry tanks: one filled with a U(93.5)-water mixture while the second tank is filled with a Pu(5) metal-water mixture. 1. Determine critical solution height for each fissile material at a fissile concentration of 100 gX/l.	**100 g/l: (U)** H=18.1 cm **100 g/l: (Pu)** H=19.2 cm	**100 g/l:PARTISN** H≈18.15 cm (U) H≈18.78 cm (Pu) **100 g/l:SCALE** H≈17.63 cm (U) H≈19.00 cm (Pu)
	2. Determine the critical solution height for each fissile material with a concentration of 150 gX/l.	**150 g/l: (U)** H=16.7 cm **150 g/l: (Pu)** H=19.0 cm	**150 g/l:PARTISN** H≈16.89 cm (U) H≈18.78 cm (Pu) **150 g/l:SCALE** H≈16.40 cm (U) H≈18.77 cm (Pu)
	3. Determine the critical solution height for each fissile material with a concentration of 50 gX/l.	**50 g/l: (U)** H=23.3 cm **50 g/l: (Pu)** H=21.1 cm	**50 g/l:PARTISN** H≈22.84 cm (U) H≈20.66 cm (Pu) **50 g/l:SCALE** H≈22.30 cm (U) H≈20.60 cm (Pu)

Table 10-2. Buckling Conversion Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
3.5.5	U(93.5)-water mixture at 100 g fissile/liter. Parametric study on *H/D* for an unreflected cylinder. Use *H/D* values of ∞, 10, 5, 2, 1, 0,9238, 0.7, 0.5, 0.25, and 0 (i.e., infinite slab thickness). See Table 3-3 in text for results and comparison with PARTISN values.	H/D = 1 Radius = 15.2 cm Height = 30.4 cm	H/D = 1 Radius = 15.5 cm Height = 31.0 cm PARTISN
3.5.6	Discussion of surface area change in Mayak 1958 process accident.	See text	No Calculations

Conclusions from Comparisons in Table 10-2.

Based on the results shown in Table 10-2, buckling conversion provides a reasonably accurate method of examining the effect of geometry change on system behavior. The first example problem in section 3.5.1 provides the equivalent spherical critical mass for the configuration involved in the 1978 ICPP accident. This allows one to compare that value with critical mass graphs as found in Reference 11 to see how much excess reactivity might be involved for a given fissile solution in a given geometry.

The second example problem in section 3.5.2 evaluates different geometries and associated leakage fractions for a Pu(5) metal-water mixture. The values rom buckling conversion are higher than those obtained from the computer calculations. In this case, it seems that the starting point from ARH-600, Reference 7 seems to be slightly higher than actual. As all the buckling conversion process is related to the starting condition, this causes the dimensions to be slightly larger than actual. However, it should be noted that estimates of axial and radial leakage fractions are quite close to those calculated in the computer analyses. For the higher concentration Pu(50 metal-water mixture in section 3.5.3, the buckling conversion values are quite close to those calculated by SCALE. PARTISN with the Hansen-Roach cross section set seems to slightly overpredict absorption for these under moderated systems (H/X about 125, while optimum moderation has an H/X of about 880).

Example problem 4 examines systems with U(93.5) and Pu(5) solutions. The values from buckling conversion are quite close to those determined by neutron transport calculations. The important take-away from this problem is that at the same fissile concentration, plutonium solutions are not always more reactive than uranium solutions. Example problem 5 in section 3.5.5 shows that the results of a buckling conversion parametric study on cylinder H/D from an infinite cylinder to an infinite slab produces similar results to those from computer calculations.

The last example problem provides a description of the effect of change in surface area and geometric buckling as solution in a large container is tipped to be poured. Although not a direct application of buckling conversion, it does show how a significant change in geometry and associated leakage area can lead to an upset condition. This illuminates how buckling conversion can be used to examine effects of geometry changes in process systems.

Table 10-3. Core-Density Method Confidence Comparison.

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
4.4.1	Pu(4.5) metal system. Calculate critical spherical, unreflected mass as changed from delta phase (15.6 g/cm^3) to alpha phase with a density of 19.8 g/cm^3.	10.43 kg Or 10.61 kg	10.4 kg (Ref. 7, Fig. III.A.6-2)
4.4.2	U(93.5) metal-H_2O system. Calculate critical spherical, unreflected mass as changed to a density of 10.0 g/cm^3 from an initial density of 18.9 g/cm^3.	15.14 cm	10.46 cm (Ref. 7, Fig. III.B.9(93.5)-2)
4.4.3	U(92.94)O_2 powder system. Calculate the critical radius for a spherical, unreflected system with a density of 6 g/cm^3, assuming that the initial density for this system was 10.845 g/cm^3.	29.65 cm	29.62 cm PARTISN
4.5.4	For $^{239}PuO_2$ system: calculate the critical mass for s spherical, unreflected systems (examine densities of 1, 3, 5, 7, and 9 g/cm^3, assuming that the initial density for this system was 11.46 g/cm^3. Compare the results to the results calculated in Section 2.6.3 (Diffusion Theory Example Problem 3).	1 g/cm^3 – 4080 kg 3 g/cm^3 – 453 kg 5 g/cm^3 – 163 kg 7 g/cm^3 – 83 kg 9 g/cm^3 – 50 kg 11.46 g/cm^3 – 32 kg	Results are essentially the same as the critical mass estimates from Section 2.6.3.
4.5.5	U(93.5)O_2 water-reflected. Calculate the spherical critical mass for a density of 5.0 g/cm^3 if the oxide had an initial density of 10.85 g/cm^3.	162.4 kg	162.4 kg PARTISN
4.5.6	Pu(5) metal system, water-reflected. Calculate spherical critical mass for a density of 15.61 g/cm^3 and for 19.8 g/cm^3.	8.31 kg	8.24 kg PARTISN 8.17 8.30kg SCALE 6.1.3
	Repeat for a density of 19.8 g/cm^3 from a density of 15.61 g/cm^3	5.88 kg	5.76 kg PARTISN 8.17 5.79kg SCALE 6.1.3

Conclusions from Comparisons in Table 10-3.

First, in section 4.4.2, the comparison of critical, spherical unreflected radius with the handbook data shows a significant discrepancy. This is indicative of the misapplication of core density conversions to systems containing hydrogen, which changes the neutron spectrum. In the Core Density Conversion method, changes in material density are assumed to have little impact on the neutron energy spectrum. However, in systems with hydrogen, this assumption is usually not correct. This example problem illustrates the importance of checking all calculations with other methods or published data.

In example 1, section 4.5.1, the comparison results indicate the applicability of the method to plutonium metal systems. In example 3, section 4.5.3, the closeness of the values indicates that for uranium oxide systems, the core-density conversion process is applicable and provides useful results.

For plutonium oxide as in section 4.5.4, the values are self-consistent depending on the value of the initial critical mass. This indicates applicability of the core density conversion method to plutonium oxide systems.

Sections 4.5.5 and 4.5.6 involve water-reflected systems, which rely on determination of the functional exponent. For the oxide problem, the calculated critical mass was right on the value determined by PARTISN, while for the plutonium metal system, the calculated value was about 1.5% higher than that determined from a SCALE calculation. This indicates that the Core Density Conversion method can be used for initial scoping calculations with both oxide and metal systems reflected with water.

10.3 CONFIDENCE IN ARRAY HAND CALCULATIONS

The example problem results presented in Sections 6 through 9 along with the corresponding comparison result are summarized in Table 10-4 through Table 10-7.

Table 10-4. Solid Angle Method Confidence Comparison.

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
6.4.1	Calculate the allowable solid angle for a 3×3×1 array of aluminum containers filled with a U(4.89)O_2F_2 and water mixture with a hydrogen-to-^{235}U (H/X) ratio of 524. The pitch is 76.52 cm and edge-to-edge (ETE) spacing is 60.96 cm.	Subcritical	Subcritical Reflected array SCALE 6.1.3 $k_{eff} = 0.6465 \pm 0.0013$
6.4.2	Reexamine the example problem in Section 8.4.1 with array units spaced 30.48 cm ETE, instead of 60.96 cm.	Subcritical	Subcritical Reflected array SCALE 6.1.3 $k_{eff} = 0.6462 \pm 0.0012$

Table 10-4. Solid Angle Method Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
6.4.3	Store plutonium solution (Pu(4)O$_2$) in a 3x3x1 unreflected planar array of 4-liter spherical bottles. The bottles are spaced 1 foot apart under normal conditions in fixed storage locations. The plutonium solution concentration can vary significantly over the range 20 gPu/l to 200 gPu/l. Will this storage arrangement be safe over this concentration range?	Subcritical	Subcritical Reflected array of Pu(4)O$_2$ at 0.20 g Pu/cm^3 SCALE 6.1.3 k_{eff} = 0..8181±0.0013
6.4.4	U(4.98)O$_2$F$_2$ solution in a 5x2x1 square lattice array of 10-inch diameter cylinders (schedule 20 pipe) each 6 feet long. Maximum 3.2 g U/cm^3 concentration. Use the solid angle criterion to estimate a safe spacing for this configuration.	Cylinder k_{eff} = 0.757 120.0 cm 47.25 inches	SCALE 6.13. k_{eff} = 0.7939±0.0013 Bare array SCALE k_{eff} = 0.8475±0.0013 Reflected array
6.4.5	1. Alpha-phase Pu(4.5) metal ingots (*L/D*=1) 4,500 gram units spaced 30 cm apart in a 3x3x1 array. Use the Solid Angle Method to determine acceptable. 2. What if the ingots have an *L/D* = 7; how does that affect the spacing?	Subcritical even with concrete reflection Also, subcritical even with concrete reflection	Subcritical Reflected array SCALE 6.1.3 k_{eff} = 0.6465±0.0013
6.4.6	U(4.98)O$_2$F$_2$ solution along corner wall array of 10-inch diameter cylinders (schedule 20 pipe) each 6 feet long. Maximum 3.2 g U/cm^3 concentration. Use the solid angle criterion to estimate a safe spacing for this configuration.	Edge-to-edge 33.5 inches 85.1 cm	Subcritical Reflected array SCALE 6.1.3 k_{eff} = 0.6462±0.0012

Conclusions from Comparisons in Table 10-4.

The solid angle method produces conservative spacings, which are limited to a minimum of 30 cm edge-to-edge (ETE). In many cases, this may be too conservative for the application, but it provides a good starting point for further analyses with neutron transport codes. Although the solid angle approach may not provide final array dimensions, its use provides significant insight into the physical interactions of units in the array. Comparing solid angles for various array positions will indicate those positions that dominate the neutron interactions among units to provide a first cut at the importance of each array location. This method was developed as a quick, empirical means of evaluating interaction among small

253

numbers of moderated fissile units and provides good information on neutron behavior for such situations.

Table 10-5. Limiting Surface Density Method Confidence Comparison.

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
7.4.1	For 2×2×2, 4x4x4, 10×10×10 and 100×100×100 arrays, what is the minimum center-to-center spacing of plutonium oxide ($^{239}PuO_2$) containers loaded with 4,500 grams of Pu per container? Assume that the Pu oxide density is 11.48 g/cm³, which is the theoretical density for PuO_2, and the Pu is pure ^{239}Pu	2×2×2 Not Applicable 4×4×4 21.4 cm 10×10×10 35.7 cm 100×100×100 114.7 cm	SCALE 6.1.3 4×4×4 20.16 cm, k_{eff} = 1.0006±0.0013 SCALE 6.1.3 10×10×10 34.36 cm, k_{eff} = 1.0007±0.0013
7.4.2	1. Using the limiting surface density method, determine the minimum center-to-center spacing for 4×4×4 and 10×10×10 arrays of 4,500 g Pu(5) metal ingots. 2. Calculate the center-to-center spacing that would give a k_{eff} = 0.8 for a 10x10x10 array of the 4,500 g Pu(5) metal ingots.	4×4×4 25.4 cm 10×10×10 42.4 cm 10×10×10 115 cm	SCALE 6.1.3 4×4×4 25.4 cm, k_{eff} = 0.9993±0.0012 SCALE 6.1.3 10×10×10 42.4 cm, k_{eff} = 0.9999±0.0013 SCALE 6.1.3 10×10×10 142 cm, k_{eff} = 0.8006±0.0012 SCALE 6.1.3 10×10×10 115 cm, k_{eff} = 0.8155±0.0012

Table 10-5. Limiting Surface Density Method Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
7.4.3	1. Using the limiting surface density method, calculate the critical mass for each array unit required for a water-reflected cubic array of fully enriched U(100) metal for a 4×4×4 array with a center-to-center spacing of 30 in. (76.2 cm). 2. After the critical mass is calculated, determine the multiplication factor for storing 20 kg of U(100) units in the 4×4×4 array.	Part 1 34.3 kg Part 2 k_{eff}= 0.835	SCALE 6.1.3 4×4×4 34.3 kg, k_{eff} = 1.0015±0.0014 SCALE 6.1.3 4×4×4 20 kg, k_{eff} = 0.8457±0.0011
7.4.3 - II	1. Using the graphical method, what would be the effect on critical array unit mass if the U(100) metal was adjusted to a more realistic material such as highly enriched uranium, U(93.2)? 2. After the critical mass is calculated, determine the multiplication factor for storing 20 kg of U(93.2) units in the 4x4x4 array.	Part 1 38.91 kg Part 2 k_{eff}= 0.801	SCALE 6.1.3 4×4×4 38.41 kg, k_{eff} = 1.0012±0.0012 SCALE 6.1.3 4×4×4 20 kg, k_{eff} = 0.8204±0.0011
7.4.4	1. Using the limiting surface density method, calculate the critical mass for each array unit required for a water-reflected cubic array of 5 kg Pu(5.2) metal units in a 4x4x4 array with a center-to-center spacing of 30 in. (76.2 cm). 2. After the critical mass is calculated, determine the multiplication factor for storing 5 kg of Pu(5.2) units in the 4x4x4 array.	Part 1 9.04 kg Part 2 k_{eff}= 0.821	SCALE 6.1.3 4×4×4 9.08 kg, k_{eff} = 1.0004±0.0012 SCALE 6.1.3 4×4×4 5 kg, k_{eff} = 0.8348±0.0011
7.4.5	Based on the results of the last example problem in Section 7.4.4 (Limiting Surface Density Example Problem 4), calculate the required array unit mass that results in a multiplication factor of 0.9 using the same limiting surface density relationships.	6.584 kg	SCALE 6.1.3 4×4×4 6.437 kg, k_{eff} = 0.9008±0.0012
7.5.1	Use the equivalence relationship derived in Section 7.5 to confirm the results of the example problem 4 from Section 7.4.4 for Pu(5.2) metal units in a 4×4×4 array.	9.032 kg	9.035 kg from example 4 section 7.4.4.

Table 10-5. Limiting Surface Density Method Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
7.6.1	Using the methodology presented in Section 7.6 and the results from Example Problem 3-II, calculate the critical mass for each array unit required for a water-reflected cubic array of fully enriched U(100) metal units in a 8x4x2 array.	35.41 kg	SCALE 6.1.3 8×4×2 35.41 kg, k_{eff} = 0.9994±0.0012
7.6.2	Part 1. Using the limiting surface density method, calculate the spherical critical mass of U(93.2) metal required for criticality in a 216-unit water-reflected cubic array (6x6x6). The center-to-center spacing ($2a_n$) of the array units is 38.1 cm.	Part 1 16.4 kg	SCALE 6.1.3 6×6×6 15.9 kg, k_{eff} = 1.0007±0.0011
	Part 2. What would be the multiplication factor of this array if the units were rearranged into a water-reflected 9×24×1 cuboidal array?	Part 2. k_{eff} = 0.858	SCALE 6.1.3 9×24×1 16.4 kg, k_{eff} = 0.8755±0.0012
	Part 3. What ^{239}Pu metal [Pu(0)] mass will result in an array multiplication factor of 0.9 for the 6×6×6	Part 3a 3.86 kg	SCALE 6.1.3 6x6x6 3.736 kg, k_{eff} = 0.9001±0.0013
	and the 9×24×1 arrays?	Part 3b 5.16 kg	SCALE 6.1.3 10×10×10 4.95 kg, k_{eff} = 0.9007±0.0013
7.8.1	Using the limiting surface density method, calculate the critical mass for each array unit required for a water-reflected cubic array of fully enriched U(100) metal for a 4x4x4 array with a center-to-center spacing of 30 in. (76.2 cm) due to a change in array density change from 18.9 g/cm^3 (limiting surface density example problem 3) to 15 g/cm^3.	47.5 kg	SCALE 6.1.3 4×4×4 46.6 kg, k_{eff} = 1.0005±0.0014

Table 10-5. Limiting Surface Density Method Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
7.9.1	1. Using the limiting surface density method, calculate the critical mass for each array unit required for a concrete-reflected cubic array of fully enriched U(100) metal for a 4×4×4 array with a center-to-center spacing of 30 in. (76.2 cm). Assume that the concrete is the Oak Ridge mixture and that there is 30.48 cm (12 in.) of concrete reflection instead of the minimum 20 cm (7.87 in.) present in the calculations for example problem 3 (Section 7.4.3). 2. After the critical mass is calculated, determine the multiplication factor for storing 20 kg of U(100) units in the 4×4×4 array.	Part 1 30.1 kg Part 2 $k_{eff} = 0.872$	SCALE 6.1.3 4×4×4 30.5 kg, $k_{eff} =$ 1.0010±0.0012 SCALE 6.1.3 4×4×4 20 kg, $k_{eff} =$ 0.8738±0.0012

Conclusions from Comparisons in Table 10-5.

Predictions of spacing required for critical arrays are conservative. Values for critical array from limiting surface density create k_{eff} values that are less than one (i.e., subcritical arrays). Calculations of masses for given k_{eff} values produce masses that are non-conservative with the actual k_{eff} values being about 2 to 3% above the expected values. Mass estimates are also non-conservative with actual masses being about 2 to 4% less than the hand calculation value. This means a higher k_{eff} for the estimated mass. The limiting surface density method covers most cases for analysis of arrays, but it requires a number of calculations. The values provided are usually within a few percent of the actual values, but they are not always on the conservative side. However, these calculations are more than sufficient as starting points in the design of array. One advantage of the limiting surface density method is the visual representation provided by the graphs of the material and geometry lines. These provide an understanding of the effects of parameter changes such as noncubic arrangement, different fissile material, and water versus concrete reflection.

Table 10-6. Surface Density Method Confidence Comparison.

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
8.4.1	Calculate the minimum spacing for a planar array of 2-liter bottles of Pu, with 5 wt % ^{240}Pu, solution, assuming a maximum concentration of 400 gPu/l? The array is assumed to be only one unit high (i.e., no stacking).	24.7 cm	SCALE 6.1.3 24.7 cm, $k_{eff} =$ 0.8888±0.0012

Table 10-6. Surface Density Method Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
8.4.2	What is the minimum center-to-center spacing for an infinite planar array of plutonium oxide ($^{239}PuO_2$) containers loaded with 4,500 grams of Pu per container? Assume that the Pu oxide density is 11.48 g/cm³, which is the theoretical density for PuO_2, that the Pu is pure ^{239}Pu, and the array is assumed to be only one unit high (i.e., no stacking).	26.6 cm	SCALE 6.1.3 26.6 cm, k_{eff} = 0.8663±0.0013
8.4.3	What is the minimum center-to-center spacing of an infinite planar array of 4,500 g Pu(5) metal ingots. For this problem, assume that the density of the Pu(5) metal ingots is the same as alpha-phase Pu, 19.75 g/cm³, and that the array is assumed to be only one unit high (i.e., no stacking). What is the minimum spacing for an array that is two units high (e.g., one unit on top of a second unit)	36.0 cm 2 layers @51.0 cm	SCALE 6.1.3 36.0 cm, k_{eff} = 0.9034±0.0014 SCALE 6.1.3 51.0 cm, k_{eff} = 0.9203±0.0013
8.4.4	1. Repeat the previous problem with delta-phase Pu, 15.6 g/cm³. What is the minimum center-to-center spacing of an infinite planar array of 4,500 g Pu(5) delta-phase metal ingots in a one unit high array? 2. Then calculate the maximum delta ingot mass if the center-to-center spacing is 20 cm (7.87 in.).	28.9 cm 2.683 kg @ 20cm	SCALE 6.1.3 28.9 cm, k_{eff} = 0.8887±0.0014 SCALE 6.1.3 20 cm, k_{eff} = 0.8679±0.0013
8.4.5	Apply the smeared density approach to the situation given in Section 6.4.4. That is, calculate the safe spacing for a 10-unit array of 10 in. diameter cylinders (schedule 20 pipe) each 6 ft long on a square lattice pattern in two rows of five. The cylinders are to contain 4.98% enriched uranyl fluoride of maximum 3.2 g U/cm³ concentration. The volume of each cylinder is 97.36 liters.	123.8 cm 48.7 in.	SCALE k_{eff} = 0.7909±0.0013 Bare array SCALE k_{eff} = 0.8450±0.0012 Reflected array

Conclusions from Comparisons in Table 10-6.

As indicated by the computer analyses, all the spacings calculated with the surface density method are well subcritical. The k_{eff} values seem to be between 0.86 and 0.91 for an infinite single layer planar array reflected by 30 cm of water on the top and bottom. When a two-layer system was analyzed (8.4.3), the k_{eff}

went up to 0.9203 for the calculated spacing. Analyses for 3-, 4-, and 5-layer systems at the appropriate calculate spacings showed k_{eff} leveling off at about 0.925 (i.e., from 0.09207±0.0012 to 0.9243±0.0012 to 0.9235±0.0012)—all appropriately subcritical. The surface density method will provide a bounding estimate of center-to-center spacing for arrays limited in one direction.

Table 10-7. Density Analog Method Confidence Comparison.

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
9.4.1	For 2×2×2, 4x4x4, 10×10×10 and 100×100×100 arrays, what is the minimum center-to-center spacing of 2-liter bottles of Pu, with 5 wt % ^{240}Pu, solution, assuming a maximum concentration of 400 gPu/l?	2×2×2 17.6 cm	SCALE 6.1.3 2×2×2 17.6 cm, k_{eff} = 08623±0.0012
		4×4×4 24.9 cm	SCALE 6.1.3 4×4×4 24.9 cm, k_{eff} = 0.9258±0.0015
		10×10×10 39.3 cm	SCALE 6.1.3 10×10×10 39.3 cm, k_{eff} = 0.9530±0.0012
9.4.2	Using the density analog method, repeat example problem in Section 8.4.2 for 2 × 2 × 2, 4 × 4 × 4, 10 × 10 × 10, and 100 × 100 × 100 arrays. Recall that each container in the array contains plutonium oxide (^{239}PuO$_2$) loaded with up to 4,500 grams of Pu.	2×2×2 17.8 cm	SCALE 6.1.3 2×2×2 17.8cm, k_{eff} = 08322±0.0012
		4×4×4 25.1 cm	SCALE 6.1.3 4×4×4 25.1 cm, k_{eff} = 0.8957±0.0012
		10×10×10 39.7 cm	SCALE 6.1.3 10×10×10 39.7 cm, k_{eff} = 0.9260±0.0012

Table 10-7. Density Analog Method Confidence Comparison (continued).

Section	Description of the Problem	Hand Calculation Result	Comparison Result from Reference or Code Package
9.4.3	Using the density analog method, repeat the example problem in Section 8.4.3 (Surface Density Example Problem 3) for 2 × 2 × 2, 4 × 4 × 4, 10 × 10 × 10, and 100 × 100 × 100 arrays. Recall that each fissile unit in the array is a 4,500 g alpha-phase Pu(5) metal ingot.	2×2×2 25.7 cm 4×4×4 36.3 cm 10×10×10 57.4 cm	SCALE 6.1.3 2×2×2 25.7 cm, k_{eff} = 0.8673±0.0013 SCALE 6.1.3 4×4×4 36.3 cm, k_{eff} = 0.9027±0.0012 SCALE 6.1.3 10×10×10 57.4 cm, k_{eff} = 0.9144±0.0013
9.4.4	Using the Density Analog Method, analyze the situation given in Section 6.4.4. That is, calculate the safe spacing for a 10-unit array of 10 in. diameter cylinders (schedule 20 pipe) each 6 feet long on a square lattice pattern in two rows of five. The cylinders are to contain 4.98% enriched uranyl fluoride of maximum 3.2 g U/cm³ concentration. From ORNL data (Reference 38), a bare stainless steel cylinder of U(4.98)O_2F_2 solution was critical with a radius of 19.55 cm and a height of 101.7 cm.	120.8 cm	SCALE k_{eff} = 0.7956±0.0011 Bare array SCALE k_{eff} = 0.8454±0.0014 Reflected array

Conclusions from Comparisons in Table 10-7.

As indicated by the computer analyses, all of the spacings calculated with the density analog method are well subcritical. Because the evaluations are based on cubic arrays, the computed k_{eff} values represent the highest values for the given number of units. Note that as the number of units increase, the k_{eff} associated with the density analog spacing also increases. For eight units, the k_{eff} values seem to be between 0.83 and 0.87, while for 1,000 units the k_{eff} values are between 0.91 and 0.95. Of course, there is a realistic limit for the number of units that can be stacked, so it is unlikely that a 10×10×10 cubic array would be stacked to a height of almost 19 ft (574 cm). Again, the density analog method is easier to use when dealing with a specific number of units, whereas the surface density method usually provides more realistically achievable results when there are either administrative or physical limits on the number of units that can be stacked.

The result from the last example problem from Section 9.4.4 is compared with results from solid angle method and the smeared thickness method in Table 9-1. That summary indicates all three methods produce very similar results for the fissionable material in the configuration analyzed.

260

10.4 COMPARISON OF THREE ARRAY TECHNIQUES ON THREE PLUTONIUM ARRAYS

Three plutonium arrays—Pu(5) solution, PuO2 powder, and Pu(5) metal ingots—were analyzed using limiting surface density, surface density, and density analog methods. This analysis highlighted the similarities and differences among the three techniques. The first significant difference is that the spacing from the limiting surface density method is for a critical array, whereas the spacings obtained from the other two methods are for subcritical arrangements. The second difference is the array configuration evaluated by the three methods. Limiting surface density analyzes a specific configuration and can be used on both cubic and non-cubic arrays to determine the critical spacing. The surface density method applies to infinite planar arrays whose height (stacking of units) is limited by either a physical control or an administrative control. The density analog method is applied to arrays with a given number of units with the bounding configuration being a cubic or near cubic arrangement of the units.

Table 10-8 shows the results from the analysis of the three plutonium arrays using the three different array techniques. All configurations were analyzed using continuous energy ENDF-7 cross sections with SCALE 6.1.3.

Table 10-8. Comparison of Three Methods.

Description of the Problem	Limiting Surface Density	Surface Density	Density Analog
Spacing of 2-liter bottles of Pu, with 5 wt % ^{240}Pu, solution, assuming a maximum concentration of 400 gPu/l?	Not Analyzed	$\infty \times \infty \times 1$ **24.7 cm,** $k_{eff} =$ 0.8888 ± 0.0012	$4 \times 4 \times 4$ **24.9 cm** $k_{eff} =$ 0.9258 ± 0.0015 $10 \times 10 \times 10$ **39.3 cm** $k_{eff} =$ 0.9530 ± 0.0012
Spacing for containers of Plutonium Oxide (^{239}PuO$_2$) loaded with up to 4,500 grams of Pu.	$4 \times 4 \times 4$ **20.16 cm** $k_{eff} =$ 1.0006 ± 0.0013 $10 \times 10 \times 10$ **34.36 cm** $k_{eff} =$ 1.0007 ± 0.0013	$\infty \times \infty \times 1$ **26.6 cm,** $k_{eff} =$ 0.8663 ± 0.0013	$4 \times 4 \times 4$ **25.1 cm** $k_{eff} =$ 0.8957 ± 0.0012 $10 \times 10 \times 10$ **39.7 cm** $k_{eff} =$ 0.9260 ± 0.0012

Table 10-8. Comparison of Three Methods (continued).

Description of the Problem	Limiting Surface Density	Surface Density	Density Analog
Spacing for array of 4,500 g alpha-phase Pu(5) metal ingots.	4×4×4 **25.4 cm** $k_{eff} =$ 0.9993 ± 0.0012	$\infty \times \infty \times 1$ **36.0 cm** $k_{eff} =$ 0.9034 ± 0.0014	4×4×4 **36.3 cm** $k_{eff} =$ 0.9027 ± 0.0012
	10×10×10 **42.4 cm** $k_{eff} =$ 0.9999 ± 0.0013	$\infty \times \infty \times 2$ **51.0 cm** $k_{eff} =$ 0.9203 ± 0.0013	10×10×10 **57.4 cm** $k_{eff} =$ 0.9144 ± 0.0013
Limiting Surface Density was also analyzed for spacing that gave $k_{eff}= 0.8$	10×10×10 **115 cm** $k_{eff} =$ 0.8155 ± 0.0012		

All three methods seem to provide realistic values for the configurations and conditions analyzed. Note that the spacings provided by surface density for a one-high infinite planar array are close to those from Density Analog for a 4×4×4 array. This shows the effect of leakage in the z-direction for the planar array.

10.5 ADDITIONAL CONFIDENCE COMPARISON RESULTS FOR ARRAYS

Some calculations were performed to demonstrate the usefulness of the hand calculation techniques. These calculations are summarized in Table 10-9. To examine the various array methods, array experiments from a benchmark evaluation, HEU-MET-FAST-023 (Reference 35) and HEU-MET-FAST-026 (Reference 36), were used to provide a comparison between the array hand calculational methods and the experimental benchmarks. This primer provides many more array examples. Cubic array experiments were used in the comparison with U(93.2) metal units.

Table 10-9. Array Hand Methods Comparison Table.

Experimental Benchmark Considered	Array Hand Method Comparison – Unit Center-to-Center Spacing (cm)				
	Surface Density Method	Density Analog Method	NB_N^2 Method	Solid Angle Method	Experimental Center-to-Center Spacing
HEU-MET-FAST-023 Case 22, 4×4×4, 10.5 kg U Metal (93.2), 15.2 cm Paraffin Reflector	63.1 (24.8 in.)	31.8 (12.5 in.)	21.9 (8.6 in.)	NA	23.8 (9.4 in.)
HEU-MET-FAST-026 Case 10, Exp b-10, 3×3×3, 15.4 kg U Metal (93.2), 15.2 cm Paraffin Reflector	77.5 (30.5 in.)	39.0 (15.4 in.)	25.3 (10.0 in.)	NA	25.7 (10.1 in.)

Table 10-9. Array Hand Methods Comparison Table (continued).

Experimental Benchmark Considered	Array Hand Method Comparison – Unit Center-to-Center Spacing (cm)				
	Surface Density Method	Density Analog Method	NB_N^2 Method	Solid Angle Method	Experimental Center-to-Center Spacing
HEU-MET-FAST-026 Case 22, Exp c-12, 3×3×3, 20.5 kg U Metal (93.2), 15.2 cm Paraffin Reflector	101.4 (39.9 in.)	51.1 (20.1 in.)	31.4 (12.4 in.)	NA	30.6 (12.0 in.)
HEU-MET-FAST-026 Case 32, Exp d-10, 3×3×3, 24.7 kg U Metal (93.2), 15.2 cm Paraffin Reflector	127.7 (50.3 in.)	64.3 (25.3 in.)	37.1 (14.6 in.)	NA	36.5 (14.4 in.)
HEU-MET-FAST-026 Case 9, Exp b-9, 3×3×3, 15.4 kg U Metal (93.2), 15.2 cm Paraffin Reflector	77.5 (30.5 in.)	39.0 (15.4 in.)	25.3 (10.0 in.)	NA	25.2 (9.9 in.)
HEU-MET-FAST-026 Case 21, Exp c-11, 3×3×3, 20.5 kg U Metal (93.2), 15.2 cm Paraffin Reflector	101.4 (39.9 in.)	51.1 (20.1 in.)	31.4 (12.4 in.)	NA	30.2 (11.9 in.)
HEU-MET-FAST-026 Case 21, Exp d-9, 3×3×3, 24.7 kg U Metal (93.2), 15.2 cm Paraffin Reflector	127.7 (50.3 in.)	64.3 (25.3 in.)	37.1 (14.6 in.)	NA	36.0 (14.2 in.)

10.6 CONCLUSIONS

Close examination of the comparisons summarized in the Section 10 tables clearly shows that the results provided by the various hand calculational methods discussed in this primer provide very good results when compared with actual dimensions, SCALE 6.1.3 results, or experimental benchmarks. Thus, hand calculations can be very effective tools for a criticality safety practitioner as a calculational tool to provide information for controls or limits for process operations or as a starting point for more complex calculations. The primer can assist the criticality safety practitioner in learning the various methods and understanding their applicability and limitations.

11. REFERENCES

1. Duderstadt, James J., and Louis J. Hamilton, *Nuclear Reactor Analysis,* John Wiley & Sons, New York, (1976), pp. 196-216.

2. Lamarsh, John R. and Anthony J. Baratta, *Introduction to Nuclear Engineering*, 3rd Edition Prentice Hall Publishing Company, Upper Saddle River, NJ, Reading, PA, (2001), pp. 230-297.

3. Wescott, C.H., "Effective Cross Section Values for Well-Moderated Thermal Reactor Spectra," AECL-1101, (January 1962).

4. Busch, R. D., "A Primer for Criticality Calculations with DANTSYS," Los Alamos National Laboratory report LA-13265 (August 1997).

5. Argonne National Laboratory, *Reactor Physics Constants,* Argonne National Laboratory document ANL-5800, 2nd Edition (July 1963).

6. McLaughlin, T.P., S.P. Monahan, N.L. Pruvost, V.V. Frolov, B.G. Ryazanov, V.I. Sviridov, "A Review of Criticality Accidents: 2000 Revision," http://www.csirc.net/10_Library/00_Reports/13638/la-13638.pdf, Los Alamos National Laboratory Report LA-13638 (May 2000).

7. Carter, R. D., G. R. Kiel, and K. R. Ridgway, "Criticality Handbook Vol. I, II, and III," Atlantic Richfield Hanford Co. Report ARH-600 (1968).

8. Jarvis, G. A., G. A. Linenberger, J. D. Orndoff & H. C. Paxton, "Two Plutonium-Metal Critical Assemblies," *Nuclear Science and Engineering*, 8:6, (December 1960), 525-531, DOI: 10.13182/NSE60-A25840G.

9. Bell, G.I., J.J. Devaney, G.E. Hansen, C.B. Mills, and W.H. Roach, "Los Alamos Group-Averaged Cross Sections," Los Alamos Scientific Laboratory report LAMS-2941 (September 1963).

10. Busch, R.D., and S.M. Bowman, "KENO V.a Primer: A Primer for Criticality Calculations with SCALE/KENO V.a Using GeeWiz," Oak Ridge National Laboratory report ORNL/TM-2005/135, (December 2005).

11. Paxton, H. C., and N. L. Pruvost, "Critical Dimensions of Systems Containing ^{235}U, ^{239}Pu, and ^{233}U, 1986 Revision," Los Alamos National Laboratory report LA-10860-MS (July 1987

12. Paxton, H. C., J. T. Thomas, D. Callahan, and E. B. Johnson, "Critical Dimensions of Systems Containing U^{235}, Pu^{239} and U^{233}," Los Alamos Scientific Laboratory and Oak Ridge National Laboratory report TID-7028 (June 1964).

13. Lutz, H.F., edited by H.J. Kroopnick, "Nuclear Criticality Safety Assessment Calculations: Part III. Calculating Nuclear Criticality in Single Units," Lawrence Livermore National Laboratory, M-164 Part 3, (June 1987).

14. Paxton, H. C., "Criticality Control in Operations with Fissile Material," Los Alamos Scientific Laboratory report LA-3366 (Rev), (November 1972).

15. Soodak, H. and E.C. Campbell, *Elementary Pile Theory,* John Wiley and Sons, New York, (1950).

16. Knief, R. A., *Nuclear Criticality Safety, Theory and Practice,* American Nuclear Society, La Grange Park, IL, (1985).

17. U.S. Atomic Energy Commission, "Reactor Handbook – Volume 1 – Physics,'" AECD-3645, Declassified Edition, (February 1955).

18. Sjöstrand, N.G., "Calculation of the Geometric Buckling for Reactors of Various Shapes," Aktiebolaget Atomenergi, AE-1, Stockholm, Sweden, (1958).

19. Murray, R.L., T.J. Hirons, Reith, R.J., and O.J. Smith, "Geometric Buckling of Polygonal Reactors," *Nucl. Sci. Eng.*, 34:1, pg. 86-87, (1968), DOI: 10.13182/NSE68-A19370.

20. Vega, R.M., T.K. Lane, J.A. Miller, and N.F. Schwers, "Reactivity Effects at the Mayak Production Association, January 2, 1958, Criticality Accident Using Serpent 2 and Openfoam," SAND2015-4236C, Sandia National Laboratories, 2015.

21. O'Dell, R. D., "Critical Size and Mass Relations as Function of Density," Los Alamos National Laboratory, unpublished data, (March 1992).

22. Stratton, W. R., "Criticality Data and Factors Affecting Criticality of Single Homogeneous Units," Los Alamos Scientific Laboratory, LA-3612 (July 1964).

23. NEA, "International Handbook of Evaluated Criticality Safety Benchmark Experiments", NEA/NSC/DOC(95)/03, OECD-NEA, Paris, France (2018).

24. Cullen, D.E., "Mass and Density, Criticality Relationships," Lawrence Livermore National Laboratory report, UCRL-ID-143496, (April 2001).

25. Fermi, E. "Critical Mass Measurements for a 25 Sphere in Tu and WC Tampers," Part B – Interpretation, Los Alamos Scientific Laboratory report, LA-442, (October 30, 1945).

26. Paxton, H.C., "Critical Masses of Fissionable Metals as Basic Nuclear Safety Data," Los Alamos Scientific Laboratory Report LA-1958 (January 1955).

27. Pruvost, N.L. and H.C. Paxton, "Nuclear Criticality Safety Guide," Los Alamos National Laboratory Report LA-12808, (1996).

28. Paxton, H.C, "Bare Critical Assemblies of Oralloy at Intermediate Concentrations of U-235," Los Alamos Scientific Laboratory Report LA-1671 (July 1954).

29. Neuer, J.J, "Critical Assembly of Uranium Metal at an Average U-235 concentration of 16-1/4%," Los Alamos Scientific Laboratory Report LA-2085 (January 1957).

30. Peterson, R.E., "Lady Godiva: An Unreflected Uranium-235 Critical Assembly." Los Alamos Scientific Laboratory Report LA-1614 (September 1953).

31. Hunt, D. C., "A Review of Criticality Safety Models Used in Evaluating Arrays of Fissile Materials," *Nucl. Technol.* **30**, 138-165 (1976).

32. C. L. Schuske, D. Dickinson & S. J. Altschuler (1974) Surface Density Method Employing Unit Shape Factor (s/v) for the Storage of Fissile Materials, *Nucl. Technol.,* **23**:2, 157-176, DOI: 10.13182/NT74-A31449 (1974).

33. Hunt, D. C., and D. Dickinson, "Comparative Calculational Evaluation of Array Criticality Models," *Nucl. Technol.* **30**, 190-214 (1976).

34. Henry, H. F., J.R. Knight, and C.E. Newlon, "General Application of a Theory of Neutron Interaction," Oak Ridge Gaseous Diffusion Plant Report K-1309, November 15, 1956.

35. Thomas, J T. Ed., "Nuclear Safety Guide TID-7016/Revision 2," U. S. Nuclear Regulatory Commission report NUREG/CR-0095 and ORNL/NUREG/CSD-6 (1978).

36. Tang, J.S., "Investigation of the Solid Angle Method Applied to Reflected Cubic Arrays," Oak Ridge National Laboratory Report, ORNL/CSD/TM-13, October 1976.

37. Thomas, J. T., "An Evaluation of the Solid Angle Method Used in Nuclear Criticality Safety," Oak Ridge National Laboratory Plant report NUREG/CR-2223, ORNL/CSD/TM-158, RC, June 1982.

38. Webster, J. W., and E.B. Johnson, "Criticality of a Single Unit of Aqueous Uranyl Fluoride Solution Enriched to 5% in U-235," Oak Ridge National Laboratory Report ORNL-TM-1195, July 1965.

39. Thomas, J. T., "Generic Array Criticality – An Analytical Representation of Reflected Arrays of Fissile Units," Oak Ridge Y-12 Plant report Y-CDC-13, UCC-ND (1973).

40. Williams, W. H., University of New Mexico Short Course, Notes for the Surface Density and Density Analogue Methods Course Module, 1985.

41. Thomas, J. T., "Surface Density and Density Analogue Models for Criticality in Arrays of Fissile Materials," *Nucl. Sci. Eng*., **62**, 424(1977).

42. Stover, T. E., J. S. Baker, M. D. Ratliff, G. C. Mitschelen, Limiting Surface Density Method Adapted to Large Arrays of Heterogeneous Shipping Packages with Non-linear Responses, *Nucl. Sci. Eng.* **190**, 178 (2018).

43. Evans, M. C., and J. R. Bowe, "Applications of the Limiting Surface Density Method to Transport and Storage of Special Nuclear Materials," Proceedings of a Topical Meeting, Jackson, Wyoming (1985), American Nuclear Society report ISBN:89448-119-3, pp. 307-321.

44. Thomas, J. T., "Uranium Metal Criticality, Monte Carlo Calculations and Nuclear Criticality Safety," Oak Ridge Y-12 Plant report Y-CDC-7, UCC-ND (1970).

45. Thomas, J. T., "The Criticality of Cubic Arrays of Fissile Material," Oak Ridge Y-12 Plant report Y-CDC-10, UCC-ND (1971).

46. Thomas, J. T., "The Effect of Reflector Location on Array Criticality," Oak Ridge Y-12 Plant report NUREG/CR-1616, ORNL/NUREG/CSD/TM-16, UCC (1980).

47. Thomas, J. T., "Remarks on Surface Density and Density Analog Representation of Array Criticality," *Trans. Am. Nucl. Soc.*, **22**, 299 (1975).

48. Monahan, S. P., "The Neutron Physics of Concrete Reflectors", 5th International Conference on Nuclear Criticality Safety, Albuquerque, NM (1995).

49. O'Dell, R. D., and D. K. Parsons, "Pu Oxide Critical Mass Estimates," ESH-6-94-289 memorandum, Los Alamos National Laboratory, ESH-6 Criticality Safety Group (December 1994).

50. Paxton, H. C., "Capsule Storage and Density Analog Techniques," Los Alamos Scientific Laboratory report LA-5930-MS (May 1975).

51. Paxton, H.C., "Density-Analog Techniques," Proceedings of the Livermore Array Symposium, CONF-680909, pages 6-11, (September 1968).

APPENDIX A. DERIVATION OF THE LIMITING SURFACE DENSITY METHOD

APPENDIX A. DERIVATION OF THE LIMITING SURFACE DENSITY METHOD

The limiting surface density (LSD) method, first developed by Joseph Thomas of Oak Ridge National Laboratory (ORNL), is discussed at length in References A1–A5. The LSD method was developed based on combining diffusion theory and density analog concepts into a new method to examine array criticality. Diffusion theory can of course be used to equate the geometric bucking for a homogeneous single unit to the material buckling for a critical system to determine the dimensions for the critical unit. For an array, the effective multiplication factor is given by the following:

$$k_{eff} = \frac{k_\infty}{1 + M^2 B^2}$$

A-1

The infinite multiplication factor represents the effective multiplication factor for an infinite array. For an infinite array, the k_∞ is only dependent upon the material properties of the array. M^2 is the neutron migration area and B^2 represents the array buckling. In an infinite array, if $M^2 B^2$ is held constant when the geometrical properties of an array are changed, then the array neutron leakage and effective multiplication factor will remain unchanged [A1]. Further, the migration area in this infinite array configuration is proportional to the inverse square of the array density, $1/\rho^2$, which is also proportional to the number in the units in the array, N, based on the density analogue technique, thus $M^2 \propto N$. For the geometric buckling, an equation can be modified from that for a single unit to be applicable for a finite array configuration:

$$B^2 = B_N^2 = \frac{\pi^2}{4(n_x a_n^x + \lambda)^2} + \frac{\pi^2}{4(n_y a_n^y + \lambda)^2} + \frac{\pi^2}{4(n_z a_n^z + \lambda)^2}$$

A-2

where

$$n_x, n_y, \text{ and } n_z \quad = \quad \text{number of array units in the x, y and z directions}$$

$$a_n^x, a_n^y, \text{ and } a_n^z \quad = \quad \text{"half-cell" dimensions (or half of the center-to-center spacing of the units in the x, y, and z directions}$$

$$\lambda \quad = \quad \text{array extrapolation length.}$$

For cubic arrays, which is the preference of Thomas' LSD method, $n_x = n_y = n_z = n$ and $a_n^x = a_n^y = a_n^z = a^n$, so equation A-2 becomes

$$B^2 = B_N^2 = \frac{3\pi^2}{4(na_n + \lambda)^2}$$

A-3

Thus, the form of this equation that considers the product, $M^2 B^2$, for a large array configuration is

$$NB_N^2 = \frac{3N\pi^2}{4(na_n + \lambda)^2} = \frac{3N\pi^2}{4\lambda^2 + 8\lambda na_n + 4n^2 a_n^2}$$

A-4

After some algebraic manipulations [A6], the NB_N^2 expression is provided by equation A-5 as follows, which is the near-final form of the LSD equation derived by Thomas:

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \sqrt{\frac{4\lambda^2 NB_N^2}{N3\pi^2}}\right)^2 \qquad \text{A-5}$$

The expression $\sqrt{\frac{4\lambda^2 NB_N^2}{3\pi^2}}$ is treated as a constant in Thomas' method, denoted as c, that has been evaluated by Thomas from a series of Monte Carlo calculations for critical array configurations and has a value of 0.55 ± 0.18.

$$NB_N^2 = \frac{n3\pi^2}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 \qquad \text{A-6}$$

To arrive at Thomas' final form of the LSD method, Eq. (A-6) must be related to the array surface density, which is essentially array unit mass divided by the area. As discussed in the LSD chapter in this document, the array unit mass is projected onto a plane that has a particular surface area. Per Reference B6, the surface area of a unit mass projected onto a plane must include the extrapolation distance, λ, for the array unit. The surface density can now be described as

$$\sigma(m) = \frac{mass}{area} = \frac{mN}{(n2a_n + 2\lambda)^2} = \frac{mN}{4(na_n + \lambda)^2} \qquad \text{A-7}$$

This surface density expression can be related to the geometric buckling for the array by rearranging equation A-4 and multiplying the expression by the array unit mass, m, as follows:

$$\sigma(m) = \frac{mNB_N^2}{3\pi^2} = \frac{mN}{4(na_n + \lambda)^2} \qquad \text{A-8}$$

The surface density, $\sigma(m)$, can now be put into the final form derived by Thomas:

$$\sigma(m) = \frac{nm}{(2a_n)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2 \qquad \text{A-9}$$

References

A1. Douglas C. Hunt, A Review of Criticality Safety Models Used in Evaluating Arrays of Fissile Materials, Nuclear Technology, 30:2, 138-165, DOI: 10.13182/NT76- A3161 (1976).

A2. J. T. Thomas, "Uranium Metal Criticality, Monte Carlo Calculations and Nuclear Criticality Safety," Y-CDC-7, Union Carbide Corporation, Oak Ridge Y-12 Plant, Nuclear Division (1970).

A3. J. T. Thomas, "The Criticality of Cubic Arrays of Fissile Material," Y-CDC-10, Union Carbide Corporation, Oak Ridge Y-12 Plant, Nuclear Division (1971).

A4. J. T. Thomas, "Generic Array Criticality: An Analytic Representation of Reflected Arrays of Fissile Units," Y-CDC-13, Union Carbide Corporation, Oak Ridge Y-12 Plant, Nuclear Division (1973).

A5. Surface Density and Density Analog Models for Criticality in Arrays of Fissile Materials, Nuclear Science and Engineering, 62:3, 424-437, DOI: 10.13182/ NSE77-A26982 (1977).

A6. Tracy E. Stover, James S. Baker, Michael D. Ratliff & Gretchen C. Mitschelen, Limiting Surface Density Method Adapted to Large Arrays of Heterogeneous Shipping Packages with Nonlinear Responses, Nuclear Science and Engineering, 190:2, 176-194, DOI: 10.1080/00295639.2017.1417344 (2018).

APPENDIX B. FRACTION CRITICAL

APPENDIX B – MULTIPLICATION FACTOR VERSUS FRACTION OF CRITICAL MASS

This appendix provides multiplication factor data for various systems to provide calculation support for using the various hand calculation methods discussed in this primer. Some of this information is extracted from Reference B1, which provides critical mass and multiplication factor data for the following metals and solutions:

- Highly Enriched Uranium (HEU) and plutonium (Pu) metal, bare and water reflected, and

- HEU and plutonium solution, bare and water reflected.

The critical masses for these systems from reference B-1 are provided in Tables B-1 and B-2. For these analyses, the following definitions are used:

- HEU: U(93.5) metal at 18.74 g/ cc

- δPu(4.5): Pu(4.5) with 1 wt.% Ga, metal alloy density = 15.61 g/cc

- δPu(20): Pu(20) with 1 wt./o Ga, metal alloy density = 15.7 g/cc

- αPu: Pu(4.5) unalloyed metal, density = 19.6 g/cc

- HEU Solution: U(93.5) metal-water mixture at various HEU concentrations

- Pu Solution: Pu(4) metal-water mixtures at various Pu concentrations

- F: Fraction of Critical Mass of Pu or HEU.

This information is used to determine the multiplication factor, k_{eff}, estimate based upon the fraction of critical mass that may be in a fissile material operation. Empirical formulae are provided to calculate this estimate. In addition to these systems, information on LEU solutions (i.e., U(5) metal-water mixtures at various U-235 concentrations) has been provided. This was not part of O'Dell's original report but is calculated for this publication. All the critical mass data, infinite multiplication factors, and effective multiplication factors have been recalculated for this report using PARTISN and Hansen-Roach cross sections.

HEU and Pu Metal Systems

Table B-1 provides critical mass data for spherical fissile metal systems. Water reflected systems are those with full water reflection (i.e., 30 cm). Figures B-1 and B-2 provide the multiplication factor data as a function of the fraction of critical mass for the HEU and Pu metal systems. Figure B-1 is for bare systems while Figure B-2 is for water reflected systems. and Pu metal systems. The k_{eff} values for the metal systems compare well to the empirical values.

Table B-1. Metal Sphere Critical Masses

Material	Critical Mass (kg)[30]	
	Unreflected	Water Reflected
HEU	53.8	24.4
δPu(4.5)	16.9	8.4
δPu(20)	19.0	9.9
αPu(4.5)	10.6	5.9

According to Reference B1, a reasonable estimate of the k_{eff} for HEU and Pu metals for both bare and water reflected configurations could be calculated with the following relationship: $k_{eff} \approx F^{0.3}$, where F is the fraction of critical mass for this system equal to the ratio of the actual fissile mass present to the critical mass for the material present (Table B-1).

This formula makes sense based on Reference B2. Thomas indicates that $k_{eff} = \left(\frac{r}{r_{crit}}\right)^{s}$ where s is 0.917 for U(93.2) and 0.916 for Pu(5.2). As the radius is proportional to volume$^{0.333}$, and mass is proportional to volume, then F $^{s/3}$. So, $k_{eff} \approx F^{0.306}$ or very close to the 0.3 found by O'Dell.

Figure B-1 shows the multiplication factor as a function of fraction critical for plutonium metal systems, both bare and reflected. As can be seen in the figures all curves lie very close to and some on top of the approximation. $k_{eff} \approx F^{0.3}$, which is indicated by the red curve. The reflected system curves are slightly above the approximation.

---

[30] Critical mass values in this table are for total Uranium and total Plutonium.
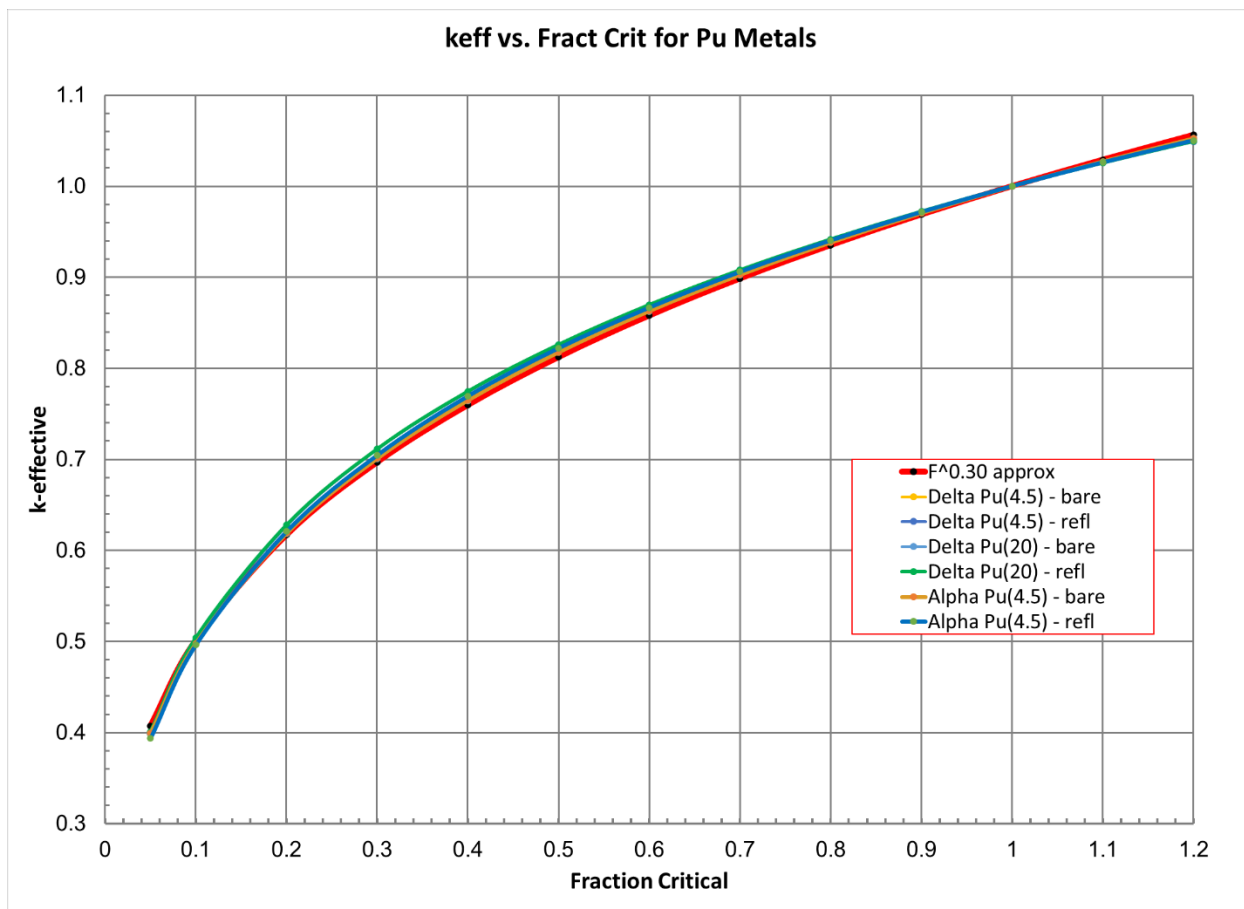
Figure B-1. k-effective versus Fraction Critical for Plutonium Metals.

Figure B-2 shows the multiplication factor as a function of fraction critical for high-enriched uranium (HEU) metal systems, both bare and reflected. As can be seen in the figures the bare curve lies very close to the approximation: $k_{eff} \approx F^{0.3}$, which is indicated by the red curve. The reflected curve is above the approximation and in fact follows the relationship, $k_{eff} \approx F^{0.274}$.
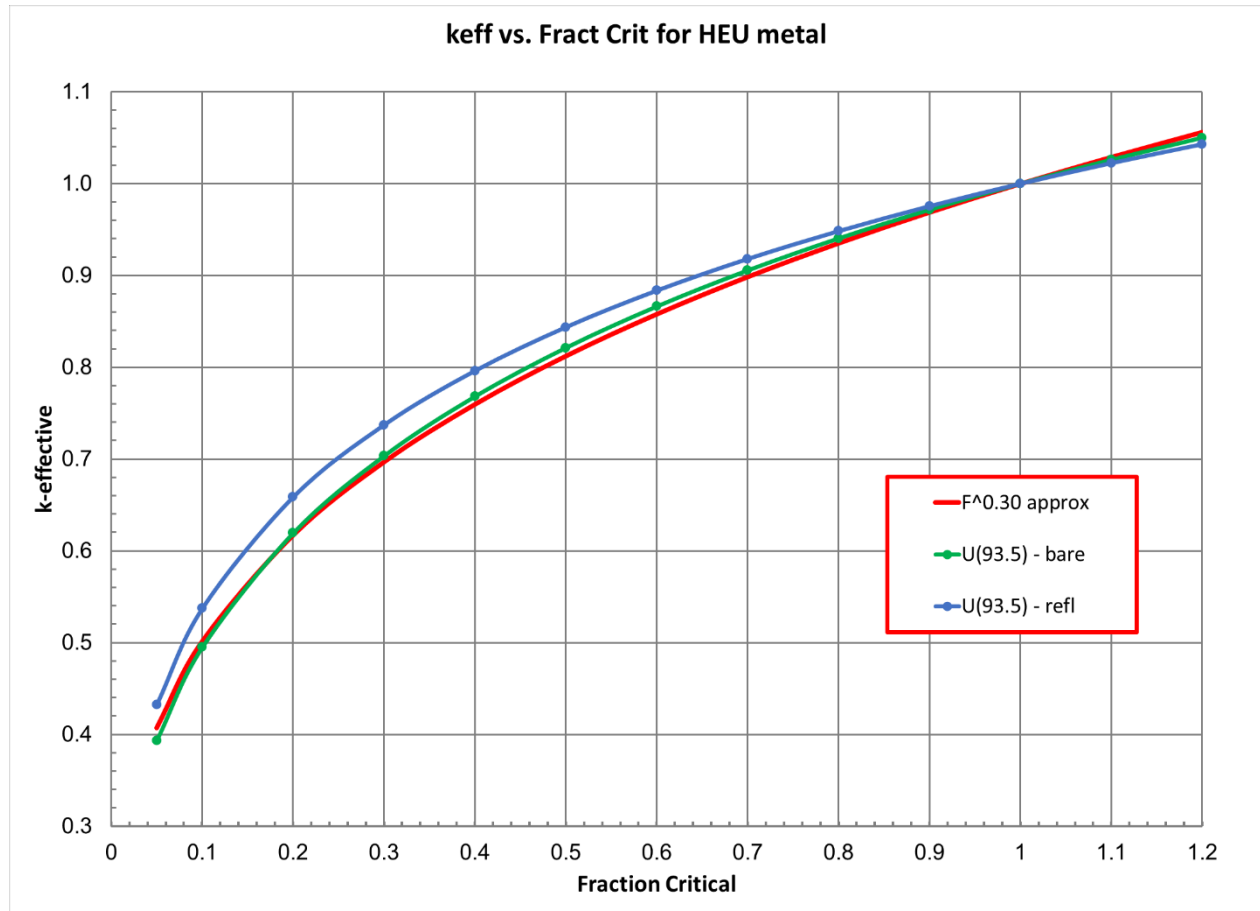

Figure B-2. k-effective versus Fraction Critical for HEU Metal.

Solutions Systems

O'Dell provides the information shown in Tables B-2 and B-3 for critical masses for spherical fissile solution systems. Table B-2 provides the information for Pu(4)-water solutions at 4 different Pu concentrations. Again, water reflected systems are those with full water reflection (i.e., 30 cm).

Table B-2. Pu Solution Sphere Critical Masses

Material	Concentration (g/liter)	Critical Mass (kg)	
		Unreflected	Water Reflected
Pu(4)	20	1.08	0.68
Pu(4)	30	1.05	0.60
Pu(4)	50	1.28	0.66
Pu(4)	200	3.97	1.80

Table B-3 provides the information for HEU-water (U(93.5)-H$_2$O) solutions at 4 different uranium concentrations. Again, water reflected systems are those with full water reflection (i.e., 30 cm).

Table B-3. HEU Solution Sphere Critical Masses

Material	Concentration (g/liter)	Critical Mass (kg)	
		Unreflected	Water Reflected
HEU	20	3.24	2.356
HEU	30	1.84	1.17
HEU	50	1.60	0.90
HEU	200	3.19	1.45

O'Dell then looks at a similar relationship to estimate the k_{eff} for HEU and Pu solutions for, again, bare and water-reflected configurations: $k_{eff} \approx F^{0.25}$, where F is the fraction of critical mass. However, as shown in Figure B-3 (for bare Pu(4) solutions) and Figure B-4 (for bare HEU solutions), there is a significant variation from the empirical fit. For this reason, it was decided to reanalyze the behavior of solution system k-effectives.
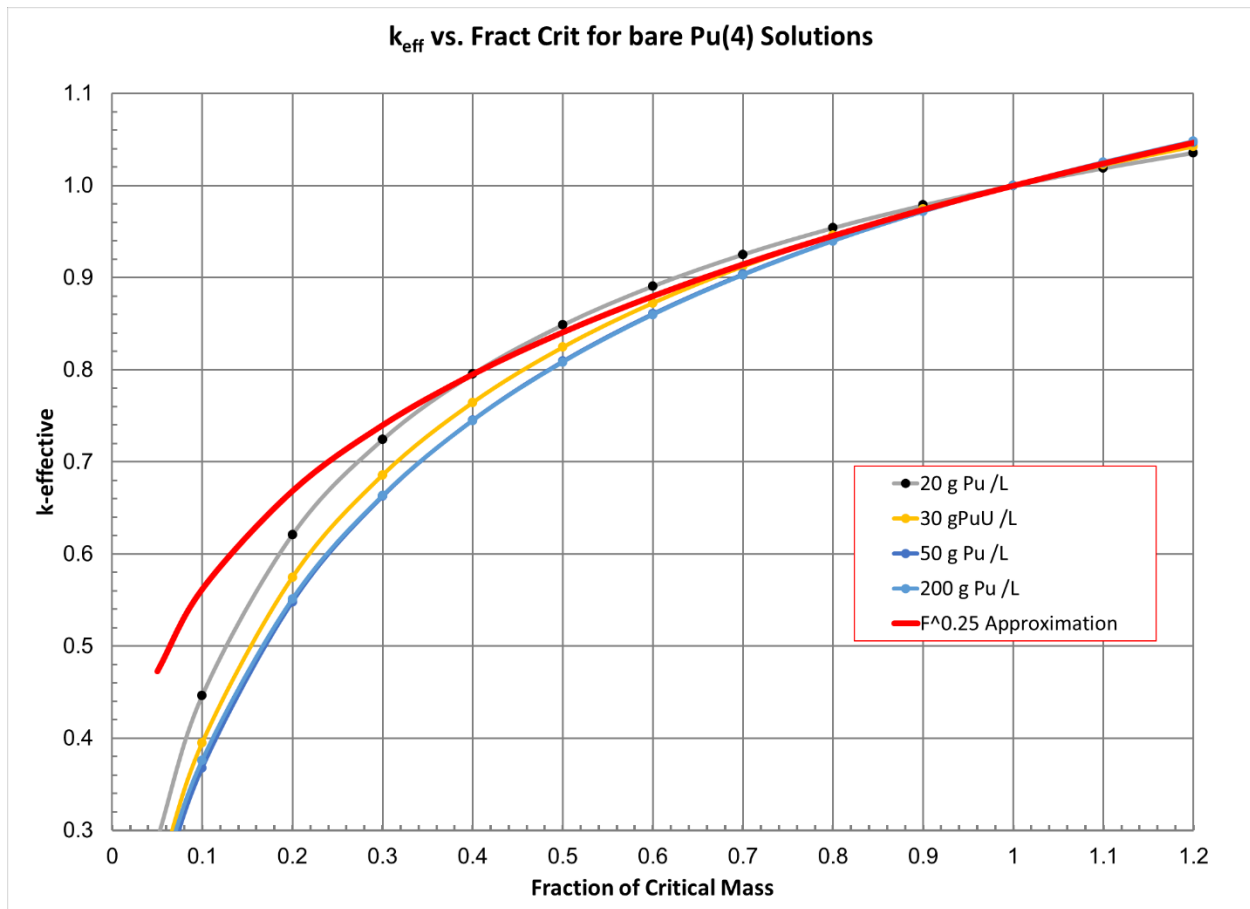
Figure B-3. k-effective versus Fraction Critical for Pu(4) Solutions.

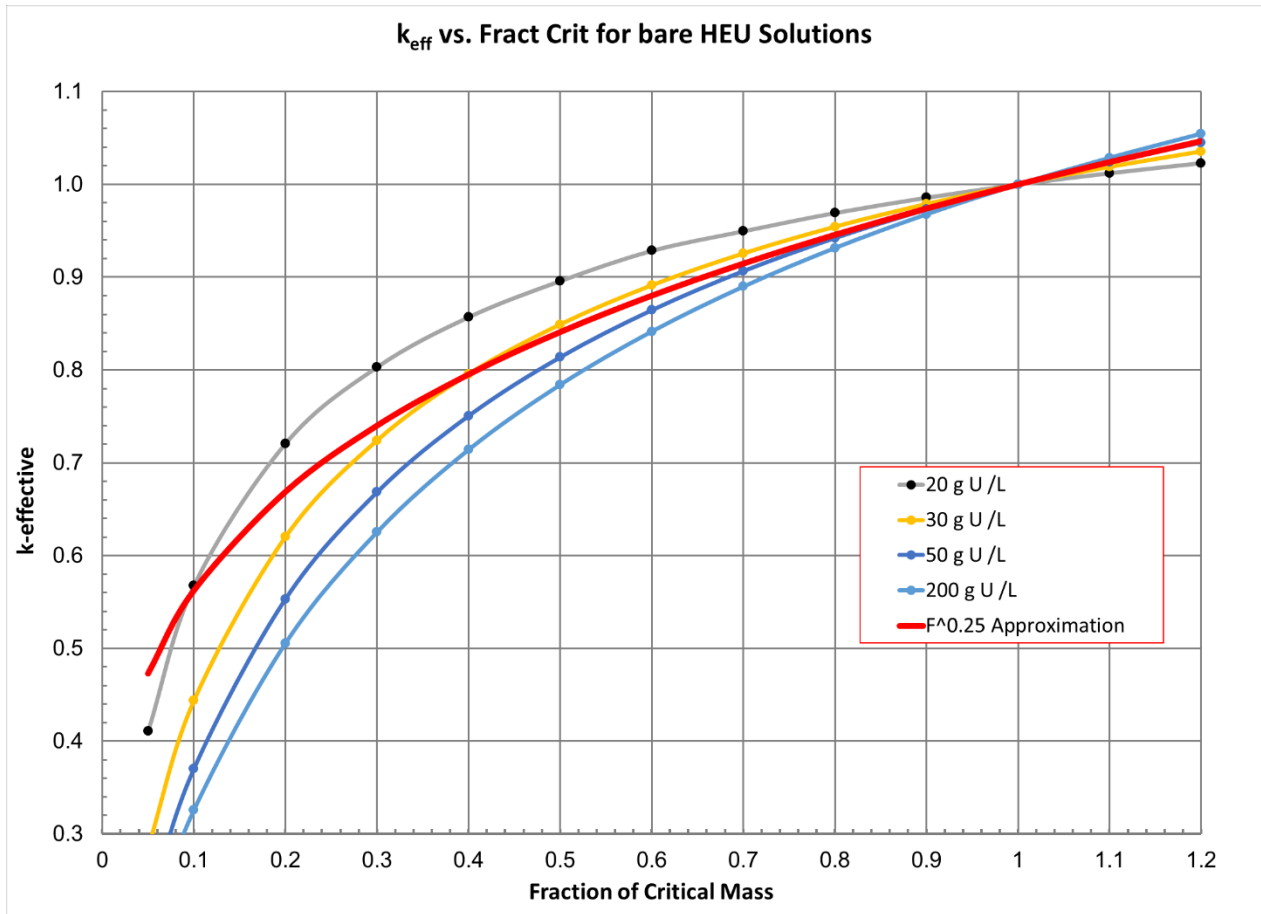Note: the 50 g Pu/L and the 200 g Pu/L curves are almost identical.

Figure B-4. k-effective versus Fraction Critical for HEU Solutions.

Examining the variation in curves for the Pu(4) solutions (figure B-3) indicates that there must be some parameter that causes one curve to have a significant different slope than another (e.g., 20 g Pu/L concentration versus 50 g Pu/L concentration) while two curves have almost identical behavior (e.g., 50 g Pu/L and 200 g Pu/L). Evaluations of the four different concentrations showed that the infinite multiplication factor, k_∞, appeared to play a major role. Table B-4 gives k_∞ for each of the four Pu(4) solution concentrations, and for each of the four U(93.5) solution concentrations. Table B-4 also provides updated critical mass values.[31]

---

[31] Although Reference B-1 provided values for total uranium mass, it is more typical to report values for U-235. Thus, Table B-4 has the critical mass values for HEU solutions reported in kg U-235, and concentrations for HEU solutions are g-U235/liter.

Table B-4. Solution Sphere Critical Masses and k_∞

Material	Concentration (g/liter)	k_∞ from ARH-600	Critical Mass (kg)[32]	
			Unreflected	Water Reflected
Pu(4)	20	1.445	1.09	0.68
Pu(4)	30	1.571	1.06	0.60
Pu(4)	50	1.671	1.29	0.67
Pu(4)	200	1.715	4.03	1.83
U(93.5)	20	1.26	2.71	1.93
U(93.5)	30	1.44	1.69	1.06
U(93.5)	50	1.63	1.54	0.86
U(93.5)	200	1.87	3.21	1.45

Note the significant difference in k_∞ between 20 g Pu /L Pu(4) solution (1.445) and 50 g Pu / L Pu(4) solution (1.671), while the values are very close for 50 g Pu /L Pu(4) solution (1.650) and 200 g Pu / L Pu(4) solution (1.715). Thus, the variation in curve shape and slope may be the result of a variation in the leakage fraction of each system.

From diffusion theory and as discussed Buckling Conversion, Chapter 3, equation 75, shows the relationship between k_{eff} and the bucklings:

$$k_{eff} = \frac{\left(1 + B_m^2 M^2\right)}{\left(1 + B_g^2 M^2\right)}$$

(B.1)

---

[32] As noted in footnote 4, most tables and figures in the literature report uranium solution concentrations and critical masses in relation to U-235 content, critical mass values in this table are for U-235 and the solution concentrations are in grams U-235 per liter. The plutonium solution concentrations and critical masses are for total plutonium.

We can use the diffusion theory definition of $k_\infty = 1 + B_m^2 M^2$ to create equation B.2.

$$k_{eff} = \frac{k_\infty}{\left(1 + B_g^2 M^2\right)}$$

(B.2)

Now we need to relate fraction critical to the bucklings.

$$F = \left(\frac{m_{geom}}{m_{crit}}\right) = \left(\frac{\rho V_{geom}}{\rho V_{crit}}\right) = \left(\frac{V_{geom}}{V_{crit}}\right)$$

$$\frac{B_m^2}{B_g^2} = \left(\frac{\left(\frac{\pi}{\tilde{R}_{crit}}\right)^2}{\left(\frac{\pi}{\tilde{R}_{geom}}\right)^2}\right) = \left(\frac{\tilde{R}_{geom}}{\tilde{R}_{crit}}\right)^2 \quad \text{for large radii,} \quad \left(\frac{\tilde{R}_{geom}}{\tilde{R}_{crit}}\right)^2 \approx \left(\frac{R_{geom}}{R_{crit}}\right)^2$$

(B.3)

$$\left(\frac{R_{geom}}{R_{crit}}\right)^2 = \left(\frac{V_{geom}^{\frac{1}{3}}}{V_{crit}^{\frac{1}{3}}}\right)^2 = \left(\frac{V_{geom}^{\frac{2}{3}}}{V_{crit}^{\frac{2}{3}}}\right) = F^{0.667} \text{ so } \frac{B_m^2}{B_g^2} \approx F^{0.667}$$

The assumption has be made that the ratio of extrapolated radii is approximately equal to the ratio of physical radii. This means that the extrapolation distance is very small compared to the radii, which is a reasonable assumption for solution systems. Now returning to equation B.2 and doing some manipulation, we find a relationship between k_{eff}, k_∞, and fraction critical.

$$k_{eff} = \frac{k_\infty}{\left(1 + B_g^2 M^2\right)} \quad \text{divide both top and bottom by } (k_\infty - 1)$$

$$k_{eff} = \frac{k_\infty/(k_\infty - 1)}{\left(\frac{1}{(k_\infty - 1)} + \frac{B_g^2 M^2}{(k_\infty - 1)}\right)} \text{ now } (k_\infty - 1) = B_m^2 M^2,$$

$$\text{so } k_{eff} = \frac{k_\infty/(k_\infty - 1)}{\left(\frac{1}{(k_\infty - 1)} + \frac{B_g^2 M^2}{B_m^2 M^2}\right)} = \frac{k_\infty/(k_\infty - 1)}{\left(\frac{1}{(k_\infty - 1)} + \frac{B_g^2}{B_m^2}\right)}$$

(B.4)

$$\text{From eqn. B.3, } \frac{B_g^2}{B_m^2} = F^{-0.667} \text{, so } k_{eff} = \frac{k_\infty/(k_\infty - 1)}{\left(\frac{1}{(k_\infty - 1)} + F^{-0.667}\right)}$$

$$\text{and multiplying by } (k_\infty - 1), k_{eff} = \frac{k_\infty/(k_\infty - 1)}{\left(\frac{1}{(k_\infty - 1)} + \frac{(k_\infty - 1)F^{-0.667}}{(k_\infty - 1)}\right)}$$

$$k_{eff} = \frac{k_\infty/(k_\infty - 1)}{\left(\frac{1}{(k_\infty - 1)} + \frac{(k_\infty - 1)F^{-0.667}}{(k_\infty - 1)}\right)} = \frac{k_\infty}{[1 + (k_\infty - 1)F^{-0.667}]}$$

(B.5)

$$\text{so } k_{eff} = f(k_\infty, F) \quad \text{and for a given } k_\infty, \ k_{eff} = F^s$$

Looking at plots of k_{eff} versus F, we see that a single exponent for F , such as 0.25 as shown in Figures B-3 and B-4, will not cover all the solution concentrations. So, for various values of k_∞, the exponent for F was determined with the behavior shown in figure B-5.
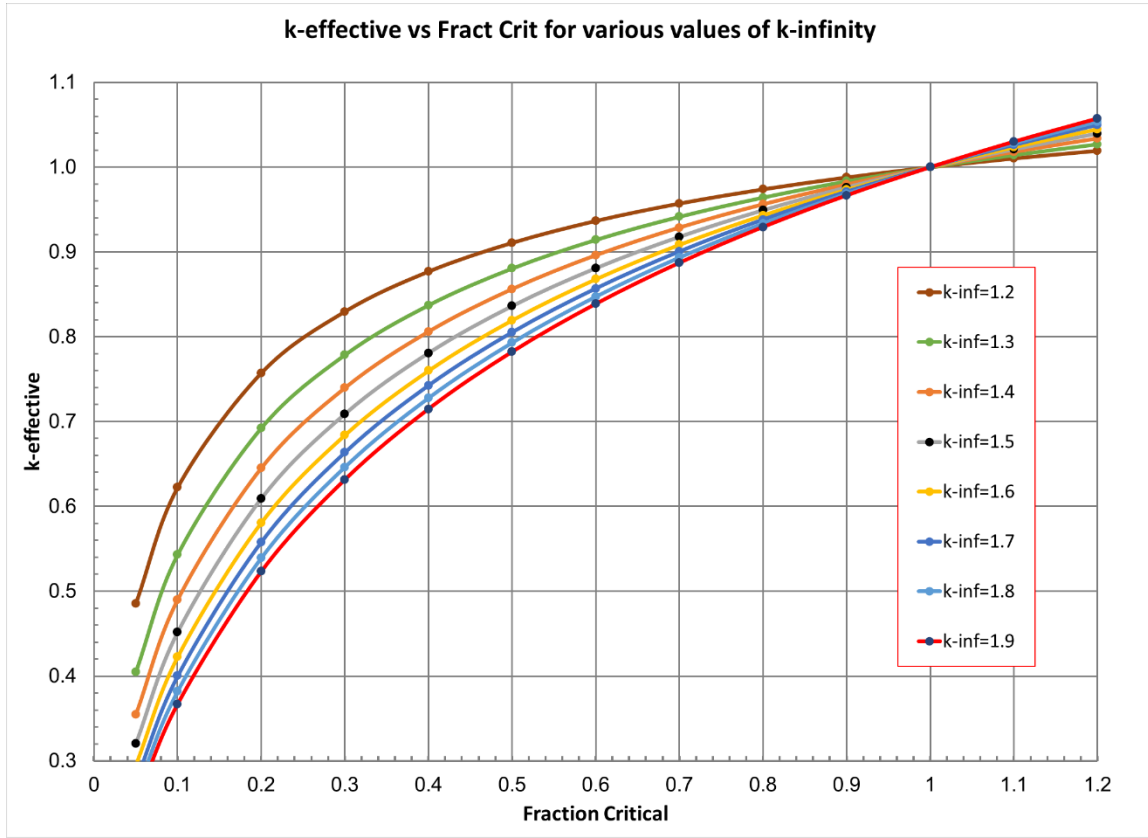

Figure B-5. k-effective versus Fraction Critical for various k_∞ values.

In evaluating the empirical fits, it was determined that for fraction critical values less than 0.3, there was wide variation in the goodness-of-fit (this was likely due to the small system sizes that conflicted with the assumption that extrapolation distance was small compared to the system radius). So empirical fits were applied to the data for fraction critical values from 0.3 to 1.2. For the bare solution systems, it was determined that:

$$s = -0.2784 \quad k_\infty^2 + 1.1768 k_\infty - 0.8649 \, so \, k_{eff} = F^s \text{ for a given } k_\infty \tag{B.6}$$

LEU Solution Systems

For this publication, critical mass values for low enriched uranium (LEU) solutions ($U(5)O_2$-H_2O) and infinite multiplication factors have been calculated and are presented in Table B-5.

Table B-5..LEU Solution Sphere Critical Masses and k_∞

Material	Concentration (g U-235/liter)	k_∞ from ARH-600, Reference B3	Critical Mass (kg U-235)	
			Unreflected	Water Reflected
$U(5)O_2$	20	1.129	6.33	4.84
$U(5)O_2$	30	1.268	3.40	2.29
$U(5)O_2$	50	1.388	3.07	1.83
$U(5)O_2$	70	1.430	3.69	2.08
$U(5)O_2$	100	1.443	5.09	3.01

It was found that the LEU bare solution systems also followed the empirical fit given as equation 3.6. For values of fraction critical greater than or equal to 0.30, the empirically determined k_{eff} was within 1 % of the calculated value for solution concentrations from 0.02 g U235 /cc through 0.10 g U235/cc..

Reflected Solution Systems

Although all three bare solution systems (Pu(4)-H_2O, U(93.5)-H_2O, and U(5)O_2-H_2O) followed the same empirical fit, this was not the case for the reflected systems. For these systems, a reflected polynomial was calculated by creating a second-order polynomial fit to the plot of ($s_{bcalc} - s_{refl}$) versus k_∞, which gave an equation of the form: $\Delta s = ck_\infty^2 + dk_\infty + e$. Then the empirical fit for the reflected exponent, s_{refl}, is:

$$s_{refl} = s_{bfit} - \Delta s = (-0.2784 - c)k_\infty^2 + (1.1768 - d)k_\infty + (-0.8649 - e)$$

(B.7)

The fits for the reflected systems are:

$$Pu(4) - H_2O : s_{refl} = -0.6234k_\infty^2 + 2.1042k_\infty - 1.5258 \quad \text{and} \quad k_{eff} = F^s$$

(B.8)

$$U(93.5) - H_2O : s_{refl} = -0.3077k_\infty^2 + 1.1732k_\infty - 0.8410 \quad \text{and} \quad k_{eff} = F^s$$

(B.9)

$$U(5)O_2 - H_2O : s_{refl} = -0.4240k_\infty^2 + 1.4661k_\infty - 1.0276 \quad \text{and} \quad k_{eff} = F^s$$

(B.10)

With these fits, all of the empirically determined keff values for fraction criticals of 0.3 or greater are within 1 % of the calculated values.

The adequacy of a single fit for bare systems results from leakage (and hence k_∞) being the dominant process. However, when reflection is added to the systems, the neutron energy spectrum is changed, so each of the three, reflected solution systems requires an individual empirical fit.

Solution System Plots

For the three types of solutions systems, plots of keff versus fraction critical are provided to demonstrate variation from a simple $k_{eff} \approx F^{0.25}$ fit.

Pu(4)-H$_2$O Solutions

Shown in Figure B-6 is the plot for a bare plutonium solution system while Figure B-7 is the plot for a plutonium solution system reflected with 30 cm of water.
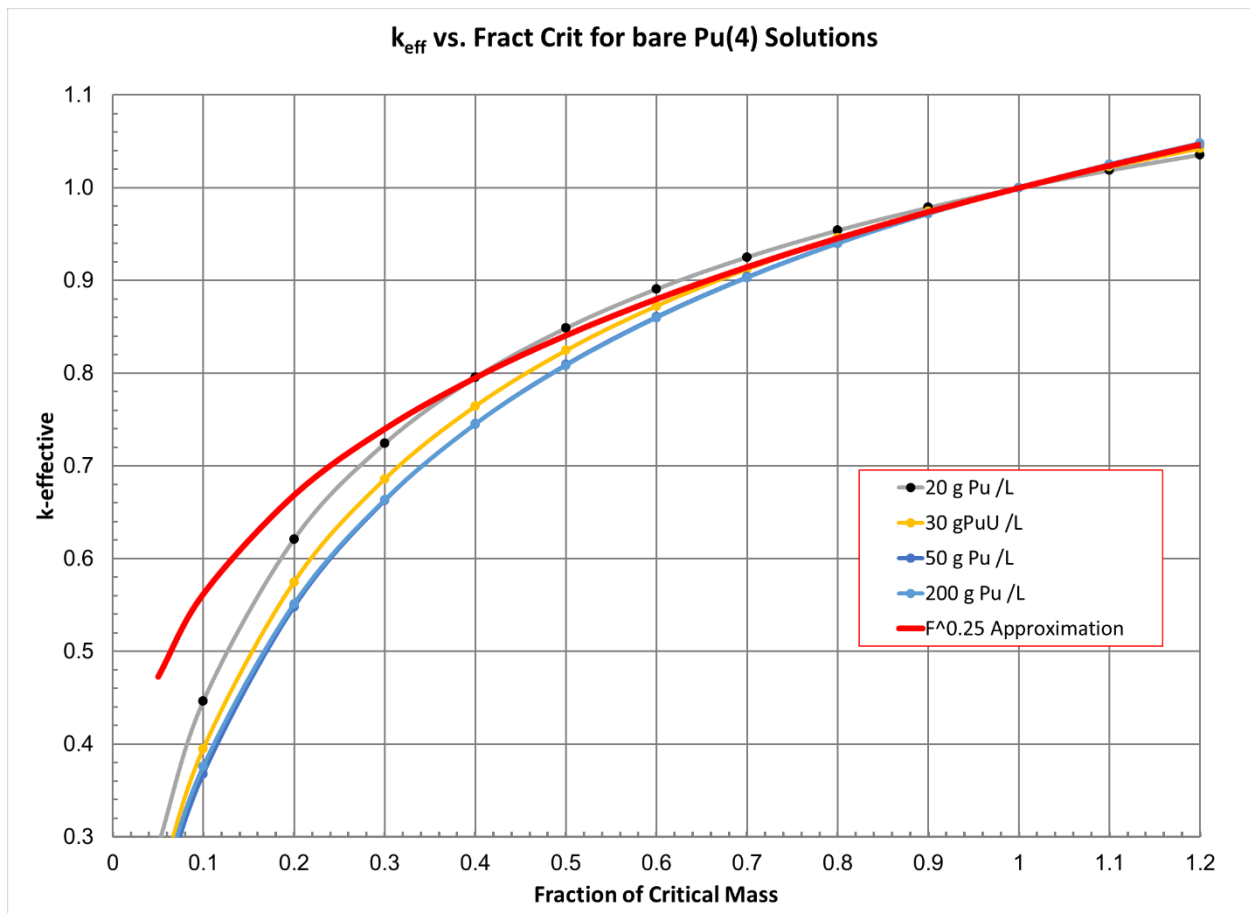

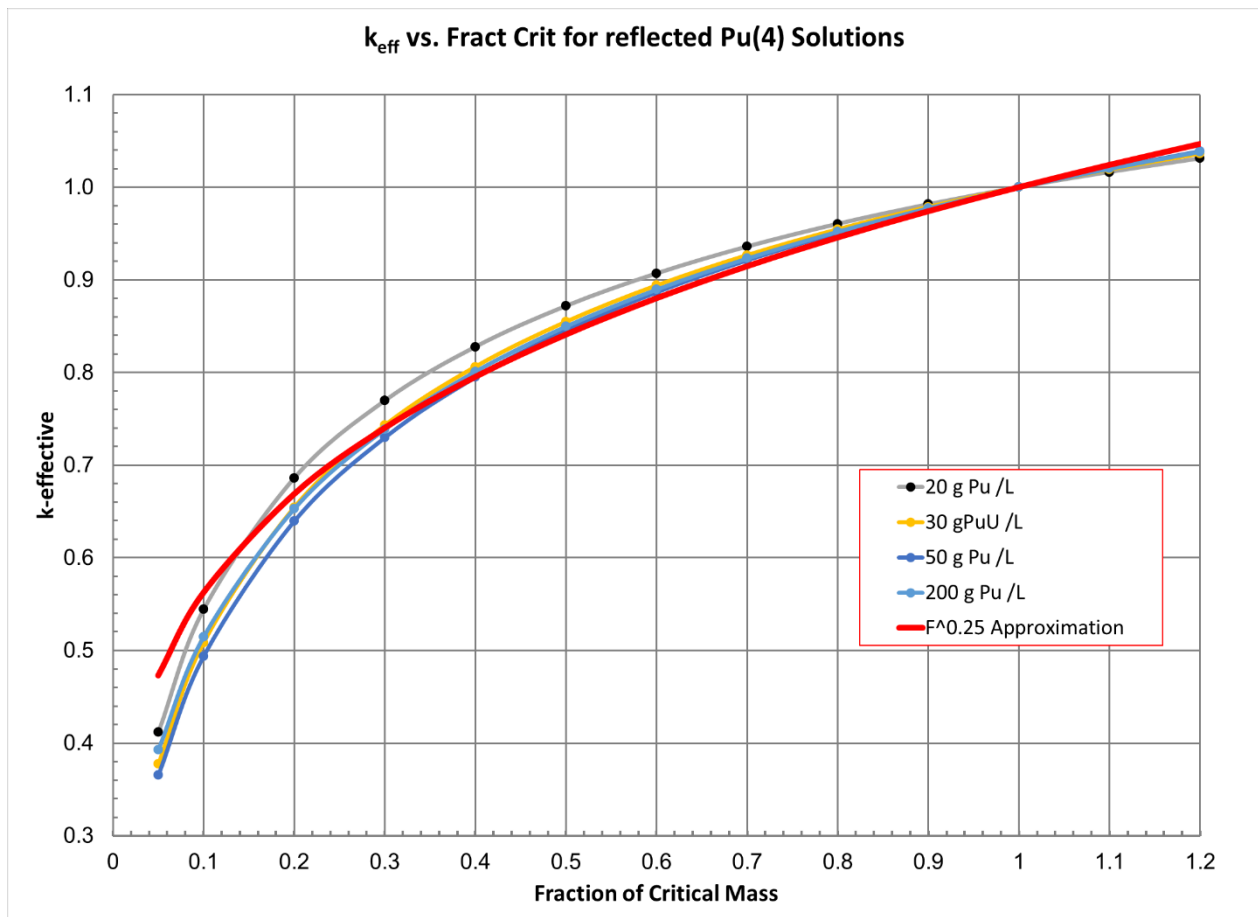**Figure B-6. k$_{eff}$ vs. Fraction of Critical Mass: Bare Pu(4) Solution**

Figure B-7. k_{eff} **vs. Fraction of Critical Mass: Reflected Pu(4) Solution**

U(93.5)-H$_2$O Solutions

Shown in Figure B-8 is the plot for a bare uranium solution system while Figure B-7 is the plot for a uranium solution system reflected with 30 cm of water.
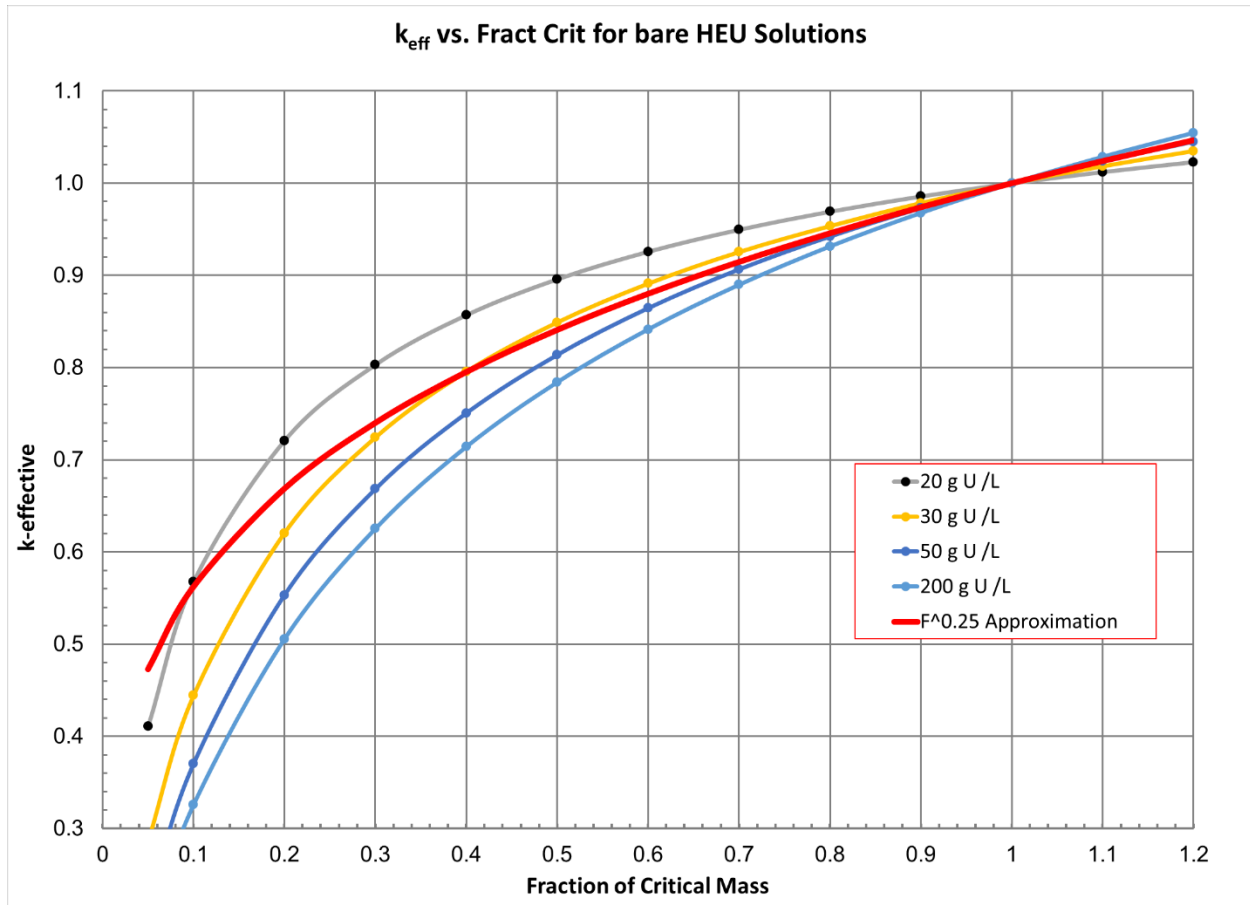

Figure B-8. k$_{eff}$ vs. Fraction of Critical Mass: Bare U(93.5) Solution
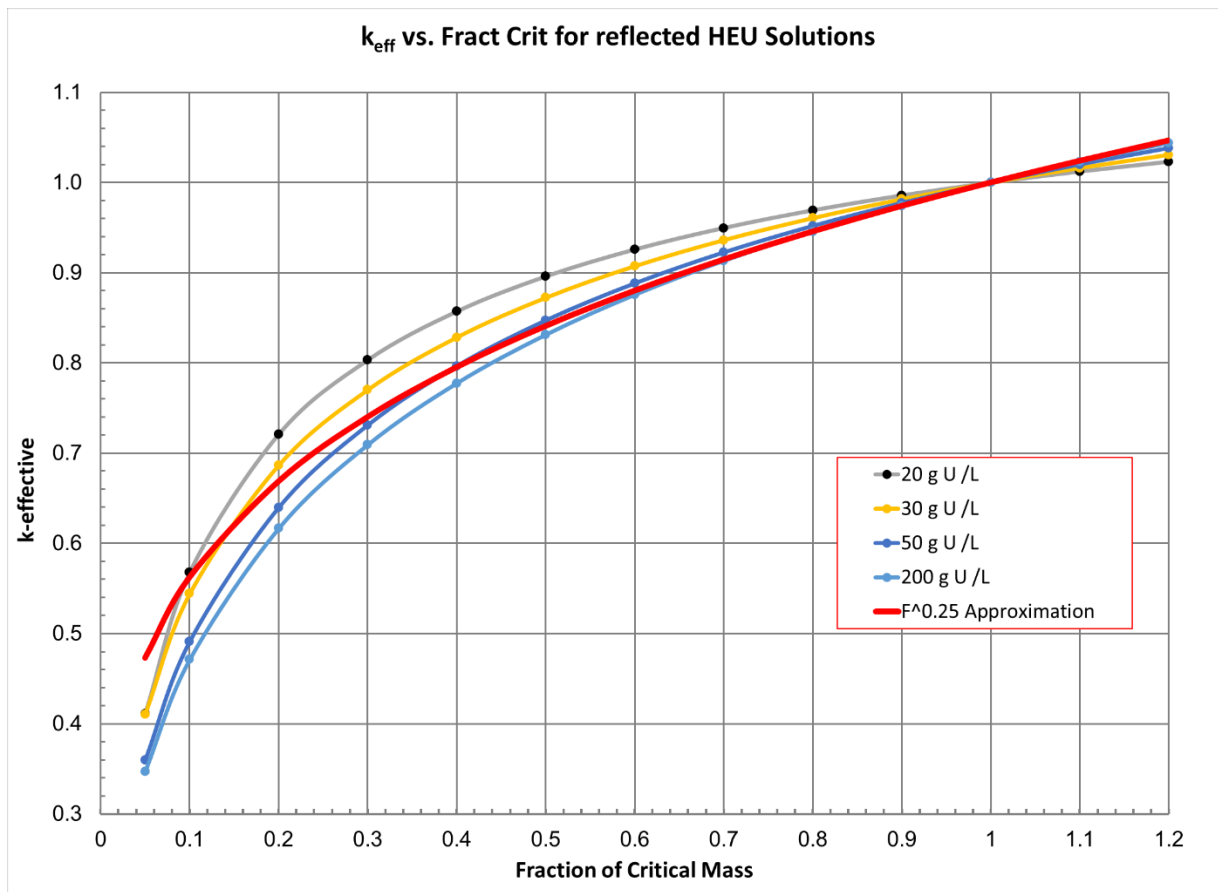
Figure B-9 k_{eff} vs. Fraction of Critical Mass: Reflected U(93.5) Solution

LEU Solution Systems

This information was not part of O'Dell's original report but is calculated for this publication. Figures B-10 and B-11 provide the multiplication factor data as a function of the fraction of critical mass for low-enriched uranium (LEU) solutions of varying concentrations. Figure B-10 is for bare systems while Figure B-11 is for water reflected systems.
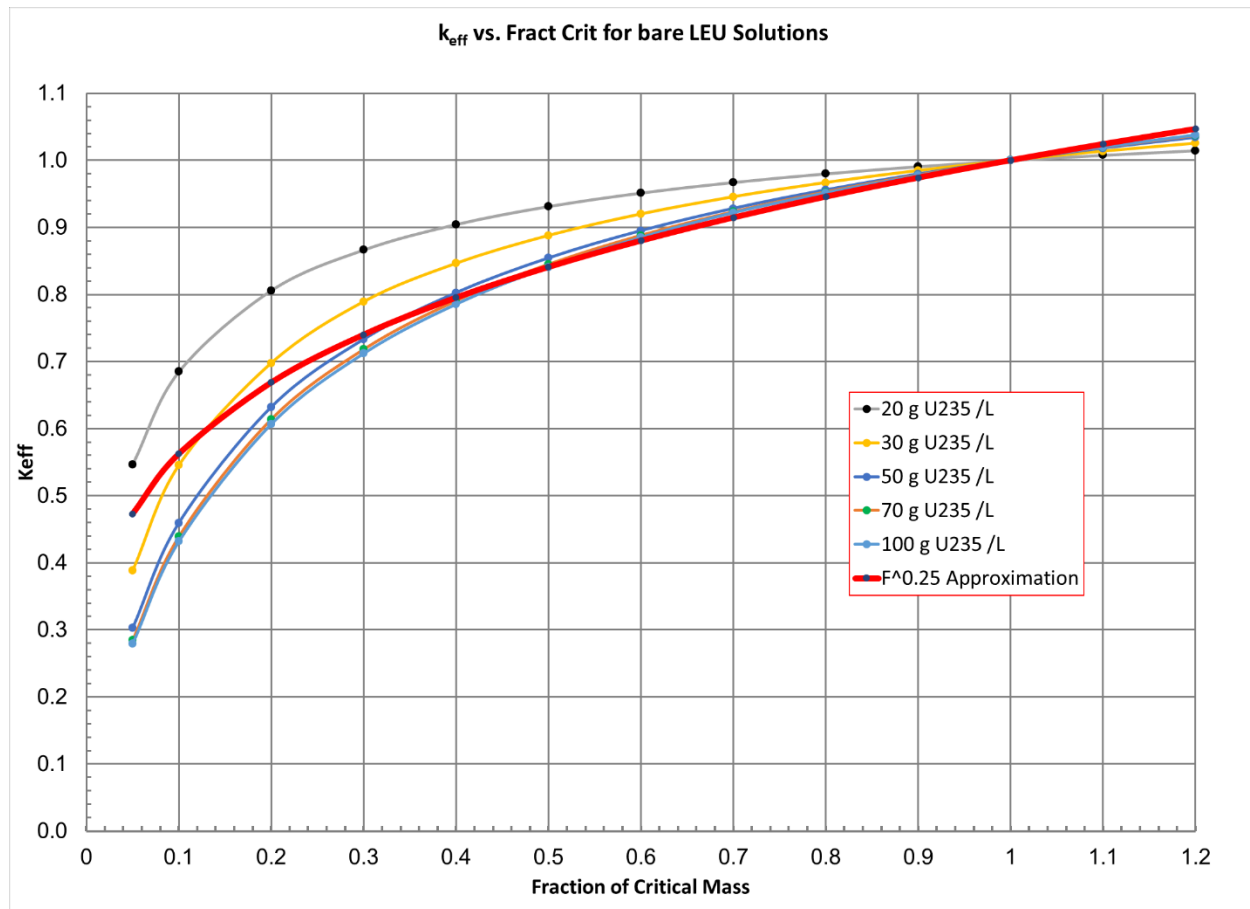

Figure B-10. k_{eff} vs. Fraction of Critical Mass: Bare LEU Solution

In Figure B-11, note the 70 gU235/L curve is hidden under the 100 gU235/L curves, also note that all three higher concentration systems (i.e., 50 gU235/L, 70 g U235/L, and 100 gU235/L) are very close throughout the entire range of fraction critical values.
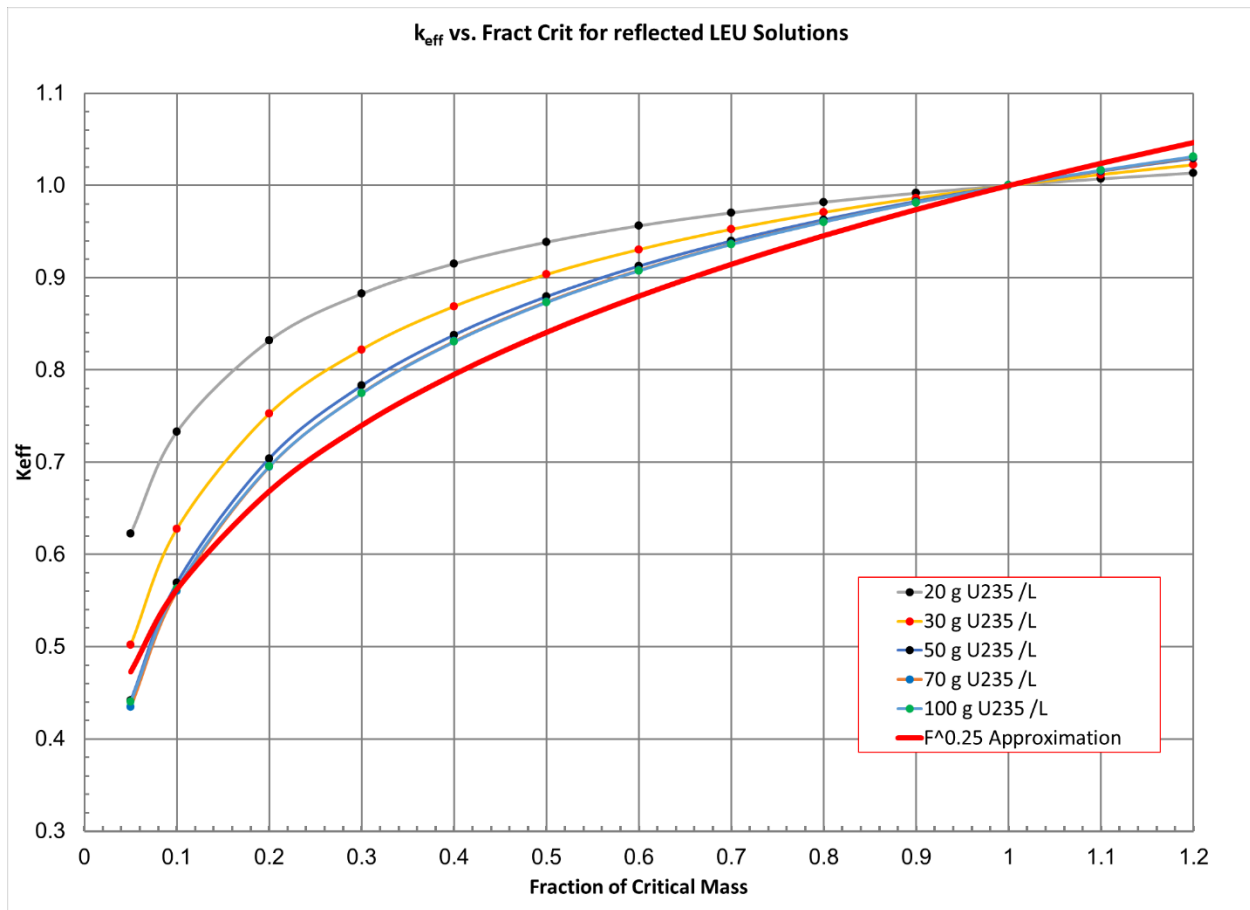

Figure B-11. k_{eff} vs. Fraction of Critical Mass: Water Reflected LEU Solution

Example Problem – Determine the k_{eff} for bare and reflected uranium systems with a fraction critical = 0.5. Compare the results for: Uranium Metal (18.74 gU/cc), HEU Solution (0.05 gU235/cc), and LEU Solution (0.05 gU235/cc).

For Uranium Metal, Table B-1 gives a critical mass of 53.8 kg U for a bare system and a critical mass of 24.4 kg U for a reflected system. For metals, the $k_{eff} \approx F^{0.3}$, so:

$$k_{eff} \approx F^{0.3} \text{ with } F = 0.5, k_{eff} \approx (0.5)^{0.3} = 0.812$$

Notice that this is the same for both bare and reflected. However, it was noted that reflected uranium metal systems tend to follow a slightly different relationship where $k_{eff} \approx F^{0.274}$, so:

$$k_{eff} \approx F^{0.274} \text{ with } F = 0.5, k_{eff} \approx (0.5)^{0.274} = 0.827$$

The computer calculated values are 0.821 for the bare system (mass = 26.9 kg U(93.5)) and 0.844 for the reflected system (mass = 12.2 kg U(93.5)); a difference of about 1% for the bare system and 2% for the reflected system.

For HEU Solutions at 0.05 gU235/cc, Table B-4 gives $k_\infty = 1.63$, a critical mass of 1.54 kg U235 for a bare system and a critical mass of 0.86 kg U235 for a reflected system. For the HEU systems, values are reported based on U-235 content. For bare solutions, the exponent is given by equation B.7:

$$s = -0.2784 \quad k_\infty^2 + 1.1768 k_\infty - 0.8649$$

With $k_\infty = 1.63$:

$$s = -0.2784(1.63)^2 + 1.1768(1.63) - 0.8649 = 0.314$$
$$k_{eff} \approx F^{0.314} \text{ with } F = 0.5, k_{eff} \approx (0.5)^{0.314} = 0.804$$

This compares with a computer calculated value of 0.814 for the bare solution system (mass = 0.77 kg U-235). For reflected HEU systems, the exponent is given by equation B.9:

$$s = -0.3077 k_\infty^2 + 1.1732 k_\infty - 0.8410$$

With $k_\infty = 1.63$:

$$s = -0.3077(1.63)^2 + 1.1732(1.63) - 0.8410 = 0.254$$
$$k_{eff} \approx F^{0.254} \text{ with } F = 0.5, k_{eff} \approx (0.5)^{0.254} = 0.839$$

This compares with a computer calculated value of 0.847 for the reflected solution system (mass = 0.43 kg U-235).

For LEU Solutions at 0.05 gU235/cc, Table B-5 gives $k_\infty = 1.388$, a critical mass of 3.07 kg U235 for a bare system and a critical mass of 1.83 kg U235 for a reflected system. For bare solutions, the exponent is given by equation B.7:

$$s = -0.2784k_\infty^2 + 1.1768k_\infty - 0.8649$$

With $k_\infty = 1.388$

$$s = -0.2784(1.388)^2 + 1.1768(1.388) - 0.8649 = 0.232$$

$$k_{eff} \approx F^{0.232} \text{with } F = 0.5, k_{eff} \approx (0.5)^{0.232} = 0.851$$

This compares with a computer calculated value of 0.854 for the bare solution system (mass = 1.535 kg U-235). For reflected LEU systems, the exponent is given by equation B.10:

$$s = -0.4240k_\infty^2 + 1.4661k_\infty - 1.0276$$

With $k_\infty = 1.388$:

$$s = -0.4240(1.388)^2 + 1.4661(1.388) - 1.0276 = 0.190$$

$$k_{eff} \approx F^{0.190} \text{with } F = 0.5, k_{eff} \approx (0.5)^{0.190} = 0.877$$

This compares with a computer calculated value of 0.879 for the reflected solution system (mass = 0.915 kg U-235).

The k_∞ values were obtained from the tables in this Appendix based on Reference B3. For systems other than those described here, k_∞ values can be obtained from Handbooks such as Reference B3 to allow the calculation of k_{eff} for systems other than those described here.

SUMMARY - Perhaps the most notable result of these analyses is the extreme nonlinearity of k_{eff} as a function of F. In particular, for low values of F (less than 0.2 of a critical mass), k_{eff} rises very quickly to values of 0.5 to 0.7. Note also that a k_{eff} of 0.9 is obtained with less than 70% of a critical mass.

References

B1. R. Douglas O'Dell, k_{eff} vs. Fraction of Critical Mass, ESH-6-96-092, Los Alamos National Laboratory, June 10, 1996.

B2. J.T. THOMAS, "Remarks on Array Criticality Techniques," Proceedings of the Livermore Array Symposium, CONF-680909, pages 67-78, (September 1968).

B3. R.D. Carter, et al., "Criticality Handbook Vol. I, II, and III," Atlantic Richfield Hanford Co. Report ARH-600 (1968).