MODULE 3.0: NUCLEAR THEORY

Introduction

Welcome to Module 3.0 of the Nuclear Criticality Safety Directed Self-Study Course! This is the third of five modules available in this directed self-study course. The purpose of this module is to assist you in describing the fission process and basic nuclear theory concepts.

This directed self-study module is designed to assist you in accomplishing the learning objectives listed at the beginning of the module. There are four sections in this module. The module has self-check questions and activities to help you assess your understanding of the concepts presented in the module. Please note there are also optional activities that are not required for completion of this module. These are noted at the beginning of the activity

Before You Begin

It is recommended that you have access to the following material:

- ☐ Trainee Guide

Complete the following prerequisite:

- ☐ There are no prerequisites to this module.

How to Complete this Module

1. Review the learning objectives.
2. Read each section within the module in sequential order.
3. Complete the self-check questions and activities within this module.
4. Check off the tracking form as you complete the self-check questions and/or activities within the module.
5. Contact your administrator as prompted for a progress review meeting.
6. Contact your administrator as prompted for any additional materials and/or specific assignments.
7. Complete all assignments related to this module.
8. Ensure that you and your administrator have dated and initialed your progress on the tracking form.

9. Go to the next assigned module.

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Learning Objectives

3.1 Upon completion of this module, you will be able to describe the fission process and basic nuclear theory concepts.

3.1.1 Define the terms:

- fissile isotopes
- fissile material
- fissile system
- fission, nuclear
- fissionable isotopes

3.1.2 Describe the fission chain reaction in terms of the following:

- energy release
- neutron production
  - number
  - energy
  - timing (prompt and delayed)
- absorption, scattering, and leakage
- radiation types and time history

3.1.3 Define k_{eff} and qualitatively state changes when parameters are changed.

3.1.4 Identify the purpose and basic features of each of the following hand calculation methods:

- buckling conversion
- age-diffusion migration area approximation
- fraction critical
- solid angle
- surface density

3.1.5 Identify the purpose and basic features of the Monte Carlo computer code KENO.

Learning Objective

When you finish this section, you will be able to:

3.1.1 Define the terms:

- fissile isotopes
- fissile material
- fissile system
- fission, nuclear
- fissionable isotopes

DEFINITIONS

These are terms that you will need to be familiar with while reviewing this module:

Fissile Isotopes
Fissile isotopes are the subset of the fissionable isotopes that will sustain a fission-chain reaction using thermal neutrons. The important isotopes ^{233}U, ^{235}U, ^{239}Pu, and ^{241}Pu are fissile isotopes. Fissile isotopes in solution or in special mixtures can absorb thermal neutrons and sustain chain reactions with much smaller masses than those usually required for sustained fission; therefore, fissile isotopes pose a greater risk of an accidental criticality.

Fissile Material
A material, other than natural uranium, that is capable of sustaining a neutron chain reaction. Source: ANSI/ANS 8.7, 1975.

Fissile System
A system containing ^{235}U, ^{239}Pu, or ^{233}U nuclei and capable of significant neutron multiplication.

Fission, Nuclear
1. Nuclear reaction in which a neutron and nucleus interact with the result that the nucleus splits into two or more parts. Fission reactions of interest here release net energy and produce neutrons that can participate in a sustained chain reaction. 2. Disintegration of a nucleus (usually Th, U, Pu, or heavier) into two (rarely more) masses of similar order of magnitude, accompanied by a large release of energy and the emission of neutrons. Although some fissions take place spontaneously, neutron-induced fissions are designated σ_f, and ν is the number of neutrons emitted per fission.

Fissionable Isotope
A fissionable isotope is any isotope capable of sustaining a neutron-induced fission-chain reaction, regardless of the neutron energy or

speed necessary to induce and sustain the reaction. For practical nuclear criticality safety purposes, these isotopes are limited to ^{233}U, ^{235}U, ^{241}Am, ^{242m}Am, ^{243}Am, ^{243}Cm, ^{244}Cm, ^{245}Cm, ^{247}Cm, ^{249}Cf, ^{251}Cf, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu. Although other isotopes of some of the above elements would sustain fission, the quantity required for a self-sustaining chain reaction is so great and/or the mass available is so small as to make a nuclear-criticality accident incredible.

Self-Check Questions 3-1

Fill in the missing words in each statement. Answers are located in the answer key section of the Trainee Guide. Choose from the following words:

fissionable	isotopes	multiplication
natural	reaction	^{235}U

1. Fissile _____ are the subset of the fissionable isotopes that will sustain a fission-chain reaction using thermal neutrons. Examples of these are ^{233}U,_____, ^{239}Pu, and ^{241}Pu.

2. Fissile material is a material other than _____ uranium that is capable of sustaining a neutron chain reaction.

3. A fissile system is a system containing ^{235}U, ^{239}Pu, or ^{233}U nuclei and capable of significant neutron _____.

4. Nuclear fission is a nuclear _____ in which a neutron and nucleus interact with the result that the nucleus splits into two or more parts.

5. A _____ isotope is capable of sustaining a neutron-induced fission-chain reaction, regardless of the neutron energy or speed necessary to induce and sustain the reaction.

You have completed this section.
Please check off your progress on the tracking form.
Go to the next section.

Learning Objectives

When you finish this section, you will be able to:

3.1.2 Describe the fission chain reaction in terms of the following:

- energy release
- neutron production
  - number
  - energy
  - timing (prompt and delayed)
- absorption, scattering, and leakage
- radiation types and time history

3.1.3 Define k_{eff} and qualitatively state changes when parameters are changed.

NUCLEAR REACTIONS

Fission Process

The fission process and its associated neutron chain reaction produces energy, which is used by licensees in:

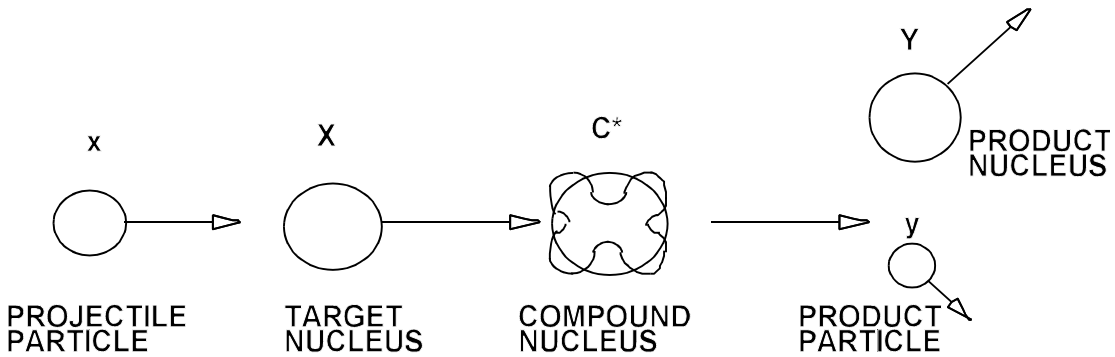
- Generation of electricity
- Propulsion
- Production of radioisotopes
- Research

Nuclear Reactions

The physics of criticality and nuclear criticality safety depends first on identification of nuclear reactions.

The basic mechanism for a nuclear reaction involves a PROJECTILE particle (x) and a TARGET nucleus (X), combining to form an unstable COMPOUND NUCLEUS (C*), which decomposes into two or more PRODUCTS (Y and y) plus excess energy in the form of radiation. See Figure 3-1.

Figure 3-1. Nuclear Reactions



The process can be written as equations:

$X + x \rightarrow C^* \rightarrow Y + y$, or
$X(x,y)Y$, or
$X(x,y)$

Mass, energy, and other considerations determine which reaction products may result; each possible reaction has a PROBABILITY of occurrence.

Neutron Reactions

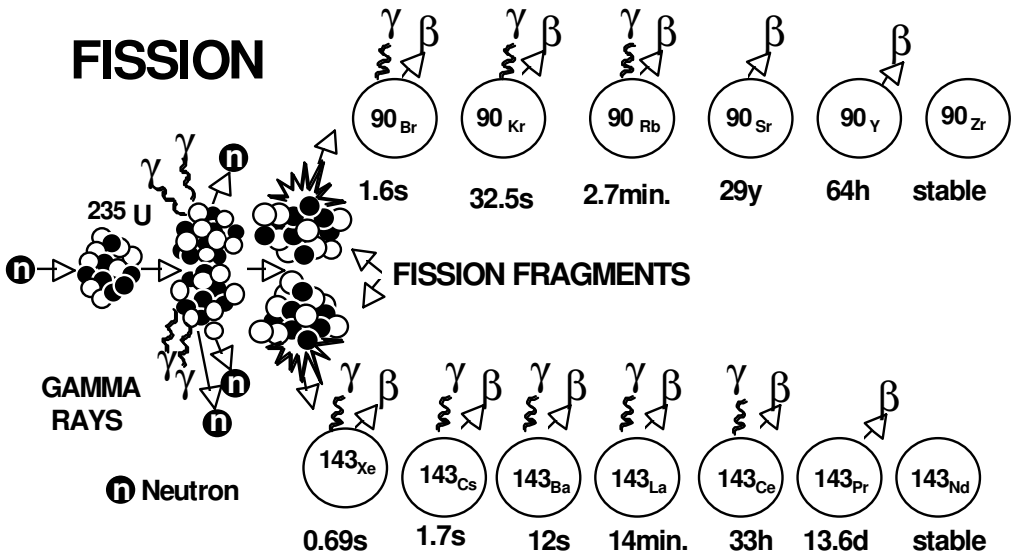
Neutron reactions are the major contributors to fission chain reactions.

- Scattering reactions start and end with a neutron but do not always reduce neutron energy (and, as shown later, change the probability of subsequent reactions).
- Absorption reactions—capture and fission—each result in the loss of the projectile neutron. In capture, the loss is permanent, while, in fission, two or more neutrons are produced.
- Must account for scattering, capture, and fission to describe a fission chain reaction.

Nuclear Fission Reaction

The fission reaction of uranium-235 is shown in Figure 3-2.

Figure 3-2. Fission Reaction of Uranium-235



The reaction has advantages and disadvantages. See Table 3-1.

Table 3-1. Advantages and Disadvantages of a Fission Reaction

Advantages	Disadvantages
Heat - Provides compact energy source	Radiation - Requires shielding, containment, and heat removal
Neutrons - Allow self-sustaining chain reaction	

Fissioning Materials

The two basic categories of materials that fission are described in Table 3-2.

Table 3-2. Categories of Materials That Fission

Category	Definition	Species	Result
Fissile	Isotopes that can be fissioned by neutrons of any energy	^{235}U, ^{233}U, ^{239}Pu, ^{241}Pu	Can sustain a fission chain reaction
Fissionable	Isotopes that can be fissioned by **HIGH** energy neutrons (but not by low energy neutrons)	^{238}U, ^{232}Th, ^{240}Pu	Can participate in a fission chain reaction

What Fissionable Material Is Present at NRC Licensee Facilities?

- The dominant fissionable material in NRC licensee fuel cycle facilities is uranium (fissile ^{235}U and non-fissile ^{238}U).
- Plutonium is present at reactor sites and storage facilities (e.g., GE-Morris) in spent fuel and will be a concern for waste management.
- ^{233}U is present only in research-related activities (e.g., high-temperature gas-cooled reactor programs).

Fission Energy Release

Fission energy release is divided among the various fission products as shown in Table 3-3.

Table 3-3. Fission Products

Fission Products		MeV	% of Energy Release
Fission Fragments (usually two)		168	84
Neutrons		5	2.5
Prompt Gamma Rays		7	3.5
Delayed Radiation	Beta Particles	8	4
	Gamma Rays	7	3.5
Radiative Capture Gammas		5	2.5
Total		200	100

Overall Heat Energy Equation

Overall heat energy from fission is produced at a rate given by the following equation:

$$3.1 \times 10^{10} \text{ fissions} \approx 1 \text{ watt-s}$$

(This expression can be used to convert total fissions or fission rate in an excursion to an equivalent energy production.)

What Are the Consequences of Fission Energy Release to a Criticality Accident?

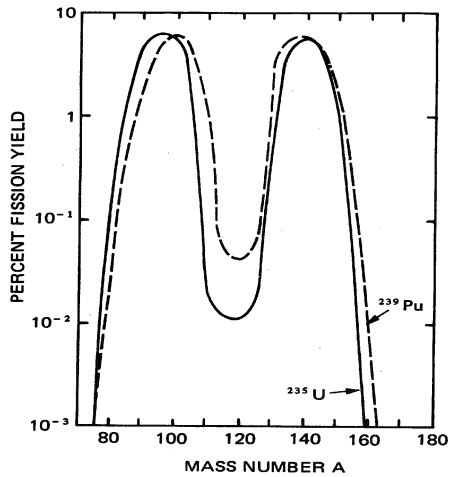
Criticality accidents have:

- Large radiation sources at the time of fission
- Delayed beta and gamma radiation, which gives rise to long-term radiation sources

Fission Fragments

When fissionable nuclei split into two FISSION FRAGMENTS, the fragments are seldom of equal mass (e.g., only 0.01% in ^{235}U). Instead, there is a range of products, as shown in the "double-humped" (bi-modal) spectrum. See Figure 3-3. (Here for ^{235}U, species in the ranges A = 90 - 100 and A = 135 - 145 may each have occurred in as many as ~7% of fissions. Overall, there are >200 species of fission products.

Figure 3-3. Double-humped (Bi-Modal) Spectrum



Consequences of Fission Products

Consequences of fission products:

- Some fission products are gaseous (iodine) and others are volatile (strontium and cesium).
- Gaseous and volatile fission products spread readily as contamination, following an accident.
- Radioactive wastes from an accident or from spent fuel are multi-species and, therefore, complex.

Fission Neutrons

Neutrons emitted from fission are characterized by:

- Number v that generally is greater than two (~2.5 for ^{235}U)
- Timing that is either:

  PROMPT - at time of fission (>99%) or
  DELAYED - following fission fragment decay (0.2%-0.7%;~0.1 seconds to 1 minute after fission)

- Energy spectrum (E):

Most probable energy	0.7 MeV
Average energy	2.0 MeV
Basic energy range	0.1 MeV to 10 MeV

Neutron Characteristics

Neutron characteristics:

- Sufficient neutrons are needed to support a self-sustaining chain reaction.
- Presence of delayed neutrons allows for control of a neutron chain reaction in reactors and the possibility of a "delayed critical" accident scenario (e.g., as described later and as may affect the design of criticality alarm systems).

Neutron Energy Considerations

Because neutrons are born fast (>0.1 MeV) but are best at causing fission when moderated to thermal energies (on the order of less than 1 eV), moderating materials like water are important to both reactor design and nuclear criticality safety.

Moderation of Neutrons

Moderation of neutrons occurs when neutrons undergo scattering reactions. Elastic scattering of neutrons with low-Z materials results in relatively large energy changes per collision. (For a neutron and hydrogen atom, the analogy is a collision of two billiard balls). With high-Z materials, small energy changes per collision occur (analogous to a billiard ball striking a bowling ball).

Moderators

Moderators include:

- WATER, which, due to its hydrogen content, can be very efficient in a relatively small volume; however, it also has significant absorption.
- DEUTERIUM (as in heavy water), BERYLLIUM, and

GRAPHITE are less efficient moderators (in terms of energy change per collision) and, thus, require successively larger volumes; however, each has much lower neutron absorption than water.

- Any of the above moderators, in the proper quantity and distribution, can reduce substantially the minimum amount of fissile material required to sustain a chain reaction.
- Elements in the range of 11<Z<83 are considered "NON-MODERATORS," which separate fissile nuclides, thereby, reducing the probability of fission.
- Heavy metals, including the fissionable materials, cause very small energy change per collision from elastic scattering.
- Inelastic scattering from some nuclides also contributes to neutron energy loss but generally in a manner of consequence only for detailed calculations.

Effects of Moderators and Non-Moderators on Critical Systems

Effects of moderators and non-moderators on critical systems:

- Hydrogen, deuterium, beryllium, and carbon are moderating materials that, when mixed, can reduce substantially the fissile material mass required to support a neutron chain reaction. Under usual conditions, only hydrogen (e.g., in water, plastic, or oil) or carbon (e.g., in organic liquids or other materials) would be expected to provide a source of accidental moderation.
- Accidental mixing of a non-moderator (e.g., aluminum powder or silicon from sand) can be expected to separate the fissile nuclides, thereby reducing the probability of fission.
- Metallic and other solid forms of fissile material do not exhibit significant moderation effects.

Neutron Balance Equation

A neutron balance equation for the fission chain reaction is as follows:

Rate of Increase in Number of Neutrons	=	Rate of Production of Neutrons	—	Rate of Absorption of Neutrons	—	Rate of Leakage of Neutrons

Accumulation = Production — Absorption — Leakage

See Table 3-4.

Table 3-4. Neutron Balance

If accumulation is:	The system is:	The neutron populations is:	The system behavior is:
=0	Critical	Steady State	Static
>0	Supercritical	Increasing	Kinetic/Dynamic
<0	Subcritical	Decreasing	Kinetic/Dynamic

CROSS SECTION

The concept of a CROSS SECTION was developed from the perception that:

Interaction Probability = n σ dx

where n = density of atoms (at/cm^3)

σ = cross-sectional area [of the target nucleus] (cm^2/at)

dx = distance traveled by neutron (cm)

However, with the determination that the interaction probability for a given material changed substantially with neutron energy, and because it was not easy to view the nucleus as changing size, the following term was defined without specific connection to physical dimensions:

$$\text{Microscopic Cross Section} = \frac{\text{Interaction Prob}}{n\ dx}$$

The unit of measurement was selected as:

1 barn [b] = 10^{-24} cm^2

The name was derived from the intended-to-be-humorous observation that such a target was "as big as the side of a barn."

Energy Dependence of Microscopic Cross Sections

ENERGY DEPENDENCE of microscopic cross sections is very complex. A few of the key features include:

POTENTIAL SCATTERING cross section is approximately the size of nucleus.

Absorption cross section over a wide energy range varies roughly as "ONE-OVER-v," which in equation form is:

$$\sigma_a(E) = \sigma_0 (v_0 / v) = \sigma_0 (E_0 / E)^{1/2}$$

Here the interaction probability is generally proportional to the "time spent near the nucleus' force field."

In the RESONANCE region, specific "energy levels" in the nucleus give rise to extremely high cross sections at rather precise neutron energies. Absorption, scattering, and fission cross sections can exhibit this trait.

Energy-Dependent Cross Sections for Uranium

The energy-dependent cross-section plots in Figure 3-4 show that:

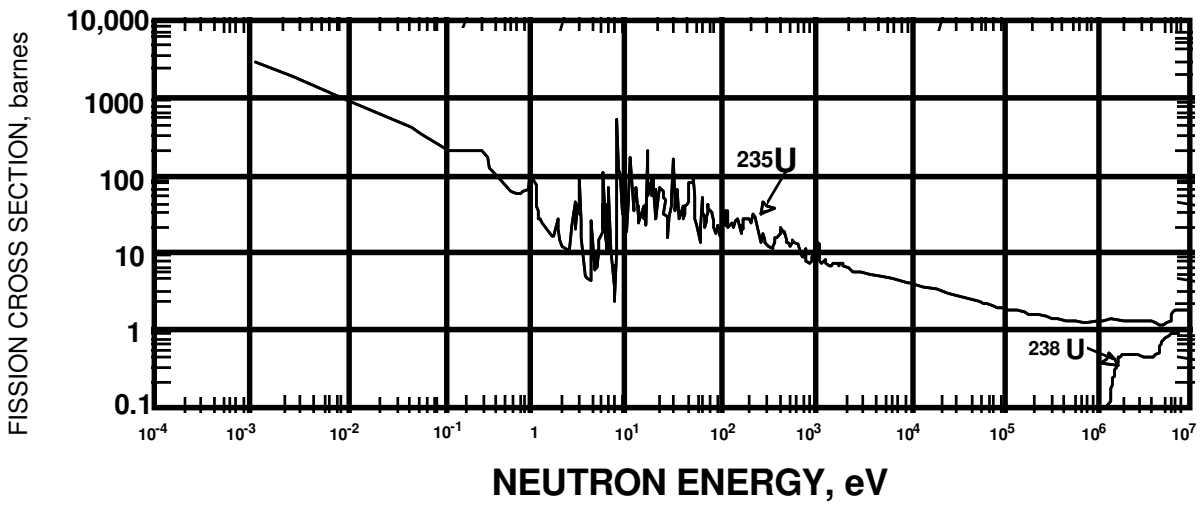
- ^{235}U has thermal and fast fission and is therefore *fissile*
- ^{238}U has fast fission only and is therefore *fissionable*, but *non-fissile*
- ^{235}U has a fission cross section several orders of magnitude greater for thermal than for fast neutrons; thus, neutron moderation can considerably increase the reaction probability.

INFINITE SYSTEM

Infinite Multiplication Factor

An initial look at developing a model for the fission chain reaction begins with consideration of an infinite system. Here, by definition, there is no leakage (the term which turns out to be very difficult to quantify), so only neutron production and absorption need be considered.

Figure 3-4. ^{235}U Fission Cross Section



The neutron balance for an infinite system compares production and absorption rates with the result, based on definitions in the previous section, that:

Production Rate ↔ Absorption Rate

$v\Sigma_f\phi$ $\Sigma_a\phi$

It is convenient to define the INFINITE MULTIPLICATION FACTOR k_∞ as:

$$k_\infty = \frac{\text{Production Rate}}{\text{Absorption Rate}} = \frac{v\Sigma_f}{\Sigma_a}$$

This expression represents the multiplication—the ratio of the neutron population in one generation of fissions to that of the previous generation—for a system with no neutron leakage (or one that is large enough that leakage can be neglected). Thus, it reflects the highest multiplication possible for a given material composition.

The definition for k_∞ is deceptively simple in appearance. Because of the complexity of reaction cross sections and the neutron flux, the parameters are essentially averaged, or "one-energy-group," values that must be calculated through a complex process like energy that which will be summarized later.

Four-Factor Formula

To look at neutron multiplication independent of the mathematical complexity, the FOUR-FACTOR FORMULA is available. It breaks down the infinite multiplication factor into four terms as shown in Table 3-5.

$$k_\infty = \epsilon\ \rho\ \eta\ f$$

Table 3-5. Four Terms of the Infinite Multiplication Factor

Symbol	Title	Definition
ϵ	Fast Fission Factor - $(\Sigma_f)_{total} / (\nu\Sigma_f)_{thermal}$	fractional augmentation for fast fission (ϵ>1)
ρ	Resonance Escape Probability - $(\Sigma_a)_{thermal} / (\Sigma_a)_{total}$	fraction of neutrons reaching thermal energies without being absorbed as fast (primarily resonance-energy) neutrons
η	Eta (Average Number of Neutrons per Thermal Fission) - $(\nu\Sigma_f)_{thermal} / (\Sigma_a)_{fuel}$	number of neutrons produced per thermal neutron absorbed in fuel
f	Thermal Utilization - $(\Sigma_a)_{fuel} / (\Sigma_a)_{thermal}$	fraction of neutrons absorbed in fissionable material

Reaction rates are considered for thermal neutrons, total (thermal + fast) neutron energy spectrum for fuel, and total (fuel + non-fuel) material compositions.

Aside from being valuable for "thinking about" the fission chain reaction, the four-factor formula was valuable in the era before high-speed computers were available.

Measurements could be made for ϵ and ρ using a neutron beam and a neutron absorber, such as cadmium, to determine thermal and total reaction rate ratios. Then η and f could be calculated because the thermal-flux distribution is well behaved mathematically and the key cross sections tend to behave "one-over-v" in this energy range. Thus, the four factors could be combined to provide a reasonable estimate of k_∞. This approach could be especially useful in predicting the effect of a change in material composition or configuration.

Heterogeneous Systems

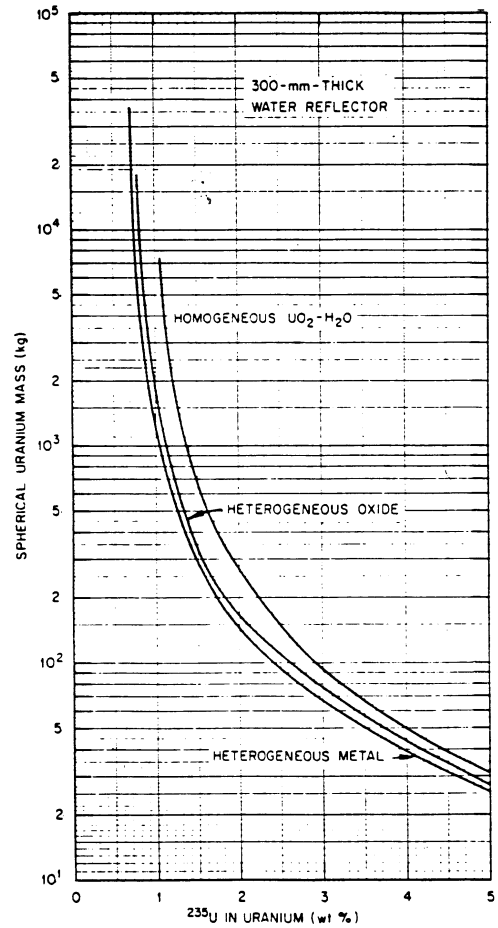
For heterogeneous systems (i.e., those where the fuel is lumped) of low-enriched fuel, the lumping increases resonance escape probability ρ with some decrease in the thermal utilization factor f. In lattices such as those used for light-water reactors, the heterogeneity is optimized such that $\triangle \rho > \triangle f$. Without lumping, homogeneous solutions of natural uranium are always subcritical (i.e., have $k_\infty < 1$).

Figure 3-5 shows critical mass of low-enriched uranium (LEU) as a function of uranium enrichment. Homogeneous and heterogeneous configurations are included.

Configurations of low-enrichment uranium are characterized by:

- Higher multiplication (lower critical mass) for optimum heterogeneous systems. This trend continues up to 6 wt% ^{235}U.
- Subcriticality of dry systems up to 5 wt%.

Figure 3-5. Critical Mass of LEU as a Function of Uranium Enrichment



FINITE SYSTEM

Neutron Balance

For the realistic finite system where the effect of leakage is considered, the neutron balance becomes:

Production ↔ Absorption + Leakage

and the EFFECTIVE MULTIPLICATION FACTOR k_{eff} is defined as:

$$k_{eff} = k = \frac{\text{Production}}{\text{Absorption} + \text{Leakage}}$$

Comparing this to the earlier definition of k_{eff}, it is clear that

$$k_{eff} < k_{\infty}$$

with the latter being the absolute maximum multiplication for a given composition in a very large system.

Comparing the definition of k_{eff} to the neutron balance, the value corresponding to each CRITICALITY STATE is:

$k_{eff} = 1$ Critical

$k_{eff} > 1$ Supercritical

$k_{eff} < 1$ Subcritical

Reactivity

An alternate view of multiplication is through REACTIVITY, which is defined as:

$$\rho = \frac{k - 1}{k}$$

where then by comparison with k_{eff}, ρ relates to the criticality states as indicated in Table 3-6.

Table 3-6. k_{eff} and ρ as Relates to Criticality State

k_{eff}	ρ	Criticality State
= 1	= 0	Critical
> 1	> 0	Supercritical
< 1	< 0	Subcritical

Nuclear Criticality Safety Practice

In nuclear criticality safety practice, the terms *multiplication* and *reactivity* are sometimes used interchangeably (except, of course, where numerical values are involved). This is especially true where a configuration of material change could be described as increasing (or decreasing) either the multiplication or reactivity. Similarly, the change could be stated as being more (or less) reactive or having higher (or lower) multiplication.

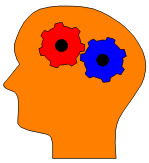
Neutron-Balance Terms

For purposes of nuclear criticality safety, the neutron balance may be controlled by changing:

- Production
- Absorption
- Leakage

A change in moderation may be noted to have a potential effect on each of the three terms.

Activity 1 - Neutron Balance



Purpose: The purpose of this activity is to identify methods for appropriate adjustment to each of the neutron balance terms (production, absorption, leakage, and moderation).

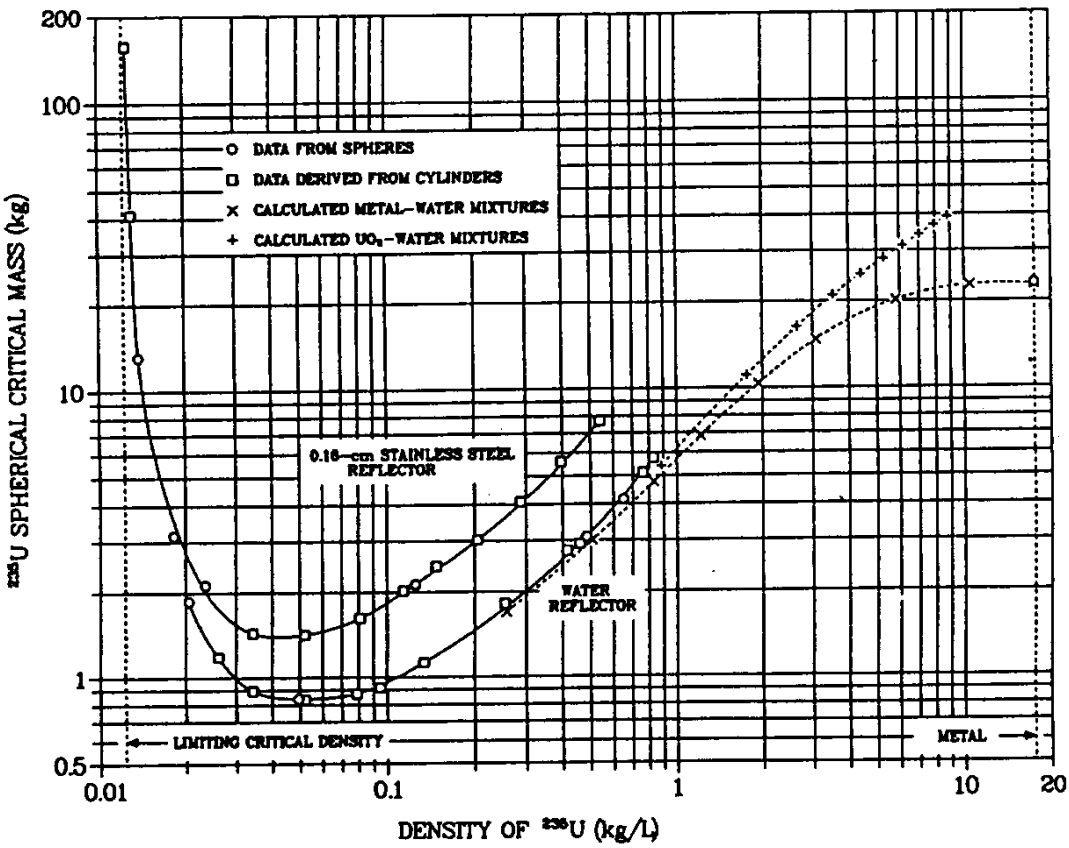
Directions: Identify methods for appropriate adjustments to each of the neutron balance terms. Answers are located in the answer key section of the Trainee Guide.

Neutron-Balance Term	Method
Production	
Absorption	
Leakage	
Moderation	

Illustrative Example

For an illustrative example, consider the variation of ^{235}U critical mass as a function of concentration. (Actual critical mass versus concentration data for ^{235}U is shown in Figure 3-6 (from LA-10860-MS [Figure 10]).

Figure 3-6. Critical Mass Versus Concentration Data for ^{235}U



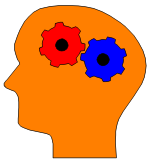
Consequences/ Impacts

Consequences/impacts:

- Masses may have two critical concentrations representing systems that are:
  - undermoderated
  - overmoderated
- There is an *optimum concentration,* where the *minimum critical mass* occurs. In this example, the latter mass is more than 25 times lower than that of the metal sphere; however, the volume is about 13 times greater (Metal: 22.8 kg ÷ 18.75 kg/liter = 1.30 liter; Solution: ~0.85 kg ÷ ~0.05 kg/liter = 17 liter; Solution ÷ Metal = 13).

  greatest at high concentration, dropping off as the system becomes more dilute (and correspondingly larger) with reduced neutron leakage from the outer boundary.
- From the standpoint of nuclear criticality safety, adding water to a solution excursion would:
  - terminate it, if the system is overmoderated
  - enhance it (i.e., make it more supercritical), if the system is undermoderated

Activity 2 - Operating Limit Values



Purpose: The purpose of this activity is to identify operating limit values.

Directions: Using data from Figure 3-6, complete the second column of the following table. Assuming that "double-batching" is a credible contingency, propose operating limit values and record the results in the third column of the table. Answers are located in the answer key section of the Trainee Guide.

Situation	^{235}U Physical Limit	^{235}U Operating Limit
Metal, fully reflected critical mass, kg		
Optimum concentration, nominal reflection critical mass, kg		
Optimum concentration, fully reflected critical mass, kg		
"Safe" concentration limit		

Results:

- Relatively large operating limits (~10 kg) can be used for processes that deal with large solid pieces of fissile material or other forms where dryness can be ensured (i.e., under verifiable "moderator control").
- Tight operating limits (~350 g) must be applied where moderator is not excluded and effective concentration is not controlled.

Self-Check Questions 3-2

Answer the following questions. Answers are located in the answer key section of the Trainee Guide.

1. The fission process and its associated neutron chain reaction produce energy that is used by licensees to do what?

2. The physics of criticality and nuclear criticality safety depends first on the identification of what?

3. What is the basic mechanism for a nuclear reaction?

4. What are some characteristics of scattering reactions?

5. What does absorption reactions–capture and fission–each result in?

6. What must you account for when describing a fission chain reaction?

7. What are the advantages and disadvantage of a fission reaction?

8. What are two categories of materials that fission and by what level of neutron energy are their isotopes fissioned?

9. What is the dominant fissionable material in NRC licensee fuel cycle facilities?

10. Fission energy release is divided among what fission products?

11. What is the equation for converting total fissions or fission rate in an excursion to an equivalent energy production.

12. What are the consequences of fission energy release to a criticality accident?

13. When fissionable nuclei split into two fission fragments, are the fragments of equal mass?

14. What are the consequences of fission products?

15. Neutrons emitted from fission are characterized by what timing?

16. What are two characteristics of neutrons as they relate to a neutron chain reaction?

17. Elastic scattering of neutrons with low-Z or high-Z materials results in what types of energy changes per collision?

18. What moderators in the proper quantity and distribution can reduce substantially the minimum amount of fissile material required to sustain a chain reaction?

19. What effect do non-moderators have in causing fissile material to sustain a chain reaction?

20. For each of the following systems, what is the status (increasing, decreasing, or steady) of their neutron populations?

If the system is:	The neutron population is:
Critical	
Supercritical	
Subcritical	

21. The concept of a cross section was developed from what perception?

22. What are some of the key features of energy dependence of microscopic cross sections?

23. The energy-dependent cross-section plots shown in Figure 3-4 for ^{235}U show what characteristics?

24. What does the infinite multiplication factor expression represent?

25. How can the four factor formula be useful?

26. Configurations of low-enrichment uranium are characterized by what?

27. Comparing the definition of k_{eff} to the neutron balance, what is the value corresponding to each criticality state below:

    $k_{eff} = 1$ Criticality state is _____
    $k_{eff} > 1$ Criticality state is _____
    $k_{eff} < 1$ Criticality state is _____

28. An alternative view of multiplication is through what?

29. For purposes of nuclear criticality safety, the neutron balance may be controlled by changing what?

30. From the standpoint of nuclear criticality safety and over-moderated and under-moderated systems, adding water to a solution excursion would do what?

You have completed this section.
Please check your progress on the tracking form.
Go to the next section.

Learning Objective

When you finish this section, you will be able to:

3.1.4 Identify the purpose and basic features of each of the following hand calculation methods:

- buckling conversion
- age-diffusion migration area approximation
- fraction critical
- solid angle
- surface density

COMPUTATIONAL METHODS

Introduction

Before the wide-spread availability of high-speed computers, hand calculation methods were the primary means for determining whether or not a fissile-material configuration was subcritical. These methods were based on correlations with experimental data and use of available calculational methods.

The computational methods for nuclear criticality are divided among the two approximations that are used to handle neutron leakage. These are diffusion theory and transport theory. Transport theory is further divided between discrete ordinates [s_n] and Monte Carlo.

Diffusion Theory

Diffusion theory, the earliest and simplest of the methods, was developed for systems where the following assumptions about the neutron population and the materials could be sustained:

- Diffusion occurs from regions of high neutron density to those of low neutron density.
- There is minimal absorption of neutrons.
- There is minimal discontinuity in neutron-reaction properties at interfaces among materials.

With these assumptions, the neutron leakage term could be cast in a form similar to that of a reaction rate as:

$$\text{Leakage} = DB^2 \phi$$

where

D = Diffusion Coefficient (*Material Property)*

B^2 = Buckling (*Geometric Property)*

and, in practice,

DB^2 = "Macroscopic Leakage Cross Section"

Thus, the neutron balance can be represented as:

$$v\Sigma_f\phi = \Sigma_a\phi + DB^2\phi$$

and

$$k_{eff} = k = \frac{v\Sigma_f}{DB^2 + \Sigma_a}$$

Calculations Used with Single Units

The hand calculation methods for single units include:

- Buckling conversion method
- Age-diffusion/migration area approximation
- Fraction critical method

These can be useful (1) for quick assessments, (2) for understanding the basic nature of some of the processes involved, and (3) as a bridge to multi-unit calculations.

Geometric Buckling

Geometric buckling (B^2) is a measure of the curvature of neutron flux. The larger the value, the greater the curvature. According to the diffusion-theory approximation, any critical configuration of a given material should have the same buckling. The BUCKLING CONVERSION METHOD was developed to provide a simple method for comparing characteristics of basic shapes. Bucklings for the basic geometries are shown in Table 3-7.

Table 3-7. Geometric Buckling Configuration

Configuration	Buckling
SPHERE	$(\pi / R)^2$ Sphere Radius = R
CYLINDER	$(2.405 / R)^2 + (\pi / H)^2$ Cylinder Radius = R Cylinder Height = H
"CUBOID" (RECTANGULAR PARALLELEPIPED)	$(\pi / A)^2 + (\pi / B)^2 + (\pi / C)^2$ Cuboid Dimensions: A, B, and C

Buckling Conversion

The method of buckling conversion, or shape conversion, equates buckling values to establish equivalent dimensions for various geometries. The buckling conversion method is used with single units.

The buckling conversion method is based on the premise that, according to diffusion theory, the buckling B^2, combined with the diffusion coefficient D, is a measure of leakage through the term DB^2. Because a reference material has a fixed D-value, geometric configurations with the same critical buckling B^2 have equivalent leakage.

Recalling that diffusion theory over predicts critical dimensions, the extrapolation distance δ is used to adjust dimensions according to:

$$R = R_{dt} - \delta$$

or

$$R_{dt} = R + \delta$$

for bare systems.

The reflected extrapolation distance δ_r is used according to:

$$R = R_{dt} - \delta_r$$

or

$$R_{dt} = R + \delta_r$$

for water-reflected systems.

With these modifications, the bucklings are adjusted such that insertion of actual dimensions provides accurate results. See Table 3-8.

NOTE:

As a "rule of thumb," $\delta \approx 2$ cm and $\delta_r \approx 6$ cm.

Using these values, knowledge of the critical dimensions of one system can be used to calculate values for another configuration.

Table 3-8. Adjusted Geometric Buckling Configuration

Configuration	Buckling
SPHERE	$(\pi / R + \delta_s)^2$ Sphere Radius = R
CYLINDER	$(2.405 / R + \delta_c)^2 + (\pi / H + 2\,\delta_c)^2$ Cylinder Radius = R Cylinder Height = H
CUBOID	$(\pi / A + 2\delta)^2 + (\pi / B + 2\delta)^2 + (\pi / C + 2\delta)^2$ Cuboid Dimensions: A, B, and C

Example

Calculate the critical radius of a sphere where a critical cylinder 20-cm diameter by 30-cm high is critical. Assume the sphere and cylinder are reflected and use δ = 6.0 cm. See Figure 3-7.

Figure 3-7. Calculations for Critical Radius

sphere cylinder

$$\left(\frac{\pi}{r_s + \delta}\right)^2 = \left(\frac{2.405}{r_c + \delta}\right)^2 + \left(\frac{\pi}{h + 2\delta}\right)^2$$

$$r_c = \frac{20\ \text{cm}}{2} = 10\ \text{cm}$$

$$\left(\frac{\pi}{r_s + 6\ \text{cm}}\right)^2 = \left(\frac{2.405}{\frac{20\ \text{cm}}{2} + 6\ \text{cm}}\right)^2 + \left(\frac{\pi}{30\ \text{cm} + 12\ \text{cm}}\right)^2$$

$$\left(\frac{\pi}{r_s + 6\ \text{cm}}\right)^2 = 2.82 \times 10^{-2}\ \text{cm}^{-2}$$

$$r_s + 6\ \text{cm} = \pi\sqrt{\frac{1}{2.82 \times 10^{-2}\ \text{cm}^{-2}}} = 18.7\ \text{cm}$$

r_s = 12.7 cm

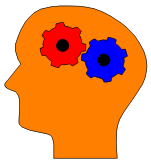
d_s = 25.4 cm

Key Points

The buckling conversion method is very simple to apply to the sphere and infinite cylinder and slab geometries, as each is characterized by a single dimension.

Application to finite cylinders and cuboids is more complex because the presence of the extrapolation distances prevents simple algebraic inversion of the equations; iterative methods are often required in these cases.

Activity 3 - Buckling Conversion*



*This is an optional activity and is not required for module completion.

Purpose: The purpose of this activity is to provide practice in performing buckling conversion hand calculations.

Directions: Read the following statement and perform the requested calculations. Space is provided for your computations. Answers are located in the answer key section of the Trainee Guide.

Reflected infinite cylinders of homogeneous 3 wt% and 5 wt% hydrogen-moderated uranium have minimum critical infinite-cylinder diameters of 34 cm and 29 cm, respectively.
Use δ_r = 6 cm.

1. Calculate the equivalent critical-sphere radius for each.

2. Calculate the volume of each sphere and compare the volumes for the two enrichments.

3. Repeat the two calculations for heterogeneous material at the same enrichments where the respective diameters are 25 cm and 22 cm. Also compare the respective volumes among the homogeneous and heterogeneous compositions.

Six-Factor Formula

The following is a modification of diffusion theory. By accounting for neutron leakage, the four-factor formula can be modified into the SIX-FACTOR FORMULA, in which the effective multiplication factor k_{eff} is:

$$k = k_{\infty} P_{fnl} P_{tnl}$$
$$k = \varepsilon p \eta f P_{fnl} P_{tnl}$$

where

P_{fnl} = Fast Non-Leakage Probability
P_{tnl} = Thermal Non-Leakage Probability

These latter two terms may be approximated by the AGE-DIFFUSION CORRELATION consisting of the two terms:

$$P_{fnl} = \exp(-B^2 \tau)$$

where

τ = (Fermi) Age

$\tau \sim \langle r^2_{sd} \rangle$ (with r a measure of average distance traveled by neutrons as they slow from fission energy)

and

$$P_{tnl} = \frac{1}{1 + L^2 B^2}$$

where

L = Thermal Diffusion Length
$L = (D_t / \Sigma_{at})^{1/2}$ (with the neutron parameters relating to thermal neutrons and the term again related to average distance of neutron travel, this time after becoming a thermal neutron)

Although the fast non-leakage probability is derived based on assumptions of a large system with continuous moderation (not a characteristic of water-moderated systems) and the thermal non-leakage probability formulation suffers from the limitations of diffusion theory in general, the expressions have been found to be a useful basis for empirical formulations.

One expression developed by combining the two terms into the MIGRATION AREA APPROXIMATION is shown in Figure 3-8.

Figure 3-8. Migration Area Approximation Formula

$$k = \frac{k_\infty \exp(-B^2 \tau)}{1 + L^2 B^2}$$

$$k = \frac{k_\infty}{1 + M^2 B^2}$$

where

$$M^2 = \tau + L^2 = \text{Migration Area}$$

Empirical tabulations of k_∞ and M^2 values that work for the equation have been prepared for a variety of materials. This allows k_{eff} to be estimated for any of the regular geometries (via the buckling B^2).

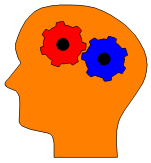
Age-Diffusion/ Migration-Area Approximation

The age-diffusion/migration-area approximation is the basis for another hand-calculation method. Using tabulated values (for example, from the ARH-600 report) for k_∞ and M^2, k_{eff} can be calculated from the age-diffusion equation. See Figure 3-9.

Figure 3-9. Age-Diffusion Formula

$$k \approx \frac{k_\infty}{1 + M^2 B^2}$$

Activity 4 - Migration-Area Approximation*



*This is an optional activity and is not required for module completion.

Purpose: The purpose of this activity is to provide practice in performing migration-area approximation hand calculations.

Directions: Read the following statements and perform the requested calculations. Answers are located in the answer key section of the Trainee Guide.

1. 4 wt%-enriched UO_2 moderated uniformly with 75 vol% water has $k_\infty = 1.395$ and $M^2 = 28.5\ cm^2$.

   For $\delta_c = 2.1$ cm, calculate k_{eff} for a can 30 inches high by 10 inches diameter.

2. Repeat the above calculation for a can 40 inches high.

3. Calculate the maximum k_{eff} for a 10-inch diameter cylinder of the reference material.

4. Assuming the reference material is optimally moderated, estimate the diameter for a favorable geometry cylinder (reflected k_{eff} = 0.90, δ = 6.0 cm).

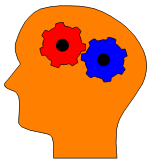
Fraction Critical Method

Another single-unit hand calculation is the fraction critical. It is sometimes applied directly (for example, setting a limit at 80% of a critical mass). It is also used in array calculations such as the surface density method described next.

One formulation for a specified material is:

$$f = \text{Fraction Critical} = \frac{\text{Mass of Uranium in Unit}}{\text{Mass of Uranium in Critical Sphere}}$$

Activity 5 - Fraction Critical*



*This is an optional activity and is not required for module completion.

Purpose: The purpose of this activity is to provide practice in performing fraction critical hand calculations.

Directions: Calculate the fraction critical. Space is provided for your computations. Answers are located in the answer key section of the Trainee Guide.

Hint:

Mass of Uranium in Unit = (Unit Volume) x (density) x (UO_2 fraction) x (U fraction in UO_2)

Mass of Uranium in Critical Sphere = (Sphere Volume) x (density) x (UO_x fraction) x (U fraction in UO_2)

$$f = \frac{\text{Mass of Uranium in Unit}}{\text{Mass of Uranium in Critical Sphere}} = \frac{\text{Unit Volume}}{\text{Critical Sphere Volume}}$$

1. The material in the 30-inch high x 10-inch diameter storage unit in the previous activity has a density of 10.96 g UO /cm^3, volume fraction of uranium dioxide of 0.25, and uranium fraction (in UO_2) of 0.88. The radius of a critical sphere of the material is 25.4 cm.

2. Repeat the calculation for a 40 inch-high storage unit.

3. Calculate the height of container with f = 0.73 (the maximum allowed by the surface density model discussed next).

Calculations Used with Arrays

The two hand calculation methods considered here for arrays are both based on correlations with experimental data and/or calculations. They predict subcritical configurations, not specific values of k_{eff}.

Uses and limitations are noted through the activities.

Surface Density Method

The surface density method judges subcriticality of a facility loading (in mass per unit area) of fissile material by comparison to that of a critical reflected infinite slab of the same material. (The following development is based on TID 7016 Rev. 2.)

Using the definition of fraction critical f provided previously:

$$\sigma = 0.54\ \sigma_0\ (1 - 1.37\ f)$$

where

σ = "Allowed" Surface Density
σ_0 = Surface Density of Critical Water-Reflected Infinite Slab
f = Fraction Critical of Unit

with the restriction that $f \leq 0.73$.

For an array of stacked units with uniform center-to-center spacing, see Figure 3-10.

$$\sigma = \frac{n\ m}{d^2}$$

where

n = Number of Units in Stack
m = Mass of Fissionable Material in Units
d = Center-to-Center Spacing (Cell Length)
[$d^2 \Rightarrow$ Area for Non-Cubic Cell]

with a minimum surface-to-surface spacing of 0.3 m.

Combining these expressions:

$$d = 1.37\ [\ n\ m\ /\sigma_0\ \ (1 - 1.37\ f)]^{1/2}$$

Although developed here for a regular array of identical units, the method is far more flexible. In practice, any units or pieces of equipment can be interchanged freely so long as each meets the surface density criteria regardless of arrangement (that is, the fraction critical limit is not exceeded and the associated area allows the surface density limit to be met). See Figure 3-11 which is an example of a calculation using the surface density method.

Figure 3-10. Surface Density Method

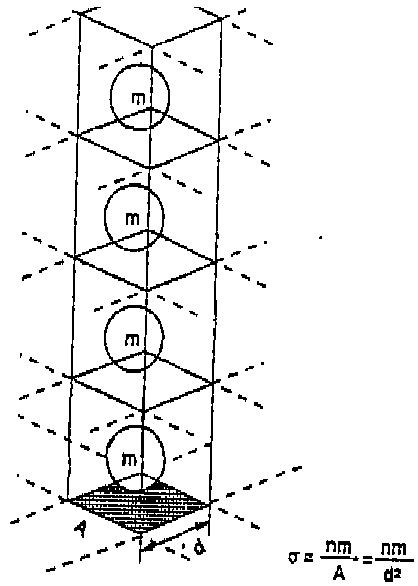


Figure 3-11. Example of Calculation Using the Surface Density Method

$$d = 1.37 \sqrt{\frac{n\ m}{\sigma_0\ (1 - 1.37f)}}$$

$$d = 1.37 \sqrt{\frac{(2)\ (10000)}{(50)\ (1 - [1.37][0.5])}}$$

d = 48.8 (cm) = 19.2 in

n = 2

m = 10 kg = 10000 g

$$\sigma_0 = 50\ \frac{g}{cm^2}$$

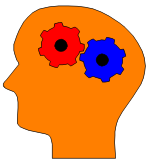
f = 0.5

Key Points

Key points for the surface density method:

- By use of the surface density method, consistent changes can be made readily (such as going from a one-high to a five-high array by modifying the floor spacing and ensuring appropriate vertical separation).
- Because the comparison is to an infinite slab, each array layer may be of unlimited extent. This is convenient, but may be excessively conservative to apply to a relatively small number of units.
- The concept of surface density is useful for picturing related physical phenomena and may still be found in safety analysis reports, even when computer calculations are the actual basis for judging subcritical configurations.

Activity 6 - Surface Density*



*This is an optional activity and is not required for module completion.

Purpose: The purpose of this activity is to provide practice in performing surface density hand calculations.

Directions: Read the following statement and perform the requested calculation. Space is provided for your computations. Answers are located in the answer key section of the Trainee Guide.

The material, whose fraction critical f was calculated in the previous activity for a 10-inch diameter x 30-inch high can, has a critical surface density of 33.0 U g/cm^2.

HINT: $d = 1.37\ [n\ m\ \delta_0\ (1 - 1.37f)]^{1/2}$

1. Determine the minimum center-to-center spacing allowed by the surface-density method for an array of one unit high.

2. Determine how the spacing would need to be modified to have the array 2 through 5 units high instead.

Solid Angle Method

The solid angle method can be used to judge subcriticality of arrays for which the k_{eff} of a single unit is known.

Interaction probability is correlated to the solid angle subtended from a central unit to all surrounding units. See Figure 3-12.

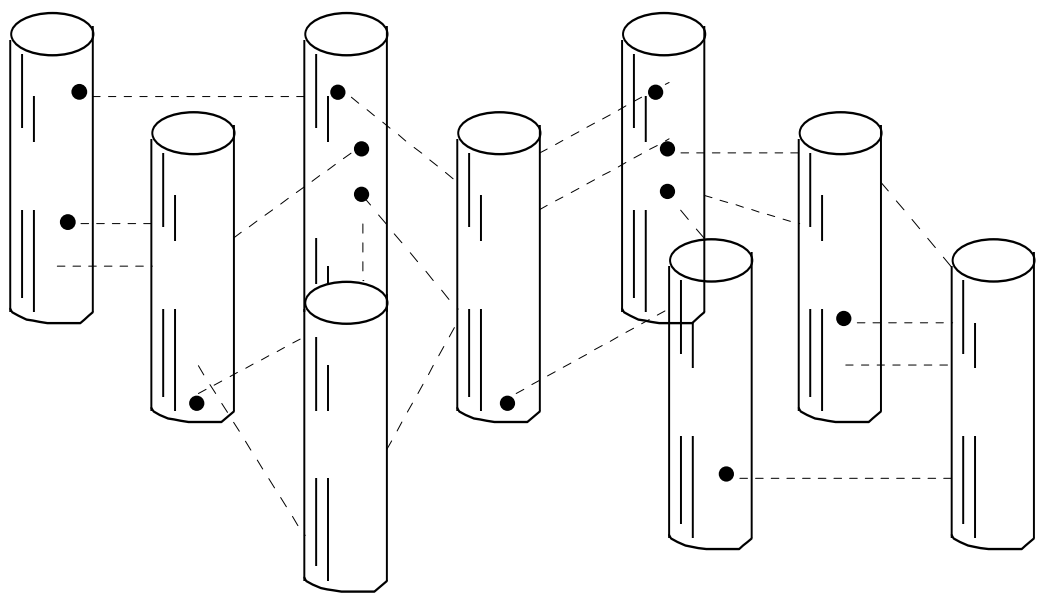
According to the formulation from TID 7016 Rev. 2.

$$\Omega_{allowed} = 9 - 10\ k_{eff}$$

where

- $k_{eff} < 0.80$
- The individual unit is subcritical when fully reflected by water.
- Center-to-center spacing is > 0.3 m.
- $\Omega_{allowed} < 6$ steradians (sr)

Figure 3-12. Solid Angle Method



Precise solid angles are complex to calculate (for example, using multiple-parameter integration). See Figure 3-13. Thus, it is common to use approximations.

One example is the "point-to-cylinder" approximation, where the solid angle is calculated from the center of a unit to a plane with the height and diameter of the cylinder tangent to it at the point closest to the central unit. See Figure 3-14.

Figure 3-13. Solid Angle Method Formula

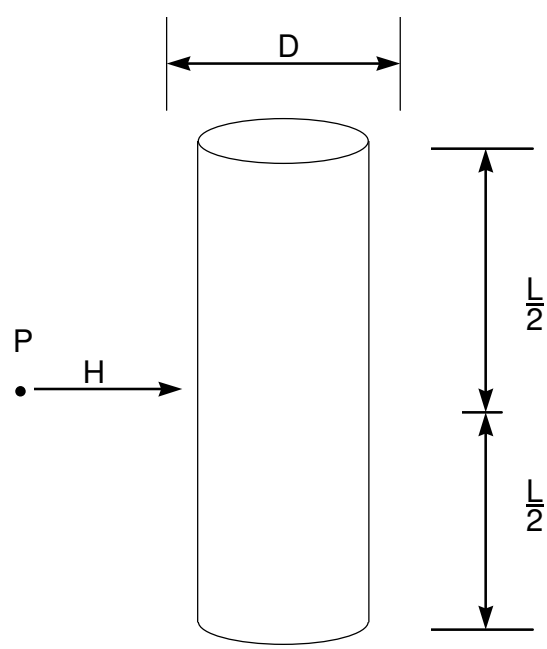
$$\Omega = \frac{LD}{H[(L/2)^2 + H^2]^{1/2}}$$

Figure 3-14. Point-to-Cylinder

$$\Omega = \frac{LD}{H\sqrt{(L/2)^2 + H^2}}$$

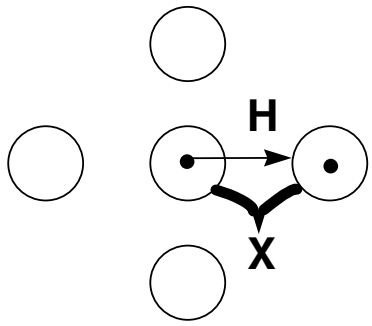
where

L = Length of the cylinder
D = Diameter of the cylinder
H = Distance from the point to the surface of the cylinder



Example This example illustrates the use of solid angle calculations.

$k_{eff} = 0.777$
$\Omega_{allowed} = 9 - 10\,(0.777) = 1.23$



L = 30 in.
D = 10 in.
H = X − D/2

$$\Omega_{allowed} = 4\,\frac{(30)\ (10)}{(x-5)\sqrt{(15)^2 + (x-5)^2}} = 4\,\frac{300}{(x-5)\sqrt{225 + (x-5)^2}} = 1.23$$

$$\frac{\Omega_{allowed}}{4} = \frac{300}{(x-5)\sqrt{225 + (x\ 5\ )^2}} = 0.3075$$

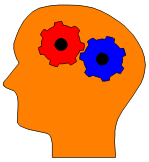
Iterative Process

x = 45	0.1756	
x = 40	0.2251	Interpolate
x = 35	0.2981	
x = 30	0.4116	34.5 inches
x = 34	0.3168	
x = 34.5	0.3073	

Key Points Key points for solid angle calculations:

- The solid angle method does not require identical units or regular spacing. Thus, it has been used for a variety of configurations with storage units and plant equipment and may still be referenced in safety analysis reports.
- The concept of neutron interaction relating to the solid angle is intuitive. Thus, the method (as noted earlier for surface density) can be a useful tool in thinking about and understanding computer calculations.
- The method is complex algebraically. Thus a small computer program is often applied.

Activity 7 - Solid Angle*



*This is an optional activity and is not required for module completion.

Purpose: The purpose of this activity is to provide practice in performing solid angle hand calculations in determining maximum k_{eff}.

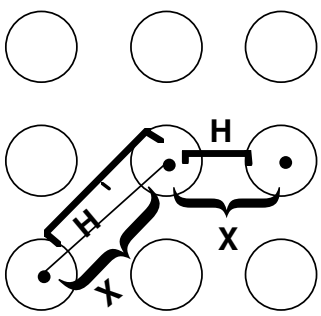
Directions: Read the following statements and perform the requested calculations. Space is provided for your computations. Answers are located in the answer key section of the Trainee Guide.

Consider a regular three-by-three array of the 10-inch diameter by 30-inch high units (described in the earlier activity using the migration-area method). Center-to-center spacing from the central unit to each of its four nearest neighbors is X = 42 inches.

Use the point-to-cylinder approximation given above to calculate solid angles.

HINT:

$$\Omega = \frac{L\ D}{H\left[\left(\frac{L}{2}\right)^2 + H^2\right]^{1/2}}$$



L = 30 in

D = 10 in

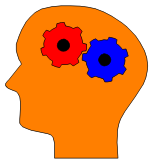
$H = X - \frac{D}{2} = X - 5$

$H^1 = X^1 - \frac{D}{2} = X^1 - 5$

1. Demonstrate that the array satisfies the solid angle criteria.

2. Determine the maximum allowed k_{eff} that the unit could have for the given spacing.

Activity 8 - Solid Angle*



*This is an optional activity and is not required for module completion.

Purpose: The purpose of this activity is to provide practice in performing solid angle hand calculations in determining allowed spacing between units.

Directions: Read the following statements and perform the requested calculations. Space is provided for your computations. Answers are located in the answer key section of the Trainee Guide.

1. Determine allowed spacing for a 10-inch diameter x 40-inch high cylindrical can.

2. What would be required to calculate a multilevel array?

Self-Check Questions 3-3

Fill in the missing words in each statement. Answers are located in the answer key section of the Trainee Guide. Choose from the following words:

buckling	identical units	shapes
conservative	infinite	slab
diffusion-theory approximation	intuitive	solid angle
extrapolation distances	leakage	subcritical
floor spacing	low	surface density
fraction critical	neutron leakage	units
high	point-to-cylinder	vertical

1. In diffusion theory, assumptions are that diffusion occurs from regions of _____ neutron density to those of _____ neutron density, that there is minimal absorption of neutrons, and that there is minimal discontinuity in neutron-reaction properties at interfaces among materials.

2. Hand calculation methods for single _____ include the buckling conversion method, age-diffusion/migration area approximation, and the fraction critical method.

3. Geometric _____ is a measure of the curvature of neutron flux.

4. According to the _____, any critical configuration of a given material should have the same buckling.

5. The buckling conversion method was developed to provide a simple method for comparing characteristics of basic _____.

6. Because a reference material has a fixed diffusion coefficient D-value, geometric configurations with the same critical buckling have equivalent _____.

7. The buckling conversion method is very simple to apply to the sphere and _____ cylinder and _____ geometries, as each is characterized by a single dimension.

8. Application to finite cylinders and cuboids is more complex because the presence of the _____ prevents simple algebraic inversion of the equations; iterative methods are often required in these cases.

9. By accounting for _____, the four-factor formula can be modified into the six-factor formula.

10. The _____ method is sometimes applied directly (for example, setting a limit at 80% of a critical mass). It is also used in array calculations, such as the surface density method.

11. The _____ method judges subcriticality of a facility loading

(in mass per unit area) of fissile material by comparison to that of a critical reflected infinite slab of the same material.

12. Use of the surface density formulation, allows consistent changes to be made readily, such as going from a one-high to a five-high array by modifying the _____ and ensuring appropriate _____ separation.

13. Because the comparison is to an infinite slab, each array layer may be of unlimited extent. This is convenient, but may be excessively _____ to apply to a relatively small number of units.

14. The concept of surface density is useful for picturing related physical phenomena and may still be found in safety analysis reports, even when computer calculations are the actual basis for judging _____ configurations.

15. The _____ method can be used to judge subcriticality of arrays for which the k_{eff} of a single unit is known.

16. One example of a solid angle calculation is the _____ approximation where the solid angle is calculated from the center of a unit to a plane with the height and diameter of the cylinder tangent to it at the point closest to the central unit.

17. The solid angle method does not require _____ or regular spacing.

18. The concept of neutron interaction relating to the solid angle is _____ .

You have completed this section.
Please check off your progress on the tracking form.
Go to the next section.

Learning Objective

When you finish this section you will be able to:

3.1.5.a Discuss the importance of validation to determining criticality safety limits.

3.1.5.b Define the two major computational methods used in criticality safety codes.

3.1.5.c Define the assumption used in Finite Difference Methods to eliminate time dependencies and the implication this assumption has on bias of these methods.

3.1.5.d Define the technique used by Monte Carlo techniques to solve the time-dependent neutron transport equation.

3.1.5.e Describe the geometry approach used in KENO and MONK and the geometry approach used in MCNP.

3.1.5.f Describe the difference between treatment of resonances in KENO versus the treatment used in MCNP and MONK.

COMPUTER CODES

Introduction

In the 21st Century, computing machines and numerical models (programs or codes) have all but replaced critical experiments or hand calculations in the determination of criticality safety limits. A few examples of these programs include XSDRNPM, DORT, TORT, KENO, MCNP, and MONK. The method selected must be versatile to encompass a wide variety of configurations/compositions and be able to reproduce all neutron processes that occur in the real systems.

Validation, Bias, and Bias Uncertainty

Per 10 CFR 70.61, computer codes used for determining nuclear criticality safety requirements must be validated against experiments of similar configurations and materials to determine a bias and bias uncertainty.

From NUREG/CR-6698:
"For use in safety related analyses, the ability of a calculational methodology to accurately predict the subcriticality of a system must be well understood. The understanding of a calculational methodology's bias in predicting subcritical systems is obtained through the validation process. Validation includes identification of the difference between calculated and experimental results. This difference, called the bias, and uncertainty associated with the bias

are used in combination with additional subcritical margin to establish an upper safety limit (USL). Subcriticality is assured if calculated results are below the USL and within the area of applicability for the validation."

As described in ANSI/ANS 8.1, a validation report will:

1) Describe the method used to validate the code in a manner which will allow independent duplication of results.
2) Describe the computer platform (hardware, software, and other support equipment).
3) Describe the code, including any options, as well as the cross section sets and any other numerical parameters.
4) Identify the experimental data.
5) List the areas of applicability. For example, metal system versus compounds; dry system versus moderated.
6) State the bias and the prescribed margin of safety over the areas of applicability.

Computational Tools

The majority of the computational tools used to calculate critical conditions can be distinguished as either Finite Difference methods or Monte Carlo methods.

Finite Difference Methods

XSDRNPM, DORT, and TORT use numerical methods that approximate the neutron transport equations by using finite difference equations. This approach produces a set of differential/algebraic equations relating the neutron flux at a point to the neutron fluxes at the surrounding points. These differential/algebraic equations include both space and energy dependences. It is important to note that these methods use the assumption that k_{eff} = 1.00 and eliminate time dependency by modifying the transport equation with a pseudo-absorption macroscopic cross section that is a function of k_{eff}. These programs assume (or allow the user to input) an initial flux distribution. The differential/algebraic equations are solved using the initial neutron flux and k_{eff} to determine a new flux and k_{eff} . The results are used to define the source distribution in a second iteration. The flux distributions are compared and the iteration repeated until convergence. However, the final k_{eff} may not equal one, and the bias and the uncertainty in the bias depend on the closeness of k_{eff} to 1.00. These programs run quickly on computers, but the approximations and flux convergence techniques used lead to unavoidable limitations.

Monte Carlo Methods

KENO, MCNP, and MONK use Monte Carlo techniques to solve the time-dependent neutron transport equation by tracking the time-dependent neutron life cycles as they interact with materials

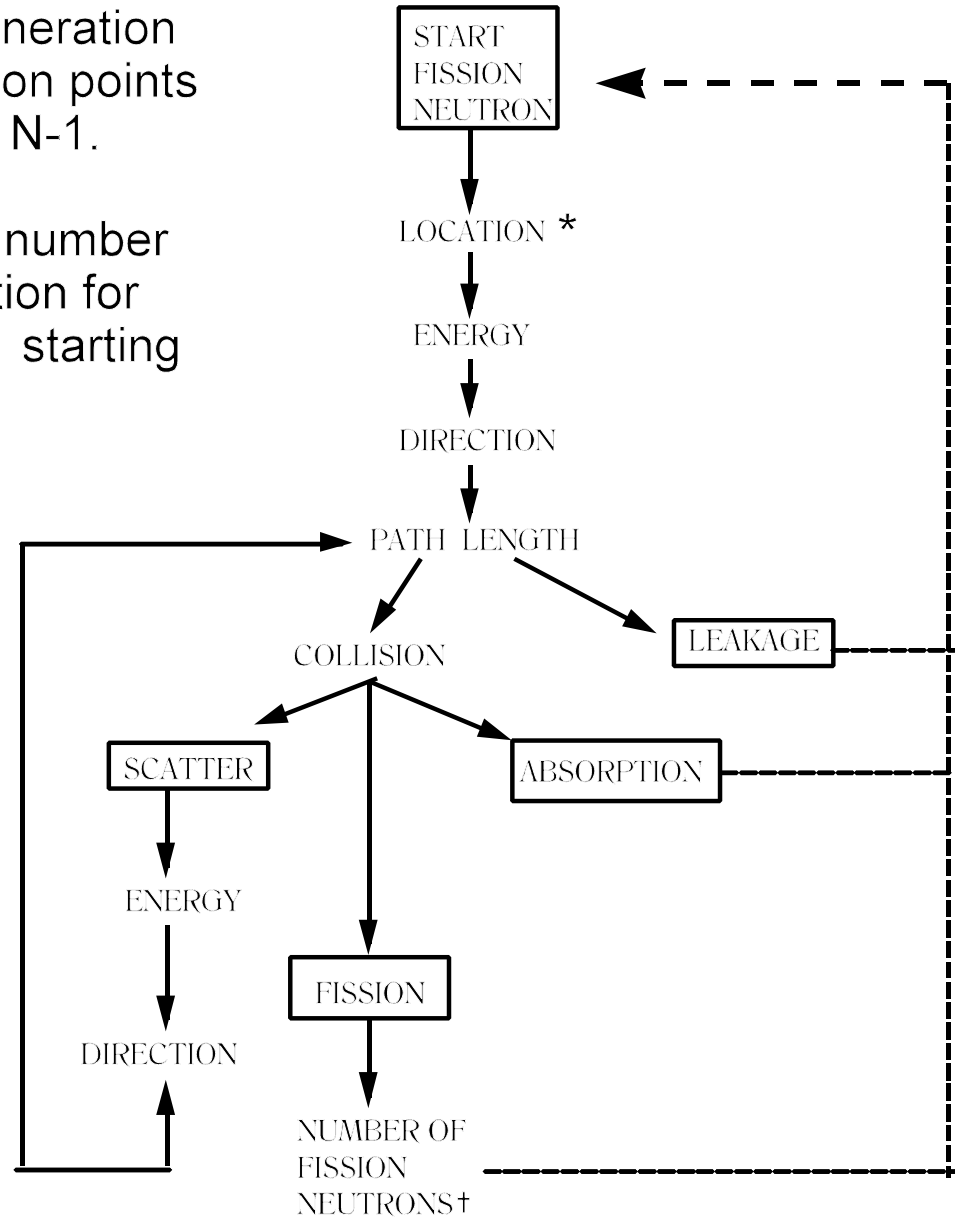
according to the physical probabilities inherent in the formulation of the neutron cross sections. Figure 3-15 is a representation of the process as it is applied in KENO. Geometric configurations and materials are specified, parameters and reaction rates are recorded, and statistical results for multiplication factor, flux, or other characteristics are developed. Statistical biasing or weighting techniques can increase the efficiency of these calculations.

In the context of nuclear criticality safety, the Monte Carlo KENO procedure is applied by developing a model that is capable of "tracking" individual (fictitious) neutrons through a material medium containing fissile and other species for each life cycle. The accuracy of the result is inversely proportional to the square root of the number of life cycles. Thus, running more tracks or groups of tracks will always improve the accuracy of your results. The life cycles are run in groups. Each group typically uses a fission source distribution based on the previous group's neutron interaction distribution. Each group is started with the same number of life cycles. Thus several measures, like the number of fission absorptions, can be used to determine a k_{eff} for each group. Typically, the initial group-to-group k_{eff} changes are large, and the cumulative k_{eff} ignore these "start-up" values. Additional groups are run until the cumulative k_{eff} has converged. The output reports a value for k_{eff} and a standard deviation (σ) value, which is a measure of confidence in the answer. The range $k_{eff} \pm \sigma$ is ascribed a 67% certainty of containing the "real" answer, while $k_{eff} \pm 2\sigma$ is ascribed a 95% certainty. These programs take more computer time to complete; however, these programs can handle complicated three-dimensional (3-D) geometries.

Figure 3-15. Monte Carlo Model KENO

* Locations for generation N based on fission points from generation N-1.

† Record neutron number and fission location for generation n + 1 starting locations.



KENO

KENO V.a is a multi-group Monte Carlo criticality program used to calculate the k_{eff} of a 3-D system. Special features include simplified data input and the ability to specify origins for spherical and cylindrical geometry regions. A large portion of the data has been assigned default values that have been found to be adequate for many problems. This feature enables the user to run a problem with a minimum of input data.

KENO V.a geometry is restricted to the use of specific shapes. These shapes are called geometry regions. Allowed shapes are cubes, cuboids (rectangular parallelepipeds), spheres, cylinders, hemispheres, and hemi-cylinders. In KENO V.a, the sense of any location with respect to a shape is defined as positive everywhere inside the shape and negative everywhere outside. These shapes must be oriented along orthogonal axes and cannot be rotated. They can be translated. Hemispheres and hemi-cylinders are not limited to half-spheres and half-cylinders; the definitive plane can be positioned by entering a chord. The value of this chord can range from the positive magnitude of the radius (giving a complete sphere or cylinder) to the negative magnitude of the radius (giving a zero volume, nonexistent sphere, or cylinder).

A major restriction applied to KENO V.a geometry is that intersections are not allowed. Furthermore, each successive geometry region must completely enclose the preceding region. To alleviate the complete enclosure restriction, KENO V.a allows multiple sets of geometry regions with each set independently governed by this restriction. Each set of these multiple geometry regions are called units. Units can be stacked together in a 3-D rectangular parallelepiped called an array or lattice just as children's blocks can be stacked. Units that are to be stacked together in this manner must have a rectangular parallelepiped outer region and the adjacent faces of adjacent units must be the same size and shape. An array can be treated as a building block and be used as a unit within another array.

The use of holes in KENO V.a allows a unit to be placed within another unit, thereby alleviating the restriction that each region within a unit must completely enclose all preceding regions within that unit. However, a hole is not allowed to intersect other holes or regions. A unit that is to be used as a hole need not have a rectangular parallelepiped as its outer boundary.

KENO V.a provides four types of boundary conditions that are accepted for performing criticality safety analyses. The default boundary condition is a vacuum where when neutrons leave they are gone forever. Three options are available for replacing the vacuum condition. The options are mirror reflection where neutrons leaving are returned as a mirror image, periodic where neutrons leaving are returned to the opposite face, and white where an isotropic return is imposed at the boundary. A fifth type of boundary condition, albedo, has not been thoroughly tested for use in criticality safety evaluations.

KENO V.a is part of the Criticality Safety Analysis Sequence (CSAS) process procedure provided with SCALE. The CSAS process cross sections are generated using the Bondarenko method (via BONAMI) and either the Nordheim integral method (via NITAWL-III) or collapsing of pointwise continuous cross sections using a problem-dependent pointwise continuous flux (via WORKER, CENTRM and PMC) to provide a resonance-corrected cross-section library based on the physical characteristics of the problem being analyzed. This cross-section library can be utilized by KENO V.a (a 3-D multi-group Monte Carlo criticality program) or XSDRNPM (a one-dimensional (1-D) discrete-ordinates code for transport analysis). The CSAS4 process procedure provides search capabilities utilizing KENO V.a. When CSAS4 is specified a parameter search is performed on k_{eff} as a function of dimensions or densities. The two basic search options offered are (1) an optimum search seeking a maximum or minimum value of k_{eff} and (2) a critical search seeking a fixed value of k_{eff} .

MCNP

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. Specific areas of application include, but are not limited to, radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, nuclear oil well logging, accelerator target design, fission and fusion reactor design, decontamination and decommissioning. The code treats an arbitrary 3-D configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori.

The geometry of MCNP treats an arbitrary 3-D configuration of user defined materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori. The orientation with respect to surfaces defining a cell is defined mathematically as any location for which the surface equation is negative is considered to be inside and any location for which the surface equation is positive is outside (i.e., a negative sign preceding a surface number means that the cell defined by that surface is a region of space having a negative sense with respect to that surface). For example, space that is outside a 3-D body (e.g., a sphere) or above or to the right of a plane has a positive sense, and vice versa. The cells are defined by the intersections, unions, and complements of the regions bounded by the surfaces. Surfaces are defined by supplying coefficients to the analytic surface equations or, for certain types of surfaces, known points on the surfaces.

Cells can be repeated using “LIKE m BUT” capabilities to repeat cell m (i.e., “like m”), but moved to a different location and/or different orientation. Lattice arrays of cells can be formed from hexahedra (solids with six faces) and hexagonal prisms (solids with eight faces)

using the “LAT” (for lattice array) capabilities. These lattice arrays extend infinitely in all directions, but can be truncated after being designated as a universe and used to fill a cell of finite dimensions.

Repeated-structure capabilities make it possible to describe, only once, the cells and surfaces of a structure that appears more than once in the geometry. One example of such a structure is a reactor core that has dozens of nearly identical fuel modules. The repeated-structure capability extends the concept of an MCNP cell. The user can specify that a cell is to be filled with something called a universe. A universe is either a lattice or an arbitrary collection of cells. A single universe, described only once, can be designated to fill each of any number of cells in the geometry. Some or all of the cells in a universe may themselves be filled with universes.

MCNP provides four types of boundary conditions that are accepted for performing criticality safety analyses. The default boundary condition is a vacuum where neutrons leaving enter a region of zero neutron importance. Three options are available for replacing the vacuum condition. The options are mirror reflection where neutrons leaving are returned as a mirror image, periodic where neutrons leaving are returned to the opposite face, and white where an isotropic return is imposed at the boundary. However, using reflective planes make it difficult (or even impossible) to get the correct answer. The user is cautioned to check the source weight and tallies to ensure that the desired result is achieved.

Point-wise cross-section data typically are used, although group-wise data also are available. For neutrons, all reactions given in a particular cross-section evaluation (such as ENDF/B-VI) are available. Resonance data is used directly to determine resonance escape probabilities that are sampled during slowing-down through the resonance energy.

MONK

The origins of MONK can be traced to a code called GEM, which came out of the post-war nuclear weapons program in the United Kingdom (UK). A more recent major program of develop was stimulated by the criticality needs of the UK reprocessing industry and resulted in the production of MONK6 in the late 1980s.

A MONK system model is assembled from simpler sub-systems using the MONK geometry package. The basic component of this package is a set of simple bodies, including the sphere, box, rod, prism, cone and torus. In MONK, the sense of any location with respect to a body is defined as positive everywhere inside the body and negative everywhere outside. These bodies can have general orientation and overlap each other if necessary. They are used as basic building blocks to form simple parts of the geometry, each part being defined quite independently of the rest of the system using local coordinates. These simple parts are then used to make more coupled parts in the

same way and so on, until the system is assembled. Hole geometries (making use of a technique called Woodcock tracking) are used extensively in MONK to provide a lot of complicated fine geometric details and to short-cut the specification of some of the commonly occurring array items.

MONK provides four types of boundary conditions that are accepted for performing criticality safety analyses. The default boundary condition is a free ("black") boundary where neutrons leaving enter a region of zero neutron importance. Three options are available for replacing the free boundary condition. The options are specular reflection where neutrons leaving are returned as a mirror image, periodic where neutrons leaving are returned to the opposite face, and a forward peaked (cos2) distribution of returning particles about the surface normal.

For criticality calculations, neutron interactions are considered in the MONK collision processing package called DICE. The standard MONK nuclear data library is a hyper-fine 8,220-group library based on UKNDL and JEF evaluations. Resonance data is used directly to determine resonance escape probabilities that are sampled during slowing down through the resonance energy. This library, together with the point-energy collision processing algorithms, provides a very detailed modeling of the physics. For comparisons to SCALE, MONK can also accept multi-group data from the SCALE libraries.

Self-Check Questions 3-4

Complete the following questions. Answers are located in the answer key section of the Trainee Guide.

1. What is importance of the validation process to determining criticality safety limits?

2. What are two major computational methods used in criticality safety codes?

3. What assumption is used in Finite Difference Methods to eliminate time dependencies and how does this assumption affect the bias of these methods?

4. How do Monte Carlo techniques solve the time-dependent neutron transport equation?

5. What geometry approach is used in KENO and MONK and what geometry approach is used in MCNP?

6. What is the difference between treatment of resonances in KENO versus the treatment used in MCNP and MONK?

Progress Review Meeting Form

It's time to schedule a progress meeting with your administrator. Review the progress meeting form on the next page. In Part III, As a Regulator, write your specific questions to discuss with the administrator.

Date Scheduled:_____**Location:**_____

I. The following suggested items should be discussed with the administrator as to how they pertain to your current position:

- Nuclear reactions
- Cross section
- Infinite systems
- Finite systems
- Computational methods:
  - Buckling conversion
  - Age-diffusion migration area approximation
  - Fraction critical
- Monte Carlo computer code KENO
- Validation report

II. Use the space below to take notes during your meeting.

III. As a Regulator:

- How are hand calculations used today?
- What other classes or short courses are available to me if I wish to learn more?
- Do we have the capability of performing computer calculations?
- How would I review an analysis provided to me and how in depth am I expected to go with it?
- Determining the reactivity of a system is one thing, but how is nuclear criticality safety implemented in the field?
- What specific computer code(s) should I be familiar with as a regulator?

Use the space below to write your specific questions.

IV. Further assignments? If yes, please note and complete. If no, initial completion of progress meeting on tracking form.

Ensure that you and your administrator have dated and initialed your progress on your tracking form for this module. Go to the module summary.

MODULE SUMMARY

The physics of criticality and nuclear criticality safety depends first on identification of nuclear reactions. Neutron reactions are the major contributors to fission chain reactions. The dominant fissionable material in NRC licensee fuel cycle facilities is uranium. Hydrogen, deuterium, beryllium, and carbon are moderating materials that, when mixed, can reduce substantially the required fissile material mass required to support a neutron chain reaction. To predict the effect of a change in material composition or configuration, numerous computational methods have been used at fuel cycle facilities. The method selected must be versatile enough to encompass a wide variety of compositions and be able to reproduce effects of all neutronic processes that occur in real systems.

Congratulations! You are ready to go to the next assigned module.