Hand Calculation Methods for Criticality Safety – A Primer

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Edited by Faith Harp, Group IM-1

About the Cover: A photograph of horizontally aligned 6" diameter tanks used to store plutonium solution at the plutonium facility at TA-55.

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Hand Calculation Methods for Criticality Safety – A Primer

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Hand Calculation Methods for Criticality Safety – A Primer

by

Douglas G. Bowen and Robert D. Busch

Abstract

The purpose of this primer is to provide an overview of the most common hand calculation methods used for criticality safety calculations. The most widely used tools available to a criticality safety 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 that a particular fissile system may be sensitive to, whereas the hand calculation methods can be used to delve into the ways each parameter may affect the reactivity of a fissile material system. Further, 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. Some time investment will be needed to master the methods that could be most useful; however, they can provide the practitioner with very 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 quicker than using a criticality code.
1. Overview of Hand Calculation Methods

1.1 Introduction

The nuclear criticality safety practitioner has many tools available 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 that a particular fissile system may be sensitive to, 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 ($\text{NB}_N^2$) method
- Solid angle method

The goal of this primer is to provide 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. Further, the hand methods can be used for parametric studies that identify which criticality safety parameters a fissile system may be sensitive to.

1.2 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 to 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. Further, 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, $k_\infty$, 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 $k_\infty$ 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.

1.3 Choosing the Appropriate Method

The biggest challenge in applying these hand calculation methods to physical problems is choosing the appropriate or best method. The discussion that accompanies each hand method includes the applicability for the particular method and its limitations. For example, if a solid chunk of plutonium or uranium metal is being machined in a particular fissile material operation, 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:

1. Overview of the method
2. Applicability of the method to solve certain problems
3. Example problems solved step-by-step

1.4 Single Unit Hand Calculations

The methods listed in Table 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.

Table 1. Single Unit Methods and Applicability Summary

<table>
<thead>
<tr>
<th>Single Unit Hand Calculation Method</th>
<th>Applicability Summary</th>
</tr>
</thead>
</table>
| 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. |
1.5 Array Hand Calculations

The methods listed in Table 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 NBx^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 2. Array Methods and Applicability Summary

<table>
<thead>
<tr>
<th>Array Hand Calculation Method</th>
<th>Applicability Summary</th>
</tr>
</thead>
</table>
| 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 (NBx^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 exists for powders, metals, up to an H/X of about 20 for some fissile materials  
  • Data exists 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 meters, 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. |

1.6 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. In the example problems presented here, many have been verified using the following code packages and data:

- MCNP5
- SCALE5, Keno V.a
- DANTSYS
- Physical Dimensions

Chapter 9 presents the results of this verification effort. The purpose for this effort is to demonstrate the usefulness and accuracy of the various hand calculation methods and assist the criticality safety practitioner choose 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, $k_\infty$, and critical dimensions for simple fissile systems
- Interpret the results provided by one-group diffusion theory

2.2 Overview of Diffusion Theory

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 this discussion 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 2).

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

In this equation, $\phi$ is the one-group or single energy neutron flux (neutrons/cm$^2$-sec), $D$ is the one-group diffusion coefficient (cm), $\Sigma_a$ is the macroscopic absorption cross-section (cm$^{-1}$), $\Sigma_f$ is macroscopic fission cross-section (cm$^{-1}$), $\nu$ 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.

For a fissile system to maintain a fission chain reaction, 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 on the basis of these production and loss effects as follows.

\[
\begin{array}{c}
\text{Net rate of gain of neutrons per unit volume} \\
\text{Rate of production of neutrons by fission per unit volume} \\
\text{Rate of loss of neutrons per unit volume by leakage and absorption}
\end{array}
\]

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$^3$).
\[
\frac{1}{v} \frac{d\phi}{dt} = -(D \nabla^2 \phi) - \Sigma_a \phi + \nu \Sigma_f \phi
\]

\[
\frac{1}{v} \frac{d\phi}{dt} = \frac{dn}{dt} = -\text{Leakage - Absorption + Production}
\]

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

\(-D \nabla^2 \phi\) 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).

\(\Sigma_a \phi\) 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).

\(\nu \Sigma_f \phi\) 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).

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

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 one-speed diffusion equation can be written as

\[-(-D \nabla^2 \phi) - \Sigma_a \phi + \nu \Sigma_f \phi = 0,\]

or if written as the neutron balance and setting \(\frac{1}{v} \frac{dn}{dt} = 0\),

\[-\text{Leakage - Absorption + Production} = 0.\]

If the diffusion equation is rearranged slightly, then

\[\nu \Sigma_f \phi = (-D \nabla^2 \phi) + \Sigma_a \phi\]

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

\[\nabla^2 \phi + \left(\frac{\nu \Sigma_f - \Sigma_a}{D}\right) \phi = 0.\]
Note that this is in the form $\nabla^2 \phi + B^2 \phi = 0$, where $B^2$ is equal to a constant,

$$
B^2 = \text{constant} = \left( \frac{\nu \Sigma_f - \Sigma_a}{D} \right).
$$

The term, $B^2$, in this form is a function of only the material properties of the system. Note that no geometric dependencies are present. 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, $B^2$, 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 one-dimensional slab (1-D), for example, the steady state diffusion equation can then be solved.

Recall from before that $\nabla^2 \phi + B^2 \phi = 0$ where $B^2$ is equal to a constant:

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

Knowing that $\nabla^2 \phi = \left( \frac{d^2 \phi}{dx^2} \right)$, the diffusion equation for a one-dimensional slab with thickness, $x$, can be rewritten as

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

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

A complete solution for the 1-D 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,
3. \[\frac{d\phi}{dx}\bigg|_{x=\text{centerline}} = 0\] (symmetry condition), and
4. $\phi(x)\bigg|_{x=\text{outside edge}} = 0$.

We need two boundary conditions for the 1-D slab, 3 and 4, to obtain a complete solution to this problem.

Figure 1 will assist with completing the solution to the 1-D slab example.
Appendix A provides an in-depth discussion of the linear extrapolation distance. On the basis of this discussion of extrapolation distance and vacuum boundary conditions, the following relationship can be defined; it states where the mathematical representation of the neutron flux is zero:

\[ X' = X + d, \]

where

\[ X = \text{one-half of the slab thickness} \]
\[ d = 2D \text{ or } 0.71 \lambda_{ir}, \text{ as defined and discussed in Appendix A}. \]

Thus, the neutron flux vanishes at the extrapolated boundary, which lies approximately 0.71\( \lambda_{ir} \) beyond the physical boundary. To take advantage of symmetry, consider the center of the slab to be at \( x = 0 \). Thus, the boundary conditions can then be used to find the diffusion theory solution.

The boundary condition is expressed as \( \frac{d\phi}{dx} \big|_{\text{centerline}} = 0 \) (symmetry condition). Thus,

\[ \phi(x) = A \cos Bx + C \sin Bx; \text{ then } \frac{d\phi}{dx} = -AB \sin Bx + CB \cos Bx \text{ at } x = 0: \]

\[ -AB \sin 0 + CB \cos(0) = 0 \]
\[ 0 + CB(1) = 0. \]

Thus, \( C = 0. \) The flux equation can then be written as follows, based on the result of applying the first boundary condition, #3.

\[ \phi(x) = A \cos Bx. \]
Now, the boundary condition, #4, can be applied to this system to complete the solution for the 1-D slab. This boundary condition is used to determine the value for $B$. 

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

Now $\cos BX' = 0$ whenever $BX' = \frac{n\pi}{2}$.

$B$ is the last variable left in this equation, so solve for $B$: $B = \frac{n\pi}{2X'}$.

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

$$B = \frac{\pi}{2X'}, \text{ where, from Figure 1, } X' = X + d,$$

$$B = \frac{\pi}{2X + 2d} = \frac{\pi}{d + 2X + d}.$$ 

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

The remaining variable to determine is the value for $A$. $A$ is the amplitude of the flux and 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 problem because two different values for $B^2$ have been defined.

$$B_m^2 = \left(\frac{\nu\Sigma_f - \Sigma_a}{D}\right) \text{ and } B_g^2 = \left(\frac{\pi}{2X'}\right)^2$$

These values for $B^2$ are not incorrect. The first definition is known as the material buckling, $B_m^2$, and is dependent on the materials in the system. The second definition is known as the geometrical buckling, $B_g^2$, and is only dependent upon the geometrical properties of the system.

If the geometric buckling, $B_g^2$, is the solution to the steady state diffusion equation, 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 only applicable 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 and material buckling can be used to identify subcritical and supercritical systems as follows.

As previously stated,

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

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

$$B_m^2 < B_g^2 \text{ then } k < 1 \text{ (Subcritical).}$$
In other words, within a fixed fissile material geometry, the geometric buckling is constrained. If more fissile material is present than will fill the geometry, the material buckling exceeds the geometric buckling and the system is supercritical. If there is less fissile material than needed to fill the geometry, 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 (\(\frac{\delta \phi}{\delta t} > 0\)), then the multiplication factor exceeds 1, which is indicative of a supercritical system. If the rate of change of the neutron flux is negative (\(\frac{\delta \phi}{\delta t} < 0\)), 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 (\(\frac{\delta \phi}{\delta t} = 0\)), then the system is at a critical condition, which indicates 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 and geometric bucklings 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.

\[
\text{Change in the Neutron Density} = \text{Production} - \text{Absorption} - \text{Leakage}
\]

or

\[
\text{Change in the Neutron Density} = \text{Function of } (\Delta B_m^2, \Delta B_g^2)
\]

### 2.2.2 Correction for Thermal Systems in One-Group Diffusion Theory

For the discussion about modified one-group diffusion theory, it is beneficial to discuss the difference between the effective multiplication factor (\(k_{\text{eff}}\)) and the infinite multiplication factor (\(k_{\infty}\)). The \(k_{\text{eff}}\) is the multiplication factor of a finite system and considers neutron leakage, neutron absorption, and neutron production. The \(k_{\infty}\) is the infinite 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, \(\nu \Sigma_f\), can be written as follows:

\[
\nu \Sigma_f = k_{\text{eff}} \Sigma_a.
\]

This relationship can be derived from the four-factor formula as follows:
Thus, the "corrected" diffusion equation can be written as follows for a finite system:

\[ k_a = \eta e pf, \]
\[ \eta f = \frac{v \Sigma_{\text{fuel}}^f}{\Sigma_u} * \frac{\Sigma_{\text{fuel}}}{\Sigma_{\text{system}}} = \frac{v \Sigma_{\text{fuel}}^f}{\Sigma_{\text{system}}}, \]

The terms \( \epsilon \) and \( p \) are correction factors to account for:

\( \epsilon \) — the increase in the number of fissions in the system caused by fast fission 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, \( \epsilon \) and \( p \) allow for a one-group equation to be generated with correction factors to consider two-group effects. In reality, 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 thermal system.

\[ \epsilon \eta \Sigma_f = k_a \Sigma_a. \]

Thus, the “corrected” diffusion equation can be written as follows for a finite system:

\[ \frac{1}{v} \frac{d\phi}{dt} = k_a \Sigma_a \phi - \Sigma_a \phi - (-D \nabla^2 \phi) \]

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,

\[ \frac{1}{v} \frac{d\phi}{dt} = \Sigma_a (k_a - 1)\phi + D \nabla^2 \phi = 0 \quad \text{or} \]

\[ \nabla^2 \phi + \frac{\Sigma_a}{D} (k_a - 1)\phi = 0. \]

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

\[ L_g = \sqrt{\frac{D}{\Sigma_a}}. \]

Substituting this into the modified one-group diffusion equation, for a steady-state system, yields

\[ \nabla^2 \phi + \left(\frac{k_a - 1}{L^2}\right) \phi = 0 \quad \text{or} \quad \nabla^2 \phi + B_m^2 \phi = 0, \]

where \( B_m^2 = \left(\frac{k_a - 1}{L^2}\right). \)
This equation can be rearranged as follows:

\[ 1 + \frac{B_m^2L_t^2}{k_-} \quad \text{or} \quad 1 = \frac{k_-}{1 + \frac{B_m^2L_t^2}{k_-}}. \]

Now, the general equation for a critical condition can be written as follows to determine the nonleakage probability expressions for a critical system:

\[ k_- P_L = 1, \]

where \( P_L \) is the nonleakage probability; therefore, if

\[ k_- P_L = 1 = \frac{k_-}{1 + \frac{B_m^2L_t^2}{k_-}} \]

then the nonleakage probability is

\[ P_L = \frac{1}{1 + \frac{B_m^2L_t^2}{k_-}}. \]

For a critical system, recall that \( B_m^2 = B_g^2 \); therefore, the nonleakage probability can be written

\[ P_L = \frac{1}{1 + \frac{B_g^2L_g^2}{k_-}}. \]

### 2.2.3 Modified One-Group Diffusion Theory

Even corrected for fast fission and resonance absorption, one-group diffusion theory still does not consider moderation 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 \( \tau \), known as the neutron age (cm\(^2\)). 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 \( \tau \), the non-thermal or fast non-leakage probability, \( P_f \), is defined as:

\[ P_f = \frac{1}{1 + \frac{B_m^2\tau}{k_-}} \]

then the six-factor formula for a critical system in modified one-group diffusion theory is

\[ k_- P_{th} P_f = 1 \quad \text{or} \quad \eta \epsilon \rho \phi P_{th} P_f = 1. \]

where \( P_{th} = \frac{1}{1 + \frac{B_m^2L_{th}^2}{k_-}} \) is the thermal non-leakage probability.
If the expressions for the nonleakage probabilities are written out, then the six-factor formula becomes:

\[
\frac{k_{\infty}}{1 + B_g^2 \tau \left(1 + B_g^2 L_{th}^2\right)} = 1 \quad \text{where} \quad L_{th}^2 = \frac{D_{th}}{\Sigma_{\alpha_h}}
\]

Now if the fourth order term in \(B_g\) is ignored, then

\[
\frac{k_{\infty}}{1 + B_g^2 \left(\tau + L_{th}^2\right)} = 1 \quad \text{or} \quad \frac{k_{\infty}}{1 + B_g^2 M^2} = 1
\]

where \(M^2 = \tau + L^2\), is the migration area.

This is the expression for a critical system in modified one-group diffusion theory.

2.3 **Applicability of One-Group Diffusion Theory**

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.

2.4 **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, this method can best be used for homogeneous systems that contain moderating materials.

2.5 **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 one another to show the usefulness and limitations of the methods for various systems.
2.5.1 Diffusion Theory Example Problem 1

Assume a slab tank (Figure 2) contains a mixture of water and pure plutonium-239 ($^{239}$Pu) with a $^{239}$Pu concentration of 100 grams per liter at 20 °C.

Using the data in Table 3, determine the following for this particular system to support the design for a slab tank that will contain a pure $^{239}$Pu solution.

1. The infinite multiplication factor, $k_{\infty}$.
2. The critical slab thickness using one-group diffusion theory.
3. The critical slab thickness for this problem using modified one-group diffusion theory.

Figure 2. Slab Tank Containing a $^{239}$Pu Metal-Water Mixture for Diffusion Theory Example Problem 1
Table 3. Diffusion Theory Example Problem 1 Data

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Parameter</th>
<th>Data Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{239}$Pu</td>
<td>$\sigma_{a}$ (2200 m/s)</td>
<td>1011.3 barns</td>
<td>2, Table II.2, pg. 643</td>
</tr>
<tr>
<td></td>
<td>$\sigma$ (2200 m/s)</td>
<td>742.5 barns</td>
<td>2, Table II.2, pg. 643</td>
</tr>
<tr>
<td></td>
<td>$\nu$</td>
<td>2.871</td>
<td>2, Table 3.4, pg. 70</td>
</tr>
<tr>
<td></td>
<td>$g_{a}$ (non-1/$v$ factor) for 20 °C</td>
<td>1.0723</td>
<td>2, Table 3.2, pg. 63</td>
</tr>
<tr>
<td></td>
<td>$g_{f}$ (non-1/$v$ factor) for 20 °C</td>
<td>1.0487</td>
<td>2, Table 3.2, pg. 63</td>
</tr>
<tr>
<td>Water</td>
<td>$\sigma_{a}$ (2200 m/s)</td>
<td>0.332 b</td>
<td>2, Table II.2, pg. 643</td>
</tr>
<tr>
<td></td>
<td>$\nu$</td>
<td>2.871</td>
<td>2, Table 3.4, pg. 70</td>
</tr>
<tr>
<td></td>
<td>$\sigma$ (2200 m/s)</td>
<td>0.28 mb</td>
<td>2, Table II.2, pg. 643</td>
</tr>
<tr>
<td></td>
<td>$\tau$</td>
<td>27 cm$^2$</td>
<td>2, Table 5.3, pg. 215</td>
</tr>
<tr>
<td></td>
<td>$D$</td>
<td>0.16 cm</td>
<td>2, Table 5.2, pg. 210</td>
</tr>
</tbody>
</table>

$D_{\text{mixture}} = D_{\text{water}}$

$\tau_{\text{mixture}} = \tau_{\text{water}}$

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.

Part 1. Because $^{239}$Pu 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 3. 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 $^{239}$Pu varies as a function of the temperature of the system.

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

For $^{239}$Pu,

$$\bar{\sigma}_{a} = \frac{\sqrt{\pi}}{2} g_{a} \sigma_{a} (2200) = 0.886 \times 1.0723 \times 1011.3 = 961 \text{ b},$$

$$\bar{\sigma}_{f} = \frac{\sqrt{\pi}}{2} g_{f} \sigma_{f} (2200) = 0.886 \times 1.0487 \times 742.5 = 690 \text{ b}.$$
For Water ($H_2O$), the cross-section adjustment for hydrogen is expressed as

$$\bar{\sigma}_{a(hyd)} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(hyd)} (2200) = 0.886 \times 1.0 \times 0.332 \text{ b} = 0.294 \text{ b}$$

and for oxygen it is expressed as

$$\bar{\sigma}_{a(ox)} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(ox)} (2200) = 0.886 \times 1.0 \times 0.28 \times 10^{-3} \text{ b} = 2.5 \times 10^{-4} \text{ b}.$$

The total for water ($H_2O$) is

$$\bar{\sigma}_{a(water)} = 2 \times \bar{\sigma}_{a(hyd)} + \bar{\sigma}_{a(ox)} = 2 \times 0.294 \text{ b} + 2.5 \times 10^{-4} \text{ b} = 0.588 \text{ b}.$$  

To calculate the macroscopic cross sections, the next step is to calculate the atom densities for $^{239}Pu$ and water; knowing the density of $^{239}Pu$, $\rho$, Avogadro's number, $N_A$, and the atomic weight of $^{239}Pu$. References 3 and 4 contain further information about calculating atom densities for various materials and compositions.

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

$$A_{Pu239} = 239.10 \text{ g/mol}$$

$$N_{Pu} = \frac{(0.1 \text{ g/cm}^3)(0.6022 \text{ atoms/cm}^2/\text{mol-b})}{239.10 \text{ g/mol}} = 2.52 \times 10^{-4} \text{ atoms/b \cdot cm}$$

Now that the $^{239}Pu$ atom density is known, calculate the volume fraction for $^{239}Pu$ and water to determine the atom density for water.

$$v_f^{^{239}Pu} = \frac{\text{Concentration}}{\text{Theoretical Density}} = \frac{0.1 \text{ g/cm}^3}{19.75 \text{ g/cm}^3} = 0.005 \text{ or } 0.5\%$$

$$v_f^{\text{Water}} = 1 - v_f^{^{239}Pu} = 1 - 0.005 = 0.995 \text{ or } 99.5\%$$

$$\rho_{H_2O} = 1.0 \frac{\text{g}}{\text{cm}^3}$$

$$N_A = 0.6022 \frac{\text{atoms \cdot cm}^2}{\text{mol-b}}$$

$$A_{H_2O} = 2 \times 1.0079 \text{ g/mol} + 15.9994 \text{ g/mol} = 18.015 \frac{\text{g}}{\text{mol}}$$

$$N_{\text{Water}} = \frac{v_f^{\text{Water}} \times \rho_{\text{Water}} \text{ g/cm}^3 \times N_A \text{ atoms/cm}^2/\text{mol-b}}{A_{H_2O} \text{ g/mol}}$$

$$N_{\text{Water}} = \frac{0.995 \times 1.0 \text{ g/cm}^3 \times 0.6022 \text{ atoms/cm}^2/\text{mol-b}}{18.015 \text{ g/mol}} = 3.326 \times 10^{-2} \frac{\text{atoms}}{b \cdot \text{cm}}$$
The macroscopic absorption and fission cross-sections can now be determined for $^{239}\text{Pu}$. References 1 and 2 provide good background information about calculating macroscopic cross sections.

$$\Sigma_f^{\text{Pu}} = N_{\text{Pu}} \times \sigma_f = 2.52 \times 10^{-4} \text{ atoms/cm} \times 690 \text{ b} = 0.1739 \text{ cm}^{-1}$$

$$\Sigma_a^{\text{Pu}} = N_{\text{Pu}} \times \sigma_a = 2.52 \times 10^{-4} \text{ atoms/cm} \times 961 \text{ b} = 0.2422 \text{ cm}^{-1}$$

$$\Sigma_{\text{water}} = N_{\text{water}} \times \sigma_{a(\text{water})} = 3.326 \times 10^{-2} \text{ atoms/cm} \times 0.588 \text{ b} = 0.196 \text{ cm}^{-1}$$

$$\therefore \Sigma_{\text{mixture}}^{\text{Pu}} = \Sigma_a^{\text{Pu}} + \Sigma_{\text{water}}^{\text{Pu}} = 0.2422 \text{ cm}^{-1} + 0.0196 \text{ cm}^{-1} = 0.2618 \text{ cm}^{-1}$$

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

$$\eta = \frac{\Sigma_f^{\text{Pu}} \times \nu}{\Sigma_a^{\text{Pu}}} = \frac{0.1739 \times 2.871}{0.2422} = 2.061,$$

$$f = \frac{\Sigma_a^{\text{Pu}}}{\Sigma_{\text{mixture}}} = \frac{0.2422}{0.2618} = 0.925.$$

Because no fertile material is present (i.e., no $^{240}\text{Pu}$ or $^{238}\text{U}$), no corrections are needed for resonance absorption or fast fission, so $k = \eta f$, which is equal to the following:

$$k = \eta f = 2.061 \times 0.925 = 1.906.$$  

This result for $k$ means that a criticality is possible for this $^{239}\text{Pu}$ and water system at the stated concentration.

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 $^{239}\text{Pu}$-water mixture. Setting up this methodology in a spreadsheet and using the “goal seek” capability provides an answer of 7.66 g Pu per liter (or 0.00766 g Pu/cm$^3$) for an infinite critical system, $k = 1$.

**Part 2.** The first step to calculate the critical slab thickness using one-group diffusion theory is to determine the diffusion length, $L^2$, and use the result to determine the value for the critical slab height.

$$L^2 = \frac{D}{\Sigma_a^{\text{mixture}}} = \frac{0.16 \text{ cm}}{0.2618 \text{ cm}^{-1}} = 0.611 \text{ cm}^2,$$

$$B^2 = \frac{k}{L^2} = \frac{1.906 - 1}{0.611 \text{ cm}^2} = 1.483 \text{ cm}^{-2}.$$

From Reference 2, Table 6.2, the buckling for an infinite slab with a thickness “a” is $B^2 = (\pi/\delta)^2$, where $\delta$ includes the extrapolation distance. Now that the buckling for this problem is known, the critical slab extrapolated thickness can be determined.
\[ B^2 = \left( \frac{\pi}{a} \right)^2, \]

\[ \hat{a} = \sqrt{\frac{\pi^2}{B^2}} = \sqrt{\frac{\pi^2}{1.483 \text{ cm}^2}} = 2.58 \text{ cm}. \]

This dimension must be corrected by subtracting the extrapolation distance, \( d \). See Appendix A for an overview on extrapolation distance. For this slab and various materials present, \( d = 2.13D \).

\[ a = \bar{a} - 2d = \bar{a} - 2 \left( 2.13 \cdot D \right) = 2.58 \text{ cm} - 2 \left( 2.13 \times 0.16 \text{ cm} \right) = 1.90 \text{ cm}. \]

Figure 3 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 \(^{239}\text{Pu}\)-water slab tank. Perhaps modified one-group diffusion theory will provide more effective results.

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

\[ B^2 = \frac{k - 1}{M^2} = \frac{k - 1}{L^2 + \tau} = \frac{1.906 - 1}{0.611 + 27} = 0.03281 \text{ cm}^{-2}, \]

\[ \hat{a} = \sqrt{\frac{\pi^2}{B^2}} = \sqrt{\frac{\pi^2}{0.03281 \text{ cm}^{-2}}} = 17.34 \text{ cm}, \]

Based on Figure 9 data, the extrapolation distance for this type of system is about 2.15 cm.

\[ a = \bar{a} - 2 \left( 2.13D \right) = 17.34 \text{ cm} - 2 \left( 2.15 \text{ cm} \right) = 13.04 \text{ cm}. \]

Note that for thermal systems (particularly those containing water), the extrapolation distance is usually around 2 cm. It is best to use figures such as Figure 9 to determine the extrapolation distance for such systems.

Based on this result, a \(^{239}\text{Pu}\)-water mixture will result in a subcritical configuration if the “infinite” slab tank thickness is less than about 17.34 cm. This result compares well with the infinite slab thickness for a Pu(0) metal-water mixture shown in Figure 3. 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.

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 problems similar to this example, as one-group diffusion theory does not consider the effects of moderation.**
Figure 3. Critical Infinite Slab Thickness for a Pu Metal-Water Mixture (Reference 5, Figure III.A.5-2)
2.5.2 Diffusion Theory Example Problem 2

It is proposed to store water solutions of uranyl sulfate (UO$_2$SO$_4$) 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$^\circ$C, and the uranium is fully enriched (i.e., no $^{238}$U is present). Table 4 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 weight percent $^{235}$U instead of fully enriched $^{235}$U.

Table 4. Diffusion Theory Example Problem 2 Data

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Parameter</th>
<th>Data Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{235}$U</td>
<td>$\sigma_a$ (2200 m/s)</td>
<td>680.8 barns</td>
<td>2, Table II.2, pg. 643</td>
</tr>
<tr>
<td></td>
<td>$\sigma_f$ (2200 m/s)</td>
<td>582.2 barns</td>
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</tr>
<tr>
<td></td>
<td>$v$</td>
<td>2.418</td>
<td>2, Table 3.4, pg. 70</td>
</tr>
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<td>$g_a$ (non-1/$v$ factor) for 20$^\circ$C</td>
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<td></td>
<td>$g_f$ (non-1/$v$ factor) for 20$^\circ$C</td>
<td>0.9759</td>
<td>2, Table 3.2, pg. 63</td>
</tr>
<tr>
<td>O in UO$_2$SO$_4$</td>
<td>$\sigma_a$ (2200 m/s)</td>
<td>0.28 mb</td>
<td>6</td>
</tr>
<tr>
<td>S in UO$_2$SO$_4$</td>
<td>$\sigma_a$ (2200 m/s)</td>
<td>0.52 b</td>
<td>6</td>
</tr>
<tr>
<td>Water</td>
<td>$\sigma_a$ (2200 m/s)</td>
<td>0.332 b</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>Hydrogen</td>
<td></td>
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</tr>
<tr>
<td></td>
<td>Oxygen</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\tau$</td>
<td>27 cm$^2$</td>
<td>2, Table 5.3, pg. 215</td>
</tr>
<tr>
<td></td>
<td>$D$</td>
<td>0.16 cm</td>
<td>2, Table 5.2, pg. 210</td>
</tr>
<tr>
<td></td>
<td>$D_{mixture} = D_{water}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\tau_{mixture} = \tau_{water}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The tank will contain mostly water with small quantities of $^{235}$U. Therefore, the diffusion coefficient and neutron age will be approximately that of water.
Part 1. Because the tank dimensions are not specified in the problem, one must assume that it is effectively infinite in size. Hence, we must calculate the infinite multiplication factor, \( k_\infty \). If the \( k_\infty \) has a value less than 1.0, the system will remain subcritical at the assumed concentration.

As stated in Section 2.5.1, because \(^{235}\text{U}\) 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 4. Thus, the absorption and fission microscopic cross sections in barns for \(^{235}\text{U}\) are adjusted as follows.

\[
\bar{\sigma}_a = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200) = 0.886 \times 0.978 \times 680.8 = 590 \text{ b}
\]

\[
\bar{\sigma}_f = \frac{\sqrt{\pi}}{2} g_f \sigma_f (2200) = 0.886 \times 0.9759 \times 582.2 = 503 \text{ b}.
\]

For sulfur,

\[
\bar{\sigma}_a = \frac{\sqrt{\pi}}{2} g_a \sigma_a (2200) = 0.886 \times 1.0 \times 0.52 = 0.461 \text{ b},
\]

For Water (\( \text{H}_2\text{O} \)), the cross-section adjustment is expressed as

\[
\bar{\sigma}_{a(\text{H}_2\text{O})} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(\text{H}_2\text{O})} (2200) = 0.886 \times 1.0 \times 0.6643 \text{ b} = 0.588 \text{ b}
\]

and for oxygen in uranyl sulfate, it is expressed as

\[
\bar{\sigma}_{a(\text{O})} = \frac{\sqrt{\pi}}{2} g_a \sigma_{a(\text{O})} (2200) = 0.886 \times 1.0 \times 0.28 \times 10^{-3} \text{ b} = 2.5 \times 10^{-4} \text{ b}.
\]

The next step is to calculate the atom densities for \(^{235}\text{U}\) and water, to calculate the macroscopic cross sections. Note that the uranium in the solution is fully enriched (100% \(^{235}\text{U}\)) and does not contain any \(^{238}\text{U}\).

\[
N_{\text{U}^{235}} = \frac{(\text{C}_{\text{U}^{235}} \text{ g} / \text{cm}^3)(N_A \text{ atoms} - \text{cm}^2 / \text{mol} - \text{b})}{(A_{\text{U}^{235}} \text{ g} / \text{mol})}
\]

\[
N_{\text{U}^{235}} = \frac{(0.03 \text{ g} / \text{cm}^3)(0.6022 \text{ atoms} - \text{cm}^2 / \text{mol} - \text{b})}{(235.04 \text{ g} / \text{mol})} = 7.69 \times 10^{-5} \text{ atoms} / \text{b} - \text{cm}
\]

\[
N_{\text{UO}_2\text{SO}_4} = 7.69 \times 10^{-5} \text{ atoms} / \text{b} - \text{cm}
\]

\[
N_0 = 6 \times N_{\text{U}^{235}} = N_{\text{UO}_2\text{SO}_4} = 6 \times (7.69 \times 10^{-5} \text{ atoms} / \text{b} - \text{cm}) = 4.614 \times 10^{-4} \text{ atoms} / \text{b} - \text{cm}
\]

\[
N_a = N_{\text{U}^{235}} = 7.69 \times 10^{-5} \text{ atoms} / \text{b} - \text{cm}
\]

Now that the \(^{235}\text{U}\) atom density is known, calculate the volume fractions for \(^{235}\text{U}\) and water to determine the atom density for water:
\[ v_{f235U} = \frac{\text{Concentration}}{\text{Theoretical Density}} = \frac{0.03 \text{ g/cm}^3}{18.9 \text{ g/cm}^3} = 0.0016 \text{ or } 0.16\% \]
\[ v_{fH2O} = 1 - v_f(235U) = 1 - 0.0016 = 0.9984 \text{ or } 99.84\% \]
\[ N_{H2O} = \frac{v_{fH2O} \times \rho_{H2O} \text{ g/cm}^3 \times N_A \text{ atoms-cm}^2/\text{mol} - b}{A_{H2O} \text{ g/mol}} \]
\[ N_{H2O} = \frac{0.9984 \times 1.0 \text{ g/cm}^3 \times 0.6022 \text{ atoms-cm}^2/\text{mol} - b}{18.015 \text{ g/mol}} \]
\[ N_{H2O} = 3.337 \times 10^{-2} \text{ atoms } b^{-1} \text{ cm} \]
\[ \Sigma_a^{H2O} = \frac{\sqrt{\pi}}{2} \times N_{H2O} \times \sigma_a^{H2O} = 3.337 \times 10^{-2} \text{ atoms } b^{-1} \text{ cm} \times 0.588 b = 0.0196 \text{ cm}^{-1}. \]

The macroscopic absorption and fission cross-sections can now be determined for 233U.

\[ \Sigma_a^{235U} = N_{235U} \times \sigma_a = 7.69 \times 10^{-5} \text{ atoms/b-cm} \times 590 b = 0.04537 \text{ cm}^{-1} \]
\[ \Sigma_f^{235U} = N_{235U} \times \sigma_f = 7.69 \times 10^{-5} \text{ atoms/b-cm} \times 503 b = 0.03868 \text{ cm}^{-1} \]
\[ \Sigma_a^{H2O} = 0.0196 \text{ cm}^{-1} \]
\[ \Sigma_a^{\text{in UO}_2\text{SO}_4} = N_a \times \sigma_a = 7.69 \times 10^{-5} \text{ atoms/b-cm} \times 0.461 b = 3.545 \times 10^{-5} \text{ cm}^{-1} \]
\[ \Sigma_a^{O\text{ in UO}_2\text{SO}_4} = N_a \times \sigma_a = 4.612 \times 10^{-4} \text{ atoms/b-cm} \times 2.48 \times 10^{-4} b = 1.1 \times 10^{-7} \text{ cm}^{-1} \]
\[ \therefore \Sigma_a^{\text{mixture}} = \Sigma_a^{235U} + \Sigma_a^{H2O} + \Sigma_a^{\text{in UO}_2\text{SO}_4} + \Sigma_a^{O\text{ in UO}_2\text{SO}_4} \]
\[ \Sigma_a^{\text{mixture}} = 0.04537 \text{ cm}^{-1} + 0.0196 \text{ cm}^{-1} + 3.545 \times 10^{-5} \text{ cm}^{-1} + 1.14 \times 10^{-7} \text{ cm}^{-1} \]
\[ \Sigma_a^{\text{mixture}} = 0.06501 \text{ cm}^{-1}. \]

Next, \( \eta \), the number of neutrons released in fission per neutron absorbed by a fissile nucleus and \( f \), the thermal utilization factor, can be calculated:

\[ \eta = \frac{\Sigma_f^{235U} \times \nu}{\Sigma_a^{235U}} = \frac{0.03868 \times 2.418}{0.04537} = 2.061 \]
\[ f = \frac{\Sigma_a^{235U}}{\Sigma_a^{\text{mixture}}} = \frac{0.04537}{0.06501} = 0.6979. \]

Because no 238U is present, the fast fission factor, \( \epsilon \), 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 235U and neutron absorption and fission in the resonance region essentially cancel each other out. Thus, the infinite multiplication factor is then \( k_\infty = \eta f. \)
\[ k_{\infty} = \eta f = 2.061 \times 0.6979 = 1.438. \]

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 can be done in a spreadsheet program to search on the concentration required to result in \( k_{\infty} = 1 \).

**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 \( \tau \) (neutron age). Then the critical infinite cylinder radius can be determined as follows.

\[
L_{th}^2 = \frac{D}{\Sigma_a} = \frac{0.16 \text{ cm}}{0.06501 \text{ cm}^{-1}} = 2.461 \text{ cm}^2
\]

\[
B_m^2 = \frac{k_{\infty} - 1}{M^2} = \frac{k_{\infty} - 1}{L^2 + \tau} = \frac{1.438 - 1}{2.461 + 27} = 0.01487 \text{ cm}^{-2}
\]

\[
\bar{R} = \sqrt{\frac{2.405^2}{B_m^2}} = \sqrt{\frac{2.405^2}{0.01487 \text{ cm}^{-2}}} = 19.7 \text{ cm}
\]

\[
R = \bar{R} - d = 19.7 \text{ cm} - 2.2 \text{ cm} = 17.5 \text{ cm}
\]

An MCNP\(^1\) calculation was performed to determine the radius for a critical, infinite cylinder of this material, which resulted in a cylinder radius of approximately 17.25 cm. Modified one-group diffusion theory provides a reasonable estimate of the critical dimensions for this moderated, thermal system. 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.

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

First, the atom densities need to be modified to reflect the presence of \(^{238}\)U. The Table 5 provides the data required for this part of the problem.

\(^1\) A General Monte Carlo N-Particle (MCNP) transport code.
Table 5. Diffusion Theory Example Problem 2 Data for Part 3

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Parameter Description</th>
<th>Data Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{238}$U</td>
<td>$\sigma_a$ (2200 m/s)</td>
<td>2.7 b</td>
<td>2, Table II.2, pg. 643</td>
</tr>
<tr>
<td></td>
<td>$\sigma_s$ (2200 m/s)</td>
<td>9.38 b</td>
<td>6, 2200 m/s elastic scattering cross section from ENDF/B-VI data</td>
</tr>
<tr>
<td></td>
<td>$g_a$ (non-1/v factor) for 20 °C</td>
<td>1.0017</td>
<td>2, Table III.2, pg. 643</td>
</tr>
<tr>
<td>$^{235}$U</td>
<td>$\sigma_a$ (2200 m/s)</td>
<td>680.8 b</td>
<td>2, Table III.2, pg. 63</td>
</tr>
<tr>
<td></td>
<td>$\sigma_s$ (2200 m/s)</td>
<td>582.2 b</td>
<td>2, Table III.2, pg. 63</td>
</tr>
<tr>
<td></td>
<td>$\sigma_s$ (2200 m/s)</td>
<td>15.48 b</td>
<td>6, 2200 m/s elastic scattering cross section from ENDF/B-VI data</td>
</tr>
<tr>
<td></td>
<td>$\nu$</td>
<td>2.418</td>
<td>2, Table III.4, pg. 70</td>
</tr>
<tr>
<td></td>
<td>$g_a$ (non-1/v factor) for 20 °C</td>
<td>0.9780</td>
<td>2, Table III.2, pg. 63</td>
</tr>
<tr>
<td></td>
<td>$g_s$ (non-1/v factor) for 20 °C</td>
<td>0.9759</td>
<td>2, Table III.2, pg. 63</td>
</tr>
<tr>
<td>O in UO$_2$SO$_4$</td>
<td>$\sigma_s$ (2200 m/s)</td>
<td>0.28 mb</td>
<td>6, 2200 m/s elastic scattering cross section from ENDF/B-VI data</td>
</tr>
<tr>
<td></td>
<td>$\sigma_s$ (2200 m/s)</td>
<td>3.76 b</td>
<td>2, Table III.2, pg. 645</td>
</tr>
<tr>
<td>S in UO$_2$SO$_4$</td>
<td>$\sigma_s$ (2200 m/s)</td>
<td>0.52 b</td>
<td>6, 2200 m/s elastic scattering cross section from ENDF/B-VI data</td>
</tr>
<tr>
<td></td>
<td>$\sigma_s$ (2200 m/s)</td>
<td>0.975 b</td>
<td>2, Table III.2, pg. 646</td>
</tr>
<tr>
<td>Water</td>
<td>Hydrogen $\sigma_a$ (2200 m/s)</td>
<td>0.332 b</td>
<td>6, 2200 m/s elastic scattering cross section from ENDF/B-VI data</td>
</tr>
<tr>
<td></td>
<td>Oxygen $\sigma_a$ (2200 m/s)</td>
<td>0.28 mb</td>
<td>6, 2200 m/s elastic scattering cross section from ENDF/B-VI data</td>
</tr>
<tr>
<td></td>
<td>Water $\sigma_a$ (2200 m/s)</td>
<td>0.6643 b</td>
<td>= 2 × 0.332 b + 0.28 × 10^{-3} b</td>
</tr>
<tr>
<td></td>
<td>Water $\sigma_s$ (2200 m/s)</td>
<td>103.0</td>
<td>2, Table III.2, pg. 647</td>
</tr>
</tbody>
</table>

Now, as in the last part of this problem, the atom densities need to be calculated to consider the effects of the $^{238}$U in the system. First, the absorption cross section must be adjusted as before for $^{235}$U because $^{238}$U is a non-1/v absorber:

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

The atom density for $^{235}$U remain unchanged as the concentration of $^{235}$U remains the same. The concentration of $^{238}$U is based on the atom density of uranium.
\[ N_{\text{en}} = 7.69 \times 10^{-8} \text{ atoms} / \text{b} \cdot \text{cm} \]

The concentration term, above, can be adjusted by dividing through by the enrichment, which is equal to 14.7 wt. % \(^{235}\text{U}\) in U:

\[
C_U = \frac{C_U^{^{235}\text{U}}}{0.147} = \frac{0.03 \text{ g/cm}^3}{0.147} = 0.204 \text{ g} \cdot \text{U/cm}^3
\]

\[
A = \left( \frac{w_{f_1} + w_{f_2}}{A_1 + A_2} \right)^{-1} = \left( \frac{0.147}{235.04} + \frac{0.853}{238.05} \right)^{-1} = 237.60 \text{ g} \cdot \text{U(14.7)/mole}
\]

\[
N_{U} = \frac{(C_U \text{ g/cm}^3)(N_A \text{ atoms/cm}^2/mol \cdot b)}{(A_U \text{ g/mol})}
\]

\[
N_{\text{en}} = \frac{(0.204 \text{ g/cm}^3)(0.6022 \text{ atoms/cm}^2/mol \cdot b)}{237.60 \text{ g/mol}} = 5.170 \times 10^{-4} \text{ atoms} / \text{b - cm}
\]

\[
N_{\text{en}} = N_U - N_{\text{en}} = 5.170 \times 10^{-4} \text{ atoms} / \text{b - cm} - 7.69 \times 10^{-5} \text{ atoms} / \text{b - cm}
\]

\[
N_{\text{en}} = 4.401 \times 10^{-4} \text{ atoms} / \text{b - cm}
\]

\[
N_{O} = 6 \times N_{U} = N_{\text{en}} = 6 \times (5.170 \times 10^{-4} \text{ atoms} / \text{b - cm}) = 3.102 \times 10^{-3} \text{ atoms} / \text{b - cm}
\]

\[
N_{S} = N_{U} = 5.170 \times 10^{-4} \text{ atoms} / \text{b - cm}.
\]

The atom densities have changed significantly compared with Part 2 of the problem because of the addition of \(^{238}\text{U}\) to the system. Thus, because the macroscopic cross sections are dependent on the atom densities, they need to be recalculated. Recall that the concentration needed for the following calculations must allow for the total uranium content in the system, not only the \(^{235}\text{U}\) content. The macroscopic absorption cross-section for water is calculated as follows:

\[
v_fU = \frac{\text{Concentration}}{\text{Theoretical Density}} = \frac{(0.204) \text{ g/cm}^3}{18.9 \text{ g/cm}^3} = 0.0108 \text{ or } 1.08\%
\]

\[
v_fH_2O = 1 - v_f(U) = 1 - 0.0108 = 0.9892 \text{ or } 98.92\%
\]

\[
N_{H_2O} = \frac{v_fH_2O \times \rho_{H_2O} \text{ g/cm}^3 \times N_A \text{ atoms/cm}^2/mol \cdot b}{A_{H_2O} \text{ g/mol}}
\]

\[
N_{H_2O} = \frac{0.9892 \times 1.0 \text{ g/cm}^3 \times 0.6022 \text{ atoms/cm}^2/mol \cdot b}{18.0152 \text{ g/mol}}
\]

\[
N_{H_2O} = 3.3066 \times 10^{-2} \text{ atoms} / \text{b - cm}
\]
\[ \Sigma_{\text{H}_2\text{O}} = N_{\text{H}_2\text{O}} \times \sigma_{\text{H}_2\text{O}} = 3.3066 \times 10^{-2} \text{ atoms} \text{ b}^{-1} \text{cm}^{-1} \times 0.588 \text{ b} = 0.01944 \text{ cm}^{-1} \]

\[ \Sigma_f^{235\text{U}} = N_f^{235\text{U}} \times \sigma_f = 7.69 \times 10^{-5} \text{ atoms} \text{ b}^{-1} \text{cm}^{-1} \times 503 \text{ b} = 0.03868 \text{ cm}^{-1} \]

\[ \Sigma_f^{238\text{U}} = N_f^{238\text{U}} \times \sigma_f = 7.69 \times 10^{-5} \text{ atoms} \text{ b}^{-1} \text{cm}^{-1} \times 590 \text{ b} = 0.04537 \text{ cm}^{-1} \]

\[ \Sigma_a^{235\text{U}} = N_a^{235\text{U}} \times \sigma_a = 4.401 \times 10^{-4} \text{ atoms} \text{ b}^{-1} \text{cm}^{-1} \times 2.40 \text{ b} = 0.001056 \text{ cm}^{-1} \]

\[ \Sigma_a^{\text{UO}_2\text{SO}_4} = N_a^{\text{UO}_2\text{SO}_4} \times \sigma_a = 5.170 \times 10^{-4} \text{ atoms} \text{ b}^{-1} \text{cm}^{-1} \times 0.461 \text{ b} = 2.383 \times 10^{-4} \text{ cm}^{-1} \]

\[ \Sigma_a^{\text{O}^{\text{UO}_2\text{SO}_4}} = N_a^{\text{O}^{\text{UO}_2\text{SO}_4}} \times \sigma_a = 3.102 \times 10^{-3} \text{ atoms} \text{ b}^{-1} \text{cm}^{-1} \times 2.48 \times 10^{-4} \text{ b} = 7.7 \times 10^{-7} \text{ cm}^{-1} \]

\[ : \Sigma_a^{\text{UO}_2\text{SO}_4} = \Sigma_a^{235\text{U}} + \Sigma_a^{238\text{U}} + \Sigma_a^{\text{UO}_2\text{SO}_4} + \Sigma_a^{\text{H}_2\text{O}} \]

\[ \Sigma_a^{\text{UO}_2\text{SO}_4} = 0.04537 \text{ cm}^{-1} + 0.001056 \text{ cm}^{-1} + 2.383 \times 10^{-4} \text{ cm}^{-1} + 7.7 \times 10^{-7} \text{ cm}^{-1} = 0.04666 \text{ cm}^{-1} \]

\[ : \Sigma_{\text{mixture}} = \Sigma_a^{\text{UO}_2\text{SO}_4} + \Sigma_a^{\text{H}_2\text{O}} \]

\[ \Sigma_{\text{mixture}} = 0.04666 \text{ cm}^{-1} + 0.01944 \text{ cm}^{-1} = 0.06610 \text{ cm}^{-1} \]

Next, \( \eta \), 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 \(^{238}\text{U}\) is very small and can be neglected in this calculation:

\[ \eta = \frac{\nu \times \Sigma_f^{235\text{U}} + \nu \times \Sigma_f^{238\text{U}}}{\Sigma_{\text{mixture}}} = \frac{2.418 \times 0.03868 + 0}{0.04666} = 2.004 \]

\[ f = \frac{\Sigma_{\text{mixture}}}{\Sigma_{\text{mixture}}} = \frac{0.04666}{0.06611} = 0.706. \]

Because this system with lower enrichment contains significant quantities of \(^{238}\text{U}\), the resonance escape probability needs to 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 \(^{238}\text{U}\) will make fewer neutrons available for subsequent fissions and reduce the system reactivity.
First, calculate the mean lethargy gain per neutron collision, \( \xi \), for the moderator and fuel mixture present in this system. From Reference 1, pg. 324, \( \xi \) is defined as follows:

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

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

\[
\xi = \frac{2}{A + \frac{2}{3}} \quad \text{for} \quad A > 10.
\]

We need to calculate \( \xi \) for the mixture of moderator and fuel.

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

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

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

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

\[
\xi_{\text{mixture}} = \frac{N_O \sigma_{_{\xi O}} + N_H \sigma_{_{\xi H}} + N_S \sigma_{_{\xi S}} + N_{^{235}U} \sigma_{_{\xi ^{235}U}} + N_{^{238}U} \sigma_{_{\xi ^{238}U}}}{N_O \sigma_{_{\xi O}} + N_H \sigma_{_{\xi H}} + N_S \sigma_{_{\xi S}} + N_{^{235}U} \sigma_{_{\xi ^{235}U}} + N_{^{238}U} \sigma_{_{\xi ^{238}U}}}
\]

\[
\xi_{\text{moderator}} = \frac{(3.3066 \times 10^{-2} \times 3.76 \times 0.12) + (2 \times 3.3066 \times 10^{-2} \times 38.0 \times 0.14) + (5.17 \times 10^{-4} \times 0.975 \times 0.061) + (7.69 \times 10^{-5} \times 15.48 \times 0.0085) + (4.401 \times 10^{-4} \times 9.38 \times 0.0084)}{(3.3066 \times 10^{-2} \times 3.76) + (2 \times 3.3066 \times 10^{-2} \times 38.0) + (5.17 \times 10^{-4} \times 0.975) + (7.69 \times 10^{-5} \times 15.48) + (4.401 \times 10^{-4} \times 9.38)}
\]

\[
\xi_{\text{mixture}} = \frac{2.528}{2.643} = 0.956
\]

Note that \( \Sigma_{moderator} = (3.3066 \times 10^{-2} \times 3.76) + (2 \times 3.3066 \times 10^{-2} \times 38.0) = 2.637 \text{ cm}^{-1} \)
Now the resonance escape probability can be calculated using the following relationship:

$$P = \exp \left[ -\frac{3.06}{\varepsilon} \left( \frac{\Sigma_{\text{moderator}}}{N_{U_{235}}} \right)^{0.472} \right] = \exp \left[ -\frac{3.06}{0.956} \left( \frac{2.637}{4.401 \times 10^{-1}} \right)^{0.472} \right] = 0.968. $$

The fast fission factor, $\varepsilon$, 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 $k_\infty = \eta \varepsilon p$.

$$k_\infty = \eta \varepsilon p = 2.004 \times 0.706 \times 1.0 \times 0.968 = 1.370 \ (Answer \ to \ Part \ 3)$$

When analyzed in DANTSYS, the $k_\infty$ was 1.368 – 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. Now the critical dimensions for this system can be determined:

$$L_{th}^2 = \frac{D}{\Sigma_a} = \frac{0.16 \text{ cm}}{0.06610 \text{ cm}^{-1}} = 2.42 \text{ cm}^2$$

$$B_m^2 = \frac{k_\infty - 1}{M^2} = \frac{1.370 - 1}{2.42 + 27} = 0.01258 \text{ cm}^{-2}$$

$$R = \sqrt{\frac{2.405^2}{B_m^2}} = \sqrt{\frac{2.405^2}{0.01258 \text{ cm}^{-2}}} = 21.4 \text{ cm}$$

$$R = R - d = 21.4 \text{ cm} - 2.2 \text{ cm} = 19.2 \text{ cm.}$$

The critical dimensions increased 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 $^{238}\text{U}$ present. When analyzed in DANTSYS, the critical radius of an infinite cylinder with 14.7 weight percent $^{235}\text{U}$ in uranyl sulfate was 19.0 cm.

---

2 DANTSYS is a code package designed to solve the discrete ordinates form of the Boltzmann transport equation in several different geometries.
2.5.3 Diffusion Theory Example Problem 3

Assume a fissile system made up of a bare sphere of Na and $^{239}\text{Pu}$ in which Pu is 30 weight percent of the core mixture. Because this system has no moderating materials present, fast neutrons dominate the system (so one-group theory is sufficient). Assume the density of the mixture is 0.8 g/cm³.

1. Using one-group diffusion theory, estimate the critical radius for this system.
2. What is the probability that a neutron will leak out of this system?

The data relevant for this problem is listed in Table 6 below.

Table 6. Diffusion Theory Example Problem 3 Data

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Parameter</th>
<th>Data Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{239}\text{Pu}$</td>
<td>$\sigma_e$ (fast)</td>
<td>2.11 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_t$ (fast)</td>
<td>1.85 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_n$ (fast)</td>
<td>6.8 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\eta$</td>
<td>2.98</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\eta$</td>
<td>2.61</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>Na</td>
<td>$\sigma_e$ (fast)</td>
<td>0.0008 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_t$ (fast)</td>
<td>0 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_n$ (fast)</td>
<td>3.3 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
</tbody>
</table>

Part 1. First, calculate the atom densities for the Pu and Na:

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

$$N_{^{239}\text{Pu}} = \frac{(0.3)(0.8 \text{ g/cm}^3)(0.6022 \text{ atoms/cm}^2/\text{mol} - \beta)}{239.05 \text{ g/mol}} = 6.05 \times 10^{-4} \text{ atoms/b-cm}$$

$$N_{\text{Na}} = \frac{(0.7)(0.8 \text{ g/cm}^3)(0.6022 \text{ atoms/cm}^2/\text{mol} - \beta)}{22.99 \text{ g/mol}} = 1.4669 \times 10^{-2} \text{ atoms/b-cm}.$$}

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

$$\Sigma^{\text{mixture}} = \Sigma^p + \Sigma^n = N_{^{239}\text{Pu}} \times \sigma_{e}^{^{239}\text{Pu}} + N_{\text{Na}} \times \sigma_{e}^{\text{Na}}$$

$$\Sigma^{\text{mixture}} = 6.05 \times 10^{-4} \text{ atoms/b-cm} \times 2.11 \text{ b } + 1.4669 \times 10^{-2} \text{ atoms/b-cm} \times 0.0008 \text{ b}$$

$$\Sigma^{\text{mixture}} = 1.288 \times 10^{-3} \text{ cm}^{-1}$$

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 all fissions occur at fast energies ($e = p = 1$).
\[ k_\infty = \eta f = \eta \times \frac{\sum_{i}^{\text{Pu}}}{\sum_{i}^{\text{mixture}}} = 2.61 \times \frac{1.276 \times 10^{-3} \text{cm}^{-1}}{1.288 \times 10^{-3} \text{cm}^{-1}} = 2.586 \]

Now, the diffusion length, \( L^2 \), can be calculated based on the result of the \( k_\infty \) calculation.

\[
\Sigma_i = \Sigma_{p} + \Sigma_{n} = N_{\text{Pu}} \times \sigma_{p}^{\text{Pu}} + N_{\text{Na}} \times \sigma_{p}^{\text{Na}}
\]

\[
\Sigma_i = (6.05 \times 10^{-4} \text{ atoms / b \cdot cm}) (6.8 b) + (1.4669 \times 10^{-2} \text{ atoms / b \cdot cm}) (3.3 b)
\]

\[
\Sigma_i = 5.25 \times 10^{-2} \text{ cm}^{-1}
\]

\[
D_{\text{mixture}} = \frac{1}{3 \Sigma_i} = \frac{1}{3 \times 5.25 \times 10^{-2} \text{ cm}^{-1}} = 6.347 \text{ cm}
\]

\[
L^2 = \frac{D_{\text{mixture}}}{\Sigma_i^{\text{mixture}}} = \frac{6.347 \text{ cm}}{1.288 \times 10^{-3} \text{ cm}^{-1}} = 4.930 \text{ cm}^2.
\]

Now, the material buckling, \( B_m^2 \), can be calculated:

\[
B_m^2 = \frac{k_\infty - 1}{L^2} = \frac{2.586 - 1}{4.930 \text{ cm}^2} = 3.22 \times 10^{-1} \text{ cm}^{-2}.
\]

The buckling is needed to determine the critical size. Notice the diffusion length, \( L^2 \), is rather large. This means that neutrons in this system diffuse or travel further on the average between collisions before being absorbed by the materials in this system, behavior which is due primarily to the very low fast absorption cross-section for sodium. Thus, it is expected that this system will be much larger than a thermal system such as a Pu metal and water mixture. The critical radius can be calculated now that the material buckling is known. Recall that the geometric and material bucklings are equal for a critical system.

\[
B_g^2 = \left( \frac{\pi}{R} \right)^2
\]

\[
R = \frac{\pi^2}{B_g^2} = \sqrt{\frac{\pi^2}{3.22 \times 10^{-1} \text{ cm}^{-2}}} = 175.1 \text{ cm}
\]

\[
R = \bar{R} - d = \bar{R} - 2.13 \times D = 175.1 \text{ cm} - 2.13 \times 6.347 \text{ cm} = 161.6 \text{ cm}.
\]

Therefore, the critical radius for a \(^{239}\text{Pu} \) and Na system is approximately 162 cm, which is a large system due to the rather low concentration of Pu in the system. The size of this system in general is related to the quantity of material present in the system. In most cases, fast systems are smaller than thermal systems but require more fissile material to achieve a critical state. In this case the extrapolation distance could be neglected because of the large size for this critical system. A DANTSYS calculation predicts a critical radius of 161.33 cm for this system, which is very close to that predicted by one-group diffusion theory. Because this is a fast, unmoderated system, one-group diffusion theory provides a reasonable estimate for the critical dimensions for this system.
Part 2. The probability that a neutron will leak out of this system can be calculated as follows. The nonleakage probability, \( P_L \), is the probability a neutron will not leak out of the system. The leakage probability is simply equal to \( 1 - P_L \) 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 from the following relationship.

\[
1 - P_L = \frac{L^2 B_m^2}{1 + L^2 B_m^2}
\]

Knowing that the following is true, a simple way to calculate the leakage probability can be determined.

\[
L^2 B_m^2 = k_n - 1
\]

Now, for a critical system, the leakage probability can be calculated:

\[
(1 - P_L) = \frac{k_n - 1}{1 + k_n - 1} = 1 - \frac{1}{k_n} = 1 - \frac{1}{2.586} = 0.613
\]

This provides the analyst with information regarding the probability that a neutron will leak out of the system instead of being absorbed within the system materials. Based on this calculation, we know that more than 61% of the neutrons will leak out of the system. This calculation illustrates that, for a critical system, the geometry, and thus the system leakage, must be such to reduce the effective multiplication factor from 2.586 to 1.0.
The Jezebel critical assembly used for experiments at Los Alamos was used to perform various critical experiments (Figure 4). Assume the assembly is made from $\delta$-phase $^{239}$Pu ($\rho = 15.61 \text{ g/cm}^3$) 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 4. The Jezebel Critical Assembly at Los Alamos
The data relevant for this problem are listed in Table 7. Note that Jezebel is an unmoderated system dominated by fast neutrons. Therefore, the first step in solving this problem is to make sure that fast neutron cross-section data are used in the calculation.

**Table 7. Diffusion Theory Example Problem 4 Data**

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Parameter</th>
<th>Data Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{239}$Pu</td>
<td>$\sigma_i$(fast)</td>
<td>2.11 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>$^{239}$Pu</td>
<td>$\sigma_f$(fast)</td>
<td>1.85 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>$^{239}$Pu</td>
<td>$\sigma_s$(fast)</td>
<td>6.8 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>$^{239}$Pu</td>
<td>$\sigma_t$(fast)</td>
<td>0.26 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>$^{239}$Pu</td>
<td>$\nu$</td>
<td>2.98</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>$^{239}$Pu</td>
<td>$\eta$</td>
<td>2.61</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
</tbody>
</table>

First, calculate the atom densities for the $^{239}$Pu so that the macroscopic cross-sections can be calculated:

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

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

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

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

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

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

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

The infinite multiplication factor, $k_\infty$, can now be calculated. Note that all fissions take place at fast energies and that only $^{239}$Pu 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.

$$k_\infty = n = \nu \times \frac{\Sigma_f}{\Sigma_a}$$

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

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 $k_\infty$ calculation.
\[ D_{239Pu} = \left( \frac{1}{3 \Sigma_{\nu}^P} \right) = \left( \frac{1}{3 \times N_{239Pu} \times \sigma_{239Pu}^\nu} \right) \]

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

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

Now, the material buckling, \( B_m^2 \), can be calculated:

\[ B_m^2 = \frac{k_m - 1}{L^2} = \frac{2.612 - 1}{15.03 \text{ cm}^2} = 0.1073 \text{ cm}^{-2}. \]

The buckling is needed to determine the critical size. Notice the diffusion length, \( L^2 \), for this system is much lower than for the Pu-Na system from the last example problem. Because the neutron absorption cross-section for a pure Pu system is greater than the Pu–Na system, neutrons will not travel as far, on the average, before being absorbed in this system. Now, for a critical system the material and geometric buckling values are equal. The critical dimensions for this system can be calculated as follows:

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

\[ \bar{R} = \sqrt{\frac{\pi^2}{B_g^2}} = \sqrt{\frac{\pi^2}{0.1073 \text{ cm}^{-2}}} = 9.59 \text{ cm} \]

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

The actual Jezebel system had a density of 15.61 g/cc, was 4.5% \(^{240}\text{Pu}\) and had a critical radius of 6.385 cm. With these cross sections and assumptions of 100% \(^{239}\text{Pu}\), this method slightly over predicts the critical radius for this type of system.
2.5.5 Diffusion Theory Example Problem 5

The Godiva I critical assembly used for experiments at Los Alamos was employed in various critical experiments (Figure 5). Assume the assembly is made from 93.5% enriched $^{235}\text{U}$ ($\rho=18.74 \text{ g/cm}^3$) 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 5. The Godiva I Critical Assembly at Los Alamos
The data relevant for this problem is listed in Table 8. Note that, like the Jezebel assembly, Godiva I is an unmoderated, fast system. Therefore, the first step in solving this problem is to make sure that fast neutron cross-section data is used in the calculation.

**Table 8. Diffusion Theory Example Problem 5 Data**

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Parameter</th>
<th>Data Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{235}$U</td>
<td>$\sigma_f$(fast)</td>
<td>1.65 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_t$(fast)</td>
<td>1.40 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_r$(fast)</td>
<td>6.80 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\nu$</td>
<td>2.60</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>$^{238}$U</td>
<td>$\sigma_f$(fast)</td>
<td>0.255 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_t$(fast)</td>
<td>0.095 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_r$(fast)</td>
<td>6.90 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\nu$</td>
<td>2.60</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
</tbody>
</table>

First, calculate the atom densities for the enriched uranium so that the macroscopic fission and absorption cross-sections can be calculated:

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

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

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

Now that the atom densities for $^{235}$U and $^{238}$U have been calculated, the macroscopic absorption and fission cross-sections can be determined for this fast system:

$$\Sigma^c_{^{235}} = N_{^{235}U} \times \sigma^c_{^{235}}$$

$$\Sigma^c_{^{235}} = 4.489 \times 10^{-2} \text{ atoms/b - cm} \times 1.65 \text{ b} = 7.407 \times 10^{-2} \text{ cm}^{-1}$$

$$\Sigma^c_{^{238}} = N_{^{238}U} \times \sigma^c_{^{238}}$$

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

$$\Sigma^f_{^{235}} = N_{^{235}U} \times \sigma^f_{^{235}}$$

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

$$\Sigma^f_{^{238}} = N_{^{238}U} \times \sigma^f_{^{238}}$$

$$\Sigma^f_{^{238}} = 3.081 \times 10^{-3} \text{ atoms/b - cm} \times 0.095 \text{ b} = 2.927 \times 10^{-4} \text{ cm}^{-1}.$$
The infinite multiplication factor, \( k_\infty \), can be determined now that the macroscopic cross-sections have been calculated. Like the previous example problem, fast neutrons dominate this system. Also, because of the small size of the system, a large fraction of the neutrons leak out of the system.

\[
k_\infty = \eta = \frac{\nu \Sigma_{f}^{\text{\textsc{nu}}U} + \nu \Sigma_{f}^{\text{\textsc{nu}}U}}{\Sigma_{a}^{\text{\textsc{nu}}U} + \Sigma_{a}^{\text{\textsc{nu}}U}} = \frac{\nu (\Sigma_{f}^{\text{\textsc{nu}}U} + \Sigma_{f}^{\text{\textsc{nu}}U})}{\Sigma_{a}^{\text{\textsc{nu}}U} + \Sigma_{a}^{\text{\textsc{nu}}U}},
\]

\[
k_\infty = \frac{2.60 \left[ 6.285 \times 10^{-2} \text{ cm}^{-1} + 2.927 \times 10^{-4} \text{ cm}^{-1} \right]}{ \left( 7.402 \times 10^{-2} \text{ cm}^{-1} \right) + \left( 7.857 \times 10^{-4} \text{ cm}^{-1} \right)} = 2.195.
\]

Now, the diffusion coefficient, \( D \), the diffusion length, \( L^2 \), and the material buckling, \( B_m^2 \), can be calculated on the basis of the result of the \( k_\infty \) calculation.

\[
D = \frac{1}{3 \Sigma_{f}^{\text{\textsc{nu}}U}} = \frac{1}{3 \left[ N_{\text{\textsc{nu}}U} \times \sigma_{f}^{\text{\textsc{nu}}U} + N_{\text{\textsc{nu}}U} \times \sigma_{a}^{\text{\textsc{nu}}U} \right]} = 1.021 \text{ cm},
\]

\[
L^2 = \frac{D}{\Sigma_{a}^{\text{\textsc{nu}}U} + \Sigma_{a}^{\text{\textsc{nu}}U}} = \frac{1.021 \text{ cm}}{7.407 \times 10^{-2} \text{ cm}^{-1} + 7.857 \times 10^{-4} \text{ cm}^{-1}} = 13.64 \text{ cm}^2.
\]

Now, the material buckling, \( B_m^2 \), can be calculated:

\[
B_m^2 = \frac{k_\infty - 1}{L^2} = \frac{2.195 - 1}{13.64 \text{ cm}^2} = 0.0876 \text{ cm}^{-2}.
\]

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 and geometric bucklings are equal.

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

\[
\bar{R} = \sqrt{\frac{\pi^2}{B_m^2}} = \sqrt{\frac{\pi^2}{0.0876 \text{ cm}^{-2}}} = 10.61 \text{ cm},
\]

\[
R = \bar{R} - d = 10.61 \text{ cm} - 2.13 \times D = 10.61 \text{ cm} - 2.13 \times 1.021 \text{ cm} = 8.44 \text{ cm}.
\]

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.
2.5.6 Diffusion Theory Example Problem 6

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 calculation. Unmoderated plutonium oxide is assumed to have a fast neutron energy spectrum; so fast data from Reference 2 and 9 are compiled in Table 9.

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Parameter</th>
<th>Data Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{239}$Pu</td>
<td>$\sigma_a$(fast)</td>
<td>2.11 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_f$(fast)</td>
<td>1.85 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\sigma_t$(fast)</td>
<td>6.8 barns</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\nu$</td>
<td>2.98</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td></td>
<td>$\eta$</td>
<td>2.61</td>
<td>2, Table 6.1, pg. 222</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>$\sigma_a$(fast)</td>
<td>0.022 barns</td>
<td>26, Table 4-30, pg. 298</td>
</tr>
<tr>
<td></td>
<td>$\sigma_t$(fast)</td>
<td>3.09 barns</td>
<td>26, Table 3-39, pg. 148</td>
</tr>
</tbody>
</table>

First, calculate the atom densities for the plutonium oxide constituents at a bulk density of 1 g/cm$^3$:

$$N = \rho_{\text{mixture}} \times N_A$$

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

$$N_{^{16}\text{O}} = N_{^{239}\text{PuO}_2} = 2.222 \times 10^{-3} \text{ atoms/b \cdot cm}$$

$$N_{\nu_0} = 2 \times N_{^{239}\text{PuO}_2} = 2 \times 2.222 \times 10^{-3} \text{ atoms/b \cdot cm} = 4.444 \times 10^{-3} \text{ atoms/b \cdot cm}$$. 

Now that the atom densities have been calculated, the macroscopic cross-sections can be determined:
\[ \Sigma_{\text{Mixture}}^k = \Sigma_{a}^{239}\text{Pu} + \Sigma_{a}^{O_2} = N_{239}\text{Pu}^a \times \sigma_{239}\text{Pu}^a + N_{O_2} \times \sigma_{O_2}^a \]

\[ \Sigma_{a}^{\text{Mixture}} = 2.222 \times 10^{-3} \text{ atoms / b} - \text{cm} \times 2.11 \text{ b} + 4.444 \times 10^{-3} \text{ atoms / b} - \text{cm} \times 0.022 \text{ b} \]

\[ \Sigma_{a}^{\text{Mixture}} = 4.688 \times 10^{-3} \text{ cm}^{-1} + 9.78 \times 10^{-5} \text{ cm}^{-1} = 4.786 \times 10^{-3} \text{ cm}^{-1}. \]

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 \( (\varepsilon = p = 1) \).

\[ k_\infty = \eta f = \eta \times \frac{\Sigma_{a}^{239}\text{Pu}}{\Sigma_{a}^{\text{Mixture}}} = 2.61 \times \frac{4.688 \times 10^{-3} \text{ cm}^{-1}}{4.786 \times 10^{-3} \text{ cm}^{-1}} = 2.557 \]

Now the diffusion length, \( L^2 \), can be calculated on the basis of the result of the \( k_\infty \) calculation.

\[ \Sigma_{v} = \Sigma_{v}^{239}\text{Pu} + \Sigma_{v}^{O_2} = N_{239}\text{Pu}^v \times \sigma_{239}\text{Pu}^v + N_{O_2} \times \sigma_{O_2}^v \]

\[ \Sigma_{v} = \left( 2.222 \times 10^{-3} \text{ atoms / b} - \text{cm} \right) \left( 6.8 \text{ b} \right) + \left( 4.444 \times 10^{-3} \text{ atoms / b} - \text{cm} \right) \left( 3.09 \text{ b} \right) \]

\[ \Sigma_{v} = 2.884 \times 10^{-2} \text{ cm}^{-1} \]

\[ D_{\text{mixture}} = \frac{1}{3 \Sigma_{v}} = \frac{1}{3 \times 2.884 \times 10^{-2}} = 11.56 \text{ cm} \]

\[ L^2 = \frac{D_{\text{mixture}}}{\Sigma_{a}^{\text{Mixture}}} = \frac{11.56 \text{ cm}}{4.786 \times 10^{-3} \text{ cm}^{-1}} = 2,415 \text{ cm}^2. \]

Now, the material buckling, \( B_m^2 \), can be calculated:

\[ B_m^2 = \frac{k_\infty - 1}{L^2} = \frac{2.557 - 1}{2,415 \text{ cm}^2} = 6.447 \times 10^{-4} \text{ cm}^{-2}. \]

The buckling is needed to determine the critical size. Notice the diffusion length, \( L^2 \), is rather large. As with the case with the Pu and Na example problem in Section 2.5.3, this means that neutrons in this system diffuse or travel farther on the average between collisions before being absorbed by the materials in this system, which is due primarily to the relatively low fast absorption cross-section for the oxygen in plutonium oxide. Thus, this system will be much larger than a thermal system such as a Pu metal and water mixture. The critical radius can be calculated now that the material buckling is known. Recall that the geometric and material bucklings are equal for a critical system.
Calculate the critical volume of a sphere based on the calculated critical radius:

\[ R = 99.1 \text{ cm} \]

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

The critical mass of PuO\(_2\) can be found simply by multiplying the critical volume by the density of the material:

\[ m = \rho \times V = 1.0 \frac{g}{cm^3} \times 4.077 \times 10^6 \text{ cm}^3 \times \frac{kg}{1000 g} = 4,077 \text{ kg}. \]

A spreadsheet can be used to quickly calculate this methodology for the desired PuO\(_2\) densities (3, 5, 7, 9, and 11.46 g/cm\(^3\)). The results of these calculations are presented in Table 10 for comparison purposes.

**Table 10. Calculation Results for Diffusion Theory Example Problem 6**

<table>
<thead>
<tr>
<th>Density of Pu (g/cm(^3))</th>
<th>Critical Spherical Radius (cm)</th>
<th>Estimated Critical Mass of PuO(_2) (kg)</th>
<th>DANTSYS Estimated Critical Mass of PuO(_2) (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>99.1</td>
<td>4,080</td>
<td>3,522</td>
</tr>
<tr>
<td>3.0</td>
<td>33.0</td>
<td>453</td>
<td>391</td>
</tr>
<tr>
<td>5.0</td>
<td>19.8</td>
<td>163</td>
<td>141</td>
</tr>
<tr>
<td>7.0</td>
<td>14.2</td>
<td>83</td>
<td>72</td>
</tr>
<tr>
<td>9.0</td>
<td>11.0</td>
<td>50</td>
<td>43.5</td>
</tr>
<tr>
<td>11.46</td>
<td>8.65</td>
<td>31</td>
<td>26.8</td>
</tr>
</tbody>
</table>

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 DANTSYS calculations was performed to compare the hand calculations with a transport calculation using the 16-group Hansen-Roach cross-section set. The results of this comparison are shown in Figure 6.
As before with Pu systems, the tabulated fast cross sections tend to over predict absorption, which results in a larger estimate of spherical critical mass.

**Figure 6. Critical Mass Comparison for Diffusion Theory Example Problem 6**
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 perform comprehensive parametric studies on criticality safety parameters for simple fissile systems.

3.2 Overview of Buckling Conversions

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 Chapter 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:

\[ D\nabla^2\phi - \Sigma_a \phi + k_{eff} \Sigma_a \phi = 0, \]

or, after some rearranging,

\[ \nabla^2\phi + \left[ \frac{(k_{eff} - 1)}{D} \right] \Sigma_u \phi = 0. \]

For neutrons with the same energy, the one group diffusion area, \( L^2 \) can be written:

\[ L^2 = \frac{D}{\Sigma_u}. \]

After substituting \( L^2 \), the diffusion equation can be written as follows:

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

where the material buckling is defined as follows:

\[ B_m^2 = \left[ \frac{(k_{eff} - 1)}{L^2} \right], \text{ for simple one-group diffusion theory and} \]
\[ B_m^2 = \left( \frac{(k_\infty - 1)}{L^2 + \tau} \right) = \left( \frac{(k_\infty - 1)}{M^2} \right), \]

for modified one-group diffusion theory. Now, at critical, \( B_m^2 = B_g^2 \), so

\[ B_g^2 \]

can be substituted back into the diffusion equation

\[ \nabla^2 \phi + B_g^2 \phi = 0 \quad \text{or} \quad B_g^2 = -\nabla^2. \]

Thus, 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, which is independent of the geometry or shape of the system. The neutron balance used to derive the diffusion approximation is:

\[ \text{Absorption + Leakage = Production.} \]

Absorption and production depend on the properties of the materials in the system and not on the geometry of the system. Therefore, for a particular 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.

The extrapolation distance, \( d \), is important when doing buckling conversions because diffusion theory assumes that the flux is zero at some point, \( d \), outside the physical dimensions of the system. Thus, the extrapolation distance must be used to reduce the predicted values for critical size to obtain an accurate estimate for the actual 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 7). Further, values for \( d \) are determined from experimental data and calculations and relevant data for various fissile systems can be found in the literature (References 5, 7, 8, and 9).
### Table 11. Geometric Buckling Expressions for Various Systems

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Geometry Illustration</th>
<th>Geometric Buckling $B_{g}^{2}$ Relationship</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere of Radius, $r$</td>
<td><img src="image" alt="Sphere Illustration" /></td>
<td>$\left(\frac{\pi}{r+d}\right)^{2}$</td>
</tr>
<tr>
<td>Cylinder of Radius, $r$, and Height, $h$</td>
<td><img src="image" alt="Cylinder Illustration" /></td>
<td>$\left(\frac{2.405}{r+d}\right)^{2} + \left(\frac{\pi}{h+2d}\right)^{2}$</td>
</tr>
<tr>
<td>Parallelepiped of Dimensions $a, b, c$</td>
<td><img src="image" alt="Parallelepiped Illustration" /></td>
<td>$\left(\frac{\pi}{a+2d}\right)^{2} + \left(\frac{\pi}{b+2d}\right)^{2} + \left(\frac{\pi}{c+2d}\right)^{2}$</td>
</tr>
<tr>
<td>Infinite Cylinder of Radius, $r$</td>
<td><img src="image" alt="Infinite Cylinder Illustration" /></td>
<td>$\left(\frac{2.405}{r+d}\right)^{2}$</td>
</tr>
<tr>
<td>Infinite Slab of Thickness, $h$</td>
<td><img src="image" alt="Infinite Slab Illustration" /></td>
<td>$\left(\frac{\pi}{h+2d}\right)^{2}$</td>
</tr>
</tbody>
</table>

**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.
3.3 Applicability of the Buckling Conversion 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 11 as long as 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, for example, is not recommended (Reference 9).
- Labeling a system as critical provides no information about the geometry or shape of the system.
- A system can be critical in simple shapes (e.g., a sphere, cylinder, or slab).
- 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.
- The technique does not guarantee that mass or volume is conserved for critical systems that have different geometries.
3.4 Example Problems

3.4.1 Buckling Conversions Example Problem 1

Deep wells are present in a glovebox (Figure 7) where each has a length of 51 in., width of 14 in. and depth of 6 in. Suspended above these wells are 6 in. (15.24 cm) diameter storage tanks, each of which contains 30 liters of Pu solution. The Pu in the metal-water mixture contains 5 weight percent $^{240}\text{Pu}$. Assume that a single 30 liter, 6 in. 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 concentration of 200 gPu per liter for 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?

![Deep wells with dimensions 51" L x 14" W x 6" D.](image1)

Figure 7. Isometric and Elevation Views of Solution Storage Tanks and Glovebox Deep Wells for Buckling Conversions 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, the 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:
Now, the critical well height for the Pu metal-water mixture can be determined by using the relationship derived previously:

\[
c = \left[ \frac{1}{(r + d)^2} - \frac{1}{(a + 2d)^2} - \frac{1}{(b + 2d)^2} \right]^{-1/2} - 2d.
\]

Solving this equation for the critical height, \( c \), results in the following expression for the critical solution height in the well:

\[
c = \left[ \frac{1}{(r + d)^2} - \frac{1}{(a + 2d)^2} - \frac{1}{(b + 2d)^2} \right]^{-1/2} - 2d.
\]

\( \text{Now that the critical slab height has been derived for this situation, critical sphere dimensions for a Pu concentration of 200 g Pu/l should be referenced to complete the calculation. Figure 8 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. Figure 9 provides a plot of the extrapolation distances for Pu metal-water mixtures with 5 weight percent }^{240}\text{Pu for various reflection conditions.}
\]

The extrapolation distance, \( d \), can be referenced from Figure 9 for this system at a concentration of 200 g Pu/l.

\[
d = d_{\text{slab}} = d_{\text{sphere}} = 2.25 \text{ cm}
\]

The critical volume for a spherical mixture of Pu metal and water for a concentration of 200 g Pu/l is:

\[V = 22.5 \text{ l.}\]

This critical, spherical volume can be converted into a critical radius:

\[r = \sqrt{\frac{3V}{4\pi}} = \sqrt{\frac{3(22.5 \text{ l})(1000 \text{ cm}^3/\text{l})}{4\pi}} = 17.5 \text{ cm.}\]

\( \text{Now the critical well height for the Pu metal-water mixture can be determined by using the relationship derived previously:}
\]

\[
c = \left[ \frac{1}{(17.5 \text{ cm} + 2.25 \text{ cm})^2} - \frac{1}{(129.54 \text{ cm} + 2 \cdot 2.25 \text{ cm})^2} - \frac{1}{(35.56 \text{ cm} + 2 \cdot 2.25 \text{ cm})^2} \right]^{-1/2} - 2(2.25 \text{ cm})
\]

\[
c = 18.5 \text{ cm.}
\]
Figure 8. Critical Volume for an Unreflected Sphere with a Pu Metal-Water Mixture with 5 Wt. % $^{240}$Pu (Reference 5, Figure III.A.9.95-3)
Figure 9. Extrapolation Distance Data for Pu Metal-Water Mixtures with 5 Wt. % $^{240}$Pu (Reference 5, Figure III.A.10.95-3)
Part 2. The critical slab height calculated in Part 1 can now be used to calculate the critical solution mass and volume required on the basis of the estimated critical height for the deep well. Knowing the Pu concentration, $\rho$, and deep well dimensions $A$, $B$ and $C$, we can calculate the critical volume and mass from the following.

The total volume and critical mass of the critical slab can be calculated as follows:

$$V = A \times B \times C = (129.54 \, cm \times 35.56 \, cm \times 18.5 \, cm)$$

$$V = 85,219 \, cm^3 = 85.2 \, l.$$ 

Thus, 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, a criticality event could not occur unless the contents of multiple tanks were to spill into the tank.
3.4.2 Buckling Conversions Example Problem 2

Calculate the water-reflected, critical radius for a cylindrical tank that has a height of 20 cm, filled with 20 g/l Pu metal-water mix. The Pu is assumed to contain 5 wt. % Pu-240. Compare this resulting critical radius with that of an infinite cylinder.

Use the buckling formulas in Table 11 to equate the geometric buckling for a sphere to that of a finite cylinder:

\[
\frac{\pi}{R_{\text{sph}} + \delta} = \left[ \frac{2.405}{R_{\text{cyl}} + \delta} \right]^2 + \left[ \frac{\pi}{H + 2\delta} \right]^2.
\]

The extrapolation distance for water-reflected Pu can be found in Figure 9, \(d = 5.65 \text{ cm}\), and, as stated in the problem description, the cylinder height, \(H\), is 20 cm. The critical radius, \(R_{\text{sph}}\), for a thick water-reflected Pu sphere for a concentration of 20 g Pu/l can be determined by finding the critical volume for this system from Figure 8 and solving for \(R_{\text{sph}}\) using the volume/radius relationship for a sphere.

\[
V_{\text{sph}} = \frac{4}{3} \pi R_{\text{sph}}^3
\]

Solve for \(R_{\text{sph}}\):

\[
R_{\text{sph}} = \left[ \frac{3}{4\pi} V_{\text{sph}} \right]^{1/3} = \left[ \frac{3}{4\pi} \left( 36.5 \frac{l}{l} \right) \left( 1000 \frac{cm^3}{l} \right) \right]^{1/3} = 20.58 \text{ cm}.
\]

Substitute the values for \(R_{\text{sph}}\) and \(H\) into the previous equation solve for \(R_{\text{cyl}}\):

\[
\left[ \frac{\pi}{20.578 + 5.65} \right]^2 = \left[ \frac{2.405}{R_{\text{cyl}} + 5.65} \right]^2 + \left[ \frac{\pi}{20 + 2 \times 5.65} \right]^2.
\]

Solve this equation for \(R_{\text{cyl}}\):

\[
\left[ \frac{2.405}{R_{\text{cyl}} + 5.65} \right]^2 = \left[ \frac{\pi}{20.58 + 5.65} \right]^2 - \left[ \frac{\pi}{20 + 2 \times 5.65} \right]^2
\]

\[
\left[ \frac{2.405}{R_{\text{cyl}} + 5.65} \right]^2 = 0.01435 - 0.01007 = 0.00428
\]

\[R_{\text{cyl}} = 31.1 \text{ cm}.
\]
It should be noted that the same extrapolation distances were used for both the sphere and the cylinder in this calculation. The height-to-diameter ratio \( H/D \) for this cylinder is \( H/D=20/30=0.667 \). Figure 16 (Reference 10, Figure 6), can be used to determine if the extrapolation distance used for the cylinder needs to be adjusted. For the cylinder considered in this example, the ratio \( (H/D)/(1+H/D)=0.25 \). The ratio of extrapolation distances for this case is approximately 1. These ratios have been empirically determined to high precision for solution cylinders of Pu solutions (Reference 10). Therefore, the extrapolation distance for a sphere is approximately equal to that of the cylinder considered for this example, thus no adjustment is required.

To calculate the critical radius for a cylinder of infinite length, the same technique can be applied by using the fourth relationship in Table 11.

Use the fourth buckling formula in Table 11 to equate the geometric buckling for a sphere to that of an infinite cylinder;

\[
\left[ \frac{\pi}{R_{\text{cyl}} + d} \right]^2 = \left[ \frac{2.405}{R_{\text{cyl}} + d} \right]^2 .
\]

The extrapolation distance for water-reflected Pu can be found in Figure 9 \((d = 5.65 \text{ cm})\). The critical radius for a thick water reflected sphere, \( R_{\text{cyl}} \), is 20.58 cm from the finite cylinder calculation. Substitute these values into the previous equation and solve for \( R_{\text{cyl}} \):

\[
\left[ \frac{\pi}{20.578 + 5.65} \right]^2 = \left[ \frac{2.405}{R_{\text{cyl}} + 5.65} \right]^2 .
\]

Solve this equation for \( R_{\text{cyl}} \):

\[
\left[ \frac{2.405}{R_{\text{cyl}} + 5.65} \right]^2 = \left[ \frac{\pi}{20.578 + 5.65} \right]^2 .
\]

\[
\left[ \frac{2.405}{R_{\text{cyl}} + 5.65} \right]^2 = 0.01435
\]

\[ R_{\text{cyl}} = 14.4 \text{ cm}. \]

Notice that the infinite cylinder has a much smaller critical radius than a short, finite cylinder. This result makes sense because a finite cylinder has axial leakage as well as radial leakage while the infinite cylinder only has radial leakage. The critical radius calculation for an infinite cylinder with Pu (5 wt. % \( ^{240}\text{Pu} \)) solution is comparable to the ANSI/ANS-8.1-1998 (Reference 18) subcritical limit of 15.4 cm for \( ^{238}\text{Pu(NO}_3)_4 \) solution at optimum concentration and thick water reflection.
3.4.3 Buckling Conversions Example Problem 3

What is the critical height for a 15 cm diameter cylinder with the same solution defined in the last example problem?

This problem can be solved with the same procedure from Section 3.4.2. As before, the geometric buckling of a critical sphere of a plutonium metal-water mixture can be set equal to the buckling relationship for a finite cylinder of radius, \( R_{cyl} \), and height, \( H \), as shown in Table 11.

\[
\left[ \frac{\pi}{R_{sph} + \lambda} \right]^2 = \left[ \frac{2.405}{R_{cyl} + \lambda} \right]^2 + \left[ \frac{\pi}{H + 2\lambda} \right]^2.
\]

As previously stated, the extrapolation distances for a sphere and cylinder are approximately the same. Thus, the extrapolation distance for the sphere was used.

The extrapolation distance for a sphere is determined from Figure 9 \((d = 5.65 \text{ cm})\), and the cylindrical radius, \( R_{cyl} \), is 7.5 cm. The spherical critical radius for a water-reflected sphere is 20.578 cm from Section 3.4.2.

\[
\left[ \frac{\pi}{20.58 + 5.65} \right]^2 = \left[ \frac{2.405}{7.5 + 5.65} \right]^2 + \left[ \frac{\pi}{H + 2 \times 5.65} \right]^2
\]

\[
\left[ \frac{\pi}{H + 2 \times 5.65} \right]^2 = 0.01435 - 0.03345
\]

\[
\left[ \frac{\pi}{H + 2 \times 5.65} \right]^2 = -0.01910.
\]

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/l (Pu with 5 wt. % \(^{239}\text{Pu}\)) solution to attain a critical state. This conclusion could also be reached from the previous analysis where a minimum 28.8 cm \((14.4 \text{ cm} \times 2)\) 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 fat, short cylindrical tanks, which makes them more inherently safe. Figure 10 illustrates that, for Pu densities less than about 1 kg/l (plutonium is in solution form), the critical diameter of an infinite cylinder will be about 15 cm (about 6 in.) for a water-reflected system. This fact is the main reason that cylindrical plutonium solution storage tanks are designed with this diameter or less to ensure, regardless of the plutonium concentration or neutron reflectors present, that criticality is impossible.
Figure 10. Estimated Critical Diameters of Infinitely Long Cylinders of Homogeneous Water-moderated Plutonium (Reference 10, Figure 33)

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 N HNO₃ and 3.1% ²³⁹Pu content of the plutonium.
3.4.4 Buckling Conversions 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 while the second tank is being filled with a plutonium metal-water mixture with 5 wt. % $^{240}$Pu (Figure 11). Both solutions have a fissile concentration of 100 g fissile/l.

Determine the critical solution height for each tank and compare the results of the two systems. Repeat this calculation with a concentration of 150 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.

The first step in the solution to this problem is to compile the data needed for each mixture.

Figures 13 and 14 provides information about the spherical critical mass and volume, respectively, for a bare U(93.2) metal-water mixture as follows:

$$M_{U(93.5)} = 1.8 \text{ kg}$$
$$V_{U(93.5)} = 18 \text{ l}$$

$$R_{U(93)} = \left[ \frac{3V_{U(93.5)}}{4\pi} \right]^{\frac{1}{3}} = \left[ \frac{3 \cdot 18 \text{ l} \cdot 1000 \text{ cm}^3}{4\pi} \right]^{\frac{1}{3}} = 16.3 \text{ cm}.$$  

Figures 8 and 12 provide the spherical critical mass and volume data, respectively, for Pu metal–water mixtures containing 5 wt. % $^{240}$Pu as follows:

$$M_{Pu(5)} = 2.25 \text{ kg}$$
$$V_{Pu(5)} = 22.5 \text{ l}$$

$$R_{Pu(5)} = \left[ \frac{3 \cdot V_{Pu(5)}}{4\pi} \right]^{\frac{1}{3}} = \left[ \frac{3 \cdot 22.5 \text{ l} \cdot 1000 \text{ cm}^3}{4\pi} \right]^{\frac{1}{3}} = 17.5 \text{ cm}.$$  

The extrapolation distances for these systems can be found as follows.

For U(93.5) metal–water mixtures at 100 gU/l, the extrapolation distance from Figure 15 is about 2 cm.

For Pu metal–water mixtures (5 wt. % $^{240}$Pu at 100 gPu/l), the extrapolation distance from Figure 9 is about 2.2 cm.
Recall that the geometric buckling for a sphere is equated to that of a cylinder as follows.

\[
\left(\frac{\pi}{R_{sph} + d}\right)^2 = \left(\frac{2.405}{R_{cyl} + d}\right)^2 + \left(\frac{\pi}{H + 2d}\right)^2.
\]

For the U(93.5) solution tank, recall that the extrapolation distance for a sphere is about the same for a cylinder (Figure 16):

\[
\left(\frac{\pi}{16.3 \text{ cm} + 2 \text{ cm}}\right)^2 = \left(\frac{2.405}{25.4 \text{ cm} + 2 \text{ cm}}\right)^2 + \left(\frac{\pi}{H + 2(2 \text{ cm})}\right)^2
\]

\[H = 17.3 \text{ cm}.
\]

For the Pu(5) solution tank, recall that the extrapolation distance for a sphere is about the same for a cylinder (Figure 16, which can be used for Pu(5) solutions as well):

\[
\left(\frac{\pi}{17.5 \text{ cm} + 2.2 \text{ cm}}\right)^2 = \left(\frac{2.405}{25.4 \text{ cm} + 2.2 \text{ cm}}\right)^2 + \left(\frac{\pi}{H + 2(2.2 \text{ cm})}\right)^2
\]

\[H = 19.1 \text{ cm}.
\]

Although the critical height difference between the plutonium and uranium and water mixtures is small (about 2 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 than for plutonium at a fissile concentration of 100-g/l.

For 150-g/l fissile concentration, the calculation proceeds as before.

Figure 13 provides information about the spherical critical mass for a bare U(93.2) metal–water mixture as follows (radius calculated based on volume):

\[M_{U(93)} = 2.55 \text{ kg}
\]

\[V_{U(93)} = 17 \text{ l}
\]

\[R_{U(93)} = 16.0 \text{ cm}.
\]

Figures 8 and 12 provide the spherical critical volume and mass data, respectively, for Pu metal–water mixtures containing 5 wt. % \(^{240}\text{Pu}\) as follows:

\[M_{Pu(5)} = 3.3 \text{ kg}
\]

\[V_{Pu(5)} = 22.0 \text{ l}
\]

\[R_{Pu(5)} = 17.4 \text{ cm}.
\]

The extrapolation distances do not change appreciably from 100 to 150 g/l concentration. Thus, the same extrapolation distances are used for this calculation.
For the U(93.5) Solution tank, recall that the extrapolation distance for a sphere is about the same for a cylinder (Figure 16):

\[
\left[ \frac{\pi}{16.0 \text{ cm} + 2 \text{ cm}} \right]^2 = \left[ \frac{2.405}{25.4 \text{ cm} + 2 \text{ cm}} \right]^2 + \left[ \frac{\pi}{H + 2(2 \text{ cm})} \right]^2
\]

\[H = 16.8 \text{ cm}.\]

For the Pu(5) solution tank and recall that the extrapolation distance for a sphere is about the same for a cylinder (Figure 16):

\[
\left[ \frac{\pi}{17.4 \text{ cm} + 2.2 \text{ cm}} \right]^2 = \left[ \frac{2.405}{25.4 \text{ cm} + 2.2 \text{ cm}} \right]^2 + \left[ \frac{\pi}{H + 2(2.2 \text{ cm})} \right]^2
\]

\[H = 19.0 \text{ cm}.\]

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 1.8 cm to 2.2 cm. It can be seen from this problem that a Pu metal-water mixture (5 wt. % $^{240}$Pu) 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.
Figure 11. KENO 3D Illustration of Tanks for Buckling Conversions Problem 4 (not to scale)
Figure 12. Spherical Critical Mass for a Plutonium-Water Mixture (5 Wt. % $^{240}\text{Pu}$)
[Reference 5, Figure III.A.6.95-3]
Fig. 10. Critical masses of homogeneous water-moderated $U(93.2)$ spheres. Solution data appear unless indicated otherwise.

Figure 13. Critical Mass for Water Moderated U(93) Spheres [Ref. 10, Figure 10]
Figure 14. Spherical Critical Volume and Mass for a Mixture of U(93.5) and Water
[Reference 5, Figure III.B.9(93.5)-2]
Figure 15. Material Buckling and Extrapolation Distances for U(93.5) and Water
[Reference 5, Figure III.B.10(93.5)-1]
Figure 16. Ratio of Cylindrical to Spherical Extrapolation Distances [Reference 10, Figure 6]
4. Core-Density Conversions

4.1 What You Will Be Able to Do

- Determine the critical dimensions of a fissile system due to 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, 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 7, page 25). Even though the dimensions of the system change, the relative number of neutrons that leak out of the system, that are absorbed or that scatter remains the same. Thus, the system remains at a critical state (Figure 17). References 7, 8, 10, 11 and 12 provide much more discussion about this hand calculation method including supporting data.

![Figure 17. Illustration of Core-Density Method Concept](image)

4.2.1 Core-Density Conversions for Bare, Homogeneous Systems

Table 12 provides the relationships from References 7 that can be useful for this method. The relationships for infinite cylinders and slabs are provided for information purposes. These relationships are not as commonly used as the relationships for spheres.
Table 12. Core-Density Conversion Relationships for Bare, Homogeneous Systems

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Critical Radius Relationship</th>
<th>Critical Volume Relationship</th>
<th>Critical Mass Relationship</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere (Final radius, r, initial radius, (r_0), etc.)</td>
<td>(\frac{r}{r_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{1}{3}})</td>
<td>(\frac{V}{V_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{3}{2}})</td>
<td>(\frac{m}{m_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{2}{3}})</td>
</tr>
<tr>
<td>Infinite Cylinder (Final radius, r, initial radius, (r_0), etc.)</td>
<td>(\frac{r}{r_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{1}{3}})</td>
<td>(\frac{V}{V_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{3}{2}})</td>
<td>(\frac{m}{m_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{2}{3}})</td>
</tr>
<tr>
<td>Infinite Slab (Final thickness, t, initial thickness, (t_0), etc.)</td>
<td>(\frac{t}{t_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{1}{3}})</td>
<td>(\frac{V}{V_0} = \left(\frac{\rho}{\rho_0}\right)^{\frac{3}{2}})</td>
<td>(\frac{m}{m_0} = \text{constant})</td>
</tr>
</tbody>
</table>

4.2.2 Core-Density Conversions for Reflected, Homogeneous System

The following relationship from References 7 and 10 can be used to determine the critical dimensions for a reflected system when the reflector density remains constant. For example, consider a water-reflected metal system (Figure 18) whose metal density changes but the water density remains the same. This relationship based on experimental data is as follows:

\[
\frac{m}{m_0} = \left(\frac{\rho}{\rho_0}\right)^{S}
\]

Where \(S\) is approximately constant over the range \(0.5 \leq \frac{r}{r_0} \leq 1.0\), where \(r\) is defined as the final radius and \(r_0\) is the initial radius of the system. The exponent, \(S\), cannot exceed a value of 2, which implies that as the density of the core approaches zero, the system dimensions approach infinity. Thus the difference between a bare system and a reflected system has no particular meaning. Further, these references provide information about determining the core-density exponent, \(S\). The example problem presented in Section 4.4.4 provides information about calculating \(S\).

Figure 18. Illustration of a Reflected, Homogenous System
4.3 Applicability of Core-Density Conversions

The Core-Density method is applicable for fissile material systems with the following characteristics and assumptions.

- The system needs to have a uniform, homogeneous composition,
- If the system is reflected, 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 (Reference 7),
- The method cannot be used if the system contains heterogeneities such as lumps of fuel or fuel rods in a reactor, and
- For reflected systems, if the reflector density changes, or if the core density changes are not uniform, 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 with a density of 19.8 g/cm\(^3\), assuming that the initial density for this system was 15.6 g/cm\(^3\).

Recall that Pu(4.5) is a system with 95.5 atom percent \(^{239}\)Pu and 4.5 atom percent \(^{240}\)Pu. The core-density conversion method can be used to calculate the bare critical mass for this system. The unreflected, spherical critical mass for Pu(4.5) system with a density of approximately 15.6 g/cm\(^3\) is approximately 16.8 kg (Reference 10, Table 32).

Using the spherical critical mass relationship in Table 12, the critical mass for this system can be calculated as follows:

\[
\frac{m}{m_0} = \left( \frac{\rho}{\rho_0} \right)^{-2}
\]

\[
m = m_0 \left( \frac{\rho}{\rho_0} \right)^{-2} = (16.8 \text{ kg}) \times \left( \frac{19.8 \text{ g/cm}^3}{15.6 \text{ g/cm}^3} \right)^{-2}
\]

\[
m = 10.4 \text{ kg.}
\]

This critical mass result is consistent with the calculated data provided in Figure 21 (Reference 5, Figure III.A.6-2), which reports the critical mass for a Pu metal system with 5 wt. % \(^{240}\)Pu and a density of 19.8 g/cm\(^3\) as approximately 10.4 kg.
4.4.2 Core-Density Example Problem 2

Calculate the critical radius for a spherical, unreflected Pu(5) metal system with a density of 9.9 g/cm$^3$, assuming that the initial density for this system was 19.8 g/cm$^3$.

Recall that Pu(5) is a system with 95 atom percent $^{239}$Pu and 5 atom percent $^{240}$Pu. The core-density conversion method can be used to calculate the bare critical mass for this system. The unreflected, spherical critical mass for Pu(3.1) system with a density of approximately 19.8 g/cm$^3$ is approximately 10.3 kg (Reference 10, Figure 31). Using either set of data will provide a good estimate for the lower density Pu(5) metal system.

Using the spherical critical mass relationship in Table 12, the critical mass for this can be calculated as follows.

The critical radius for a Pu metal sphere with a critical mass of 10.3 kg for a density of 19.8 g/cm$^3$ is:

$$r = \left( \frac{3 \cdot V}{4\pi} \right)^{\frac{1}{3}} = \left[ 3 \cdot \left( \frac{10300 \text{ g}}{19.8 \text{ g/cm}^3} \right) \right]^{\frac{1}{3}} = 5.0 \text{ cm}$$

$$\frac{r}{r_0} = \left( \frac{\rho}{\rho_0} \right)^{-1}$$

$$r = r_0 \left( \frac{\rho}{\rho_0} \right)^{-1} = \left( 5.0 \text{ cm} \right) \times \left( \frac{9.9 \text{ g/cm}^3}{19.8 \text{ g/cm}^3} \right)^{-1}$$

$$r = 10.0 \text{ cm}.$$  

This result is consistent with the results of a Keno V.a calculation for this system, where the critical radius was calculated to be approximately 10.1 cm.
4.4.3 Core-Density Example Problem 3

Calculate the critical mass for a spherical, unreflected $^{239}\text{PuO}_2$ system with a density 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 2.5.6 (Diffusion Theory Example Problem 6).

Recall that the critical mass for an unmoderated $^{239}\text{PuO}_2$ system was calculated in Section 2.5.6, using diffusion theory, as approximately 31 kg. Using the critical mass relationship from Table 12 for a spherical system, the critical mass for this unmoderated system can be calculated for the densities of interest. The same procedure used in Sections 4.5.1 and 4.5.2 is used to calculate the critical masses for this system:

$$m = m_0 \left( \frac{\rho}{\rho_0} \right)^{-2}$$

$$m = m_0 \left( \frac{\rho}{\rho_0} \right)^{-2} = (31 \text{ kg}) \times \left( \frac{1.0 \text{ g/cm}^3}{11.46 \text{ g/cm}^3} \right)^{-2}$$

$$m = 4084 \text{ kg}.$$  

This calculation is repeated for the other densities of interest. The resulting critical mass estimates for the system are summarized in Table 13.

<table>
<thead>
<tr>
<th>Density of Pu (g/cm$^3$)</th>
<th>Critical Spherical Radius (cm)</th>
<th>Estimated Critical Mass of PuO$_2$ (kg) (One-Group Diffusion Theory)</th>
<th>Estimated Critical Mass of PuO$_2$ (kg) (Core-Density Method)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>99.1</td>
<td>4,080</td>
<td>4,084</td>
</tr>
<tr>
<td>3.0</td>
<td>33.0</td>
<td>453</td>
<td>453</td>
</tr>
<tr>
<td>5.0</td>
<td>19.8</td>
<td>163</td>
<td>163</td>
</tr>
<tr>
<td>7.0</td>
<td>14.2</td>
<td>83</td>
<td>83</td>
</tr>
<tr>
<td>9.0</td>
<td>11.0</td>
<td>50</td>
<td>50</td>
</tr>
</tbody>
</table>

Notice that the results are essentially the same as the critical mass estimates from Section 2.5.6. As long as the initial critical mass is known with some confidence and the applicability of this technique is valid (Section 4.3), the critical mass estimates at other densities can be estimated very accurately with the core-density method.

---

$^3$ The diffusion theory value is used, as it is consistent with the diffusion theory critical mass values shown in Table 10 and those used for comparison in Table 13.
4.4.4 Core-Density Example Problem 4

Calculate the water-reflected critical mass for a spherical, Pu(5) metal system with a density of 15.75 g/cm$^3$ if the Pu core had an initial density of 19.8 g/cm$^3$.

This system is different than Core-Density example problem 3 because this problem has a uniform density reflector surrounding the Pu. The core-density conversion relationship for a constant density reflector can be used to calculate the resulting critical mass for this case:

$$\frac{m}{m_o} = \left( \frac{\rho}{\rho_o} \right)^{-S}.$$

The critical mass of a water reflected sphere of Pu(5.2) at 19.74 g/cc is 5.8 kg (Reference 10, Table 32), while from section 4.5.1, the unreflected critical mass is 10.4 kg. Figure 19 can be used to determine the core-density exponent, $S$, for this system:

$$ \frac{r_{\text{reflected}}}{r_{\text{unreflected}}} = \left( \frac{m_{\text{reflected}}}{m_{\text{unreflected}}} \right)^{1/3} = \left( \frac{5.8}{10.4} \right)^{1/3} = 0.823 $$

From Figure 19, the value for the core density exponent (denoted in Figure 18 as $n$) is approximately 1.5.

$$m = m_o \left( \frac{\rho}{\rho_o} \right)^{-1.5} = 5.8 \text{ kg} \times \left( \frac{15.75 \text{ g/cm}^3}{19.8 \text{ g/cm}^3} \right)^{-1.5}$$

$$m = 8.2 \text{ kg.}$$

This result is very close to the experimental data provided in Reference 10, Figure 35, which reports the critical mass for a water-reflected Pu(5) metal system with a density of 15.75 g/cm$^3$ as approximately 8 kg. Furthermore, the results of a Keno V.a calculation concluded that the critical mass for this system is about 8.25 kg.
Figure 19. Density Exponent Plot of Unmoderated Spherical Cores in Constant Density Reflectors (Reference 10, Figure 8)
5. Surface Density Method

5.1 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 units of irregular shapes, such as equipment items with fissile material present, stored on a process floor.

- Comprehensive parametric studies on various array parameters (fissile mass, spacing, array size, etc.).

5.2 Surface Density Method Overview

This particular 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 particular facility via an engineered or administrative control. Information beyond that covered in this section can be found in References 13, 14, 15, 16, and 17. The method was derived from the limiting surface density method, experimental and calculated critical data (Reference 33). 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 is used by projecting the fissile material mass of the array units onto an area of a plane (Reference 13) and comparing 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 20 illustrates this concept.

The average surface density, $\overline{\sigma}$, 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 13) was derived from limiting surface density relationships (Reference 23, 24, and 25). Chapter 7 provides a more comprehensive description of the limiting surface density method. The 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 33 for the surface density method is shown below.
Begin with the limiting surface density relationship for the array material characteristics:

\[ \sigma(m) = c_2 (m_0 - m) \text{ or after factoring out an } m_0, \sigma(m) = c_2 m_0 \left( 1 - \frac{m}{m_0} \right). \]

The limiting surface density relationship for the array geometric characteristics can be written as follows:

\[ \sigma(m) = \frac{nm}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2. \]

The surface density method assumes an infinite planar array that is of finite height (i.e., \( n \) units high). Thus, the 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:

\[ \sigma(m) = \frac{nm}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{\infty}} \right)^2 = \frac{nm}{(2a_n)^2} \left( 1 - 0 \right)^2 = \frac{nm}{(2a_n)^2}. \]

This relationship can be simplified more by knowing that the quantity \( 2a_n \) is equivalent to the center-to-center spacing between array units, \( d \).

\[ \sigma(m) = \frac{nm}{d^2}. \]

Solving this equation 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, \( \sigma \), which is dependent upon the material characteristics of the array:

\[ d = \left[ \frac{nm}{\sigma} \right]^{\frac{1}{2}}. \]

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 the following limiting surface density relationship after some simplification earlier. The expression is also known as the allowed surface density:

\[ \sigma(m) = c_2 m_0 \left( 1 - \frac{m}{m_0} \right). \]

The fraction of a critical mass, \( f \), present at each location in the array is: \( f = \frac{m}{m_0} \). The surface density method requires that the fraction critical, \( f \), not exceed a value of 0.73. In Section 7.3.1, the effective multiplication factor, \( k_{eff} \), is defined as follows.
\[ k_{\text{eff}} = \left( \frac{m}{m_0} \right)^{\frac{1}{3}} = (f)^{\frac{1}{3}}. \]

For \( f = 0.73 \), the \( k_{\text{eff}} = (0.73)^{\frac{1}{3}} = 0.9 \). Thus, each unit in the array must not exceed this value. This safety margin can be incorporated into the allowed surface density for the array.

\[ \sigma(m) = c_2 m_0 \left( 1 - 1.37 \frac{m}{m_0} \right) = c_2 m_0 \left( 1 - 1.37f \right). \]

If \( f \) were equal to 0.73, the allowed surface density for that array would be zero:

\[ \sigma(m) = c_2 m_0 \left( 1 - 1.37 \times 0.73 \right) = c_2 m_0 \left( 1 - 1.37 \times 0.73 \right) = c_2 m_0 \left( 1 - 1 \right) = 0. \]

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 simplified and 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 \( m = 0 \):

\[ \sigma(0) = c_2 m_0 \left( 1 - 1.37 \left( \frac{0}{m_0} \right) \right) = c_2 m_0. \]

The allowed surface density when the array unit mass is zero, \( \sigma(0) \), is also denoted \( \sigma_0 \), so the allowed surface density relationship can be written as follows.

\[ \sigma(m) = \sigma_0 \left( 1 - 1.37f \right). \]

Now, the expression in Reference 13, Eq. 4.5, defines the allowed surface density, with a coefficient that limits the allowed surface density to 54\% of the allowed surface density:

\[ \sigma(m) = 0.54 \sigma_0 \left( 1 - 1.37f \right). \]

This coefficient 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. This relationship can be substituted into the relationship for the center-to-center spacing that was previously derived with limiting surface density relationships. 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. The center-to-center spacing between array units for the surface density method was defined previously as:
\[ d = \left[ \frac{nm}{\sigma(m)} \right]^{\frac{1}{2}}. \]

Substitute the expression for the allowed surface density that was just determined from Reference 13 and the following expression for \( d \) is determined.

\[ \sigma(m) = 0.54\sigma_0 \left( 1 - 1.37f \right) \]

\[ d = \left[ \frac{nm}{0.54\sigma_0 \left( 1 - 1.37f \right)} \right]^{\frac{1}{2}} = 1.37 \left[ \frac{nm}{\sigma_0 \left( 1 - 1.37f \right)} \right]^{\frac{1}{2}}. \]

Each of the variables for \( d \) is defined below for Thomas’ representation of the surface density method (Reference 13):

\( \sigma_0 \) – 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).
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.

**Fissile 6x4x2 Array**

**Figure 20. Illustration of the Surface Density Method**
5.3 Applicability of the Surface Density Method

The surface density method can be used for a variety of fissile materials and array configurations, and it is applicable for the following situations:

- 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. The calculated array center-to-center spacing will result in a subcritical array configuration.

- This method, as described above, is applicable to infinite planar arrays reflected by water at least 155 mm thick or its nuclear equivalent (Reference 13). Guidance for applying this method with arrays located next to concrete reflectors can be found in Reference 16. The example problems consider arrays with water reflection only.

- This method can be used in situations where the fissile units have irregular geometries such as where equipment containing fissile materials is stored on a process floor (Reference 9). 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 array unit and array shape are discussed in greater detail in References 13 and 16.

- 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.
5.4 Surface Density Method Example Problems

5.4.1 Surface Density Example Problem 1

Calculate the minimum spacing for a planar array of 2-liter bottles of Pu, with 5-wt. % $^{240}\text{Pu}$, 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 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. From Figure 21, the critical, unreflected spherical mass of Pu at 400 gPu/L with 5 wt. % $^{240}\text{Pu}$ is about 9 kg, and the corresponding critical, unreflected spherical volume is 22.5 L from Figure 8.

The surface density of a water-reflected slab, $\sigma_o$, 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) solution system can be estimated from Figure 22 as 2.7 in. or 6.86 cm.

$$\sigma_o = 6.86 \text{ cm} \times 400 \text{ gPu/l} \times 0.001 \text{ l/cm}^3$$

$$\sigma_o = 2.74 \text{ gPu/cm}^2.$$ 

The mass of Pu in each bottle of solution is

$$2 \text{ l/bottle} \times 400 \text{ gPu/l} = 800 \text{ g Pu per bottle.}$$

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:

$$m = 400 \text{ gPu/L} \times 22.5 \text{ L} = 9 \text{ kg}$$ (this is equal to the Pu critical mass for a system with 5 wt. % $^{240}\text{Pu}$ from Figure 21 for this concentration).

Now, $f$ can be calculated as follows:

$$f = \frac{\text{mass of Pu in a 2 L bottle}}{\text{critical mass of unreflected Pu(5) metal-water mixture}}$$

$$f = \frac{800 \text{ gPu}}{9000 \text{ gPu}} = 0.089.$$
Knowing $\sigma_o$ and $f$, the center-to-center spacing can be determined for an infinite array stacked one unit high ($n = 1$):

$$d = 1.37 \left[ \frac{nm}{\sigma_o (1 - 1.37f)} \right]^{1/2}$$

$$d = 1.37 \times \left[ \frac{1 \times 800 \text{ gPu}}{2.74 \text{ gPu/cm}^2 (1 - 1.37 \times 0.089)} \right]^{1/2}$$

$$d = 25.0 \text{ cm (9.8 in.)}.$$ 

Therefore, as a limit, the center-to-center spacing for this one-unit-high, infinite array of Pu solution bottles containing 5 wt. % $^{240}\text{Pu}$ should not be less than 25.0 cm (about 10 in.).
Figure 21. Spherical Critical Mass of an Unreflected Mixture of Plutonium and Water (Reference 5, Figure III.A.6-2)
Figure 22. Critical Infinite Slab Thickness of a Mixture of Plutonium and Water (Reference 5, Figure III.A.5-3)
5.4.2 Surface Density Example Problem 2

What is the minimum center-to-center spacing for an infinite planar array of plutonium oxide (\(^{239}\text{PuO}_2\)) containers loaded with 4,500 grams of Pu per container? Assume that the Pu oxide density is 11.48 g/cm\(^3\), which is the theoretical density for PuO\(_2\); that the Pu is pure \(^{239}\text{Pu}\); and that 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 \(f\), 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, \(\sigma_o\).

The value of \(\sigma_o\) can be determined by taking the product of the slab height of an infinite, water-reflected slab and the theoretical Pu density. The water-reflected, infinite slab thickness for a \(^{239}\text{PuO}_2\) system can be determined via Reference 18, Table 4, as 1.4 cm (0.55 in.) for Pu oxide that contains less than 1.5 wt. % water at theoretical density.

\[
\sigma_o = 1.4 \text{ cm} \times 11.48 \text{ gPuO}_2 / \text{cm}^3
\]
\[
\sigma_o = 16.07 \text{ gPuO}_2 / \text{cm}^2.
\]

Next, \(f\) needs to be calculated based on the critical mass of an unreflected sphere of \(^{239}\text{PuO}_2\) and water. From Reference 19, the critical, unreflected spherical mass of \(^{239}\text{PuO}_2\) at 11.48 gPuO\(_2\)/cm\(^3\) is about 26,700 g.

The value of \(f\) can be calculated as follows:

\[
f = \frac{\text{mass of } ^{239}\text{PuO}_2}{\text{critical mass of unreflected } ^{239}\text{PuO}_2 \text{ system at theoretical density}}
\]
\[
f = \frac{5102 \text{ gPu}}{26700 \text{ gPu}} = 0.192.
\]

Knowing \(\sigma_o\) and \(f\), the center-to-center spacing can be calculated for an infinite array stacked one unit high \((n = 1)\):

\[
d = 1.37 \left[ \frac{nm}{\sigma_o \left( 1 - 1.37f \right)} \right]^{1/2}
\]
\[
d = 1.37 \times \left[ \frac{1 \times 5102 \text{ gPuO}_2}{16.07 \text{ gPu/cm}^2 \left( 1 - 1.37 \times 0.192 \right)} \right]^{1/2}
\]
\[
d = 28.4 \text{ cm (11.2 in.).}
\]
Therefore, as a limit, the center-to-center spacing for this one-unit-high, infinite array of $^{239}\text{PuO}_2$ containers is about 28 cm (11.2 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 40.2 cm (15.3 in.), which is somewhat intuitive because of the presence of additional fissile material in the array requires a larger spacing.

The full water reflection only makes the limited dimension have zero leakage, making it effectively infinite (Figure 23).

Figure 23. Illustration of the Surface Density Water Reflection Assumptions
5.4.3 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 value of $\sigma_o$ can be determined by taking the product of the slab height of an infinite, water-reflected slab and the material density. The water-reflected, infinite slab thickness for an alpha-phase Pu(3.1) metal system can be determined via Reference 10, 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 $^{240}\text{Pu}$ content for this case results in more of the fissile $^{239}\text{Pu}$ isotope being present; thus, the slab thickness used will be conservative. (A KENO V.a calculation gives ~0.835 cm for a pure $^{239}\text{Pu}$ infinite slab). Now, calculate the surface density for the water-reflected, infinite slab.

$$\sigma_o = 0.82 \text{ cm} \times 19.75 \text{ gPu/cm}^3$$

$$\sigma_o = 16.20 \text{ gPu/cm}^2.$$

Next, $f$ needs to be calculated based on the critical mass of an unreflected sphere of Pu(5) metal-water. From Figure 21, the critical, unreflected spherical mass of Pu metal with 5 wt. % $^{240}\text{Pu}$ at 19.75 gPu/cm³ is about 10,300 g.

The value of $f$ can be calculated as follows:

$$f = \frac{\text{mass of Pu(5) metal per container}}{\text{critical mass of a unreflected Pu(5) metal system at theoretical density}}$$

$$f = \frac{4500 \text{ gPu}}{10300 \text{ gPu}} = 0.437.$$

Knowing $\sigma_o$ and $f$, the center-to-center spacing can be determined for an infinite array stacked one unit high ($n = 1$):

$$d = 1.37 \left[ \frac{nm}{\sigma_o (1 - 1.37f)} \right]^{1/2}$$

$$d = 1.37 \times \left[ \frac{1 \times 4500 \text{ gPu}}{16.20 \text{ gPu/cm}^2 (1 - 1.37 \times 0.437)} \right]^{1/2}$$

$$d = 36.0 \text{ cm (14.2 in.).}$$
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 cm (14 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 51 cm (20 in.).
6. Density Analog Method

6.1 What You Will Be Able to Do

- Determine the center-to-center spacing between fissile 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.

- Comprehensive parametric studies on various array parameters (fissile mass, spacing, array size, etc.).

6.2 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 13, 16, and 17. 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 16). This method was developed in the 1940s to consider the storage of weapon capsules in various array configurations (Reference 20). 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 similar to 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. Although the surface density method does limit the array dimension in one dimension, 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. 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 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.

As for the surface density method, the Thomas formulation of the density analog method (Reference 13) was derived from limiting surface density relationships (Reference 23, 24, and 25). 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 (Section 7.3.1). A simplified derivation from Reference 33 is shown below.
As before, the limiting surface density relationship for the array material characteristics can be written as:

\[ \sigma(m) = c_2(m_0 - m) \text{ or after factoring out an } m_0, \quad \sigma(m) = c_2 m_0 \left(1 - \frac{m}{m_0}\right). \]

The limiting surface density relationship for the array geometric characteristics can be written as:

\[ \sigma(m) = \frac{nm}{(2a_n)^2} \left(1 - \frac{c}{\sqrt{N}}\right)^2. \]

See the limiting surface density discussion in Chapter 7 for more information about these relationships. The density analog method formulation from Reference 13 defines the array unit center-to-center spacing, \( d \), for a cubic array. Thus, the relationships can be modified to reflect this type of array. The limiting surface density method assumes that the array size is at least 64 units in size (at least a 4×4×4 array).

As shown for the surface density method, the center-to-center spacing between array units for a large array as a function of the number of units vertically, \( n \), the array unit mass, \( m \), and the limiting value of the surface density for the array, \( \sigma \), (dependent upon the material characteristics of the array) is defined as:

\[ d^2 = \left[ \frac{nm}{\sigma}\right]. \]

Also, as defined in the surface density method, as the array unit mass approaches zero (\( m = 0 \)), the allowed surface density approaches that for a water-reflected slab known as the critical surface density, \( \sigma_c \):

\[ \sigma(m) = c_2 m_0 \left(1 - \frac{m}{m_0}\right) \]

\[ \sigma(0) = \sigma_c = c_2 m_0 \left(1 - \frac{0}{m_0}\right) = c_2 m_0. \]

The next step of the derivation is to equate the allowed surface density relationships for the array geometric and material characteristics and substitute the characteristics for large cubic arrays. Equating the limiting surface density relationships for the array material and geometry characteristics:
\[
\sigma(m) = c_2m_0\left(1 - \frac{m}{m_0}\right) = \frac{nm}{(2a_\delta)^2}\left(1 - \frac{c}{\sqrt{N}}\right)^2.
\]

After some simplification as previously defined, the following relationship is obtained. This is similar to the surface density method derivation in the last chapter. Recall the relationships for the fraction critical, \(f\), and the center-to-center spacing, \(d\), and that \(\left(1 - \frac{c}{\sqrt{N}}\right)^2\) approaches 1 for a large number of array units, \(N\).

\[
\sigma_0(1 - f) = \frac{nm}{d^2}.
\]

For the surface density method, the maximum multiplication factor for an array unit is 0.9. This corresponds to a fraction critical of 0.73. Thus, \(1.37f\) ensures that the multiplication factor of the individual array units will be less than 0.9, which indicates that each unit will remain subcritical in isolation. Incorporating this and solving for the center-to-center spacing results in the following.

\[
d^2 = \frac{nm}{\sigma_0(1 - 1.37f)}.
\]

The density analog method (Thomas’ methodology from Reference 13) assumes a cubic array \((n\times n \times n)\) for the total number of units, equal to \(n^3 = N\). The center-to-center spacing between array units is equal to \(d\) (\(d = 2a_\delta\)) and the volume of a unit cell is \(V = d^3\). A relationship that compares the array density to the allowed surface density is derived below.

Continue with the previously defined equation and cube both sides of the equation.

\[
(d^3)^2 = \left[\frac{nm}{\sigma_0(1 - 1.37f)}\right]^3
\]

Substitute the definition for the array unit volume and the number of units in the array.

\[
V^2 = \left[\frac{m}{\sigma_0(1 - 1.37f)}\right]^3 N, \text{ solve for } N:
\]

\[
N = \left[\frac{\sigma_0(1 - 1.37f)}{m}\right]^3 V^2. \text{ This is similar to equation 4.7 in Reference 13. This equation can be used to determine the subcritical limits for array configurations for any shape (Reference 9). Continuing the derivation results in the following:}
\]
This method is applicable for the following situations.

6.3 representation of the surface density method (Reference 13):

\[ n^3 = \left( \frac{\sigma_0(1-1.37f)}{m} \right)^3 (d^3)^2, \]

Rearrange:

\[ (d^2)^3 = n^3 \left( \frac{m}{\sigma_0(1-1.37f)} \right)^3 = \left[ \frac{nm}{\sigma_0(1-1.37f)} \right]^3, \]

Simplify this relationship and solve for \( d \):

\[ d^2 = \left[ \frac{nm}{\sigma_0(1-1.37f)} \right], \]

\[ d = \left[ \frac{nm}{\sigma_0(1-1.37f)} \right]^{0.5}. \] This is similar to equation 4.8 in Reference 13.

The following relationship represents Thomas' representation of the density analog method. The coefficient (2.1 or 0.69) in the expression, as in the surface density relationship, represents experimental and calculational data for cubic arrangements of fissile materials. The final expressions for the center-to-center spacing, \( d \), between array units are listed below.

\[ d = \left[ \frac{nm}{2.1\sigma_0(1-1.37f)} \right]^{\frac{1}{2}} \equiv 0.69 \left[ \frac{nm}{\sigma_0(1-1.37f)} \right]^{\frac{1}{2}}. \]

Each of the variables for this center-to-center spacing relationship, \( d \), is defined below for Thomas' representation of the surface density method (Reference 13):

where

- \( n \) – the number of fissile units in any dimension which is equal to \( N^{1/3} \),
- \( \sigma_0 \) – the surface density of the water-reflected infinite slab (g/cm²) as defined previously,
- \( f \) – the ratio of the mass of a unit in the array to the critical mass of the unreflected sphere of the same fissile material, and
- \( m \) – the fissile material mass (g).

6.3 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.

- This method, as described above, is applicable to cubic arrays reflected by water at least 200 mm thick or its nuclear equivalent (Reference 13). Guidance for applying this method with arrays located next to concrete reflectors can be found in Reference 16.
- This method can be used in 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 9). 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 array unit and array shape are discussed in greater detail in References 13 and 16. The example problems consider arrays with water reflection only.
- 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.

6.4 Density Analog Method Example Problems

The following example problems illustrate the use of the density analog method. The 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.
6.4.1 Density Analog Example Problem 1

Using the density analog method, repeat the example problem in Section 5.4.1 for 2×2×2, 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 5.4.1, the values of $\sigma_o$ and $f$ are the same, because the system has not changed; only the method we are going to use to calculate the center-to-center spacing between units has changed. So, the values of $\sigma_o$ and $f$ are summarized below.

$$\sigma_o = 2.74 \text{ gPu/cm}^2$$

$$f = 0.089.$$  

Knowing $\sigma_o$ and $f$, the center-to-center spacing using the density analog method can be determined as follows.

Start with the density analog relationship for a cubic array:

$$d = \left[ \frac{nm}{2.1 \sigma_o (1-1.37f)} \right]^{1/2}$$

For the smallest array, 2×2×2:

$$d = \left[ \frac{2 \times 800 \text{ gPu}}{2.1 \times 2.74 \text{ gPu/cm}^2 (1-1.37 \times 0.089)} \right]^{1/2}$$

$$d = 17.8 \text{ cm (7 in.)}$$

For a 10×10×10 array:

$$d = \left[ \frac{10 \times 800 \text{ gPu}}{2.1 \times 2.74 \text{ gPu/cm}^2 (1-1.37 \times 0.089)} \right]^{1/2}$$

$$d = 39.8 \text{ cm (~15.7 in.)}$$

While for a 100×100×100 array:

$$d = \left[ \frac{100 \times 800 \text{ gPu}}{2.1 \times 2.74 \text{ gPu/cm}^2 (1-1.37 \times 0.089)} \right]^{1/2}$$

$$d = 126 \text{ cm (~50 in.)}.$$
In Section 5.4.1, the surface density method provided a center-to-center spacing between fissile units of about 25 cm (~10 in.). This is for an infinite number of Pu solution bottles in a planar array that is limited one unit high with no stacking ($\infty \times \infty \times 1$). In contrast, the density analog results for the $2 \times 2 \times 2$, $10 \times 10 \times 10$ and $100 \times 100 \times 100$ arrays demonstrate that, as one would expect, the center-to-center spacing would increase as the array got larger indicating the array is more reactive as the total number of units increase. 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 $2 \times 2 \times 2$, $10 \times 10 \times 10$ and $100 \times 100 \times 100$ arrays respectively. 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.
6.4.2 Density Analog Example Problem 2

Using the density analog method, repeat example problem in Section 5.4.2 for 2x2x2, 10x10x10 and 100x100x100 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 5.4.2, the values of \(\sigma_o\) 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 \(\sigma_o\) and \(f\) are summarized below:

\[
\sigma_o = 16.07 \text{ gPu/cm}^2
\]

\[
f = 0.169.
\]

Knowing \(\sigma_o\) and \(f\), the center-to-center spacing using the density analog method can be determined as follows:

Again, start with the density analog relationship:

\[
d = \left[\frac{nm}{2.1\sigma_o (1-1.37f)}\right]^{1/2}
\]

For the 2x2x2 array:

\[
d = \left[\frac{2 \times 4500 \text{ gPu}}{2.1 \times 16.07 \text{ gPu/cm}^2 (1-1.37 \times 0.169)}\right]^{1/2}
\]

\[
d = 18.6 \text{ cm (~7.3 in.)}
\]

For the 10x10x10 array:

\[
d = \left[\frac{10 \times 4500 \text{ gPu}}{2.1 \times 16.07 \text{ gPu/cm}^2 (1-1.37 \times 0.169)}\right]^{1/2}
\]

\[
d = 41.6 \text{ cm (~16.4 in.)}
\]

For the 100x100x100 array:

\[
d = \left[\frac{100 \times 4500 \text{ gPu}}{2.1 \times 16.07 \text{ gPu/cm}^2 (1-1.37 \times 0.169)}\right]^{1/2}
\]

\[
d = 132 \text{ cm (~52 in.)}
\]
Consider a situation in a fissile material storage area where 1,000 Pu oxide containers are stored in a 50x20x1 array. The density analog method for this example recommends a spacing of 41.6 cm (~16 in.) for 1,000 units arranged in a 10x10x10 array. This result would bound the 50x20x1 array because 1,000 units in a cubic array (10x10x10) is the most reactive array configuration. Spreading the 1,000 units out in any other configuration is less reactive than the 10x10x10 result. 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 28.4 cm (11.2 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 this method allows a much closer spacing, more than 13 cm (5.2 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.
6.4.3 Density Analog Example Problem 3

Using the density analog method, repeat the example problem in Section 5.4.3 (Surface Density Example Problem 3) for \(2 \times 2\), \(10 \times 10\) and \(100 \times 100\) arrays. Recall that each fissile unit in the array is a 4,500 g Pu(5) metal ingot.

From the example problem in Section 5.4.3, the values of \(\sigma_o\) 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 \(\sigma_o\) and \(f\) are summarized below:

\[
\sigma_o = 16.20 \text{ gPu / cm}^2
\]

\[
f = 0.437.
\]

Knowing \(\sigma_o\) and \(f\), the center-to-center spacing using the density analog method can be determined as follows.

Once again, begin with the density analog relationship:

\[
d = \left[ \frac{nm}{2.1\sigma_o(1-1.37f)} \right]^{1/2}
\]

For the \(2 \times 2 \times 2\) array:

\[
d = \left[ \frac{2 \times 4500 \text{ gPu}}{2.1 \times 16.20 \text{ gPu / cm}^2 (1-1.37 \times 0.437)} \right]^{1/2}
\]

\[
d = 25.7 \text{ cm (~10.1 in.)}
\]

For the \(10 \times 10 \times 10\) array:

\[
d = \left[ \frac{10 \times 4500 \text{ gPu}}{2.1 \times 16.20 \text{ gPu / cm}^2 (1-1.37 \times 0.437)} \right]^{1/2}
\]

\[
d = 57.4 \text{ cm (~22.6 in.)}
\]
For the $100 \times 100 \times 100$ array:

$$d = \left( \frac{100 \times 4500 \ gPu}{2.1 \times 16.20 \ gPu / cm^2 \left( 1 - 1.37 \times 0.437 \right)} \right)^{1/2}$$

$$d = 182 \ cm \ (\sim 72 \ in.).$$

As one would expect, the Pu metal ingots require more spacing than the Pu solution bottles in Section 6.4.1 or the Pu oxide containers in Section 6.4.2 because of the higher fissile mass that is present. Also, the surface density method for the same problem (Section 5.4.3) results in a center-to-center spacing of 36.0 cm (14.2 in.) for an $\left( \infty \times \infty \times 1 \right)$ 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, 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.
7. Limiting Surface Density ($NB_{N^2}$) 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 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 ($NB_{N^2}$) Method Overview

This method was developed to allow for complex array analyses to be performed without doing expensive computer calculations. Although codes may be advantageous these days, the limiting surface density or $NB_{N^2}$ technique is still a very comprehensive and valid technique with which to analyze various array configurations. The $NB_{N^2}$ method combines the density analog method and diffusion theory into a thorough method for performing array criticality calculations (Reference 21).

The geometric buckling for a single unit is expanded analogously for a cubic array, which can then be expanded to arrays of various shapes. This method can also be used to substitute other fissile array units and reflector materials. Because this method is such a comprehensive one, it can be more difficult than the other array methods to understand and apply, initially. However, it is the most comprehensive and flexible of the array methods presented here. This method is easily adapted to a spreadsheet or computer code, where quick parametric studies on the factors affecting criticality safety can be performed. A brief overview of this method is provided in this section for the analyst to quickly become familiar with the method to perform array calculations. Additional derivations and variations of the method are described in significantly more detail in References 21–27.

Typically, the $NB_{N^2}$ method is used to determine critical spacing of units with a given mass. Then this information is used to determine allowable masses or spacing based on a desired $k_{eff}$. The $NB_{N^2}$ method was developed from a combination of diffusion theory and of the density analog method. For arrays consisting of the same fissile material units with the same $k_{eff}$ the basic premise for this method is that the number of neutrons that leak out of the array boundary is constant (Reference 9). Reference 21 provides a very detailed derivation that is an excellent supplement to the discussions in References 23, 24, and 25. For this method to be applicable, the array must have at least 64 units (Figures 24 and 25).
The limiting surface density, $\sigma(m)$, for a cubic array is based on air-spaced, spherical units with a thick water reflector at the outside array boundary (Figure 24), and for a cubic array, $\sigma(m)$, is defined by the following relationship:

$$\sigma(m) = \frac{n_z m}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2,$$

where

- $n_z$ – the least number of units along an array edge (= minimum ($n_x$, $n_y$, $n_z$)), which is equal to $\sqrt[3]{N}$ for a cubic array,
- $m$ – 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 26,
- $c$ – an empirically determined constant (Reference 25) equal to $0.55 \pm 0.18$, and
- $N$ – the total number of fissile units in the array.

The term, $n_z m / (2a_n)^2$, represents the surface density (g/cm$^2$) of a stack of $n_z$ units with mass $m$ and a center-to-center spacing $2a_n$ as illustrated in Figure 27.

Figure 24. Keno 3D Illustration of a 64-unit Array with a Thick Water Reflector
Figure 25. Illustration of a 64-unit Cubic Array

Figure 26. Illustration of the Center-to-Center Spacing between Array Units
This relationship is mainly dependent on the geometrical properties of the array. Another relationship can be defined that is dependent upon the material properties of the array units based on experimental observations:

\[ \sigma(m) = c_2 \left( m_o - m \right) \]

where

- \( c_2 \) — a constant that depends on all of the material properties of the arrays except for the mass, \( m \), and is also equal to the slope of the “material-line” discussed later (cm\(^{-2}\)) (Table 14 provides values for this constant for various fissile systems),
- \( m_o \) — the critical mass (kg) of an unreflected, single fissile unit in the array (Figure 28), and
- \( m \) — the mass (kg) of a fissile unit in the array (Figure 28).
Both of these expressions for $\sigma(m)$ are linear relationships with the independent variable being fissile unit mass, $m$, and the dependent variable, the surface density, $\sigma(m)$. These expressions 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:

$$
\sigma(m) = \frac{n_z m}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 \quad \text{and} \quad \sigma(m) = c_2 (m_o - m).
$$

Dividing these equations by $m$ results in the following:

$$
\frac{\sigma(m)}{m} = \frac{n_z}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 \quad \text{and} \quad \frac{\sigma(m)}{m} = c_2 \left( \frac{m_o}{m} - 1 \right).
$$

Equating these two relationships results in the following:

$$
\frac{\sigma(m)}{m} = \frac{n_z}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 = c_2 \left( \frac{m_o}{m} - 1 \right).
$$

This relationship can be used to solve for the fissile material mass, $m$, or array unit center-to-center spacing, $2a_n$, required for the array to achieve a critical state. These relationships are defined below.
The array unit mass, $m$, is required for a critical array:

$$m = m_o \left[ \frac{n^2_z}{c_2 (2a_n)^2 \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1} \right]^{1/2}.$$  

The array unit center-to-center spacing, $2a_n$, is required for a critical array:

$$d = \left( 2a_n \right) = \left[ \frac{n^2_z \left( 1 - \frac{c}{\sqrt{N}} \right)^2}{c_2 \left( \frac{m_n}{m} - 1 \right)} \right] \frac{1}{2}.$$  

Because the geometrical and material expressions for the limiting surface density, $\sigma(m)$, 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 29 illustrates that the $m$ is the independent variable and $\sigma(m)$ is the dependent variable, while the expression in front of the variable, $m$, defines the slope of the line.

Figure 29. Illustration of the Limiting Surface Method
7.3 Applicability of the Limiting Surface Density Method

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 or its nuclear equivalent. Guidance for applying this method with arrays located next to concrete reflectors can be found in Reference 16.

- Arrays of units of any shape can be treated provided the data for $c_2$ and $m_o$ are available (Reference 17).

- 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 14 does 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 21 and 24 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 in order to ultimately end up with the configuration of interest may involve a significant number of calculations (see example problems for the limiting surface density method in Reference 9), which can introduce opportunities for error.
<table>
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<th>Material</th>
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<th>Characteristic Constant, c₂, for Criticality of Water-Reflected Arrays (10⁻³ cm²)</th>
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<td>0.854 ± 0.007</td>
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<tr>
<td>4</td>
<td>Oxide, U(93.2)O₂</td>
<td>3</td>
<td>63.59</td>
<td>0.758 ± 0.008</td>
</tr>
<tr>
<td>5</td>
<td>Oxide, U(93.2)O₂</td>
<td>10</td>
<td>31.43</td>
<td>0.778 ± 0.007</td>
</tr>
<tr>
<td>6</td>
<td>Oxide, U(93.2)O₂</td>
<td>20</td>
<td>17.34</td>
<td>0.805 ± 0.004</td>
</tr>
<tr>
<td>7</td>
<td>Metal, U(80)</td>
<td>0</td>
<td>69.89</td>
<td>1.359 ± 0.012</td>
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<tr>
<td>8</td>
<td>Oxide, U(80)O₂</td>
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<td>111.36</td>
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<td>9</td>
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<td>20</td>
<td>18.67</td>
<td>0.779 ± 0.005</td>
</tr>
<tr>
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<td>1.192 ± 0.018</td>
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<td>0.723 ± 0.006</td>
</tr>
<tr>
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<td>0.686 ± 0.006</td>
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<tr>
<td>15</td>
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<tr>
<td>18</td>
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<tr>
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<tr>
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<td>0.744 ± 0.005</td>
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<tr>
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<td>Metal, Pu(0)⁵</td>
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<td>9.95</td>
<td>4.356 ± 0.112</td>
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<tr>
<td>29</td>
<td>Oxide, Pu(0)O₂</td>
<td>0.4</td>
<td>26.66</td>
<td>1.542 ± 0.015</td>
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<tr>
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<td>1.113 ± 0.010</td>
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<td>3</td>
<td>32.78</td>
<td>1.097 ± 0.011</td>
</tr>
</tbody>
</table>

⁴ 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).

⁵ 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).
<table>
<thead>
<tr>
<th>No.</th>
<th>Material</th>
<th>H/X</th>
<th>Spherical Unit Unreflected Critical Mass, m₀ (kg)</th>
<th>Characteristic Constant, c₂, for Criticality of Water-Reflected Arrays (10⁻³ cm⁻²)</th>
</tr>
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<td></td>
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<td>c₂</td>
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</tr>
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<td>0.947</td>
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<td>Metal, U(93.2)-10 wt. % Mo</td>
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<td>73.06</td>
<td>1.305</td>
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</table>

### 7.3.1 Calculating the Multiplication Factor of an Array

A useful relationship developed by Thomas (References 21 and 25) for calculating the effective multiplication factor, $k_{eff}$, for array configuration is given by the following relationship.

This expression is a function of the unit mass before and after a change to the mass of an array unit. In this equation, $m'$ is the mass of a spherical fissile unit in a critical array and $m$ is the mass of a spherical fissile unit in a subcritical array, while $r'$ and $r$ represent the spherical critical and subcritical radii for these fissile units in the array, respectively.

$$k_{eff} = \left( \frac{m \text{ in subcritical array}}{m' \text{ in critical array}} \right)^{\frac{1}{3}} = \left( \frac{m}{m'} \right)^{\frac{1}{3}}$$

By substituting the expression for the fissile material density, this equation can be rearranged to be a function of only the unit radius. Recall that the volume of a sphere is equal to $V = \frac{4}{3}\pi r^3$:

$$\rho = \frac{\text{mass}}{\text{Volume}} = \frac{m}{V} = \frac{m}{\frac{4}{3} \pi r^3}$$

Solve for $m$ and substitute into the previous relationship for the multiplication factor (note that the spacing between array units and the material density, $\rho$, does not change as it is the same fissile material for both units):
\[ m = \frac{4}{3} \pi r^3 \rho, \]

\[ k_{\text{eff}} = \left( \frac{m}{m'} \right)^{\frac{2}{3}} = \left( \frac{4}{3} \pi r^3 \rho \right)^{\frac{2}{3}} = \left( \frac{\text{subcritical spherical radius of unit}}{\text{critical spherical radius of unit}} \right)^{\frac{2}{3}} = \frac{r}{r'}, \]

The use of this relationship will be illustrated in the example problems to follow. Also, this expression for the \( k_{\text{eff}} \) of an array can be used to derive relationships for the center-to-center spacing, \( d \), between array units, and the \( k_{\text{eff}} \) 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 \( k_{\text{eff}} \) relationship in Section 7.3.1, expressions for the center-to-center spacing, \( d \), can be derived as a function of the desired \( k_{\text{eff}} \) for a particular array configuration.

Begin the derivation with the expression for the \( k_{\text{eff}} \) for an array as defined in Section 7.3.1.

\[ k_{\text{eff}} = \left( \frac{\text{mass in subcritical array}}{\text{mass in critical array}} \right)^{\frac{1}{3}} = \left( \frac{m}{m'} \right)^{\frac{1}{3}}, \quad \text{or} \quad k_{\text{eff}}^3 = \frac{m}{m'}. \]

Recall the center-to-center spacing, \( d \), for a critical array is given by:

\[ d = \left[ \frac{n_c \left( 1 - \frac{c}{\sqrt{N}} \right)}{c_2 \left( \frac{m_0}{m} - 1 \right)} \right]^{\frac{1}{2}}, \quad \text{where} \quad \frac{m_0}{m} = \frac{\text{critical mass}}{\text{mass in a subcritical unit}}. \]

The following product can be performed to determine the ratio of the unreflected critical mass of an array unit to the array unit mass in a critical array.

\[ \frac{m_0}{m} \times k_{\text{eff}}^3 = \frac{m_0}{m} \times \frac{m}{m'} = \frac{m_0}{m'} = \left[ \frac{\text{unreflected critical mass of an array unit}}{\text{array unit mass in a critical array}} \right]. \]

The limiting surface density relationship defined in Section 7.2 to determine the array unit mass required for a critical array is given by the following relationship:

\[ m' = m_0 \left[ \frac{n_c}{c_2 d^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1 \right]^{\frac{1}{2}}, \quad \text{so this can be rewritten by substituting the in ratio defined above:} \]

\[ \frac{m_0}{m'} = \left[ \frac{n_c}{c_2 d^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1 \right] = \frac{m_0}{m} \times k_{\text{eff}}^3. \]
Substitute the limiting surface density expression for the center-to-center spacing, \( d \), between array units in a critical array with the array unit mass, \( m' \), that results in a critical array. This results in the following expression:

\[
\frac{m_0}{m'} = \left[ \frac{n_z}{c_2} \left( \frac{m_0}{m'} - 1 \right) \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1 \right]^{1/2} = \frac{m_0}{m'} - 1 + 1 = \frac{m_0}{m'}
\]

So, \( d_0 \) is the critical spacing for \( m' \). The center-to-center spacing, \( d_0 \), for a critical array can be written as follows:

\[
d_0 = \left\{ \frac{n_z}{c_2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 \right\}^{1/2}
\]

Replacing \( m' \) with \( m \) (\( m < m' \)) and retaining the spacing, \( d_0 \), will produce an array with a \( k_{\text{eff}} < 1 \).

\[
m' = \frac{m}{k_{\text{eff}}^3}
\]

Substitute this expression into the critical array center-to-center spacing:

\[
d_0 = \left\{ \frac{n_z}{c_2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 \right\}^{1/2} = \left\{ \frac{n_z}{c_2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 \right\}^{1/2} = \frac{n_z}{c_2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 \left[ \frac{m_0}{m} k_{\text{eff}}^3 - 1 \right]
\]
Solving for $m$, the array unit mass required for an array $k_{\text{eff}}$:

$$m = \frac{k_{\text{eff}}^3 m_0}{\left[ \frac{n_z}{c^2 d_0^2 \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1} \right]}.$$

### 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 Chapter 7. Other relationships are defined to consider changes in array unit density, for example, and will be considered in subsequent sections. For this section, $d$, represents the center-to-center spacing for a critical array and $d_0$ represents the center-to-center spacing for an array with a particular $k_{\text{eff}}$.

- Array unit center-to-center spacing, $d$, in a critical array:

$$d_0 = \left[ \frac{n_z}{c^2} \left( \frac{1}{m_0/m' - 1} \right) \right]^{-\frac{1}{2}}$$

where $m_0/m'$ is unreflected, spherical critical array unit mass array unit mass required for a critical array.

- Array unit center-to-center spacing, $d$, as a function of the array $k_{\text{eff}}$:

$$d = \left( 2a_n \right) = \left[ \frac{n_z}{c^2} \left( \frac{1}{m_0 \left( \frac{k_{\text{eff}}^3}{m_0} \right) - 1} \right) \right]^{-\frac{1}{2}}$$

where $m_0$ is unreflected critical array unit mass array unit mass for desired $k_{\text{eff}}$.

- Array $k_{\text{eff}}$ as a function of array unit mass, $m$:

$$k_{\text{eff}} = \left[ \frac{n_z}{c^2 d^2 \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1} \right]^{-\frac{1}{2}}$$

where $m_0/m$ is array unit mass for desired $k_{\text{eff}}$ unreflected critical array unit mass.

- Array unit mass, $m$, required for a desired array $k_{\text{eff}}$:

$$m = \frac{k_{\text{eff}}^3 m_0}{\left[ \frac{n_z}{c^2 d_0^2 \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1} \right]}.$$
7.4  Example Problems for Limiting Surface Density

Using the graphical technique, as illustrated in Figure 29, 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 14 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) have been provided in Chapter 9.
7.4.1 Limiting Surface Density Example Problem 1

Using the limiting surface density method, repeat example problem in Section 5.4.2 (Surface Density Example Problem 2) for 2×2×2, 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.

The limiting surface density relationships were developed from array configurations with more than 64 units. Thus, this method should not be used for the 2×2×2 array; however the other cubic arrays, the 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 derived as follows.

Recall that the center-to-center spacing between array units for a critical array is given by the following relationship for arrays with more than 64 units:

$$d = \left(2a_n\right) = \left[ \frac{n_z \left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_z \left(\frac{m}{m-1}\right)} \right]^{\frac{1}{2}}$$

Where:

- $m_0$ = 26.66 kg for $^{239}$PuO$_2$ oxide with an H/X = 0.4 (Table 14),
- $m$ = 4.5 kg from the problem description,
- $n_z$ = 10 and 100 from the problem description,
- $c_2$ = 0.001542 cm$^{-2}$ (Table 14),
- $N$ = equal to $n^3$=1,000 and 1,000,000, and
- $c$ = 0.55, defined previously.

Note that there is a small quantity of moisture in the critical mass and $c_2$ data listed in Table 14. This fact should not affect the result much because a small quantity of moisture only tends to reduce 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 result.

The 10×10×10 cubic array center-to-center spacing is given by:

$$d = \left(2a_n\right) = \left[ \frac{10 \left(1 - \frac{0.55}{\sqrt{1000}}\right)^2}{0.001542 \text{ cm}^{-2} \left(\frac{26.66 \text{ kg}}{4.5 \text{ kg}} - 1\right)} \right]^{\frac{1}{2}}$$

$$d = \left(2a_n\right) = 35.7 \text{ cm} \sim 14 \text{ in.}.$$
This spacing of PuO₂ units would make the 10×10×10 cubic array critical. The result from Section 6.4.2 for the 10×10×10 array was about 41.6 cm (16.4 in.), which is for a subcritical array configuration. The density analog relationships have some safety margin built into the center-to-center spacing expression provided by Reference 13.

For a 100×100×100 array, one would expect that the critical, center-to-center spacing be much larger than that for the 10×10×10 array. The 100×100×100 cubic array center-to-center spacing is given by:

\[
d = \left(2a_n\right) = \frac{100\left(1 - \frac{0.55}{\sqrt{1,000,000}}\right)^2}{0.001542 \text{ cm}^2\left(\frac{26.66 \text{ kg}}{4.5 \text{ kg}} - 1\right)}
\]

\[
d = \left(2a_n\right) = 114.7 \text{ cm (~45 in.)}
\]

This is significantly more spacing between units than for the 10×10×10 case. The result from Section 6.4.2 for the 100×100×100 array is 132 cm (~52 in.), which will provide a subcritical spacing for the array. Because of the incorporated safety margin, the density analog and surface density methods will provide a larger center-to-center spacing than the limiting surface density method.

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 10×10×10 array, the surface density is:

\[
\frac{n \times m}{d^2} = \frac{10 \times 4.5 \text{ kg}}{\left(35.7 \text{ cm}\right)^2} = 35.3 \text{ g/cm}^2,
\]

while the surface density for the 100×100×100 array is:

\[
\frac{n \times m}{d^2} = \frac{100 \times 4.5 \text{ kg}}{\left(114.7 \text{ cm}\right)^2} = 34.2 \text{ g/cm}^2.
\]

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 that is dependent upon the material properties of the array:

\[
\sigma(m) = c_2(m_s - m), \text{ where } c_2, m_s \text{ and } m \text{ are previously defined. Substituting these values into this relationship results in the same limiting surface density value:}
\]

\[
\sigma(m) = 1.542 \times 10^{-3} \text{ cm}^{-2} \times (26.68 \text{ kg} - 4.5 \text{ kg}) \times \left(\frac{1000 \text{ g}}{\text{kg}}\right),
\]

\[
\sigma(m) = 34.2 \text{ g/cm}^2.
\]
7.4.2 Limiting Surface Density Example Problem 2

Using the limiting surface density method, repeat the example problem in Section 5.4.3 (Surface Density Example Problem 3) for 10×10×10 and a 100×100×100 arrays. Recall that each fissile unit in the array is a 4,500 g Pu(5) metal ingot.

Recall that the center-to-center spacing between array units for a critical array is given by the following relationship for arrays with more than 64 units:

\[
d = (2a_n) = \left[ \frac{n_z \left( 1 - \frac{c}{\sqrt{N}} \right) - c_2 \left( \frac{m - 1}{m} \right)}{c_2} \right]^{\frac{1}{2}},
\]

Where:

- \(m_o\) = 10.34 kg for Pu(5.2) metal (Table 14),
- \(m\) = 4.5 kg from the problem description,
- \(n_z\) = 10 and 100 from the problem description,
- \(c_2\) = 0.004138 cm\(^{-2}\) (Table 14),
- \(N\) = equal to \(n^3 = 1,000\) and \(1,000,000\), and
- \(c\) = 0.55, defined previously.

Note that the data from Table 14 for Pu metal is for Pu(5.2), which contains 5.2 atom percent \(^{240}\)Pu. 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.

10×10×10 cubic array center-to-center spacing:

\[
d = (2a_n) = \left[ \frac{10 \left( 1 - \frac{0.55}{\sqrt{1000}} \right)}{0.004138 \ cm^{-2} \left( \frac{10.34 \ kg}{4.5 \ kg} - 1 \right)} \right]^{\frac{1}{2}}
\]

\[
d = (2a_n) = 42.4 \ cm \ (22.6 \ in.)
\]

This is the spacing of 4.5 kg Pu(5.2) metal units required to keep the 10×10×10 cubic array critical. The result from Section 6.4.3 for the 10×10×10 array was about 57.4 cm (22.6 in.), which represents a subcritical center-to-center spacing result. In contrast, the limiting surface density will provide a center-to-center spacing for a critical array.
For a 100×100×100 array, one would expect that the critical, center-to-center spacing would be much larger than the 10×10×10 array.

The 100×100×100 cubic array center-to-center spacing is given by:

\[
d = \left(2a_n\right) = \frac{100 \left(1 - \frac{0.55}{\sqrt{1,000,000}}\right)^2}{0.004138 \text{ cm}^{-2} \left(\frac{10.34 \text{ kg}}{4.5 \text{ kg}}\right)^3 - 1}^{\frac{1}{2}}
\]

\[d = \left(2a_n\right) = 136.4 \text{ cm} (~54 \text{ in.})\]

This is significantly more spacing between units than that for the 10×10×10 case. 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 \(k_{\text{eff}}\) relationships in Section 7.3.1 can be used to determine the array unit mass for a desired multiplication factor. Also, a relationship was derived for this Primer to consider the array unit center-to-center spacing as a function of the array \(k_{\text{eff}}\) (Section 7.3.2). Thus, if a criticality safety engineer wanted a center-to-center spacing result that resulted in an array \(k_{\text{eff}}\) of 0.8, the following calculation could be done.

For a subcritical array, the center-to-spacing between array units is given by the following equation from Section 7.3.2 and 7.3.3:

\[
d = \left(2a_n\right) = \left[\frac{n_z \left(1 - \frac{c}{\sqrt{N}}\right)^2}{c_z \left(\frac{m}{m_{\text{unreflected critical array unit mass}}}k_{\text{eff}}^3\right) - 1}\right]^{\frac{1}{2}}
\]

where \(\frac{m_0}{m} = \text{unreflected critical array unit mass over array unit mass for desired } k_{\text{eff}}\).

For the 100×100×100 array:

\[
d = \left(2a_n\right) = \frac{100 \left(1 - \frac{0.55}{\sqrt{1,000,000}}\right)^2}{0.004138 \text{ cm}^{-2} \left(\frac{10.34 \text{ kg}}{4.5 \text{ kg}}\right)^3 - 1}^{\frac{1}{2}}
\]

\[d = 370 \text{ cm} (~146 \text{ in.})\]

Thus, to maintain a subcritical configuration for this large array size, it makes sense that the array units should be spaced much further apart than for the critical array.
7.4.3 Limiting Surface Density Example Problem 3

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). After the critical mass is calculated, determine the multiplication factor for storing 20 kg of U(100) units in the 4x4x4 array.

Non-graphical solution

For a 4x4x4 cubic array with the given spacing:

- \( n = n_x = n_y = n_z = 4 \)
- \( a_x = a_y = a_z = 30/2 = 15 \) in. (38.1 cm)

The following relationship for a cubic array can be used to determine the critical mass per unit to maintain the array in a critical condition for U(100) metal units.

\[
m = m_0 \left[ \frac{n_z}{c_z (2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1 \right]^{-1},
\]

where

- \( m_0 = 45.68 \) kg from Table 14,
- \( n_z = 4 \) from the assumptions specified above,
- \( a_n = 15 \) in. (38.1 cm) from the assumptions specified above,
- \( c_z = 0.001806 \) cm\(^{-2} \) from Table 14,
- \( N \) equal to \( n^3 = 64 \), and
- \( c = 0.55 \), defined previously.

Substituting the values for each variable into the array critical mass relationship provides the following result:

\[
m = \left( 45.68 \text{ kg} \right) \left[ \frac{4}{\left( 0.001806 \text{ cm}^2 \right) \left( 2 \times 38.1 \text{ cm} \right)^2} \left( 1 - \frac{0.55}{\sqrt{64}} \right)^2 + 1 \right]^{-1}
\]

\[m = 34.3 \text{ kg}.
\]

This is the mass of U(100) metal required in each array unit to keep the 4x4x4 cubic array critical. 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 below where \( m \) is the desired unit mass to be stored (20 kg) and \( m' \) is the calculated critical mass in the array as calculated above:

\[
k_{eff} = \left( \frac{m}{m'} \right) = \left( \frac{20}{34.3} \right) = 0.84
\]

With 30 in. (76.2 cm) spacing between units, this array configuration will remain subcritical.
Graphical solution

Geometry Line: \( \sigma(m) = \frac{n_m}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 = \frac{4m}{(2 \times 38.1 \text{ cm})^2} \left( 1 - \frac{0.55}{\sqrt{64}} \right)^2 \)

\( \sigma(m) = 5.974 \times 10^{-4} \text{ m} \) or \( \frac{\sigma(m)}{m} = 5.974 \times 10^{-4} \)

Material Line: \( \sigma(m) = c_z (m_o - m) \)

\( \sigma(m) = 1.806 \times 10^{-3} (45.68 - m) \) or \( \frac{\sigma(m)}{m} = 1.806 \times 10^{-3} \left( \frac{45.68}{m} - 1 \right) \)

Equating the geometrical and material relationships results in the following:

\( \frac{\sigma(m)}{m} = 5.974 \times 10^{-4} = 1.806 \times 10^{-3} \left( \frac{45.68}{m} - 1 \right) \).
Note that the graphical solution (Figure 30) illustrates a solution for the array critical unit mass at about 34.3 kg, which corresponds to a limiting surface density of about 20 g/cm². To verify the graphical solution, the following calculation can be done.

The stack surface density is given as: \( \sigma_s = \frac{n \times m}{d^2} \),

and the limiting surface density is: \( \sigma_{ls} = \sigma_s \left( 1 - \frac{0.55}{\sqrt{n^2}} \right)^2 \).

The stack surface density is given as: \( \sigma_s = \frac{4 \times 34.33 \text{ kg}}{(76.2 \text{ cm})^2} = 23.65 \text{ g/cm}^2 \),

and the limiting surface density is: \( \sigma_{ls} = \sigma_s \left( 1 - \frac{0.55}{\sqrt{4^2}} \right)^2 = 20.5 \text{ g/cm}^2 \),

which matches the value derived from Figure 30.
7.4.4 Limiting Surface Density Example Problem 4

Using the limiting surface density method, repeat the example problem in Section 7.4.3 (Limiting Surface Density Example Problem 3) for 5 kg Pu(5.2) metal array units. Recall that the array considered in Section 7.4.3 contained U(100) metal units.

Non-graphical solution:

\[ m = m_o \left[ \frac{n_z}{c_z(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1 \right]^{-1}, \]

where

- \( m_o = 10.336 \text{ kg} \) (Table 14),
- \( n = 4 \) from the assumptions specified above,
- \( a_n = 15 \text{ in.} \) from the assumptions specified above,
- \( c_z = 0.004138 \text{ cm}^{-2} \) (Table 14),
- \( N = \) equal to \( n^3 = 64 \), and
- \( c = 0.55 \), defined previously.

Substituting the values for each variable into the array critical mass relationship provides the following result:

\[ m = (10.336 \text{ kg}) \left[ \frac{4}{(0.004138 \text{ cm}^{-2})(2 \times 38.1 \text{ cm})^2} \left( 1 - \frac{0.55}{\sqrt{64}} \right)^2 + 1 \right]^{-1} \]

\[ m = 9.03 \text{ kg}. \]

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 U(100) metal system in the last example problem.

Now, the multiplication factor can be calculated if one is interested in storing 5 kg Pu(5.2) metal units in each array location. The resulting multiplication factor 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:

\[ k_{eff} = \left( \frac{m}{m'} \right)^{\frac{1}{3}} = \left( \frac{5}{9.03} \right)^{\frac{1}{3}} = 0.82. \]

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 last 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: \[
\sigma(m) = \frac{n_m m}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 = \frac{4m}{(2 \times 38.1 \text{ cm})^2} \left( 1 - \frac{0.55}{\sqrt{64}} \right)^2
\]

\[
\sigma(m) = 5.974 \times 10^{-4} \text{ m} \quad \text{or} \quad \frac{\sigma(m)}{m} = 5.974 \times 10^{-4}
\]

Material Line for Pu(5.2): \[
\sigma(m) = c_2 (m - m_o)
\]

\[
\sigma(m) = 4.138 \times 10^{-3} (10.336 - m) \quad \text{or} \quad \frac{\sigma(m)}{m} = 4.138 \times 10^{-3} \left( \frac{10.336}{m} - 1 \right)
\]

Equating the geometrical and material relationships results in the following:

\[
\frac{\sigma(m)}{m} = 5.974 \times 10^{-4} = 4.138 \times 10^{-3} \left( \frac{10.336}{m} - 1 \right).
\]

---

Figure 31. Solution for Limiting Surface Density Example Problem 4
Note that the graphical solution (Figure 31) 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/cm$^2$. This plot clearly shows how much more reactive Pu(5.2) metal is compared to U(100) metal as demonstrated by the much lower array unit mass required to result in about the same multiplication factor, keeping the array geometry constant.
7.4.5 Limiting Surface Density Example Problem 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. Recall that the array considered in Section 7.4.4 contained Pu(5.2) metal array units.

The first step for this problem is to calculate the mass required for this array to have a multiplication factor of 0.9 as follows.

Use the multiplication factor relationship to solve for the mass, \( m \), that will result in the mass of a Pu unit in the array and that will result in a multiplication factor of 0.9.

\[
k_{\text{eff}} = \left( \frac{m}{m'} \right)^{\frac{1}{3}}
\]

\[
\frac{m}{m'} = k_{\text{eff}}^3
\]

\[
m = m' k_{\text{eff}}^3
\]

\[
m = 9.03 \times \left( 0.9 \right)^3 = 6.58 \text{ kg.}
\]

The critical mass relationship from the last example problem can be modified algebraically to solve for the center-to-center spacing between array units. The modifications are shown below and recall the critical mass for each array unit is 9.03 kg from the last example problem.
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 25). This array condition will be true if the following is true.

\[
\frac{\sigma(m)}{m} = \frac{\sigma(m')}{m'}.
\]

In this relationship, the variables \(m\) and \(m'\) represent the different masses or different materials in the same array configuration (i.e., \(a_n\), \(N\) and \(n_z\) represent the geometrical configuration of the array, which do not change). One can derive an equivalence relationship for this situation as follows.

\[
\frac{\sigma(m)}{m} = \frac{\sigma(m')}{m'}
\]

Geometry Line:

\[
\frac{\sigma(m)}{m} = \frac{n_z}{(2a_n)^2} \left(1 - \frac{c}{\sqrt{N}}\right)^2
\]

Material Line:

\[
\frac{\sigma(m)}{m} = c_2 \left\{ \frac{m}{m} - 1 \right\}
\]

Substitute these expressions into the "equivalence relationship":

\[
\frac{n_z}{(2a_n)^2} \left(1 - \frac{c}{\sqrt{N}}\right)^2 \frac{c_2 \left\{ m - 1 \right\}}{m} = \frac{n_z}{(2a_n)^2} \left(1 - \frac{c}{\sqrt{N}}\right)^2 \frac{c_2 \left\{ m' - 1 \right\}}{m'}
\]

Again, because the geometrical characteristics for this situation do not change, the variables \(n_z\), \(a_n\), and \(N\) do not change. Thus, this relationship can be simplified in the following two steps:

\[
1 = \frac{c_2 \left\{ m - 1 \right\}}{c_2 \left\{ m' - 1 \right\}}
\]
\[ c_2' \left( \frac{m_0'}{m'} - 1 \right) = c_2 \left( \frac{m_0}{m} - 1 \right) \]

Solve for the new critical unit mass, \( m' \):

\[ m' = m_0' \left[ \frac{c_2}{c_2'} \left( \frac{m_0}{m} - 1 \right) + 1 \right]^{-1} \]

Thus, this relationship can be used to consider an “equivalent” mass of a different fissile material in order to maintain criticality of the array.
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 from Section 7.4.4 (Limiting Surface Density Example Problem 4).

The values for the characteristic constants, \( c_2 \) and \( c'_2 \) and the bare, spherical critical masses can be found in Table 14.

\[
m_0' = 10.34 \text{ kg for Pu}(5.2) \text{ metal},
\]
\[
c'_2 = 4.136 \times 10^{-3} \text{ cm}^{-2} \text{ for Pu}(5.2) \text{ metal},
\]
\[
m = 34.30 \text{ kg for U}(100) \text{ metal (result from example problem in Section 7.4.3)},
\]
\[
m_0 = 45.68 \text{ kg for U}(100) \text{ metal and }
\]
\[
c_2 = 1.806 \times 10^{-3} \text{ cm}^{-2} \text{ for U}(100) \text{ metal}.
\]

The equivalence relationship from Section 7.5 can be used to find the equivalent mass of Pu(5.2) in the critical 4\( \times \)4\( \times \)4 array of U(100) metal units:

\[
m' = m_0' \left[ \frac{c_2}{c'_2} \left( \frac{m}{m_0} - 1 \right) + 1 \right]^{-1}
\]

\[
m' = 10.34 \text{ kg} \left[ \frac{1.806 \times 10^{-3}}{4.136 \times 10^{-3}} \left( \frac{45.68 \text{ kg}}{34.30 \text{ kg}} - 1 \right) + 1 \right]^{-1}
\]

\[
m' = 9.03 \text{ kg}.
\]

This is the same critical mass as calculated in Section 7.4.4, which represents the mass of Pu(5.2) metal units that would be required to maintain criticality of the 4\( \times \)4\( \times \)4 array. Using the equivalence relationship, the analyst can calculate the equivalent mass needed for a critical array keeping all of the geometrical characteristics of the array constant.
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 32). 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, either the unit mass must increase, the distance between units be reduced or the number of units in the array be increased.

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 32), 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 25, can be used to make adjustments to the array shape.

![4x4x4 Array](image1)

![8x4x2 Array](image2)

**Figure 32. Illustration of Two Different 64-Unit Arrays**

In most facilities that have 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 32. 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, $R$, to use in subsequent calculations in order to determine the new characteristics the units in the new array must have to remain in a critical configuration. The shape factor, $R$, is defined as follows.
The surface area for a noncubic array 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:

\[
S_{nc} = (2a_n)^2 \left[ n_x n_y + n_x n_z + n_y n_z \right]
\]

\[
V_{nc} = (2a_n)^3 \left[ n_x n_y n_z \right].
\]

Now, calculate the surface-area-to-volume ratio for the non-cubic array:

\[
\frac{S_{nc}}{V_{nc}} = \frac{1}{2a_n} \left( \frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z} \right).
\]

For a cubic array, the surface-area-to-volume ratio where \( n \) is equal for each side of the array (recall that \( N = n^3 \) or \( n = \sqrt[3]{N} \)) is given by:

\[
\frac{S_c}{V_c} = \frac{1}{2a_n} \left( \frac{1}{n} + \frac{1}{n} + \frac{1}{n} \right) = \frac{1}{2a_n} \left( \frac{3}{n} \right) = \frac{1}{2a_n} \left( \frac{3}{\sqrt[3]{N}} \right).
\]

Now, the shape factor, \( R \), can be defined as

\[
R = \left( \frac{S}{V} \right) = \sqrt[3]{N} \left( \frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z} \right).
\]

It should be noted that \( N \) is independent of the array shape and does not have to be an integer value. According to Reference 16, the maximum value that \( R \) can have is 5.34. Calculationally, if \( R \) exceeds this value, 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, \( c_2' \) can be calculated that accounts for the increased neutron leakage for the non-cubic array. The following relationship was developed by Thomas (Reference 25) 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.

\[
c_2' = \frac{4n_z'}{n_z} \left( \frac{c_z}{5R^{0.672} - 1} \right),
\]

where \( n_z' \) is the least number of units along an array edge, which is equal to \( \sqrt[3]{N} \) or \( n_z \) in the noncubic array configuration, \( R \) is the shape factor (not to exceed 5.34), and \( c_z \) are previously defined.

This relationship was developed for 10.4 kg, U(93.2) metal units in a 512-unit array (Reference 16) 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 this step is complete.
7.6.1 Limiting Surface Density Example Problem 7

Repeat the example problem in Section 7.4.3 for an 8 \times 4 \times 2 array, using the methodology presented in Section 7.6. Recall that the array considered in Section 7.4.3 contained U(100) metal units.

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 \times 4 \times 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 limiting surface density was developed based on experiments involving arrays of U(93.2) metal units. This solution will involve the graphical solution done previously.

Step 1

Assume a 4 \times 4 \times 4 cubic array:

- \( n = n_x = n_y = n_z = 4 \)
- \( a_n = a_x = a_y = a_z = 15 \text{ in. (38.1 cm)} \).

The following relationship for a cubic array can be used to determine the critical mass per unit in order 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:

- \( m_0 = 52.1 \text{ kg from Table 14} \),
- \( c_2 = 0.001762 \text{ cm}^{-2} \text{ from Table 14} \),
- \( N = \) equal to \( n^3 = 64 \), and
- \( c = 0.55 \).

Geometry Line:

\[
\sigma(m) = \frac{n_m}{(2a_n^2)} \left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{4m}{(2\times38.1 \text{ cm})^2} \left(1 - \frac{0.55}{\sqrt{64}}\right)^2
\]

\( \sigma(m) = 5.974 \times 10^{-4} m \quad \text{or} \quad \frac{\sigma(m)}{m} = 5.974 \times 10^{-4} \text{ cm}^{-2} \)

Material Line:

\[
\sigma(m) = c_2(m_o - m)
\]

\( \sigma(m) = 1.762 \times 10^{-3} (52.1 - m) \quad \text{or} \quad \frac{\sigma(m)}{m} = 1.762 \times 10^{-3} \left( \frac{52.1}{m} - 1 \right) \text{ cm}^{-2} \)
Equating the geometrical and material relationships results in the following:

\[
\frac{\sigma(m)}{m} = 5.974 \times 10^{-4} = 1.762 \times 10^{-3} \left( \frac{52.1}{m} - 1 \right)
\]

\[m = 38.9 \text{ kg.} \]

Note that the graphical solution (Figure 33) illustrates a solution for the array critical unit mass at about 39.5 kg, which corresponds to a limiting surface density of about 23 g/cm².

**Step 2**

The next step is to compute the shape factor and determine \(c_2\) that considers the increased leakage due to changing the shape of the array from a cubic \((4 \times 4 \times 4)\) to non-cubic in shape \((8 \times 4 \times 2)\).

The shape factor, \(R\), can be calculated as follows:

\[
R = \frac{\sqrt[3]{N}}{3} \left( \frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z} \right)
\]

\[
R = \frac{\sqrt[3]{64}}{3} \left( \frac{1}{8} + \frac{1}{4} + \frac{1}{2} \right) = 1.167.
\]
With \( R \) calculated, \( c'_2 \) can be calculated from this relationship from Section 7.6:

\[
c'_2 = \frac{4n'_2}{n_2} \left( \frac{c_2}{5R^{0.672} - 1} \right)
\]

\[
c'_2 = \frac{4 \times 2}{4} \left( \frac{1.762 \times 10^{-3}}{5(1.167)^{0.672} - 1} \right) = 1.005 \times 10^{-3}.
\]

Because the geometric characteristics of the array have changed, \( \sigma(m) \) can be calculated by taking the ratio of the limiting surface density relationships before and after the array transformation was made.

The ratio of the limiting surface density relationships can be calculated as follows. Note that the variables \( a_n, m_b \) 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\( \times \)4\( \times \)4 array (Figure 34) to an 8\( \times \)4\( \times \)2 array:

\[
\frac{n'_2}{n_2} \cdot \frac{(2a_n)^2 \left( 1 - \frac{c}{\sqrt{N}} \right)^2}{(2a_n')^2 \left( 1 - \frac{c'}{\sqrt{N}} \right)^2} = \frac{c_2' \left( \frac{m}{m'} - 1 \right)}{c_2 \left( \frac{m}{m} - 1 \right)}
\]

The simplified relationship is as follows:

\[
\frac{n'_2}{n_2} = \frac{c_2' \left( \frac{m}{m'} - 1 \right)}{c_2 \left( \frac{m}{m} - 1 \right)}
\]

Solve for the new critical unit mass, \( m' \):

\[
m' = m_a \left[ \frac{5R^{-0.672}}{4} - 1 \left( \frac{m}{m} - 1 \right) + 1 \right]^{-1} \quad \text{or} \quad m' = m_a \left[ \frac{c_2' \left( \frac{m}{m'} - 1 \right)}{c_2 \left( \frac{m}{m} - 1 \right)} + 1 \right]^{-1}
\]

\[
m' = 52.1 \left[ \frac{5(1.167)^{-0.672}}{4} - 1 \left( \frac{52.1}{38.9} - 1 \right) + 1 \right]^{-1} = 40.16 \text{ kg}
\]

\[
m' = 52.1 \left[ \frac{1.762 \times 10^{-3}}{1.005 \times 10^{-3}} \left( \frac{2}{4} \right) \left( \frac{52.1}{38.9} - 1 \right) + 1 \right]^{-1} = 40.16 \text{ kg}.
\]

This corresponds to the mass of U(93.2) metal units required to keep the 8\( \times \)4\( \times \)2 array in a critical state after the array was transformed from a 4\( \times \)4\( \times \)4 array (Figure 34).
Figure 34. Transformation of a U(93.2) Metal 4x4x4 Array to an 8x4x2 Array

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 8x4x2 array in a critical state based on the results for a U(93.2) metal system. First, the $c_2$ value for U(100) metal needs to be calculated because the data that will be used from Table 14 apply to cubic arrays, not a cuboidal, 8x4x2, array. The following approach can be taken to calculate $c_2$ for the 8x4x2 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 4x4x4 array to an 8x4x2 array.

For the U(93.2) array:

$$
\left( \frac{c_2'}{c_2} \right)_{8x4x2\ U(93.2)} = \frac{4n'}{n_z} \left( \frac{c_2}{5R^{-0.672} - 1} \right)
$$

For the U(100) array:

$$
\left( \frac{c_2'}{c_2} \right)_{8x4x2\ U(100)} = \frac{4n'}{n_z} \left( \frac{c_2}{5R^{-0.672} - 1} \right)
$$
Calculating the ratio of these two relationships results in the following:

\[
\left( \frac{c_2'}{c_2} \right)_{8 \times 4 \times 2 \ \text{U}(93.2)} \cdot \frac{4n'}{n} \left( \frac{c_2}{c_2} \right)_{4 \times 4 \times 4 \ \text{U}(93.2) \ - \ 1} = \left( \frac{c_2'}{c_2} \right)_{8 \times 4 \times 2 \ \text{U}(100)} \cdot \frac{4n'}{n} \left( \frac{c_2}{c_2} \right)_{4 \times 4 \times 4 \ \text{U}(100) \ - \ 1}
\]

Because the geometric properties of the array will not change for the fissile material transformation from U(93.2) to U(100) metal units, the previous relationship can be simplified to the following ratio of \( c_2 \) values.

\[
\left( \frac{c_2'}{c_2} \right)_{8 \times 4 \times 2 \ \text{U}(93.2)} = \left( \frac{c_2'}{c_2} \right)_{8 \times 4 \times 2 \ \text{U}(100)} \left( \frac{c_2}{c_2} \right)_{4 \times 4 \times 4 \ \text{U}(100)} \left( \frac{c_2}{c_2} \right)_{4 \times 4 \times 4 \ \text{U}(93.2) \ - \ 1}
\]

Rearranging the ratio provides the following result that can be used to calculate the \( c_2 \) value for the U(100) \( 8 \times 4 \times 2 \) array:

\[
\left( \frac{c_2}{c_2} \right)_{8 \times 4 \times 2 \ \text{U}(100)} = \left( \frac{c_2}{c_2} \right)_{8 \times 4 \times 2 \ \text{U}(93.2)} \left( \frac{c_2}{c_2} \right)_{4 \times 4 \times 4 \ \text{U}(100)} \left( \frac{c_2}{c_2} \right)_{4 \times 4 \times 4 \ \text{U}(93.2) \ - \ 1}
\]

\[
\left( \frac{c_2}{c_2} \right)_{8 \times 4 \times 2 \ \text{U}(100)} = 1.005 \times 10^{-3} \ \text{cm}^{-2} \left( \frac{1.806 \times 10^{-3} \ \text{cm}^{-2}}{1.762 \times 10^{-3} \ \text{cm}^{-2}} \right) = 1.030 \times 10^{-3} \ \text{cm}^{-2}
\]

The mass required to maintain criticality of the \( 8 \times 4 \times 2 \) array with U(100) metal units can now be determined using the equivalence relationship defined previously.

The equivalence relationship from Section 7.5 is defined as

\[
m' = m \left[ \frac{c_2}{c_2} \left( \frac{m}{m} - 1 \right) + 1 \right]^{-1}
\]

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Substitute the relevant variable values:

\[ m_0' = 45.68 \text{ kg} \text{ for U(100) metal with } H/U = 0 \text{ (Table 14)}, \]
\[ c_2' = 1.030 \times 10^{-3} \text{ cm}^2 \text{ for U(100) metal with } H/U=0 \text{ for the } 8 \times 4 \times 2 \text{ array, calculated above,} \]
\[ m = 40.16 \text{ kg} \text{ corresponding to the critical unit mass for U(93.2) metal units calculated previously,} \]
\[ c_2 = 1.762 \times 10^{-3} \text{ cm}^2 \text{ for U(93.2) metal (Table 14), and} \]
\[ m_0 = 52.1 \text{ kg} \text{ for U(93.2) metal from the last step.} \]

The final result is:

\[ m' = 45.68 \text{ kg} \left[ \frac{1.005 \times 10^{-3} \text{ cm}^2}{1.030 \times 10^{-3} \text{ cm}^2} \left( \frac{52.1 \text{ kg}}{40.16 \text{ kg}} - 1 \right) + 1 \right]^{-1} = 35.41 \text{ kg}. \]

This is the mass required to maintain array criticality in an 8\times4\times2 configuration with U(100) metal units. The graphical solution is illustrated in Figure 35.

![Figure 35. Graphical Solution for an 8\times4\times2 Array with U(100) Metal Units](image)
7.6.2  Limiting Surface Density Example Problem 8

This problem will be split into several parts to demonstrate the strength of the limiting surface density 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. The center-to-center spacing \( (2a_n) \) of the array units is 38.1 cm.

Geometry Line: \[ \sigma(m) = \frac{n_m}{(2a_n)^2} \left( 1 - \frac{c}{\sqrt{N}} \right)^2 = \frac{6m}{(38.1 \text{ cm})^2} \left( 1 - \frac{0.55}{\sqrt{216}} \right)^2 \]

\[ \sigma(m) = 3.830 \times 10^{-3} \text{ m} \quad \text{or} \quad \frac{\sigma(m)}{m} = 3.830 \times 10^{-3} \]

Material Line: \[ \sigma(m) = c_z (m_o - m) \text{ where } c_z = 1.762 \times 10^{-3} \text{ cm}^{-2} \text{ and } m_o = 52.1 \text{ kg} \text{ from Table 14.} \]

\[ \sigma(m) = 1.762 \times 10^{-3} (52.1 - m) \quad \text{or} \quad \frac{\sigma(m)}{m} = 1.762 \times 10^{-3} \left( \frac{52.1}{m} - 1 \right) \]

Equating the geometrical and material relationships results in the following:

\[ \frac{\sigma(m)}{m} = 3.830 \times 10^{-3} = 1.762 \times 10^{-3} \left( \frac{52.1}{m} - 1 \right) \]

\[ m = 16.4 \text{ kg} \]

This result is consistent with the graphical solution as shown in Figure 36.
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 $c_2'$ and new value for $\sigma' (m)/m$ 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:

$$R = \frac{3\sqrt[3]{N}}{3} \left( \frac{1}{n_x} + \frac{1}{n_y} + \frac{1}{n_z} \right)$$

$$R = \frac{\sqrt[3]{216}}{3} \left( \frac{1}{24} + \frac{1}{9} + \frac{1}{1} \right) = 2.306.$$
With $R$ calculated, $c'_2$ can be calculated from this relationship from Section 7.6:

$$c'_2 = \frac{4n'_2}{n_z} \left( \frac{c_2}{5R^{-0.672} - 1} \right)$$

$$c'_2 = \frac{4 \times 1}{6} \left( \frac{1.762 \times 10^{-3}}{5(2.306)^{-0.672} - 1} \right) = 6.343 \times 10^{-4}.$$

Now, calculate the value for $\sigma'(m)/m$ 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.

$$\frac{\sigma(m')}{m'} = \frac{n_z}{n} \frac{\sigma(m)}{m} \quad \frac{\sigma(m')}{m'} = \frac{1}{6} \left( 3.83 \times 10^{-3} \text{ kg/cm}^2 \right) = 6.383 \times 10^{-4} \text{ kg/cm}^2.$$

Substitute this value into the limiting surface density (material line):

$$\frac{\sigma(m')}{m'} = c'_2 \left( \frac{m'_2}{m'} - 1 \right) = 6.383 \times 10^{-4}.$$

The type of fissile material in the array units have not changed. Therefore, $m_0 = 52.1$ kg.

Solve for $m'$:

$$m' = \left( \frac{c'_2 m_0}{6.383 \times 10^{-4} \text{ cm}^2 + c'_2} \right)$$

$$m' = \left( \frac{6.343 \times 10^{-4} \text{ cm}^2 \times 52.1 \text{ kg}}{6.383 \times 10^{-4} \text{ cm}^2 + 6.343 \times 10^{-4} \text{ cm}^2} \right) = 26.0 \text{ kg}.$$

This is consistent with the graphical solution shown in Figure 37.
Figure 37. Solution for the Change from a 6×6×6 Array to a 9×24×1 Array

The multiplication factor can now be calculated using the relationships in Section 7.3.1.

\[ k_{\text{eff}} = \left( \frac{m}{m'} \right)^{\frac{1}{3}} = \left( \frac{16.4}{26.0} \right)^{\frac{1}{3}} \]

\[ k_{\text{eff}} = 0.86. \]

**Part 3. What \(^{239}\text{Pu}\) metal (\(\text{Pu}[0]\)) 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 \(^{239}\text{Pu}\) 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 \(\text{Pu}(0)\) metal.
Geometry Line:

\[ \sigma(m) = \frac{n_m}{(2a_n)^2} \left(1 - \frac{c}{\sqrt{N}}\right)^2 = \frac{6m}{(38.1 \text{ cm})^2} \left(1 - \frac{0.55}{\sqrt{216}}\right)^2 \]

\( \sigma(m) = 3.830 \times 10^{-3} m \) or \( \frac{\sigma(m)}{m} = 3.830 \times 10^{-3} \)

Material Line:

\[ \sigma(m) = c_2 (m_o - m) \]

\( \sigma(m) = 4.356 \times 10^{-3} (9.95 - m) \) or \( \frac{\sigma(m)}{m} = 4.356 \times 10^{-3} \left(\frac{9.95}{m} - 1\right) \)

For this case, the geometry line is unchanged. The material line changes due because of the fissile material change.

Equating the geometrical and material relationships results in the following:

\[ \frac{\sigma(m)}{m} = 3.830 \times 10^{-3} = 4.356 \times 10^{-3} \left(\frac{9.95}{m} - 1\right) \]

\( m = 5.29 \text{ kg.} \)

This array unit mass corresponds to a critical array as shown in Figure 38.
Figure 38. Solution for Pu(0) metal 6x6x6 Critical Array

The array unit mass needed to result in a $k_{\text{eff}}$ of 0.9 and can be calculated as follows:

$$k_{\text{eff}} = \left( \frac{m}{m'} \right)^{\frac{1}{3}}.$$

Rearrange this equation to solve for $m$, and recall that $m$ is the mass of a spherical unit in the subcritical array while $m'$ is the mass of a spherical unit in a critical array:

$$m' = m k_{\text{eff}}^3 = \left(5.29 \text{ kg} \right) \left(0.9\right)^3 = 3.86 \text{ kg}.$$

Thus, for the 6x6x6 array, units of 3.86 kg Pu(0) metal array units will result in a $k_{\text{eff}}$ of 0.9.

For the 9x24x1 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 6x6x6 array to a 9x24x1 array. Thus, using the same approach discussed in Section 7.6, a relationship can be derived to determine a new $c_2$ for the 9x24x1 array for a Pu(0) metal system.
The ratio of the limiting surface density relationships can be calculated as follows. Note that the variables \( a_s, m_0, n_x, c, \) 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 \( 6 \times 6 \times 6 \) to an \( 9 \times 24 \times 1 \) array.

For the U(93.2) array:

\[
\left( \frac{c_2}{n_x} \right)_{9 \times 24 \times 1, \text{U}(93.2)} = \frac{4n'}{n_x} \left( \frac{c_2}{6 \times 6 \times 6, \text{U}(93.2)} \right) \left( \frac{2}{5R^{-0.672} - 1} \right)
\]

For the Pu(0) array:

\[
\left( \frac{c_2}{n_x} \right)_{9 \times 24 \times 1, \text{Pu}(0)} = \frac{4n'}{n_x} \left( \frac{c_2}{6 \times 6 \times 6, \text{Pu}(0)} \right) \left( \frac{2}{5R^{-0.672} - 1} \right)
\]

The simplified relationship:

\[
\left( \frac{c_2}{n_x} \right)_{9 \times 24 \times 1, \text{U}(93.2)} \left( \frac{c_2}{6 \times 6 \times 6, \text{Pu}(0)} \right) = \left( \frac{c_2}{6 \times 6 \times 6, \text{U}(93.2)} \right) \left( \frac{c_2}{6 \times 6 \times 6, \text{Pu}(0)} \right)
\]

Solve for \( \left( \frac{c_2}{n_x} \right)_{9 \times 24 \times 1, \text{Pu}(0)} \):

\[
\left( \frac{c_2}{n_x} \right)_{9 \times 24 \times 1, \text{Pu}(0)} = \left( \frac{4.356 \times 10^{-3} \text{cm}^{-2}}{1.762 \times 10^{-3} \text{cm}^{-2}} \right) \left( \frac{6.343 \times 10^{-4} \text{cm}^{-2}}{6.343 \times 10^{-4} \text{cm}^{-2}} \right)
\]

\[
\left( \frac{c_2}{n_x} \right)_{9 \times 24 \times 1, \text{Pu}(0)} = 1.568 \times 10^{-3} \text{cm}^{-2}.
\]

Based on the fact that the value for \( \sigma(m)/m \) is constant for the \( 9 \times 24 \times 1 \) array calculation in Part 2, the new \( c_2 \) value can be used to calculate the critical array mass (Figure 39) for the \( 9 \times 24 \times 1 \) array for the Pu(0) metal system.
The material line can be written as: \[ \left( \frac{c_2'}{b_{Pu(0)}} \right) \left( \frac{m_0}{m'} - 1 \right) = 6.383 \times 10^{-4} \]

The geometry line for a \( 9 \times 24 \times 1 \) array is \[ \frac{\sigma(m)}{m} = 6.383 \times 10^{-4} \] :

Equating the material and geometry lines and solving for \( m' \):

\[
\left( 1.568 \times 10^{-3} \text{ cm}^{-2} \right) \left( 9.95 \right) - \left( 1.568 \times 10^{-3} \right) m' = \left( 6.383 \times 10^{-4} \right) m' \\
m' = \frac{\left( 1.568 \times 10^{-3} \text{ cm}^{-2} \right) \left( 9.95 \text{ kg} \right)}{\left( 6.383 \times 10^{-4} \text{ cm}^{-2} + 1.568 \times 10^{-3} \text{ cm}^{-2} \right)} = 7.07 \text{ kg}.
\]

Figure 39. Solution for a Pu(0) Metal 9x24x1 Critical Array

This mass corresponds to the array unit Pu(0) metal mass required to maintain the \( 9 \times 24 \times 1 \) array in a critical state. The mass necessary to result in multiplication factor of 0.9 can now be calculated:

\[ m' = m k_{eff}^3 = \left( 7.07 \text{ kg} \right) \left( 0.9 \right)^3 = 5.15 \text{ kg}. \]
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, 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, \(0.3 \leq H/D \leq 3\), the limiting surface density method will 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 \(\sigma(m) = c_2(m_0 - m)\), as discussed in Reference 25. However, as the Figure 40 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, 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 an \(H/D\) of 0.3 (also within range of applicability), which is due to the significant increase in the neutron leakage for 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 40 shows, the 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 40 as \(c_2'\)) for segment #2 for the \(H/D\) of 0.2, is calculated via the Thomas methodology (Reference 25), 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 40, 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 40. Critical Water-Reflected Cubic Arrays of U(93.2) Metal Cylinders with Various Height-to-Diameter Ratios
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 \((\rho = 19.75 \text{ g/cm}^3)\) that were replaced with delta-phase plutonium ingots \((\rho = 15.75 \text{ g/cm}^3)\). The core density conversion from Chapter 4 can be used to determine the new value for \( c_2 \) as a result of the density change:

\[
\frac{m_0'}{m_0} = \left( \frac{\rho'}{\rho} \right)^2,
\]

where \( m_0' \) and \( \rho' \) represent the unreflected critical mass and density, respectively, for the new fissile material shape, and \( m_0 \) and \( \rho \) represent the unreflected critical mass and density for the original, spherical unit.

Then, noting that for the spherical and different shape, the limiting surface density where \( m = 0 \), \( \sigma(0) \) is equal for both cases:

\[
\sigma(0) = \sigma(0)' = c_2 m_0 = c_2' m_0'.
\]

Solving for the new characteristic constant, \( c_2' \),

\[
\frac{c_2'}{c_2} = \left( \frac{m_0'}{m_0} \right) = \left( \frac{\rho'}{\rho} \right)^2.
\]

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 in invariant, whereas the material line changes along with the density change. The effect of a change in the characteristic constant, \( c_2 \) to \( c_2' \), 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, 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 \( a_n, m_0 \) 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 \( \rho \) to \( \rho' \).
\[
\begin{align*}
\frac{\alpha_2}{m_m} = \frac{m_m}{m} & \quad \frac{n_n}{(2a_n)^2} \left( \frac{N - c}{\sqrt{N}} \right)^2 \quad \frac{n_n}{(2a_n)^2} \left( \frac{N - c}{\sqrt{N}} \right) \\
\frac{\alpha_2}{m_m'} = \frac{m_m'}{m'} & \quad \frac{n_n'}{(2a_n')^2} \left( \frac{N' - c}{\sqrt{N'}} \right)^2 \quad \frac{n_n'}{(2a_n')^2} \left( \frac{N' - c}{\sqrt{N'}} \right)
\end{align*}
\]

Simplifying this relationship results in the following:

\[
\begin{align*}
\frac{\alpha_2}{m_m} = \frac{n_n}{(2a_n)^2} \left( \frac{\sqrt{N} - c}{\sqrt{N}} \right)^2 \quad \frac{n_n}{(2a_n)^2} \left( \frac{\sqrt{N} - c}{\sqrt{N}} \right) \\
\frac{\alpha_2}{m_m'} = \frac{n_n'}{(2a_n')^2} \left( \frac{\sqrt{N'} - c}{\sqrt{N'}} \right)^2 \quad \frac{n_n'}{(2a_n')^2} \left( \frac{\sqrt{N'} - c}{\sqrt{N'}} \right)
\end{align*}
\]

These simplifications yield equation 7 of Reference 25 which relates different critical arrays and fissile materials, including changes to the fissile material density.

\[
\begin{align*}
\frac{\alpha_2}{m_m} = \frac{n_n}{(2a_n)^2} \left( \frac{\sqrt{N} - c}{\sqrt{N}} \right)^2 \quad \frac{n_n}{(2a_n)^2} \left( \frac{\sqrt{N} - c}{\sqrt{N}} \right) \\
\frac{\alpha_2}{m_m'} = \frac{n_n'}{(2a_n')^2} \left( \frac{\sqrt{N'} - c}{\sqrt{N'}} \right)^2 \quad \frac{n_n'}{(2a_n')^2} \left( \frac{\sqrt{N'} - c}{\sqrt{N'}} \right)
\end{align*}
\]

Recall that: \(\frac{\alpha_2}{\alpha_2'} = \left( \frac{\rho}{\rho'} \right)^2\). Substituting this ratio into the previous relationship and, after some simplification, results in the following, final equation for the resulting fissile unit mass, \(m'\), that results in a critical array after the density change. This equation is equation 19 in Reference 25.

\[
\frac{m}{m'} = \frac{m}{m_0} \left( \frac{\rho'}{\rho} \right)^2 + \frac{1 - m}{m_0} \left( \frac{\alpha_n n_n' \sqrt{N - c}}{\alpha_n n_n' \sqrt{N' - c}} \right)^2.
\]

This is a very useful equation that shows how the array unit mass, center-to-center spacing or total number of units needs to change to maintain a critical array configuration. Only changes to the fissile array unit mass necessary to maintain a critical array due to a change in fissile material density is examined in detail here.
Notice that for only a fissile material density change in the array, only the material properties of the array will change. The physical characteristics of array \((N, N', a_n, a'_n, n_z\) and \(n'_z\)) will remain constant. Thus,

\[
\left(\frac{a'_n n'_z \sqrt{N - c}}{a_n n_z \sqrt{N' - c}}\right)^2 = 1.
\]

Substitute this result into the equation and solve for \(m'\). This relationship shows that the mass required to maintain the array in a critical state increases for a reduction in the fissile material density and decreases when the density is increased. These trends are illustrated in Figure 41.

\[
m' = m \left[ \frac{m}{m_0} \left( \frac{\rho'}{\rho} \right)^2 + \left( 1 - \frac{m}{m_0} \right) \right].
\]

Reference 25 provides additional information about fissile material density changes in array configurations.

![Graph showing density change in a critical 4x4x4 array with U(100) metal units](image)

**Figure 41. Density Change in a Critical 4x4x4 Array with U(100) Metal Units**
7.8.1 Limiting Surface Density Example Problem 9

Repeat the example problem in Section 7.4.3 (limiting surface density example problem 3) for a density change from 18.9 g/cm$^3$ to 15 g/cm$^3$. Recall that Section 7.4.3 considered an array that contained U(100) metal units.

From Reference 25, the critical array unit fissile mass of an array that has an array unit density change can be determined by the following relationship:

$$\frac{m}{m'} = \frac{m}{m_0} \left( \frac{\rho'}{\rho} \right)^2 + \left( 1 - \frac{m}{m_0} \right) \left( \frac{a_n \sqrt{N - c}}{a_n' \sqrt{N' - c}} \right)^2.$$

Notice that $a_n$, $a_n'$, $n_1$, $n_2$, $N$, and $N'$ depend upon the geometric array characteristics only. Because the geometrical characteristics of the array are unchanged, the term on the right is equal to unity, and the relationship can be solved for the new critical array unit mass after the fissile unit density change:

$$\frac{m}{m'} = \frac{m}{m_0} \left( \frac{\rho'}{\rho} \right)^2 + \left( 1 - \frac{m}{m_0} \right).$$

$$m' = m \left[ \frac{m}{m_0} \left( \frac{\rho'}{\rho} \right)^2 + \left( 1 - \frac{m}{m_0} \right) \right]^{-1}.$$

Next, substitute the unreflected critical mass, $m_0$, the critical mass for the initial density, $m$, ($m = 34.3$ kg from the results from Section 7.4.3) and the initial and final fissile material densities, $\rho$ and $\rho'$, respectively, as follows:

$$m' = 34.3 \left[ \frac{34.3}{45.686} \left( \frac{15}{18.9} \right)^2 + \left( 1 - \frac{34.3}{45.686} \right) \right]^{-1},$$

$$m' = 47.5 \text{ kg}.$$

Figure 42 illustrates this solution.
7.8.2 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 instead. Depending upon the thickness of concrete considered in the analysis, this may result in a reduction or increase in the array unit mass that is required to maintain the array in a critical state. The 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 25) 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 25, 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 14), the ratio of $c_2$ for concrete and water can be calculated for each concrete thickness. These ratios are listed in Table 15. Reference 25 provides a $c_2$ value for a similar array of Pu(94.8) metal units.
Table 15. Comparison of U(93.2) Metal Arrays with Water and Concrete Reflectors

<table>
<thead>
<tr>
<th>Concrete Thickness (cm)</th>
<th>$c_2$ for the 216-unit U(93.2) Metal Units Reflected by This Thickness of Concrete ($\times 10^{-3}$ cm$^2$)</th>
<th>$c_2$ for the 216-unit U(93.2) Metal Units Reflected by Water ($\times 10^{-3}$ cm$^2$)</th>
<th>Ratio of $c_2$ for Concrete and Water, $\frac{c_2(\text{concrete})}{c_2(\text{water})}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.16</td>
<td>2.007</td>
<td></td>
<td>1.139</td>
</tr>
<tr>
<td>12.70</td>
<td>1.694</td>
<td></td>
<td>0.961</td>
</tr>
<tr>
<td>15.24</td>
<td>1.432</td>
<td></td>
<td>0.813</td>
</tr>
<tr>
<td>20.32</td>
<td>1.240</td>
<td></td>
<td>0.704</td>
</tr>
<tr>
<td>25.40</td>
<td>1.156</td>
<td></td>
<td>0.656</td>
</tr>
<tr>
<td>30.48</td>
<td>1.128</td>
<td></td>
<td>0.640</td>
</tr>
<tr>
<td>30.48 for Pu(94.8)</td>
<td>3.050</td>
<td></td>
<td>1.333</td>
</tr>
<tr>
<td>40.64</td>
<td>1.085</td>
<td></td>
<td>0.616</td>
</tr>
</tbody>
</table>

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 28) based, primarily, on the water content of the concrete. Thomas used Oak Ridge concrete for the $c_2$ calculations listed in Table 15. Oak Ridge concrete has a water content of about 5.53 weight percent, where the water content ranges from 2.97 for Magnuson concrete to 10.99 weight percent for Hanford concrete (Reference 28). The water content of the various types on concrete should be considered before the Table 15 data are used in a calculation, if this information is known.
7.8.3 Limiting Surface Density Example Problem 10

Calculate the critical mass for each array unit required for the water-reflected cubic array from the limiting surface density example problem 3 (Section 7.4.3) for fully enriched U(100) metal, assuming 30.48 cm (12 in.) of concrete reflection instead of 20 cm (7.87 in.) of water reflection. Assume that the concrete is the Oak Ridge mixture.

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 (20 cm thick) to a concreted reflected array results in a change in the array unit mass required to maintain array criticality.

Non-graphical solution

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:

- \( m_0 = 45.686 \) kg from Table 14,
- \( n_z = 4 \) from the assumptions specified above,
- \( a_n = 15 \) in. (38.1 cm) from the assumptions specified above,
- \( c_2 = 1.806 \times 10^{-3} \) cm\(^{-2} \) from Table 14 for U(100) metal for a 12 in. thick water reflector,
- \( N = n^3 = 64 \), and
- \( c = 0.55 \), defined previously.

Before the mass is calculated, determine \( c_2 \) corresponding to the concrete reflected array.

From Table 15, the \( c_2 \) concrete-to-water ratio for 12 in. of Oak Ridge concrete reflection is 0.640:

\[
\frac{c_2(\text{concrete})}{c_2(\text{water})} = 0.640
\]

or

\[
c_2(\text{concrete}) = 0.640 \times c_2(\text{water})
\]

\[
c_2(\text{concrete}) = 0.640 \times 1.806 \times 10^{-3} \text{ cm}^{-2} = 1.156 \times 10^{-3} \text{ cm}^{-2}.
\]

Substituting the values for each variable into the array critical mass relationship provides the following result:
\[ m = m \left[ \frac{n}{c_{\text{concrete}}(2a_n)^2 \left( 1 - \frac{c}{\sqrt{N}} \right)^2 + 1} \right]^{-1} \]

\[ m = (45.686 \text{ kg}) \left[ \frac{4}{(1.156 \times 10^{-3} \text{ cm}^{-2}) \cdot (2 \times 38.1 \text{ cm})^2 \left( 1 - \frac{0.55}{\sqrt{64}} \right)^2 + 1} \right]^{-1} \]

\[ m = 30.1 \text{ kg}. \]

This is the mass of U(100) metal required in each array unit to keep the 4x4x4 cubic array critical, which is about 5 kg less U(100) metal per array unit because of the change from a 12 in. water reflector to a 12 in. concrete reflector. 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 below where \( m \) is the desired unit to be stored (20 kg) and \( m' \) is the calculated critical mass in the array as calculated above:

\[ k_{\text{eff}} = \left( \frac{m}{m'} \right)^{\frac{1}{3}} = \left( \frac{20}{30.1} \right)^{\frac{1}{3}} = 0.87. \]

With 1-ft spacing between units, this array configuration will remain subcritical, although the multiplication is about 3% higher for a concrete reflected system.

**Graphical Solution**

**Geometry Line:**

\[ \sigma(m) = \frac{n m}{(2a_n)^2 \left( 1 - \frac{c}{\sqrt{N}} \right)^2} = \frac{4m}{(2 \times 38.1 \text{ cm})^2 \left( 1 - \frac{0.55}{\sqrt{64}} \right)^2} \]

\[ \sigma(m) = 5.974 \times 10^{-4} \text{ m} \quad \text{or} \quad \frac{\sigma(m)}{m} = 5.974 \times 10^{-4} \]

**Material Line:**

\[ \sigma(m) = c_{\text{concrete}}(m_c - m) \]

\[ \sigma(m) = 1.156 \times 10^{-3} \left( 45.686 - m \right) \quad \text{or} \quad \frac{\sigma(m)}{m} = 1.156 \times 10^{-3} \left( \frac{45.686}{m} - 1 \right) \]

Equating the geometrical and material relationships results in the following:

\[ \frac{\sigma(m)}{m} = 5.974 \times 10^{-4} = 1.156 \times 10^{-3} \left( \frac{45.686}{m} - 1 \right) \].
Figure 43. Solution for Limiting Surface Density Example Problem 10

Note that the graphical solution (Figure 43) illustrates a solution for the array critical unit mass at about 30 kg, which corresponds to a limiting surface density of about 17 g/cm².
8. Solid Angle Method

8.1 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

8.2 Solid Angle Method Overview

This method is a technique that has been around for many years. The basic idea behind this method is that the multiplication factor for fissile materials in an array configuration depends upon 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 intersect another unit, which can 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 (Reference 9).

This technique has developed by accumulating a great deal of experimental data in aqueous solutions and the developing of a correlation that is dependent upon the reactivity of the individual units in the array and the maximum solid angle subtended at the central fissile unit by the other fissile units in the array. References 5, 13, 15, 34, and 35 provide additional information about the development of this method for use in array calculations.

The critical data used to develop this method resulted in the following correlation for use in array calculations:

\[ \Omega_{\text{allowable}} = 9 - 10k_{\text{eff}}. \]

The variable \( \Omega_{\text{allowable}} \) represents the allowable solid angle that may be subtended at the center fissile unit of the array, and the multiplication factor, \( k_{\text{eff}} \), is 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 44 illustrates the allowable solid angle as a function of the multiplication factor for the array units under consideration.
The solid angle between array units is calculated using the applicable method from Table 16. 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 16 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 13, Figure 4.2, and will not be included here.
Table 16. Solid Angle Approximate Formulas (Reference 13)

<table>
<thead>
<tr>
<th>Point-to-Sphere</th>
<th>Point-to-Cylinder</th>
<th>Point-to-Arbitrary Shape</th>
</tr>
</thead>
</table>

$$\Omega = 2\pi \left( 1 - \frac{1}{\sqrt{1 + \left( \frac{R}{H} \right)^2}} \right)$$

where

- $R =$ Radius of the sphere.
- $H =$ Distance from the point to the surface of the sphere.

$$\Omega = \frac{LD}{H\sqrt{\left( \frac{L}{2} \right)^2 + H^2}}$$

where

- $L =$ Length of the cylinder
- $D =$ Diameter of the cylinder
- $H =$ Distance from the point to the surface of the cylinder.

$$\Omega = \frac{\text{Cross Sectional Area}}{H^2}$$

<table>
<thead>
<tr>
<th>Point-to-Plane</th>
<th>Point-to-Disk</th>
</tr>
</thead>
</table>

$$\Omega = \sin^{-1} \left( \frac{AB}{\sqrt{A^2 + H^2 \sqrt{B^2 + H^2}}} \right)$$

where

- $A =$ Length of one side of the plane
- $B =$ Length of the other side of the plane
- $H =$ Perpendicular distance from the point to the plane.

If the point, $P$, is directly above the center of the plane (not directly over a corner as shown in the figure) with dimensions $2A \times 2B$, multiply $\Omega$ by 4 to obtain the solid angle.

$$\Omega = 2\pi \left( 1 - \frac{1}{\sqrt{1 + \left( \frac{R}{H} \right)^2}} \right) \leq \frac{\pi R^2}{H^2}$$

where

- $R =$ Radius of the disk
- $H =$ Distance from the point $P$ to the surface of the disk.
8.3 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 spectrum should be cautioned that the results obtained from the solid angle method can be non-conservative (Reference 13).
- 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.
- The allowed solid angle according to the method shall not exceed 6 steradians, and
- 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 13). 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 can be considered bounded by this criterion. Guidance for more concrete reflection than is found in Reference 13.

Figure 44 illustrates the applicability, as discussed above, for the solid angle method. 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 44.

8.4 Solid Angle Method Example Problems

The example problems for the solid angle method will be included in a future revision of this document. The authors have decided to study the history behind the solid angle method in more detail to ensure that example problems provided are as accurate and practical as possible.
9. Establishing Confidence in Hand Calculation Methods

9.1 Summary of Hand Calculation Results

The purpose of this section is to summarize the results of each of the foregoing example problems in order to compare the results 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.

9.2 Confidence in Single Unit Hand Calculations

The example problem results presented in Chapters 1 through 4 along with the corresponding comparison results are summarized in Tables 17, 18, and 19.
Table 17. Diffusion Theory Confidence Comparison

<table>
<thead>
<tr>
<th>Section</th>
<th>Description of the Problem</th>
<th>Hand Calculation Result</th>
<th>Comparison Result from Reference or Code Package</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5.1</td>
<td>A slab tank contains a mixture of water and pure $^{239}$Pu with a $^{239}$Pu concentration of 100 grams per liter at 20 °C. Using modified one-group diffusion theory, estimate the critical slab thickness.</td>
<td>13.04 cm</td>
<td>14.2 cm (Ref. 5, Figure III.A.5.2)</td>
</tr>
<tr>
<td>2.5.2</td>
<td>It is proposed to store water solutions of uranyl sulfate ($\text{UO}_2\text{SO}_4$) with a concentration of 30 g $^{235}$U/l of the Sulfate. Assume the temperature of the solution is 20 °C, and the uranium is fully enriched. Part 2: Calculate the critical cylindrical tank radius using modified one-group diffusion theory. Part 3: Repeat part 2 if the enrichment was 14.7 wt. % U-235 instead of fully enriched uranium.</td>
<td>Part 2: 17.5 cm</td>
<td>Part 2: ~17.25 cm (MCNP5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Part 3: 19.2 cm</td>
<td>Part 3: ~19.0 cm (DANTSYS)</td>
</tr>
<tr>
<td>2.5.3</td>
<td>Assume a fissile system made up of a bare sphere of Na and $^{239}$Pu in which Pu is 30 weight percent of the core mixture. Because this system has no moderating materials present, fast neutrons dominate the system (so one-group theory is sufficient). Part 1: Using one-group diffusion theory, estimate the critical radius for this system.</td>
<td>161.6 cm</td>
<td>~161.3 cm (DANTSYS)</td>
</tr>
<tr>
<td>2.5.4</td>
<td>The Jezebel critical assembly used for experiments at Los Alamos was used to perform various critical experiments (see Figure 4). Assume the assembly is made from δ-phase $^{239}$Pu ($\rho = 15.45$ 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.</td>
<td>6.93 cm</td>
<td>6.385 cm (Actual Dimension)</td>
</tr>
<tr>
<td>2.5.5</td>
<td>The Godiva critical assembly used for experiments at Los Alamos was employed in various critical experiments (see Figure 5). Assume the assembly is made from 93% enriched $^{235}$U ($\rho = 18.9$ 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.</td>
<td>8.44 cm</td>
<td>8.6 cm (Actual Dimension)</td>
</tr>
<tr>
<td>2.5.6</td>
<td>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$^3$.</td>
<td>1 g/cm$^3$ – 4080 kg</td>
<td>1 g/cm$^3$ – 3522 kg</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3 g/cm$^3$ – 453 kg</td>
<td>3 g/cm$^3$ – 391 kg</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5 g/cm$^3$ – 163 kg</td>
<td>5 g/cm$^3$ – 141 kg</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7 g/cm$^3$ – 83 kg</td>
<td>7 g/cm$^3$ – 72 kg</td>
</tr>
<tr>
<td></td>
<td></td>
<td>9 g/cm$^3$ – 50 kg</td>
<td>9 g/cm$^3$ – 43.5 kg</td>
</tr>
<tr>
<td></td>
<td></td>
<td>11.46 g/cm$^3$ – 31 kg</td>
<td>11.46 g/cm$^3$ – 26.8 kg (DANTSYS)</td>
</tr>
</tbody>
</table>
## Table 18. Buckling Conversion Confidence Comparison

<table>
<thead>
<tr>
<th>Section</th>
<th>Description of the Problem</th>
<th>Hand Calculation Result</th>
<th>Comparison Result from Reference or Code Package</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4.1</td>
<td>Determine the critical solution height in the deep well for a Pu(5) concentration of 200 gPu/l 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.)</td>
<td>18.5 cm</td>
<td>15.24 cm (Ref. 5, Fig. III.A.5.95-3 for an infinite slab)</td>
</tr>
<tr>
<td>3.4.2</td>
<td>Calculate the water-reflected, critical radius for a cylindrical tank that has a height of 20 cm, filled with 20 g/l Pu(5) metal-water mix.</td>
<td>31.1 cm</td>
<td>~32.3 cm (MCNP5)</td>
</tr>
<tr>
<td>3.4.3</td>
<td>Calculate the critical height for a 15 cm diameter cylinder for the same solution from Section 3.4.2.</td>
<td>3.4.4</td>
<td>This configuration will always remain subcritical.</td>
</tr>
<tr>
<td>3.4.4</td>
<td>Two cylindrical, unfavorable geometry tanks are being filled with a fissile solution. The first tank is filled with a U(93.5)-water mixture while the second tank is filled with a Pu metal-water mixture containing 5 wt. % $^{239}$Pu. Both solutions have a fissile concentration of 100 gU/l. Determine the critical solution height for each tank and compare the results of the two systems. Repeat this calculation with a concentration of 150 gU/l.</td>
<td>100 g/l: H=17.3 cm (U) H=19.1 cm (Pu) 150 g/l: H=16.8 cm (U) H=19.0 cm (Pu)</td>
<td>100 g/l: H≈17.8 cm (U) H≈18.8 cm (Pu) 150 g/l: H≈16.5 cm (U) H≈18.6 cm (Pu) (SCALE5, Keno V.a)</td>
</tr>
</tbody>
</table>

## Table 19. Core-Density Method Confidence Comparison

<table>
<thead>
<tr>
<th>Section</th>
<th>Description of the Problem</th>
<th>Hand Calculation Result</th>
<th>Comparison Result from Reference or Code Package</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.4.1</td>
<td>Calculate the critical mass for spherical, unreflected Pu(4.5) metal system with a density of 19.8 g/cm$^3$, assuming that the initial density for this system was 15.6 g/cm$^3$.</td>
<td>10.4 kg</td>
<td>10.4 kg (Ref. 5, Fig. III.A.6-2)</td>
</tr>
<tr>
<td>4.4.2</td>
<td>Calculate the critical radius for spherical, unreflected Pu(5) metal system with a density of 9.9 g/cm$^3$ assuming that the initial density for this system was 19.8 g/cm$^3$.</td>
<td>10.0 cm</td>
<td>10.1 cm (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>4.4.3</td>
<td>Calculate the critical mass for a spherical, unreflected $^{238}$PuO$_2$ system with a density of 1, 3, 5, 7, and 9 g/cm$^3$, assuming that the initial density for this system was 11.46 g/cm$^3$.</td>
<td>1 g/cm$^3$ – 4084 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</td>
<td>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 (Diffusion Theory Calculations from Section 2.5.6)</td>
</tr>
<tr>
<td>4.4.4</td>
<td>Calculate the water-reflected critical mass for a spherical, Pu(5) metal system with a density of 15.75 g/cm$^3$ if the Pu core had an initial density of 19.8 g/cm$^3$.</td>
<td>8.2 kg</td>
<td>8.25 kg (SCALE5, Keno V.a)</td>
</tr>
</tbody>
</table>
9.3 Confidence in Array Hand Calculations

The example problem results presented in Chapters 5 through 7 along with the corresponding comparison result are summarized in Tables 20, 21, and 22. The solid angle method chapter did not have example problems to include in this comparison exercise.

Table 20. Surface Density Method Confidence Comparison

<table>
<thead>
<tr>
<th>Section</th>
<th>Description of the Problem</th>
<th>Hand Calculation Result</th>
<th>Comparison Result from Reference or Code Package (Critical Spacing)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.4.1</td>
<td>What is the minimum spacing for a planar array of 2-liter bottles of Pu, with 5 wt. % $^{240}\text{Pu}$, solution, assuming a maximum concentration of 400 gPu/l? The array is assumed to be only one unit high (i.e., no stacking).</td>
<td>25.0 cm $k_{\text{eff}} \approx 0.89^6$</td>
<td>$\sim 23.1$ cm (SCALE5, Keno V.a, 238-group ENDF/B-V library)</td>
</tr>
<tr>
<td>5.4.2</td>
<td>What is the minimum center-to-center spacing for an infinite planar array of plutonium oxide ($^{239}\text{PuO}_2$) containers loaded with 4,500 grams of Pu per container?</td>
<td>28.4 cm $k_{\text{eff}} \approx 0.88$</td>
<td>$\sim 19.5$ cm (SCALE5, Keno V.a, 238-group ENDF/B-V library)</td>
</tr>
<tr>
<td>5.4.3</td>
<td>What is the minimum center-to-center spacing of an infinite planar array of 4,500 g Pu(5) metal ingots.</td>
<td>36.0 cm $k_{\text{eff}} \approx 0.88$</td>
<td>$\sim 25.0$ cm (SCALE5, Keno V.a, 238-group ENDF/B-V library)</td>
</tr>
</tbody>
</table>

6 This represents the $k_{\text{eff}}$ for the hand calculated spacing result based on a SCALE5, Keno V.a calculation.
## Table 21. Density Analog Method Confidence Comparison

<table>
<thead>
<tr>
<th>Section</th>
<th>Description of the Problem</th>
<th>Hand Calculation Result</th>
<th>Comparison Result from Reference or Code Package (Critical Spacing)</th>
</tr>
</thead>
</table>
| 6.4.1   | Using the density analog method, repeat the example problem in Section 5.4.1 for $2 \times 2$, $10 \times 10$ and $100 \times 100 \times 100$ 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. | $2 \times 2 \times 2$  
17.8 cm$^2$  
10$\times$10$\times$10  
39.8 cm  
k$_{eff} = 0.968$  
100$\times$100$\times$100  
126 cm | $2 \times 2 \times 2$  
No minimum spacing  
required, k$_{eff} = 0.94$  
with no spacing  
$10 \times 10 \times 10$  
~36.5 cm  
$100 \times 100 \times 100$  
~108.0 cm  
(SCALE5, Keno V.a) |
| 6.4.2   | Using the density analog method, repeat the example problem in Section 5.4.2 for $2 \times 2$, $10 \times 10$ and $100 \times 100 \times 100$ arrays. Recall that each container in the array contains Pu oxide ($^{239}$PuO$_2$) loaded with up to 4,500 grams of Pu. | $2 \times 2 \times 2$  
18.6 cm  
10$\times$10$\times$10  
41.6 cm  
k$_{eff} \approx 0.88$  
100$\times$100$\times$100  
132 cm | $2 \times 2 \times 2$  
~10.6 cm  
$10 \times 10 \times 10$  
~34.0 cm  
$100 \times 100 \times 100$  
~109.6 cm  
(SCALE5, Keno V.a) |
| 6.4.3   | Using the density analog method, repeat the example problem in Section 5.4.3 for $2 \times 2$, $10 \times 10$ and $100 \times 100 \times 100$ arrays. Recall that each fissile unit in the array is a 4,500 g Pu(5) metal ingot. | $2 \times 2 \times 2$  
25.7 cm  
10$\times$10$\times$10  
57.4 cm  
k$_{eff} \approx 0.91$  
100$\times$100$\times$100  
182 cm | $2 \times 2 \times 2$  
~15.0 cm  
$10 \times 10 \times 10$  
~41.7 cm  
$100 \times 100 \times 100$  
~137.0 cm  
(SCALE5, Keno V.a) |

7 The density analog method provides a center-to-center spacing between solution units in the array that is more reactive than similar arrays with metal units. Thus, some care should be exercised when using this method with thermal systems.

8 This represents the $k_{eff}$ for the hand calculated spacing result based on a SCALE5, Keno V.a calculation.
### Table 22. Limiting Surface Density Method Confidence Comparison

<table>
<thead>
<tr>
<th>Section</th>
<th>Description of the Problem</th>
<th>Hand Calculation Result</th>
<th>Comparison Result from Reference or Code Package&lt;sup&gt;9&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.4.1 (EP 1)</td>
<td>Repeat example problem in Section 5.4.2 for 2×2×2, 10×10×10 and 100×100×100 arrays. Recall that each container in the array contains Pu oxide ((^{239})PuO(_2)) loaded with up to 4,500 grams of Pu.</td>
<td>2×2×2, Not Applicable 10×10×10 35.7 cm 100×100×100 114.7 cm</td>
<td>2×2×2, ~10.6 cm 10×10×10 ~34.0 cm 100×100×100 ~109.6 cm (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.4.2 (EP 2)</td>
<td>Repeat the example problem in Section 5.4.3 for 2×2×2, 10×10×10 and 100×100×100 arrays. Recall that each fissile unit in the array is a 4,500 g Pu(5) metal ingot.</td>
<td>2×2×2, Not Applicable 10×10×10 42.4 cm 100×100×100 136.4 cm</td>
<td>2×2×2, ~15.0 cm 10×10×10 ~41.7 cm 100×100×100 ~137.0 cm (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.4.3 (EP 3)</td>
<td>Calculate the critical mass for each array unit required for a water-reflected cubic array of fully enriched U(100) metal units spaced 30 in. (76.2 cm) center-to-center. After the critical mass is calculated, determine the multiplication factor for storing 20 kg of U(100) units in the 4×4×4 array.</td>
<td>34.3 kg (k_{\text{eff}} = 0.84)</td>
<td>~34.3 kg (k_{\text{eff}} = 0.85) (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.4.4 (EP 4)</td>
<td>Calculate the critical mass for each array unit required for a water-reflected cubic array of Pu(5.2) metal units spaced 30 in. (76.2 cm) center-to-center. After the critical mass is calculated, determine the multiplication factor for 5 kg Pu(5.2) metal array units.</td>
<td>9.03 kg (k_{\text{eff}} = 0.82)</td>
<td>~8.93 kg (k_{\text{eff}} = 0.83) (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.4.5 (EP 5)</td>
<td>Based on the results of the last example problem in Section 7.4.4, calculate the required center-to-center spacing between array units to provide a multiplication factor of 0.9.</td>
<td>(m = 6.58 \text{ kg} \quad k_{\text{eff}} = 0.90)</td>
<td>(m = 6.58 \text{ kg} \quad k_{\text{eff}} = 0.91) (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.5.1 (EP 6)</td>
<td>Repeat the example problem in Section 7.4.4 for an 8×4×2 array, using the methodology presented in Section 7.4 for U(100) metal units.</td>
<td>9.03 kg (k_{\text{eff}} = 0.83)</td>
<td>~8.93 kg (k_{\text{eff}} = 0.83) (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.6.1 (EP 7)</td>
<td>Repeat the example problem in Section 7.4.3 for an 8×4×2 array, using the methodology presented in Section 7.6 for U(100) metal units.</td>
<td>35.9 kg</td>
<td>35.9 cm (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.6.2 (EP 8)</td>
<td><strong>Part 1.</strong> Calculate the spherical critical mass of U(93.2) metal required for criticality in a 216-unit water-reflected cubic array. The center-to-center spacing (2a) of the array units is 38.1 cm. <strong>Part 2.</strong> What would be the multiplication factor of this array if the units were rearranged into a water-reflected 9×24×1 cuboidal array? <strong>Part 3.</strong> 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?</td>
<td>16.4 kg (k_{\text{eff}} = 0.86) 3.86 kg (6×6×6) (k_{\text{eff}} = 0.9) 5.15 kg (9×24×1) (k_{\text{eff}} = 0.9)</td>
<td>16.0 kg (k_{\text{eff}} = 0.87) 3.86 kg (6×6×6) (k_{\text{eff}} = 0.9) 5.15 kg (9×24×1) (k_{\text{eff}} = 0.91) (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.6.3 (EP 9)</td>
<td>Repeat the example problem in Section 7.2.4 for a density change from 18.9 g/cm(^3) to 15 g/cm(^3).</td>
<td>~47.3 kg (SCALE5, Keno V.a)</td>
<td>~47.3 kg (SCALE5, Keno V.a)</td>
</tr>
<tr>
<td>7.7.3 (EP 9)</td>
<td>Calculate the critical mass for each array unit required for the water-reflected cubic array from the limiting surface density example problem 3 (Section 7.3.4) for fully enriched U(100) metal, assuming 12 in. of concrete reflection instead of 7.8 in. of water reflection (20 cm as assumed by the limiting surface density method).</td>
<td>30.1 kg (k_{\text{eff}} = 0.87)</td>
<td>30.3 kg (k_{\text{eff}} = 0.88) (SCALE5, Keno V.a)</td>
</tr>
</tbody>
</table>

*The spacing result provided is for a critical array unless otherwise stated in the example problem.*

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### 9.4 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 22. To examine the various array methods, array experiments from a benchmark evaluation, HEU-MET-FAST-023 (Reference 30) and HEU-MET-FAST-026 (Reference 31), was used to provide a comparison between the array hand calculation 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 23. Array Hand Methods Comparison Table

<table>
<thead>
<tr>
<th>Experimental Benchmark Considered</th>
<th>Array Hand Method Comparison – Unit Center-to-Center Spacing (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Surface Density Method(^{10})</td>
</tr>
<tr>
<td>HEU-MET-FAST-023</td>
<td></td>
</tr>
<tr>
<td>Case 22, 4x4x4, 10.5 kg U Metal (93.2), 15.2 cm Paraffin Reflector</td>
<td>63.1 (24.8 in.)</td>
</tr>
<tr>
<td>HEU-MET-FAST-026</td>
<td></td>
</tr>
<tr>
<td>Case 10, Exp b-10, 3x3x3, 15.4 kg U Metal (93.2), 15.2 cm Paraffin Reflector</td>
<td>77.5 (30.5 in.)</td>
</tr>
<tr>
<td>HEU-MET-FAST-026</td>
<td></td>
</tr>
<tr>
<td>Case 22, Exp c-12, 3x3x3, 20.5 kg U Metal (93.2), 15.2 cm Paraffin Reflector</td>
<td>101.4 (39.9 in.)</td>
</tr>
<tr>
<td>HEU-MET-FAST-026</td>
<td></td>
</tr>
<tr>
<td>Case 32, Exp d-10, 3x3x3, 24.7 kg U Metal (93.2), 15.2 cm Paraffin Reflector</td>
<td>127.7 (50.3 in.)</td>
</tr>
<tr>
<td>HEU-MET-FAST-026</td>
<td></td>
</tr>
<tr>
<td>Case 9, Exp b-9, 3x3x3, 15.4 kg U Metal (93.2), 15.2 cm Paraffin Reflector</td>
<td>77.5 (30.5 in.)</td>
</tr>
<tr>
<td>HEU-MET-FAST-026</td>
<td></td>
</tr>
<tr>
<td>Case 21, Exp c-11, 3x3x3, 20.5 kg U Metal (93.2), 15.2 cm Paraffin Reflector</td>
<td>101.4 (39.9 in.)</td>
</tr>
<tr>
<td>HEU-MET-FAST-026</td>
<td></td>
</tr>
<tr>
<td>Case 21, Exp d-9, 3x3x3, 24.7 kg U Metal (93.2), 15.2 cm Paraffin Reflector</td>
<td>127.7 (50.3 in.)</td>
</tr>
</tbody>
</table>

Note that although most of these benchmarks do not comply with the limiting surface density requirement of 64 or more units, the results are still quite good. The limiting surface density method will generally give good results for all array sizes, but the user must be aware that unless the limiting value is approached (i.e., 64 or more units in the array), the results are not necessarily the most limiting.

\(^{10}\) The surface density method considers an infinite planar array with a height corresponding to stack height of the array considered in the experiment. The method provides a subcritical center-to-center spacing result.

\(^{11}\) The density analog method considers a cubic array configuration. The method provides a subcritical center-to-center spacing result.

\(^{12}\) The limiting surface density method, NB\(n^2\), provides a center-to-center spacing that results in a critical array configuration.
9.5 Conclusions

Close examination of the comparisons summarized in the Section 9 tables clearly show that the results provided by the various hand calculation methods discussed in this primer provide very good results when compared with actual dimensions, MCNP5 or Keno V.a results, or experimental benchmarks. Thus, hand calculations can be very effective tools for a criticality safety practitioner as a calculation 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 to learn how to use the various methods and understand their applicability and limitations.
10. References


11. Appendix A - Linear Extrapolation Distance for Diffusion Theory Hand Calculations

11.1 Introduction

The following information provides an in-depth discussion about linear extrapolation distance to support the discussion in Chapter 2 about hand calculation methods using one-group and modified one-group diffusion theories.

11.2 Discussion

In transport theory, the flux has angular dependence so the neutron currents can be accurately calculated. However, in diffusion theory, it is assumed that the flux is isotropic, which means that there is no way of calculating the flux at a vacuum boundary, as illustrated in Figure 45.

![Figure 45. Illustration of Fissile Material/Vacuum Boundary](image)

Because it is not known whether the neutron flux is not actually zero in the vacuum, a mathematical assumption can be made that indicates the flux approaches zero at some point in the vacuum. To find the point at which the flux will be defined as zero, known as the linear extrapolation distance, the slope of the flux at the boundary can be extrapolated to the point where the flux is equal to zero. Figure 46 shows the flux profile at the boundary of a system.

![Figure 46. Illustration of the Slope of the Neutron Flux at the System Boundary](image)
From diffusion theory, it can be shown that the extrapolation distance, $d$ (cm), can be defined by the following where $D$ is the diffusion coefficient (cm).

$$d = 2 \times D$$

Because the diffusion coefficient, $D$, can be related to the transport mean free path, the extrapolation distance, $d$, can be related to the transport mean free path.

$$D = \frac{\lambda_{tr}}{3}; \text{ therefore, the extrapolation distance can be rewritten as}$$

$$d = \frac{2 \times \lambda_{tr}}{3} = 2 \times D$$

A more refined transport analysis indicates that

$$d = 0.71 \times \lambda_{tr} = \frac{0.71}{\Sigma_{tr}}, \text{ where the macroscopic transport cross section is defined as}$$

$$\lambda_{tr} = \frac{1}{\Sigma_{tr}}.$$

Recall that $\lambda_{tr} = \left[ \Sigma_{tr} \right]^{-1} = \left[ \Sigma_i - \mu_0 \Sigma_s \right]^{-1},$

where $\mu_0$ represents the average scattering angle cosine.

Thus, the neutron flux mathematically vanishes at the extrapolated boundary, which lies at $0.71 \lambda_{tr}$ beyond the physical boundary for the fissile material as illustrated above. The transport macroscopic cross section and transport mean free paths consider anisotropic scattering processes taking place in a fissile system where neutrons are diffusing from locations in the system with a high neutron density to locations with lower neutron densities (Reference 1). In most thermal systems, $\Sigma_{tr}$ is about 0.2 to 0.4 cm$^{-1}$; therefore, the extrapolation distance, $d$, ranges from about 1 to 3.5 cm.
12. 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. This information (Reference 32) 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 are provided from Reference 32 in Tables 24 and 25. 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.

**Table 24. Metal Sphere Critical Masses**

<table>
<thead>
<tr>
<th>Material</th>
<th>Critical Mass (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Unreflected</td>
</tr>
<tr>
<td>HEU</td>
<td>53.8</td>
</tr>
<tr>
<td>δPu(4.5)</td>
<td>17.0</td>
</tr>
<tr>
<td>δPu(20)</td>
<td>19.0</td>
</tr>
<tr>
<td>αPu(4.5)</td>
<td>10.6</td>
</tr>
</tbody>
</table>

**Table 25. Solution Sphere Critical Masses**

<table>
<thead>
<tr>
<th>Material</th>
<th>Concentration (g/liter)</th>
<th>Critical Mass (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Unreflected</td>
<td>Water Reflected</td>
</tr>
<tr>
<td>HEU</td>
<td>20</td>
<td>3.24</td>
</tr>
<tr>
<td>HEU</td>
<td>30</td>
<td>1.84</td>
</tr>
<tr>
<td>HEU</td>
<td>50</td>
<td>1.60</td>
</tr>
<tr>
<td>HEU</td>
<td>200</td>
<td>3.19</td>
</tr>
<tr>
<td>Pu(4)</td>
<td>20</td>
<td>1.08</td>
</tr>
<tr>
<td>Pu(4)</td>
<td>30</td>
<td>1.05</td>
</tr>
<tr>
<td>Pu(4)</td>
<td>50</td>
<td>1.28</td>
</tr>
<tr>
<td>Pu(4)</td>
<td>200</td>
<td>3.97</td>
</tr>
</tbody>
</table>

According to Reference 32, 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:

$$k_{eff} = \delta^{0.3}$$

where $\delta$ 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 (Tables 24).

Also, Reference 32 also defines the relationship to provide an estimate of the $k_{eff}$ for HEU and Pu solutions, for, again, bare and water-reflected configurations.
\[ k_{\text{eff}} = 3^{0.25} \], where \( \exists \) is the fraction of critical mass for this system equal to, as before, the ratio of the actual fissile mass present to the critical mass for the material present (Tables 25).

Figures 47–52 provide the multiplication factor data as a function of the fraction of critical mass for the HEU and Pu metal or solution systems. The metal systems compare well to the empirical value for the multiplication factor; however, the solutions tend to vary significantly at lower critical mass fractions. Based on the calculations provided in addition to the empirical data, one can estimate the multiplication factor sufficiently to provide assistance for hand calculations in most cases. Curve fits for low enriched uranium would be useful; however, that information has not yet been compiled.

Figure 47. \( k_{\text{eff}} \) vs. Fraction of Critical Mass: Unreflected HEU and Pu Metal
Figure 48. $k_{\text{eff}}$ vs. Fraction of Critical Mass: Water Reflected HEU and Pu Metal

Figure 49. $k_{\text{eff}}$ vs. Fraction of Critical Mass: Bare HEU Solution
Figure 50. $k_{\text{eff}}$ vs. Fraction of Critical Mass: Water Reflected HEU Solution

Figure 51. $k_{\text{eff}}$ vs. Fraction of Critical Mass: Bare Pu Solution
Figure 52. $k_{\text{eff}}$ vs. Fraction of Critical Mass: Water Reflected Pu Solution