

*Criticality Calculations with MCNP™:
A Primer*

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by

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ABSTRACT

The purpose of this Primer is to assist the nuclear criticality safety analyst to perform computer calculations using the Monte Carlo code MCNP. Because of the closure of many experimental facilities, reliance on computer simulation is increasing. Often the analyst has little experience with specific codes available at his/her facility. This Primer helps the analyst understand and use the MCNP Monte Carlo code for nuclear criticality analyses. It assumes no knowledge of or particular experience with Monte Carlo codes in general or with MCNP in particular. The document begins with a Quickstart chapter that introduces the basic concepts of using MCNP. The following chapters expand on those ideas, presenting a range of problems from simple cylinders to 3-dimensional lattices for calculating keff confidence intervals. Input files and results for all problems are included. The Primer can be used alone, but its best use is in conjunction with the MCNP4A manual. After completing the Primer, a criticality analyst should be capable of performing and understanding a majority of the calculations that will arise in the field of nuclear criticality safety.

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INTRODUCTION

With the closure of many experimental facilities, the nuclear criticality safety analyst increasingly is required to rely on computer calculations to identify safe limits for the handling and storage of fissile materials. However, in many cases, the analyst has little experience with the specific codes available at his/her facility. This Primer will help you, the analyst, understand and use the MCNP Monte Carlo code for nuclear criticality safety analyses. It assumes that you have a college education in a technical field. There is no assumption of familiarity with Monte Carlo codes in general or with MCNP in particular. Appendix A gives an introduction to Monte Carlo techniques. The primer is designed to teach by example, with each example illustrating two or three features of MCNP that are useful in criticality analyses.

Beginning with a Quickstart chapter, the primer gives an overview of the basic requirements for MCNP input and allows you to run a simple criticality problem with MCNP. This chapter is not designed to explain either the input or the MCNP options in detail; but rather it introduces basic concepts that are further explained in following chapters. Each chapter begins with a list of basic objectives that identify the goal of the chapter, and a list of the individual MCNP features that are covered in detail in the unique chapter example problems. It is expected that on completion of the primer you will be comfortable using MCNP in criticality calculations and will be capable of handling 80 to 90 percent of the situations that normally arise in a facility. The primer provides a set of basic input files that you can selectively modify to fit the particular problem at hand.

Although much of the information to do an analysis is provided for you in the primer, there is no substitute for understanding your problem and the theory of neutron interactions. The MCNP code is capable only of analyzing the problem as it is specified; it will not necessarily identify inaccurate modeling of the geometry, nor will it know when the wrong material has been specified. Remember that a single calculation of k_{eff} and its associated confidence interval with MCNP or any other code is meaningless without an understanding of the context of the problem, the quality of the solution, and a reasonable idea of what the result should be.

The primer provides a starting point for the criticality analyst using MCNP. Complete descriptions are provided in the MCNP manual. Although the primer is self-contained, it is intended as a companion volume to the MCNP manual. The primer provides specific examples of using MCNP for criticality analyses while the manual provides information on the use of MCNP in all aspects of particle transport calculations. The primer also contains a number of appendices that give the user additional general information on Monte Carlo techniques, the default cross sections available with MCNP, surface descriptions, and other reference data. This information is provided in appendices so as not to obscure the basic information illustrated in each example.

To make the primer easy to use, there is a standard set of notation that you need to know. The text is set in Palatino type. Information that you type into an input file is set in Courier. Characters in the Courier font represent commands, keywords, or data that would be used as computer input. Because the primer often references the MCNP manual, these references will be set in braces, e.g. {see MCNP Manual Chapter xx}. Material presented in a grey box is provided for more in-depth discussions of general MCNP concepts.

It is hoped that you find the primer useful and easy to read. As with most manuals, you will get the most out of it if you start with Chapter One and proceed through the rest of the chapters in order. Each chapter assumes that you know and are comfortable with the concepts discussed in the previous chapters. Although it may be tempting to pick up the primer and immediately go to the example problem that is similar to your analysis requirement, this approach will not provide you with the background or the confidence in your analysis that is necessary for safe implementation of procedures and limits. There is no substitute for a thorough understanding of the techniques used in an MCNP analysis. A little extra time spent going through the primer and doing the examples will save many hours of confusion and embarrassment later. After studying the primer, you will find it a valuable tool to help make good, solid criticality analyses with MCNP.

Chapter 1

MCNP *Quickstart*

1.1 WHAT YOU WILL BE ABLE TO DO:

- Interpret an MCNP input file.
- Set up and run a simple criticality problem on MCNP.
- Interpret k_{eff} information from MCNP output.

1.2 MCNP INPUT FILE FORMAT

The MCNP input file describes the problem geometry, specifies the materials and the source, and defines the results you desire from the calculation. The geometry is constructed by defining cells that are bounded by one or more surfaces. Cells can be filled with a material or be void.

An MCNP input file has three major sections: cell cards, surface cards, and data cards. A one-line title card precedes the cell card section. Note: The word “card” is used throughout this document and in the MCNP manual to describe a single line of input of up to 80 characters. A section consists of one or more cards. Figure 1–1 shows the input file structure.

```
Title Card  
Cell Cards  
.....  
.....  
Blank Line Delimiter  
Surface Cards  
.....  
.....  
Blank Line Delimiter  
Data Cards  
.....  
.....  
Blank Line Terminator (optional)
```

Figure 1–1. MCNP input file structure.

1.2.A Title Card

The title card is the first card in an MCNP input file and can be 80 characters long. It often contains information about the problem being modeled. This title is echoed in various places throughout the MCNP output. It also serves as a label to distinguish among input files.

1.2.B General Card Format

The cards in each section can be in any order and alphabetic characters can be upper, lower, or mixed case. MCNP uses a blank line delimiter to denote separation between the three different sections. In this chapter only, we will use a ¶ to identify these blank lines.

The general format for the cell, surface, and data cards is the same. The cell or surface number or data card name must begin within the first five columns. Card entries must be separated by one or more blanks. Input lines cannot exceed 80 columns. The following are some special characters used for comments and card continuation.

<u>Character</u>	<u>Placement</u>	<u>Function</u>
C	Columns 1-5 Followed by at least one blank.	Denotes a comment line. Can be any line in an input file after the title card.
\$	After input data on a line	Anything that follows this character is a comment.
&	After input data	Data on the next line is a continuation and can be in columns 1-80.
blanks	Columns 1-5	Blanks in the first 5 columns indicate continuation of the previously named card.

1.2.C Cell Cards

The first section after the title card is for the cell cards and has no blank line delimiter at the front of it. Cells are used to define the shape and material content of physical space. The specific format for a cell card is:

j m d geom params

j = Cell number, starting in columns 1-5.

m = Material number (0 if cell is a void).

d = Cell material density:

No entry if the cell is a void.

Positive entry = atom density (atoms/b-cm).

Negative entry = mass density (g/cc).

geom = List of all signed surface numbers and Boolean operators that
specify a cell.

params = Optional specification of cell parameters.

The cell number, j, is an integer from 1 to 99999. The material number, m, is also an integer from 1 to 99999 that determines what material is present in the cell. The composition of a specific material is defined in the data card section. A positive entry for the cell material density, d, indicates an atomic density in *atoms per barn-centimeter*. A negative entry indicates a mass density in *grams per cubic centimeter*. The geometry specification, geom, consists of signed surface numbers combined with Boolean operators to describe how regions of space are bounded by those surfaces. Surfaces are the geometric shapes used to form the boundaries of the problem being modeled. The optional params feature allows cell parameters to be specified on the cell card line instead of in the data card section. For example, the importance card (imp:n) specifies the relative cell importance for neutrons, one entry for each cell of the problem. The imp:n card can go in the data card section or it can be placed on the cell card line at the end of the list of surfaces. The imp:n card will be discussed more thoroughly in the following chapters. [Chapter 3 of the MCNP manual provides a full explanation of the params option.]

Figure 1-2 is an example of a cell card. The optional comment card has a C in column 1, followed by a blank and the comment itself. The second line shows the cell number (4) followed by the material number (1) and the material density ($1.234\text{e-}3$). Because $1.234\text{e-}3$ is positive, the density of material 1 is in units of *atoms per barn-cm*. The -2 indicates that cell 4 is bounded only by surface 2. Surface 2 is defined in the surface card section. The negative sign preceding the surface number means that cell 4 is the region of space that has a negative sense with respect to surface 2.

```
C  Cell Card
4  1  1.234e-3  -2  imp:n=1
```

Figure 1-2. Cell card example.

1.2.D Surface Cards

The specific format for a surface card is:

```
j      a      list
```

j = Surface number, starting in columns 1-5. (1-99999)

a = Surface mnemonic. (plane, sphere, cylinder, etc.)

list = Numbers that describe the surface.
(dimensions, radius, etc., in cm)

Figure 1-3 is an example of a surface card. The number of this surface is 1. The mnemonic cz defines an infinite cylinder centered on the z-axis, with a radius of 20.0 cm. The \$ terminates data entry and everything that follows, *infinite z cylinder*, is interpreted as a comment, providing the user with more detail.

```
1      cz 20.0  $ infinite z cylinder
```

Figure 1-3. Surface card example.

1.2.E Data Cards

The format of the data card section is the same as the cell and surface card sections. The data card name must begin in columns 1-5. At least one blank must separate the data card name and the data entries. Specifying both a criticality calculation source and material cards is most important for criticality analysis. These are only three of many available MCNP data cards. {See chapter 3 of the MCNP manual.}

All criticality calculations must have a kcode card. The kcode card format is shown below.

kcode nsrck rkk ikz kct

kcode = Card name for criticality calculation.

Starts in columns 1-5.

nsrck = Number of neutrons per cycle.

rkk = Initial guess for k_{eff} .

ikz = Number of cycles skipped before accumulating data.

kct = Total number of cycles to be run.

Figure 1-4 is an example of a kcode card. The problem will be run with 1000 neutrons per cycle and an initial guess for k_{eff} of 1.0. Fifteen cycles will be skipped before k_{eff} data accumulation begins, and a total of 115 cycles will be run.

kcode 1000 1.0 15 115

Figure 1-4. Example of kcode card.

Criticality problems often use a ksrc card to specify the initial spatial fission distribution. Other methods to specify starting fission source locations will be discussed in a later chapter. The ksrc format is shown in Figure 1-5. A fission source point will be placed at the point with coordinates (x_k , y_k , z_k). As many source points as needed can be placed within the problem geometry. At least one of the source points must be within a region of fissile material for the problem to run. The ksrc card format is:

ksrc x1 y1 z1 x2 y2 z2 ... xn yn zn

ksrc = Card name for initial fission source location. Starts in columns 1-5.

x_k y_k z_k = Location of the kth initial fission source point.

Figure 1-5 shows an example of a ksrc card. Two initial fission source points are used. The first is located at the coordinates (1, 0, 0) and the second at (12, 3, 9).

ksrc 1 0 0 12 3 9

Figure 1-5. Example of ksrc card.

Next we discuss the material card. The format of the material, or m card, is:

mn zaid₁ fraction₁ zaid₂ fraction₂

mn = Material card name (m) followed immediately by the material number (n) on the cell card. Starts in columns 1-5.

zaid = Atomic number followed by the atomic mass of the isotope.

fraction = Nuclide fraction.

(+) Atom fraction

(-) Weight fraction

An example of a material card where two isotopes of plutonium are used is shown in Figure 1-6. The material number *n* is an integer from 1 to 99999. Each material can be composed of many isotopes. Default cross sections will be used for all materials throughout this document. {Chapter 3 and Appendix G of the MCNP manual describe how to choose cross sections from different libraries.}


```

m1      94239 2.442e-2
        94240 1.673e-3

```

Figure 1–6. Data card with material format in atom fractions.

The first `zaid` is 94239 followed by the atom fraction. The atomic number is 94, plutonium. The atomic mass is 239 corresponding to the 239 isotope of plutonium. A second isotope in the material begins immediately after the first using the same format and so on until all material components have been described. Notice that the material data is continued on a second line. If a continuation line is desired or required, make sure the data begins after the fifth column of the next line, or end the previous line with an ampersand (&). Because the fractions are entered as positive numbers, the units are atoms/b-cm. If the atom or weight fractions do not add to unity, MCNP will automatically renormalize them.

1.3 EXAMPLE PROBLEM

This introduction should provide enough information to run a simple example problem. It is our intent that you gain confidence in using MCNP right away, so we walk through this sample problem step by step, explaining each line of input. For the present it is important that you enter this problem exactly as we describe it. As you gain more experience with MCNP, you may find other ways to set up input files that are more logical to you. For example, you may find it easier to work out the surface cards before doing the cell cards.

1.3.A Problem Description

This problem is a bare sphere of plutonium metal with a coating of nickel (also known as the Jezebel reactor). Experimental parameters are:

delta-phase Pu metal sphere: radius	= 6.38493 cm	
N ₂₃₉ = Atom density of Pu-239	= 3.7047e-2	atoms/b-cm
N ₂₄₀ = Atom density of Pu-240	= 1.751e-3	atoms/b-cm
N ₂₄₁ = Atom density of Pu-241	= 1.17e-4	atoms/b-cm
N _{Ga} = Atom density of Ga	= 1.375e-3	atoms/b-cm
Spherical nickel coating: Thickness	= 0.0127 cm	
N _{Ni} = Atom density of Ni	= 9.1322e-2	atoms/b-cm

Now you are ready to begin entering the example problem. First open a new file named `example1`. All text shown in the `courier` font is what you need to type in. Each new card, as it is discussed, is indicated by an arrow in the left margin. The first line in the file must be the title card, which is followed by the three major sections of an MCNP input file (cells, surfaces, and data).

1.3.B Title Card

A one line title card is required and can be up to 80 characters in length. There is no blank line between the title card and the cell cards.

→ Jezebel problem. Bare plutonium sphere w/nickel shell

1.3.C Cell Cards

The problem requires description of the plutonium sphere and a nickel shell, as shown in Figure 1-7. We will enter the plutonium cell information first. The comment card shows how it helps make the input file easier to follow. The cell number is 1 and the material number is 1. The material density, $4.0290\text{e-}2$, is the sum of the material densities of the plutonium isotopes present in the sphere. Because $4.0290\text{e-}2$ is positive, the units are *atoms/b-cm*. The next entry, -1 , indicates that cell 1 (inside the sphere) is all space having a negative sense with respect to surface 1. The `imp:n=1` says this cell has an importance (*imp*) for neutrons (*:n*) of 1.

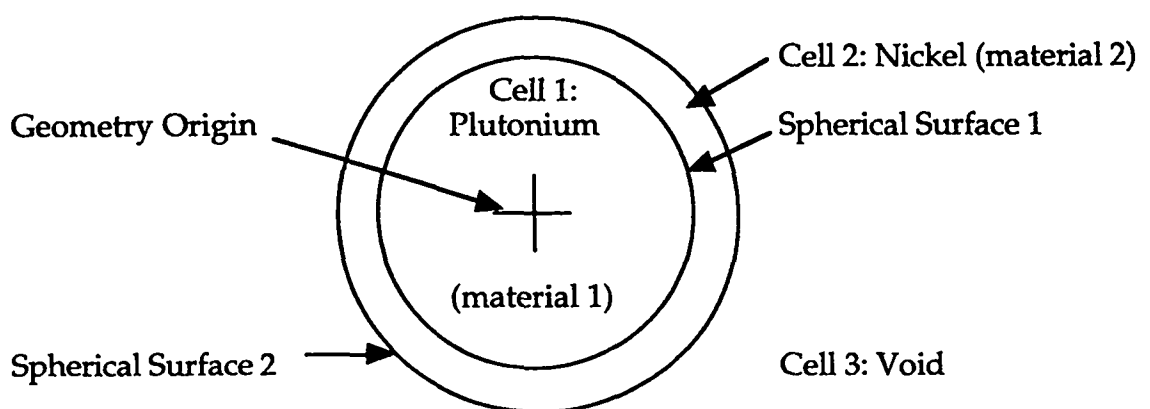


Figure 1-7. Bare plutonium sphere geometry.

```

Jezebel problem. Bare plutonium sphere w/nickel shell
C      Cell Cards
→ 1    1  4.0290e-2   -1   imp:n=1

```

Next we will enter information about the nickel shell encasing the plutonium. The cell number is 2, and the material number is 2. Again, the material atom density, $9.1322\text{e-}2$, is positive, so the units are *atoms/b-cm*. The next two entries, 1 -2, define cell 2 as all space that has a positive sense with respect to surface 1 and a negative sense with respect to surface 2 (outside sphere 1 and inside sphere 2). A surface number with no sign is interpreted as positive. A +1 entry would also be accepted. Cell 2 also has a neutron importance of 1 (imp:n=1).

```

Jezebel problem. Bare plutonium sphere w/nickel shell
C      Cell Cards
1    1  4.0290e-2   -1   imp:n=1
→ 2    2  9.1322e-2   1 -2   imp:n=1

```

To complete the cell card section we must define all space outside the plutonium/nickel system. The cell number is 3 and the material number is 0, indicating a void. The next entry, 2, defines cell 3 as all space that has a positive sense with respect to surface 2 (outside of sphere 2). As there is no outer boundary, this makes cell 3 an infinite cell. Cell 3 has a neutron importance of zero (imp:n=0). This infinite cell defines an outside world for the problem. When particles enter a cell of zero importance, they are assumed to have escaped the problem and are terminated. {A complete explanation of the importance card can be found in Chapter 3 of the MNCP manual.} A blank line delimiter concludes the cell card section.

```

Jezebel problem. Bare plutonium sphere w/nickel shell
C      Cell Cards
1    1  4.0290e-2   -1   imp:n=1
2    2  9.1322e-2   1 -2   imp:n=1
→ 3    0              2   imp:n=0
→

```

1.3.D Surface Cards

Two spherical surfaces are required for the geometry of this problem. The first sphere, surface 1, encloses the plutonium material. It is a sphere centered at the origin 0,0,0; therefore the so surface mnemonic is used. A sphere radius, 6.38493 cm in this case, is needed to complete the information on surface card 1. Appendix F of this document provides a list of the 29 surface mnemonics available.

```
Jezebel problem. Bare plutonium sphere w/nickel shell
C      Cell Cards
1      1  4.0290e-2 -1      imp:n=1
2      2  9.1322e-2  1 -2   imp:n=1
3      0                      2   imp:n=0
b
C      Surface Cards
→ 1      so  6.38493
```

The second sphere, surface 2, also is centered at the origin, but it has radius of 6.39763 cm. The inner surface of the nickel shell corresponds exactly to the outer surface of the plutonium sphere, which is already defined as surface 1. A blank line concludes the surface card section.

```
Jezebel problem. Bare plutonium sphere w/nickel shell
C      Cell Cards
1      1  4.0290e-2 -1      imp:n=1
2      2  9.1322e-2  1 -2   imp:n=1
3      0                      2   imp:n=0
b
C      Surface Cards
→ 1      so  6.38493
→ 2      so  6.39763
→ b
```

1.3.E Data Cards

This example illustrates a criticality calculation, so the kcode card is required. The number of neutrons per k_{eff} cycle is 1000. The number of source neutrons depends on the system and the number of cycles being run. An initial estimate of k_{eff} is 1.0 because this example's final result is expected to be very close to critical. We will skip 15 k_{eff} cycles to allow the spatial fission source to settle to an equilibrium before k_{eff} values are used for averaging for the final k_{eff} estimate. A total of 115 k_{eff} cycles will be run.

```
Jezebel problem. Bare plutonium sphere w/nickel shell
C    Cell Cards
1    1  4.0290e-2 -1      imp:n=1
2    2  9.1322e-2  1 -2   imp:n=1
3    0                      2   imp:n=0
h
C    Surface Cards
1    so  6.38493
2    so  6.39763
h
C    Data Cards
→ kcode 1000 1.0 15 115
```

The entries on the ksrc card place one fission source point at (0, 0, 0), the center of the plutonium sphere. For the first k_{eff} cycle, 1000 neutrons with a fission energy distribution will start at the origin. More source points can be used but are not necessary for this example.

```
Jezebel problem. Bare plutonium sphere w/nickel shell
C    Cell Cards
1    1  4.0290e-2 -1      imp:n=1
2    2  9.1322e-2  1 -2   imp:n=1
3    0                      2   imp:n=0
h
C    Surface Cards
1    so  6.38493
2    so  6.39763
h
C    Data Cards
→ kcode 1000 1.0 15 115
→ ksrc  0 0 0
```

The last information needed for this problem is a description of our materials. Material 1, in cell 1, is plutonium, and material 2, in cell 2, is nickel. The material number on the m card is the same as the material number used on the cell card. Material 1, m1, has three isotopes of plutonium and one of gallium. The zaid of Pu-239 is 94239, followed by the nuclide atom fraction ($3.7047e-2$). The other isotopes are treated in the same manner. Because of the length of the m1 data card line, a continuation card is required. Blanks in columns 1-5 indicate this line is a continuation of the last card.

```

Jezebel problem. Bare plutonium sphere w/nickel shell
C      Cell Cards
1      1  4.0290e-2 -1      imp:n=1
2      2  9.1322e-2  1 -2   imp:n=1
3      0              2     imp:n=0
b
C      Surface Cards
1      so  6.38493
2      so  6.39763
b
C      Data Cards
kcode 1000 1.0 15 115
ksrc   0 0 0
→ m1    94239 3.7047e-2 94240 1.751e-3
→      94241 1.17e-4   31000 1.375e-3

```

Material 2, m2, is the nickel that coats the plutonium. The zaid of nickel is 28000, followed by the nuclide atom fraction (1.0). The three zeros following the atomic number (28) indicate that this cross-section evaluation is for elemental nickel, where the five stable nickel isotopes are combined into one cross-section set. The optional blank line terminator indicates the end of the data card section and the end of the input file.

```

Jezebel problem. Bare plutonium sphere w/nickel shell
C      Cell Cards
1      1  4.0290e-2 -1          imp:n=1
2      2  9.1322e-2  1 -2      imp:n=1
3      0                      2      imp:n=0
␣
C      Surface Cards
1      so  6.38493
2      so  6.39763
␣
C      Data Cards
kcode 1000 1.0 15 115
ksrc   0 0 0
m1      94239 3.7047e-2          94240 1.751e-3
        94241 1.17e-4           31000 1.375e-3
→ m2      28000 1.0
→ ␣      (optional blank line terminator)

```

The input required to run this example is complete. Now you are ready to run MCNP. Save your input as a file called `example1`.

1.4 RUNNING MCNP

We will assume that MCNP has been installed on the machine you are using. The default names of the input and output files are `INP` and `OUTP`, respectively. To run MCNP with different file names, type `mcnp inp=` and then the filename of the example problem followed by `outp=` and the name of the output file.

```
mcnp inp=example1 outp=exlout
```

MCNP writes information to the screen about how the calculation is progressing. Once the calculation is complete, check the output file to see your results. The run time for this problem should be on the order of minutes or less.

1.4.A Output

First, let's assume the run was successful. There is a significant amount of information contained in the output file, but right now we are interested in the k_{eff} results. Therefore, we will skip past most of the information.

Output skipped over...

1. Echo of input file.
2. Description of cell densities and masses.
3. Material and cross-section information.
4. k_{eff} estimator cycles.
5. Neutron creation and loss summary table.
6. Neutron activity per cell.

After the "Neutron Activity Per Cell" you will see...

```
keff results for: Jezebel problem. Bare plutonium sphere w/nickel shell
```

This is the beginning of the criticality calculation evaluation summary table. Check to see that the cycle values of the three estimators for k_{eff} – $k(\text{collision})$, $k(\text{absorption})$, and $k(\text{track length})$ – appear normally distributed at the 95 or 99 percent confidence level. See that all the cells with fissionable material have been sampled. The final estimated combined k_{eff} , in the dashed box, should be very close to 1 (0.9968 computed on a SPARC 1 at the University of New Mexico.) The combined k_{eff} and standard deviation can be used to form a confidence interval for the problem. If your results are similar to these then you have successfully created the input file and run MCNP.

If your input did not run successfully, you can look at the FATAL ERROR messages in the `ex1out` file. They are also displayed at the terminal. These error messages should not be ignored because they often indicate an incorrectly specified calculation. FATAL ERRORS must be corrected before the problem will run.

MCNP also provides WARNING messages to inform you of possible problems. For example, this calculation has the WARNING message: "neutron energy cutoff is below some cross-section tables." The lower energy limit for most neutron cross-section data is 10^{-11} MeV. The default problem energy cutoff is 0 MeV, clearly below the lowest energy data point. In all room temperature energy ($2.5 \cdot 10^{-8}$ MeV) problems, this message can be ignored. All WARNING messages from an MCNP calculation should be examined and understood to be certain that a problem of concern has not been detected. However, a problem will run with WARNING messages.

1.5 SUMMARY

This chapter has helped you to:

- Interpret an MCNP input file.
- Set up and run a criticality problem with MCNP.
- Interpret neutron multiplication information from MCNP output.
{See the MCNP manual, Chapter 5, Section IV, for an annotated partial listing emphasizing the criticality aspects of the output from a criticality calculation.}

Now that you have successfully run MCNP, you are ready to learn about the more complex options available with MCNP. The following chapters present these options in a format similar to the *Quickstart* chapter.

Chapter 2:

Reflected Systems

In the Quickstart chapter you ran a simple problem with MCNP and gained some confidence in using the code. This chapter provides a more detailed explanation of the commands used in the Quickstart chapter. Example problems are taken from LA-10860 and represent computational models of criticality benchmark experiments. Each example problem is selected to focus on two or three specific MCNP commands.

2.1 WHAT YOU WILL BE ABLE TO DO:

- Interpret the sense of a surface.
- Use the Boolean intersection, union, and complement geometry operators.
- Define a multicell problem.

2.2 PROBLEM DESCRIPTION

This set of examples uses a plutonium metal cylinder and examines it in three different configurations (LA-10860 p. 101). The three configurations are a bare (unreflected) system and two natural uranium reflected systems: one with a radial reflector and one with both a radial and an axial reflector. In each configuration the central cylinder of plutonium has a diameter of 9.87 cm while the height of the plutonium cylinder varies with the reflection conditions. The plutonium material is the same for each configuration; therefore, the plutonium atom density (N_{239}) is the same for all three analyses. Note that for many materials both a mass density (g/cc) and an atom density (atoms/b-cm) are provided. Either is sufficient to describe materials in MCNP.

2.3 CONFIGURATION 1

The bare plutonium cylinder is modeled first. This example discusses the sense of a surface and the Boolean intersection and union geometry operators. The data for this example follows.

Plutonium Material

Delta phase Pu metal (100 percent Pu-239)

$\rho = 15.8 \text{ g/cc}$

$N_{239} = 3.9802\text{e-}2 \text{ atoms/b-cm}$

Configuration I. *Bare Plutonium Metal System*

Plutonium cylinder:

Radius = 4.935 cm

Height = 17.273 cm

2.3.A Geometry

The setup for this problem will be done in a different order than found in an MCNP input file. Recall that the cell cards precede the surface cards, but it is often easier to begin by defining the surfaces first. We will then combine these surfaces to form the cells. Figure 2-1 shows the cylindrical geometry for Configuration 1.

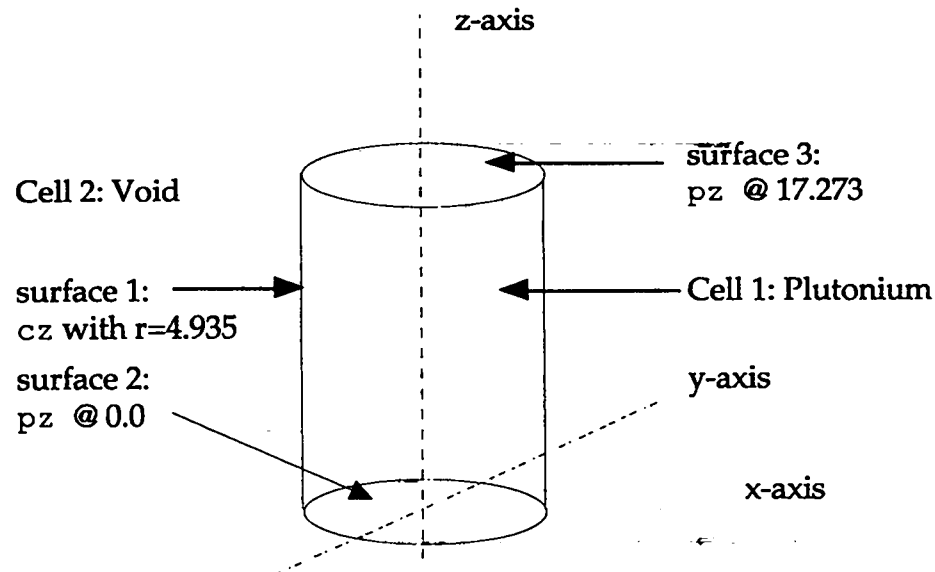


Figure 2-1. Configuration 1 geometry.

Surfaces

MCNP has 29 different types of surfaces, but the primary ones used for criticality safety are spheres, planes, and cylinders. All surfaces except the sphere and torus are infinite in extent. Therefore, the surfaces must be combined to define finite shapes that enclose volumes called cells. For example, a cylinder in MCNP is infinite in height, so a top plane and a bottom plane are required to make the cylinder finite. As configuration 1 involves a finite cylinder, we will need three surfaces (an infinite cylinder and two infinite planes) to create this shape. Figure 2-2 shows the combination of surfaces for configuration 1, and Figure 2-3 shows the MCNP input for these surfaces. Defining an infinite cylinder requires choosing an axis and radius. A cylinder symmetric about the z -axis, cz , called surface 1, will be used here. From the problem description, the radius of the infinite cylinder is 4.935 cm. Two planes perpendicular to the z -axis, pz , will be used to limit the cylinder's height. For our example, we have chosen the bottom plane, surface 2, to cross the z -axis at $z=0$. The top plane, surface 3, will cross the z -axis at $z=17.273$. When the surfaces are combined they create a finite cylinder with a height of 17.273 cm.

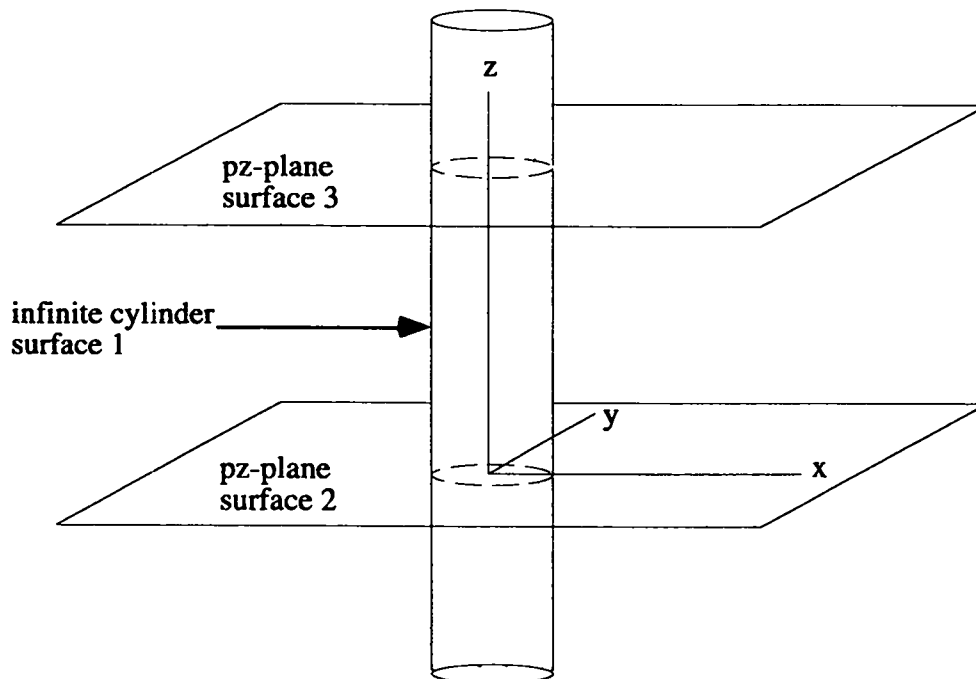


Figure 2-2. Configuration 1 surface combinations.

C	Surface Cards	
1	cz	4.935
2	pz	0
3	pz	17.273

Figure 2-3. Configuration 1 surface cards.

Cells

Now that the surface cards are defined, the geometric cells can be defined. Cells are defined by identifying individual surfaces and combining these surfaces using the Boolean *intersection*, *union*, and *complement* operators. The two cells for configuration 1 are shown in Figure 2-1. The cell cards are shown in Figure 2-4. Remember, the first card of the input file is the problem title card.

Cell 1 is the plutonium cylinder and is assigned material number 1. The gram density, taken from the problem description, follows the material number. Recall from the first chapter that a gram density is entered as a negative number.

Problem 2A. Bare Pu Cylinder					
C	Cell Cards				
1	1	-15.8	-1	2	-3 imp:n=1
2	0		1	-2:3	imp:n=0

Figure 2-4. Configuration 1 cell cards.

Surface Sense

An important concept you need to understand when combining surfaces is the *sense* of all points in a cell with respect to a bounding surface. The *sense* is a sign associated with a surface that specifies which side of a surface a cell is on. Suppose that $f(x,y,z)=0$ is the equation of a surface. Choose a point (x,y,z) and put that point into the equation of the surface. If the sign of the result is *negative*, the point is said to have a *negative sense* with respect to the surface. If the result is *positive*, the point is said to have a *positive sense* with respect to the surface. If the result is zero, the point is on the surface.

For example, assume a plane intersects the x-axis at $x=2$. The MCNP equation for this plane is $x-2=0$. In this case, y and z can have any value, so the only coordinate we are concerned with is the x coordinate. Choose a point, say $x=5$, and substitute it into the equation: $5-2=3$, which is positive. Therefore, the point $x=5$ has a *positive sense* with respect to the plane at $x=2$. You do not have to evaluate an equation every time you define a cell.

For commonly used simple surfaces, space that is:

inside a sphere, cylinder, or cone has a **negative** sense;
outside a sphere, cylinder, or cone has a **positive** sense;
above or to the right of a plane has a **positive** sense;
below or to the left of a plane has a **negative** sense.

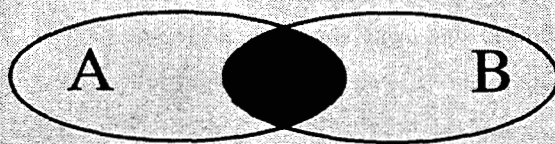
{For more detail see Chapter 1 of the MCNP manual.}

Continuing with cell 1, the plutonium is contained inside the cylinder, therefore the sense of surface 1, the infinite cylinder, with respect to (wrt) cell 1 is negative, -1. Cell 1 now needs to be restricted to the region above surface 2 and below surface 3. Using the rules stated above, the sense of surface 2 is positive, and the sense of surface 3 is negative wrt cell 1. This combination of three surfaces is entered on the cell 1 card after the material density. The blanks between the surface numbers, -1 2 -3, define intersections of the space inside the cylinder and above the lower plane and below the upper plane. A neutron importance of 1 completes this cell description.

MCNP requires that you define all space, so the only remaining geometry to be defined for this example is the outside world, cell 2. The outside world is everything outside the plutonium cylinder. The material number is zero because this cell is a void. Remember, a void has no material density entry. To define the region of space that is the outside world, we need to introduce the **union** operator.

Intersections and Unions

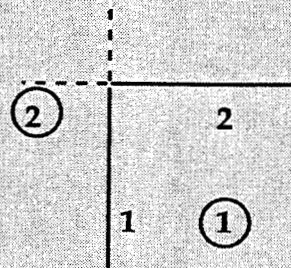
The **intersection** operator in MCNP is simply a blank space between two surface numbers on a cell card. Assume you have two regions of space, A and B. The region of space containing points that belong to both A and B is called the **intersection** of A and B, written A B. The shaded area below represents A B. Because it is a binary Boolean operator, the **intersection** can be considered multiplicative.



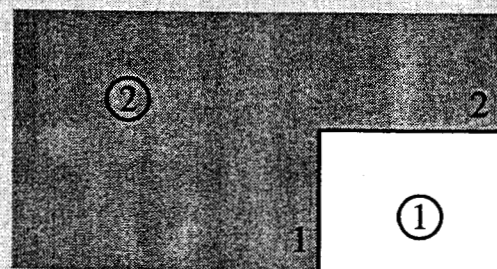
A region containing points that belong to A alone or to B alone or to both A and B is called a **union** of A and B. The union operator is indicated by a colon (:). The shaded region below represents the **union** of A and B ($A:B$). Because it is a binary Boolean operator, the **union** can be considered additive.



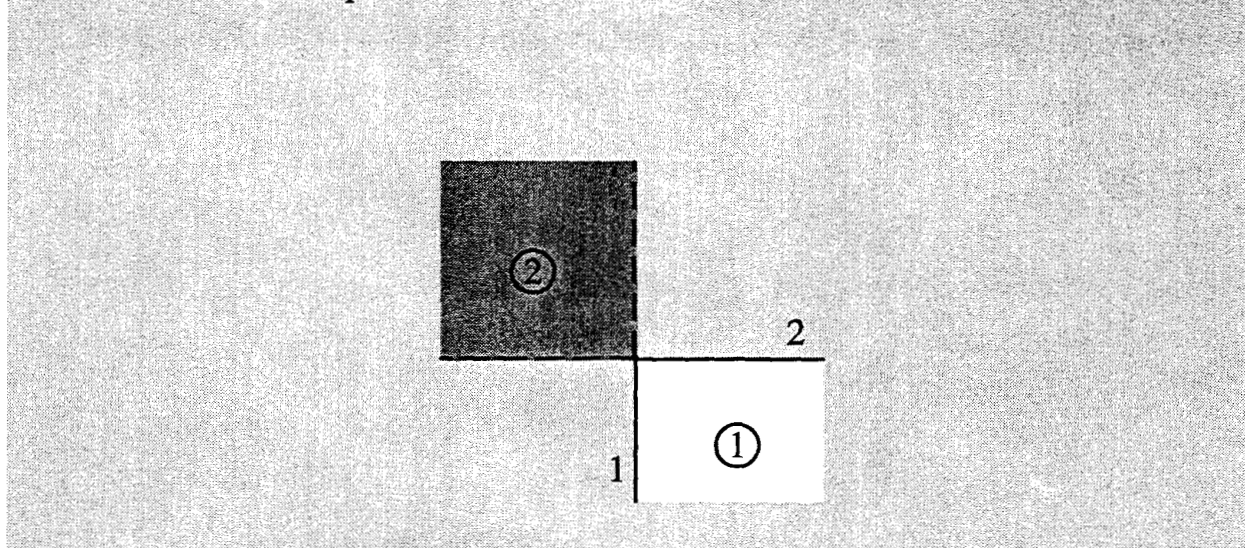
Consider two planes that meet to form two cells. Cell numbers are circled.



Cell 1 is the region below surface 2, that is, with a negative sense, that is also in common with (intersected with) everything to the right of surface 1, that is, with a the positive sense. Therefore, the surfaces defining cell 1 are written $1 - 2$. Cell 2 is everything to the left (negative sense) of surface 1 **plus** everything above (positive sense) surface 2. Therefore, the surfaces defining cell 2 are written $-1 : 2$. Cells 1 and 2 are illustrated below.



If cell 2 were specified as -1 2, that would be the space to the left of surface 1 that is in common with the space above surface 2, illustrated below.



The **union** operator is what we use to define the "rest of the world" in configuration 1. Therefore, the sense of the surfaces in cell 2 is opposite to those defining cell 1 and the Boolean intersection operator is replaced by the **union**, 1:-2:3. Figure 2-4 illustrates the format of the cell 2 card in this example. The cell is assigned an importance of zero. Any particles entering cell 2 need to be terminated because once particles leave the cylinder they have no chance of returning.

2.3.B Materials

Now that the geometry of the system is defined, we need to identify the material. This example requires only plutonium-239, which has an atomic number of 94 and an atomic weight of 239. The default cross-section evaluation for this isotope is selected by entering only 94239. Figure 2-5 shows the material card required. The procedure to define a material was described in the first chapter. The only thing new is the use of an atom fraction for the plutonium. Material 1 is 100 percent plutonium-239, so the atom fraction is 1.

```
C      Data Cards
m1     94239 1.0
```

Figure 2-5. Configuration 1 material specification.

2.3.C MCNP Criticality Controls

A kcode card is required to run a criticality calculation. We will specify 1000 neutrons per cycle, an initial guess for k_{eff} of 1.0, 15 cycles will be skipped, and a total of 115 cycles will be run. For this example, a single fission source point is placed near the center of the plutonium cylinder using the ksrc card. Figure 2-6 shows these two cards for this problem.

```
kcode 1000 1.0 15 115
ksrc 0 0 8.6
```

Figure 2-6. Configuration 1 criticality control cards.

A criticality source is different from a fixed source because the fission source locations change from cycle to cycle. A cycle is the completion of the number of histories requested by the first entry on the kcode card. The initial ksrc source is used only for the first k_{eff} cycle. A new spatial fission source is generated during each cycle and is used as the source for the next cycle.

2.3.D Configuration 1 MCNP Input File

The input required for this example problem is complete. Do not forget the required blank line delimiters between sections when entering this information. After entering the data, your input file should appear as follows:

```
Problem 2A. Bare Pu Cylinder
C    Cell Cards
1    1  -15.8          -1 2 -3 imp:n=1
2    0                  1:-2:3 imp:n=0

C    Surface Cards
1    cz    4.935
2    pz    0
3    pz    17.273

C    Data Cards
m1    94239 1
kcode 1000 1.0 15 115
ksrc 0 0 8.6
```

The problem can be run by typing...

```
mcnp inp=file1 outp=file2 runtpe=file3
```

where inp, outp, and runtpe are the default names for the input file, the output file, and the binary results file, respectively. The runtpe file is useful for plotting problem results and for continuing a calculation as discussed in later chapters of the Primer.

The name option is useful for automatically naming files. It uses the inp name as the base and appends the appropriate letter (o for outp and r for runtpe).

```
mcnp name=prob2a
```

produces an outp file named prob2ao and a runtpe file prob2ar.

2.3.E Output

At this time we are only interested in looking at the k_{eff} result in the output. Recall from the first chapter that there is a good deal of information to be skipped to find

```
final estimated combined collision/absorption/track-length keff.
```

Your result should be close to 1.00. The result on a SPARC 1 at University of New Mexico was 1.0101 with an estimated standard deviation of 0.0018. If your result is not close to ours, check your input to make sure your surface dimensions are correct and that material densities are correctly entered on the cell cards.

2.4 CONFIGURATION 2

The second problem in this chapter takes configuration 1 and adds a radial natural uranium reflector. This example introduces how to define cells within cells.

Natural Uranium Radial Reflector

$$\rho = 18.80 \text{ g/cc}$$

Configuration II. *Plutonium Metal , Radially Reflected by Uranium*

Plutonium cylinder:	Radius = 4.935 cm
	Height = 6.909 cm

Uranium reflector thickness:	5.0 cm
Uranium reflector height:	6.909 cm

2.4.A Geometry

The setup process is the same as for configuration 1. Surface cards will be defined first and then used to create the cell cards. Figure 2-7 shows the geometry setup for configuration 2. (Note that the cylinder has been changed to be symmetric about the x-axis.)

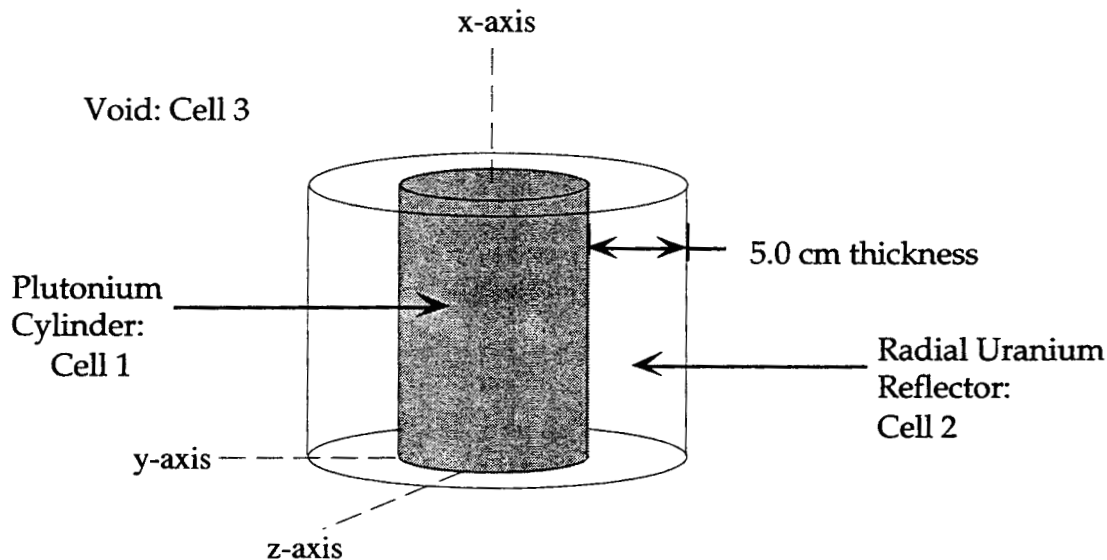


Figure 2-7. Configuration 2 geometry.

Surfaces

Before continuing, try to create the surface cards for this configuration on your own and check them with Figure 2-8. If you encounter difficulty, read the surface card description that follows.

Beginning with the plutonium cylinder, the problem description specifies a radius of 4.935 cm (the same as configuration 1). This time a cylinder on the x-axis, cx , will be used as surface 1. Two planes perpendicular to the x-axis, px , are needed to give the cylinder a finite height of 6.909 cm. Surfaces 2 and 3 are chosen so that the distance between them is 6.909 cm.

Another cylinder must be defined for a radial uranium reflector that has a thickness of 5 cm. A second cylinder on the x-axis, cx , with a radius of $4.935 \text{ cm} + 5.0 \text{ cm} = 9.935 \text{ cm}$ is used. Because there is no reflection on the top or bottom of this system, the reflector region is the same height as the plutonium cell, so we can use the two planes already defined (surfaces 2 and 3) to make the reflector finite in

height. Figure 2-8 shows the surface cards required for this example. The \$ is used to include comments on cards as appropriate.

C	Surface Cards			
1	cx	4.935	\$	Pu cylinder
2	px	0	\$	bottom
3	px	6.909	\$	top
4	cx	9.935	\$	U reflector

Figure 2-8. Configuration 2 surface cards.

Cells

The four surfaces now can be used to build the plutonium and uranium cells. Figure 2-9 shows the cell cards for this example. We call the plutonium cylinder cell 1, assign it material 1 with a material density entered with a negative sign indicating g/cc. The intersection operator is used to combine the surfaces. An importance of 1 is assigned to this cell.

We call the uranium reflector cell 2 and assign it material number 2. The material density, 18.80 g/cc is entered with a negative sign indicating g/cc. Next, we enter the bounding surfaces using the **intersection** operator. Recalling the rules of surface sense, the reflector is the space outside surface 1 (positive sense) and the space inside surface 4 (negative sense) and the space between surfaces 2 and 3, 1 -4 2 -3. The importance of this cell is 1.

The last cell is the outside world. As in configuration 1, we use the **union** operator. Cell 3 is all space outside surface 4 or below surface 2 or above surface 3. The union of these surfaces, 4 :-2:3, defines cell 3. Our outside world is now all space except the plutonium and uranium. An importance of zero is assigned to this cell, terminating any neutrons entering this region. The cell cards required for configuration 2 are complete.

C	Cell Cards				
1	1	-15.8	-1	2 -3	imp:n=1
2	2	-18.8	1	-4 2 -3	imp:n=1
3	0		4:-2:3		imp:n=0

Figure 2-9. Configuration 2 cell cards.

2.4.B Materials

Configuration 2 requires two materials: plutonium and natural uranium. Figure 2-10 shows the material cards for this example. Material 1, plutonium-239, is the same as in configuration 1. For the reflector we have natural uranium, which consists of U-235 and U-238. These isotopes will be entered as atom fractions. U-238 is the first isotope entered because it is the most abundant. The atomic number of uranium is 92 and 238 represents the 238 isotope. The atom percent is taken from the Chart of the Nuclides. The U-235 isotope is entered in the same manner.

```
C      Data Cards
m1     94239 1.0
m2     92238 0.992745 92235 0.007200
```

Figure 2-10. Configuration 2 material cards.

Normalization of Atom Fractions

The atom fractions of the two uranium isotopes do not add to exactly 1.00. When this occurs, MCNP renormalizes the values. For example, if you have trace elements in a material that you do not include in the material card, the atom fractions will not add up to exactly 1.0. MCNP will then add up the specific fractions and renormalize them to sum to 1.0. A WARNING message informs you that the fractions did not add to one or to the density on the cell card.

2.4.C MCNP Criticality Controls

The entries on the required kcode card do not change from configuration 1. Because we made the cylinder shorter, we will move the initial source point closer to the center of the cylinder at 3.5 cm on the x-axis. Figure 2-11 shows the criticality controls for this example.

```
kcode 1000 1.0 15 115
ksrc 3.5 0 0
```

Figure 2-11. Configuration 2 criticality control cards.

2.4.D Configuration 2 MCNP Input File

The input for this problem is complete. Double check your input for entry errors and do not forget the blank-line delimiters between sections. After you have entered this information, the input file should appear as follows:

```
Configuration 2, Pu cylinder, radial U(nat) reflector
C      Cell Cards
1      1  -15.8          -1  2  -3          imp:n=1
2      2  -18.8          1  -4  2  -3        imp:n=1
3      0                  4:-2:3          imp:n=0

C      Surface Cards
1      cx  4.935         $  Pu cylinder
2      px  0             $  bottom
3      px  6.909         $  top
4      cx  9.935         $  U reflector

C      Data Cards
m1      94239 1.0
m2      92238 0.992745 92235 0.007200
kcode 1000 1.0 15 115
ksrc 3.5 0 0
```

2.4.E Output

Scan through the output and find the...

final estimated combined collision/absorption/track-length keff.

Your result should be subcritical. The radial reflector is not sufficient to give you a critical mass for this configuration. The result on a SPARC 1 at University of New Mexico was 0.8859 with an estimated standard deviation of 0.0022. If your result is not close to ours, check your input to make sure your surface dimensions are correct, and check the material densities in the cell cards. If the run was successful, continue on to configuration 3.

2.5 CONFIGURATION 3

In this third example we show how to use the Boolean complement operator, #. Configuration 3 is the same as configuration 2 with an axial reflector added.

Natural Uranium Reflector

$$\rho = 18.80 \text{ g/cc}$$

Configuration III. *Plutonium Metal , Fully Reflected by Uranium*

Plutonium cylinder:	Radius = 4.935 cm
	Height = 6.909 cm

Uranium reflector thickness:	5.0 cm radially
	5.0 cm axially

2.5.A Geometry

The geometry setup for this problem is similar to configuration 2. Figure 2-12 shows the geometry for configuration 3. Note we are still using an x-axis cylinder for configuration 3 although y-axis or z-axis cylinders would work just as well.

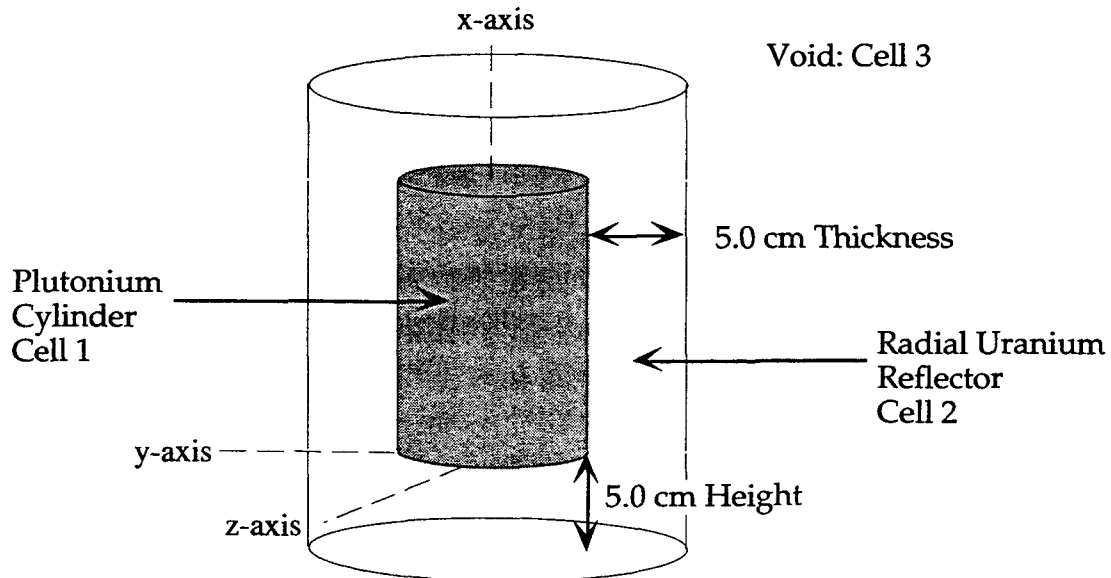


Figure 2-12. Configuration 3 geometry.

Surfaces

Two px planes need to be added to the surface card section to bound the new axial uranium reflector. Figure 2-13 shows the surface cards for configuration 3, where surfaces 5 and 6 are new. Comments can be added to the surface cards for clarification.

C	Surface Cards	
1	cx	4.935
2	px	0
3	px	6.909
4	cx	9.935
5	px	-5.0
6	px	11.909

Figure 2-13. Configuration 3 surface cards.

Cells

Because the plutonium cylinder is the same size as in the other two configurations, cell 1 does not change. Cell 2 will be defined differently in configuration 3 than it was in configuration 2: we will use the Boolean complement operator, #.

Complement Operator

The complement operator, #, is a short-hand cell-specifying method that implicitly uses the intersection and union operators. It can be thought of as saying "not in." For example, let's look at the cell cards for configuration 1 again.

C	Cell Cards	
1	1 -15.8	-1 2 -3 imp:n=1
2	0	1:-2:3 imp:n=0

Cell 2 defines the outside world using the union of three surfaces (1:-2:3). Cell 2 also could be specified using the complement operator. The outside world is everything except cell 1, so we can define cell 2 as all space that is "not in" cell 1, or #1.

C	Cell Cards	
1	1 -15.8	-1 2 -3 imp:n=1
2	0	#1 imp:n=0

In this simple example the complement operator changes intersections to unions and reverses the senses of the surfaces of cell 1.

Returning to configuration 3, we can define cell 2 as the region of space inside surface 4 and below surface 6 and above surface 5, that is "not in" cell 1, -4 -6 5 #1. This method may be easier than defining cell 2 explicitly, -4 -6 5 (1:-2:3). However, in more complicated problems, using the complement operator can cause the run time to increase significantly. Figure 2-14 shows the cell cards for configuration 3.

C	Cell Cards					
1	1	-15.8	-1	2	-3	imp:n=1
2	2	-18.8	-4	-6	5 #1	imp:n=1
3	0			4:-5:6		imp:n=0

Figure 2-14. Configuration 3 cell cards.

2.5.B Materials

There is no change in the material cards from configuration 2. Figure 2-15 shows the m cards used in configuration 3.

C	Data Cards				
m1	94239	1			
m2	92238	0.992745	92235	0.007200	

Figure 2-15. Configuration 3 material cards.

2.5.C MCNP Criticality Controls

The kcode and ksrc cards are not changed from configuration 2. Figure 2-16 shows the controls used in configuration 3.

kcode	1000	1.0	15	115
ksrc	3.5	0	0	

Figure 2-16. Configuration 3 criticality control cards.

2.5.D Configuration 3 MCNP Input File

The input for configuration 3 is complete and should appear as follows. Do not forget the blank line delimiters at the end of sections.

Configuration 3, Pu cylinder with U(nat) reflector

C Cell Cards

```
1     1   -15.8   -1   2   -3            imp:n=1
2     2   -18.8   -4   -6   5   #1        imp:n=1
3     0                4:-5:6            imp:n=0
```

C Surface Cards

```
1     cx     4.935
2     px     0
3     px     6.909
4     cx     9.935
5     px     -5.0
6     px     11.909
```

C Data Cards

```
m1     94239 1
m2     92238 0.992745   92235 0.007200
kcode 1000 1.0 15 115
ksrc   3.5 0 0
```

2.5.E Output

Scan through the output file and find the

final estimated combined collision/absorption/track-length keff.

Your result should be close to 1. The result on a SPARC 1 at the University of New Mexico was 1.027 with an estimated standard deviation of 0.002.

2.6 SUMMARY

This chapter presented you with three examples designed to teach the basic geometry concepts and Boolean geometry operations used to define cells. We discussed the sense of surfaces and the union, intersection, and complement operators. You have also learned how to model multicell problems. The information presented in this chapter will help you to model the more complex problems presented in the following chapters.

Chapter 3

$S(\alpha,\beta)$ Thermal Neutron Treatment for Moderators

This chapter presents the use of $S(\alpha,\beta)$ thermal neutron cross sections for use with problems containing hydrogenous and other moderating material. It also demonstrates how to handle a void region that is not defined as the “rest of the world.” An explanation of the basic features of the MCNP k_{eff} output is provided.

3.1 WHAT YOU WILL BE ABLE TO DO:

- Use and understand $S(\alpha,\beta)$ thermal neutron treatment.
- Understand the order of geometry operations on cell cards.
- See effects of $S(\alpha,\beta)$ treatment.
- Interpret k_{eff} output.

3.2 $S(\alpha,\beta)$ THERMAL NEUTRON TREATMENT

Let's begin with a description of why we use $S(\alpha,\beta)$ cross-sections. When the neutron energy drops below a few eV, the thermal motion of scattering nuclei strongly affects collisions. The simplest model to account for this effect is the free gas model that assumes the nuclei are present in the form of a monatomic gas. This is the MCNP default for thermal neutron interactions. In reality, most nuclei will be present as components of molecules in liquids or solids. For bound nuclei, energy can be stored in vibrations and rotations. The binding of individual nuclei will affect the interaction between thermal neutrons and that material. The $S(\alpha,\beta)$ cross sections are used to account for the bound effects of the nuclei. It is important to recognize that the binding effects for hydrogen in water are different than for hydrogen in polyethylene. MCNP has different $S(\alpha,\beta)$ data for hydrogen, as well as other elements. See Appendix D of this Primer for available default cross-sections.

3.3 PROBLEM DESCRIPTION

This example is a bare (unreflected) $\text{U}(4.89)\text{O}_2\text{F}_2$ solution cylinder (LA-10860 p.32). The solution has a radius of 20.12 cm and a height of 100.0 cm. An aluminum tank with a thickness of 0.1587 cm on the sides and bottom, and a height of 110.0 cm contains the solution. There is no lid on the tank. The region from the top of the solution to the top of the aluminum tank is void. The data for this problem follows:

U(4.89)O₂F₂ Solution Composition:

N_{235}	$= 1.0889\text{e-}4$ atoms/b-cm	Solution height	$= 100$ cm
N_{238}	$= 2.0909\text{e-}3$ atoms/b-cm		
N_{Fluorine}	$= 4.3996\text{e-}3$ atoms/b-cm		
N_{Hydrogen}	$= 5.7058\text{e-}2$ atoms/b-cm		
N_{Oxygen}	$= 3.2929\text{e-}2$ atoms/b-cm		
N_{total}	$= 9.6586\text{e-}2$ atoms/b-cm		

Aluminum Container:

$$\rho = 2.70 \text{ g/cc}$$

Tank thickness	$= 0.1587$ cm
Bottom thickness	$= 0.1587$ cm
Inside height	$= 110.0$ cm
Inside Radius	$= 20.12$ cm

Appendix B shows how the atom densities for this problem were calculated.

3.4 EXAMPLE 3 SETUP

3.4.A Geometry

Figure 3-1 shows the geometry for this example.

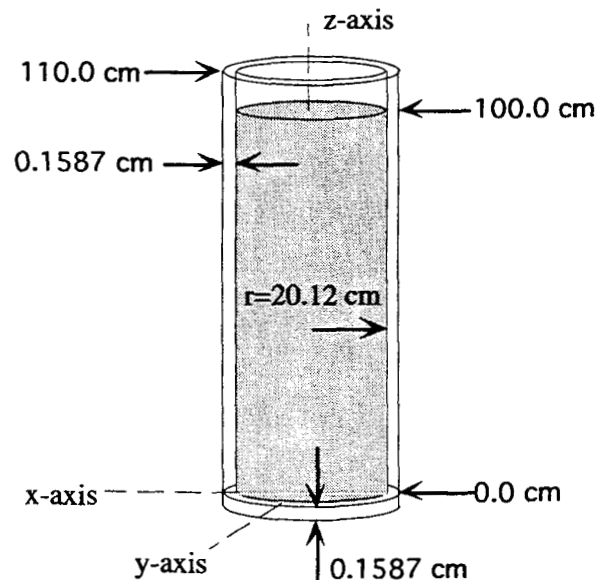


Figure 3-1. Example 3 geometry.

Surfaces

This example again uses cylinders and planes to construct the model. We want to look at how these surfaces are arranged. On your own, try to define the surfaces using what you have learned. Refer to the problem description for the dimensions of the problem. So your problem matches ours, set up your cylinders and planes on the z-axis with the bottom plane (surface 6) of the aluminum container at $z = -0.1587$. Once you are finished, the surface cards should be similar to those in Figure 3-2. Figure 3-3 shows a diagram of the tank with the surfaces and cells labeled.

C	Surface Cards
1	cz 20.12
2	cz 20.2787
3	pz 0.0
4	pz 100.0
5	pz 110.0
6	pz -0.1587

Figure 3-2. Example 3 surface cards.

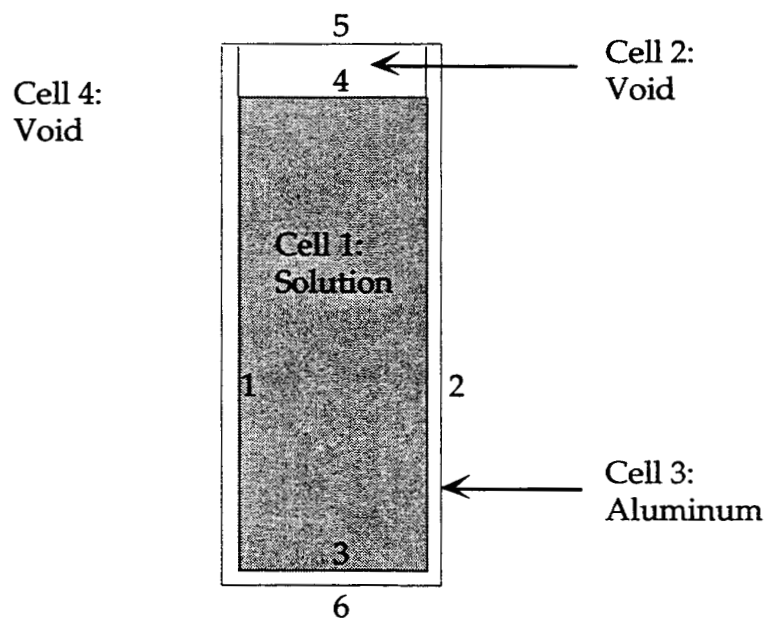


Figure 3-3. Example 3 cells and surfaces.

Cells

The cell card section begins with the problem title card,

Example Problem 3. S(alpha, beta) Treatment.

Cell 1 contains material 1 (the uranium solution) and is assigned a neutron importance of 1. It is everything inside the cylinder (surface 1), and above the plane at 0.0 (surface 3), and below the plane at 100.0 (surface 4); i.e., -1 3 -4.

Cell 2 is the region above the top of the uranium solution and below the top of the aluminum container, described as inside surface 1, and above surface 4, and below surface 5, written as -1 4 -5. This is a void, so the material number is zero. This cell should not be assigned an importance of zero because there is a slight chance of neutrons entering this cell and then returning to the solution by scattering off of the aluminum container. Therefore, it is assigned an importance of 1.

Order of Operation

In some problems it may be necessary to use parentheses to group the ordering of geometric operations. The order of operation is the same as the order of operation followed in mathematics, where the **union** operator is the same as addition and the **intersection** operator is multiplication. MCNP first clears parentheses, doing intersections before unions, from left to right. For example, if you had three spheres, 1, 2, and 3, and you want the intersection of space inside of surfaces 2 and 3 to be unioned with the space inside of surface 1. For the geometry shown in case 1 below, here are two ways it could be written.

-1:-3 -2 is equivalent to -1: (-3 -2)

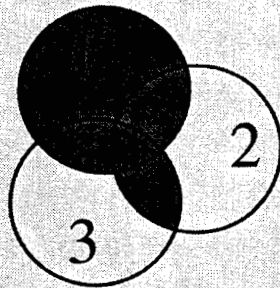
These expressions are equivalent because, with or without the parentheses, MCNP will perform the intersection of surfaces 2 and 3 before the union with surface 1.

An example of when parentheses change the evaluation of the expression...

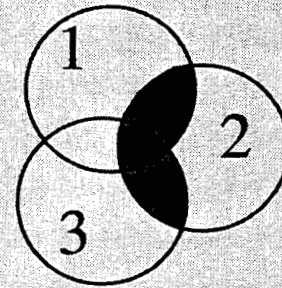
$-1:-3 -2$

is not equivalent to

$(-1:-3) -2$



Case 1



Case 2

In case 2, the parentheses are cleared first. The space inside surface 1 is added to the space inside surface 3, and that region is intersected with the space inside surface 2. In case 1, the space inside surface 3 is intersected with the space inside surface 2, and that region is added to the space inside surface 1. As illustrated, the parentheses around the union operator creates a much different geometry.

Remember, the order of operations is the same as doing simple algebra. Perform operations in parentheses first, doing intersections before unions, from left to right.

Continuing with our example, cell 3 is the aluminum container. You can describe the aluminum container in at least three ways. We show one way here by treating the container as a combination of an aluminum shell plus a bottom disk. The axial region (1 -2 -5 3) is unioned with (or added to) the bottom region of aluminum (-2 -3 6), written (1 -2 -5 3) : (-2 -3 6). Cell 4 is the "rest of the world" void cell. The union operator is used again to describe everything outside of the solution and aluminum container. The cell cards for this geometry are shown in Figure 3-4.

Example Problem 3. S(alpha, beta) Treatment						
C	Cell Cards					
1	1	9.6586e-2	-1	3 -4		imp:n=1
2	0		-1	4 -5		imp:n=1
3	2	-2.7	(1 -2 -5 3) :	(-2 -3 6)		imp:n=1
4	0		2:5:-6			imp:n=0

Figure 3-4. Example 3 cell cards.

Alternative Cell 3 Descriptions

Convince yourself that the two alternative descriptions of cell 3 that follow are correct.

```
3  2  -2.7  -5  1  -2  3
```

```
5  2  -2.7  -2  -3  6
```

or

```
3  2  -2.7  (1:-3)  -5  -2  6
```

3.4.B Materials

Material 1 is the uranium solution. The uranium is in the form of UO_2F_2 in water (H_2O), so we have two oxygen concentrations. The two have been combined in this case but can be left separate. Following the m1 card is the S(α,β) card (mt1) that specifies that the S(α,β) cross section data for hydrogen are to be applied to material 1. The light water identifier, lwtr, tells the code to apply the S(α,β) treatment to the hydrogen present in material 1 and treat it as if bound in light water instead of as a free gas. {Appendix G of the MCNP manual gives a complete listing of available S(α,β) materials.}

Aluminum, which has an atomic number of 13 and an atomic weight of 27, is material 2. The zaid is 13027. *The atomic weight is always input as three integers so a zero must precede any atomic weight between 10 and 99 while two zeros must precede atomic weights less than 10.* Aluminum is the only isotope being used in material 2 so we can enter an atom fraction of 1; 100 percent of the material is aluminum. Figure 3-5 shows the material cards for this problem.

C Data Cards

```
m1  1001  5.7058e-2  8016  3.2929e-2
    9019  4.3996e-3  92238  2.0911e-3
    92235  1.0889e-4
mt1  lwtr
m2  13027  1
```

Figure 3-5. Example 3 material cards.

3.4.C MCNP Criticality Controls

The kcode card is identical to our previous examples. On the ksrc card, we will put the source at approximately the center of the solution, or at the coordinates (0, 0, 50.0). Figure 3-6 shows the controls for this example.

```
kcode 1000 1.0 15 115  
ksrc 0 0 50.0
```

Figure 3-6. Example 3 control cards.

Setting the Criticality Problem Controls

The following discussion presents guidelines for performing criticality calculations. Each problem should be examined to assess if these guidelines are appropriate. The Monte Carlo method can exhibit a small bias in the calculated k_{eff} . If at least 500 neutrons per k_{eff} cycle are used, this bias should not be a factor in MCNP results. The larger the number of neutrons per k_{eff} cycle requested in the first entry on the kcode card, the smaller the bias. Therefore, it is wise to run as many neutron histories as you can afford, combined with using at least 100 active k_{eff} cycles. One hundred is a large enough number of active cycles to determine that the problem appears to be behaving normally and the fission source is converged. At least 30 active cycles are required by MCNP to produce the final table of k_{eff} results. Fewer active cycles do not provide enough information to assess the quality of the calculation. In addition, the creation of confidence intervals not provided by MCNP is more difficult with a smaller number of cycles because the number of degrees of freedom in the k_{eff} result must be taken into account carefully.

There is no maximum number of cycles that can be calculated. The number of active cycles should not become so large that the estimated standard deviation in the final k_{eff} result becomes much smaller than the very small bias in k_{eff} . Typically, 100 to 500 active k_{eff} cycles should be acceptable.

The initial guess of k_{eff} (the second entry on the `kcode` card) only affects the creation of fission source points for the second k_{eff} cycle. A severe underestimate of the initial guess will result in the creation of too many source points and vice versa. Source points in future cycles are unaffected by the initial guess of k_{eff} .

Enough k_{eff} cycles must be declared to be inactive (the third entry on the `kcode` card) so that the calculated spatial fission source has converged. The closer the initial source approximates the converged spatial shape, the fewer cycles you need to skip. Point sources can be specified easily using the `ksrc` card. It is wise to put at least one point into each fissionable region, especially for largely-spaced array elements. Reactor problems that have thousands of fuel rods do not require as many initial points because the rods are in close proximity to one another. It is usually best to skip at least 10 k_{eff} cycles for a `ksrc` initial source.

A uniform source can be created using the source definition `sdef` card and usually requires that fewer k_{eff} cycles be skipped. The best initial source distribution is from an `SRCTP` file from a previous calculation of a similar system. This file is automatically created by MCNP for every criticality calculation. Even fewer k_{eff} cycles usually can be skipped in this case. [See Chapter 2, Section VIII, in the MCNP manual for more discussion of these topics.]

3.4.D Example 3 MCNP Input File

This completes the input requirements for example 3. Your completed input file should resemble the following. Do not forget the blank line delimiters.

```

Example Problem 3. S(alpha, beta) Treatment
C    Cell Cards
1    1  9.6586e-2    -1 3 -4                imp:n=1
2    0                -1 4 -5                imp:n=1
3    2  -2.7          (1 -2 -5 3):(-2 -3 6)    imp:n=1
4    0                2:5:-6                imp:n=0

C    Surface Cards
1    cz  20.12
2    cz  20.2787
3    pz  0.0
4    pz  100.0
5    pz  110.0
6    pz  -0.1587

```

```

C   Data Cards
m1   1001  5.7058e-2  8016  3.2929e-2
      9019  4.3996e-3  92238 2.0909e-3
      92235 1.0889e-4
mt1   lwtr
m2   13027 1
kcode 1000 1.0 15  115
ksrc   0 0 50.0

```

3.4.E Output

After successfully running the problem, you should get a k_{eff} of approximately 1.0 (0.9978 with an estimated standard deviation of 0.0027 on a SPARC 1 at the University of New Mexico). If you run the same problem without the $S(\alpha,\beta)$ treatment you will see a noticeable difference in k_{eff} (0.9823 with an estimated standard deviation of 0.0025 on a SPARC 1 at the University of New Mexico). Much larger differences are possible, depending on the problem. It is not our intent to say $S(\alpha,\beta)$ treatment must be used for materials for which evaluations do not exist. However, for the majority of criticality calculations, it is **strongly** recommended that the appropriate $S(\alpha,\beta)$ cross sections be used. We want to stress the fact that you must analyze the system you are modeling and decide which method is appropriate for what you are analyzing.

A situation may arise where you would want $S(\alpha,\beta)$ thermal treatment but the cross sections for that material do not exist. Lucite ($\text{C}_4\text{H}_6\text{O}_2$) is an example. The thermal treatment should be used for this material, but $S(\alpha,\beta)$ cross sections for Lucite do not exist. You can run the problem with the free gas treatment or make an $S(\alpha,\beta)$ substitution on the mt card. Polyethylene or water $S(\alpha,\beta)$ data for hydrogen could be used. $S(\alpha,\beta)$ cross sections are available for both of these. Polyethylene would probably be the best substitution because both polyethylene and Lucite are linked hydrocarbons and solids. You should run all reasonable options available and choose the most conservative result.

We refer to the use of the $S(\alpha,\beta)$ thermal neutron cross sections for problems at room temperature. While most criticality applications will make use of the room temperature evaluations, there may be a need for cross sections at different temperatures. The MCNP cross section library contains many thermal neutron cross sections for materials at varying temperatures.

3.5 MCNP k_{eff} OUTPUT

Examine the dashed box on the "keff results for:" page. This box will be produced for at least 30 active cycles as long as at least one k_{eff} estimator set of values appears normally distributed at the 99% confidence level. The final result in the box is the estimated value of k_{eff} using a combination of the three individual estimators along with its estimated standard deviation. Estimated 68%, 95% and 99% confidence intervals are given in the box.

Final k_{eff} Estimator Confidence Interval

Calculating k_{eff} consists of estimating the average number of fission neutrons produced in one fission generation per fission neutron born. A fission generation is the life of fission neutrons from birth to death by escape, parasitic capture, or absorption leading to fission. The computational equivalent of a fission generation in MCNP is the k_{eff} cycle. The number of neutrons calculated in each k_{eff} cycle is specified by the first entry on the kcode card. As these fission neutrons are born, transported, and terminated in a k_{eff} cycle, the fission source points are created for the next k_{eff} cycle. It is essential that enough k_{eff} cycles are skipped, using the third entry on the kcode card, before k_{eff} values are accumulated so that the fission source distribution has converged to the correct spatial shape. A poorer initial spatial distribution requires that more k_{eff} cycles be skipped before convergence is achieved.

MCNP uses three different methods for calculating k_{eff} from each neutron random walk in a cycle: absorption, collision, and track length. [See Chapter 2, Section VIII, of the MCNP manual for more details.] Because no one k_{eff} estimator is optimal for all problems, MCNP uses a statistical combination of all three to provide a combined k_{eff} estimate. In general, the combined k_{eff} estimate is the best one to use and is the result enclosed in the dashed box in the output. Always examine all the k_{eff} results on the k_{eff} results page. If one k_{eff} estimator produces a more conservative result from the calculation, this result can be used.

The combined k_{eff} estimate is usually between the extreme k_{eff} values. Occasionally when the three k_{eff} estimators are highly positively correlated, the

combined k_{eff} estimate will lie outside the extreme values. This behavior is expected because if one k_{eff} estimator is above the precise k_{eff} result, the others are likely also to be above that result because of the positive correlation. The reverse is also true. It is extremely important to emphasize that the k_{eff} result from a Monte Carlo criticality calculation is a confidence interval for k_{eff} that is formed by adding and subtracting a multiple of the final *estimated* standard deviation from the final *estimated* k_{eff} . A properly formed confidence interval from a valid calculation should include the precise k_{eff} result the fraction of the time used to create the confidence interval. The fraction of the time determines the multiplier of the *estimated* standard deviation. There will always be some probability that the precise result lies outside of the confidence interval. MCNP provides the *estimated* final k_{eff} confidence intervals at the 68%, 95%, and 99% levels when at least 30 active k_{eff} cycles have been calculated. [Further discussion on many aspects of k_{eff} confidence intervals are described in the MCNP manual, Chapter 2, Section VIII.]

Returning to our problem, examine the first three lines after the title card on the "keff results for:" page. The first line describes the initial source used. The second line provides information about the criticality problem defined on the kcode card. The third line shows what was actually run for this problem.

the initial fission neutron source distribution used the 1 source points that were input on the ksrc card.

the criticality problem was scheduled to skip 15 cycles and run a total of 115 cycles with nominally 1000 neutrons per cycle.

this problem has run 15 inactive cycles with 14919 neutron histories and 100 active cycles with 99850 neutron histories.

Continuing on, the fourth line tells you if the problem finished. The fifth line is extremely important because it states whether or not all cells containing fissionable material were sampled. If all the cells containing fissionable material were not sampled, a warning message will be printed with a list of the cells that were not sampled. Such a calculation should probably be rerun with more settling cycles, and/or a different initial spatial source distribution to ensure sampling of all cells with fissionable material.

this calculation has completed the requested number of k_{eff} cycles using a total of 114769 fission neutron source histories.

all cells with fissionable material were sampled and had fission neutron source points.

The next part of the output describes the results of the normality checks for each of the three k_{eff} estimators. The number of neutrons per cycle is usually large enough so that the individual k_{eff} estimators will appear to be distributed as though they were sampled from a normal distribution. MCNP checks to see if the k_{eff} values appear to be normally distributed, first at the 95% confidence level, and, if not, then at the 99% confidence interval. A WARNING is printed if an estimator appears not to be normally distributed at the 99% level. This situation is equivalent to a 99% confidence interval not including the precise answer, which will occur 1% of the time.

It is unlikely that all three of the k_{eff} estimators will not appear normally distributed at the same time. MCNP will not print the dashed box results in this case, although the results are available elsewhere in the output. Additional information is supplied in the output to assist the user in determining the cause of this behavior. One situation that can cause this behavior to occur is when the fission neutron source has not converged. Even when all three sets of k_{eff} data appear not to be normally distributed, it is still possible that each of the three *average* k_{eff} results would be normally distributed if many independent calculations were made. The user is cautioned to examine the problem output carefully to assess the possible cause(s) for the nonnormal behavior. Additional independent calculations can be made, if necessary, using the dbcn card. {See Chapter 3 and Chapter 5 of the MCNP manual for more information.}

Continuing a Calculation From RUNTPE and Customizing the OUTP File

An MCNP calculation can be continued for more k_{eff} cycles by using the RUNTPE file that is generated automatically for all problems. RUNTPE contains all of the problem information and the calculated results, including the fission source point information for the next cycle. The input file for a continued run requires only the following two cards:

```
continue
kcode      1000 1.0 10 210
```

Only the fourth entry on the kcode card is used. It sets a new upper limit to the total number of active cycles to be run in the calculation. Runs can be continued any number of times. The MCNP execution line for a continue run is:

```
mcnp c inp=filename1 runtpe=filename2
```

where filename1 is the input file shown above and filename2 is the name of the RUNTPE file. If you lose the output file from a calculation, it can be regenerated from the RUNTPE with the following continuation input file:

```
continue
nps -1
```

The length of the OUTP file can be controlled by the print card. A print card followed by no entries provides all of the MCNP output possible. Numerical entries can include or exclude selected print table numbers from the output. { See Chapter 3 of the MCNP manual. }

3.6 SUMMARY

After completing the first three chapters of this Primer you should be able to model successfully any simple system that does not involve repeated structures or arrays. After running a problem you should be able to determine from the output whether or not the run was successful.

The main objective of this chapter was to demonstrate and show the effects of $S(\alpha,\beta)$ thermal neutron cross sections. In the field of criticality safety, you will find that in most cases the appropriate $S(\alpha,\beta)$ cross sections should be used, but it is up to you to determine which set of cross sections will give the best analysis of the problem. When possible, multiple runs should be done to understand the system and to know what is driving the system. Remember, the $S(\alpha,\beta)$ thermal neutron cross sections used in this chapter are at room temperature. If needed, other temperatures neutron cross sections are provided in the MCNP cross section library.

This chapter gave a description of some of the statistical output features of MCNP for criticality purposes that helps you determine if a run is statistically a success or if it should be rerun.

Chapter 4

Simple Repeated Structures

This chapter is designed to introduce the repeated structure capability of MCNP. A cell can be defined in one location and easily be repeated at different locations with different properties, if desired. Square and triangular lattice arrays are described in later chapters.

4.1 WHAT YOU WILL BE ABLE TO DO

- Use the universe (u) and fill cards.
- Use the like m but card.
- Use the trcl card.
- Use the 2-D color geometry plotting capability.

4.2 PROBLEM DESCRIPTION

This example consists of two identical $\text{U}(93.4)\text{O}_2\text{F}_2$ solution cylinders inside a water tank (LA-10860 p. 123). Assume the water reflector density is 1 g/cc and has a minimum thickness of 20 cm except on one side of the first cylinder where the thickness is only 10 cm. The height of the water is at the top of the open aluminum containers. The data for this problem is:

Uranium Solution

$$N_{235} = 1.1760\text{e-}3 \text{ (0.48 g/cc)}$$

$$N_{238} = 8.2051\text{e-}5$$

$$N_{\text{Oxygen}} = 3.3621\text{e-}2$$

$$N_{\text{Hydrogen}} = 6.2210\text{e-}2$$

$$N_{\text{Fluorine}} = 2.5161\text{e-}3$$

$$N_{\text{Total}} = 9.9605\text{e-}2$$

$$\text{Solution height} = 70.2 \text{ cm}$$

$$\text{Diameter} = 12.7 \text{ cm}$$

Aluminum Container

$$\rho = 2.7 \text{ g/cc}$$

$$\text{Height} = 80.0 \text{ cm}$$

$$\text{Surface separation} = 4.0 \text{ cm}$$

$$\text{Inner diameter} = 12.7 \text{ cm}$$

$$\text{Thickness} = 0.15 \text{ cm}$$

4.3 EXAMPLE 4 SETUP

4.3.A Geometry

Figure 4-1 shows the geometry setup for this example.

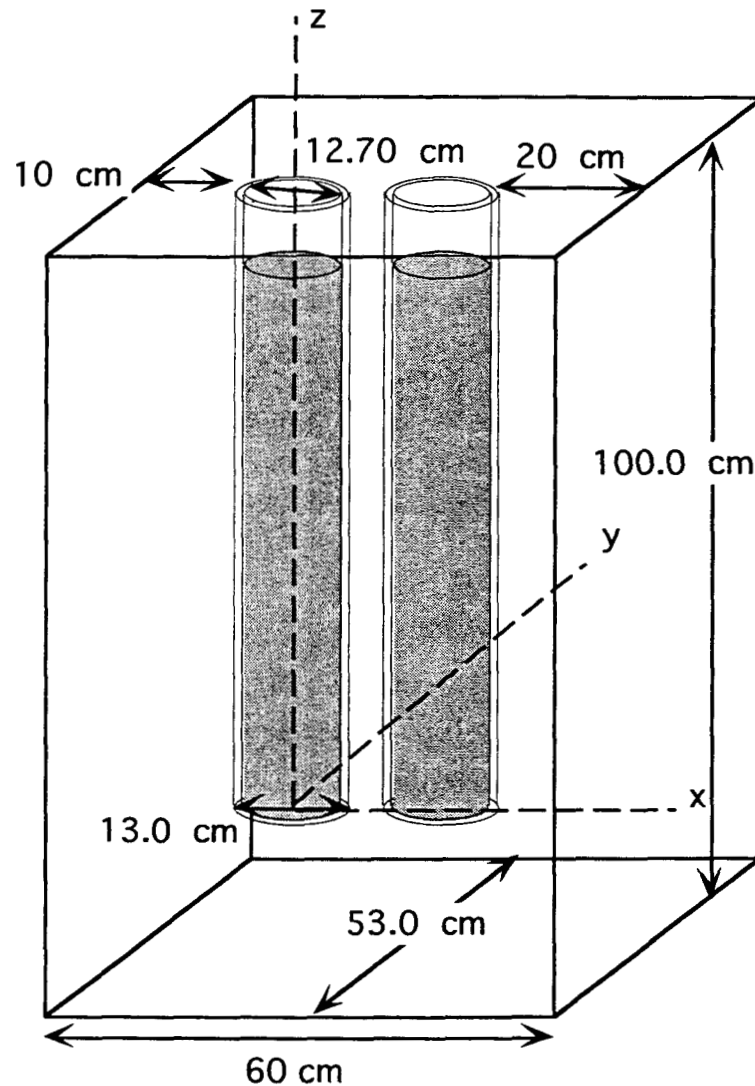


Figure 4-1. Example 4 geometry.

Surfaces

The focus of this chapter is repeated structures so we will define and use surfaces to create one solution cylinder. This solution cylinder, shown in Figure 4-2, requires six surfaces (four planes and two cylinders). We will repeat the first cylinder to form the second cylinder using the `like m` but `command`. Figure 4-3 shows all the surfaces used in example 4. The first six surfaces are used for the cylinder and the last five are used for the water reflector description.

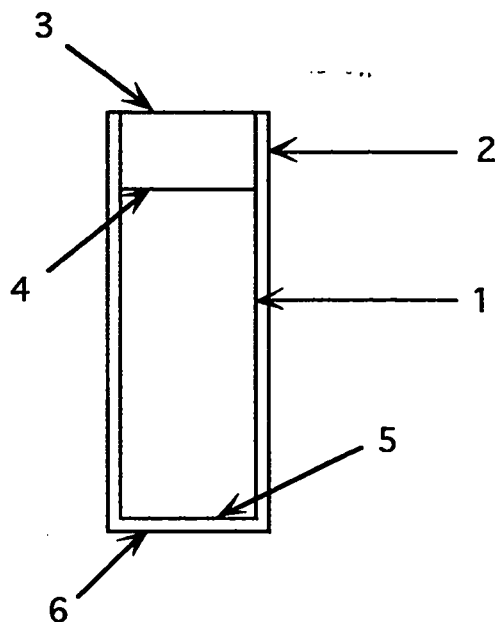


Figure 4-2. Solution cylinder surfaces.

```

C Surface Cards
1  cz 6.35 $ Solution radius
2  cz 6.50
3  pz 80.0 $ Top of container
4  pz 70.2 $ Top of solution
5  pz 0.0
6  pz -0.15
7  pz -20.15 $ Bottom of tank
C Sides of tank
8  px -16.5
9  px 43.5
10 py -26.5
11 py 26.5
    
```

Figure 4-3. Example 4 surface cards.

Cells

We begin the input file in Figure 4-4 with the title card for the problem: Example4, Repeated structures. The problem description tells us we have two identical solution cylinders. Both solution cylinders will be defined with the use of like m but card and universe (u) and fill cards. Cells 1, 2, and 3, the uranium solution, void region above the uranium solution, and aluminum container, respectively, will be defined as part of the same universe.

The Universe Concept

A universe is either a lattice or an arbitrary collection of cells that, once defined, can be used to fill other cells within a geometry. Another way to think of it is to look out a window at the sky. You can see part of the sky but not all of it because of the window edges. There is essentially an infinite amount of sky but you are limited to what the window allows you to see. The window is the filled cell and the sky is the universe that fills the cell.

In this chapter the universe will be a collection of cells. In other words, several cells will be defined to be in a universe and another cell will be filled with that universe. (Lattices will be explained in later chapters of the primer.)

Recalling the card format from Chapter 1, the universe card is entered in the `params` section of the cell card. Universe numbers are arbitrary integers chosen by the user. There are two rules when using universes.

1. The cells of a universe can be finite or infinite but must completely fill all of the space within the cell that the universe is specified to fill.
2. The surfaces of a filled cell and surfaces of the filling universe must never coincide.

If you want to model several open canisters that are half-filled with a solution, such as example 4, the `u` and `fill` cards make this easy. With the two rules stated above in mind, let's create an open cylinder partially filled with solution as a universe. We will use the surfaces already defined in Figure 4-3. The solution, aluminum canister, and void region above the solution will be defined as universe 3. These three cells are analogous to the sky that we use to fill the window. The first cell of universe 3 is the uranium solution. The solution includes all points that have a negative sense with respect to surface 1 intersected with the negative sense of surface 4, and intersected with the positive sense of surface 5.

```
1 1 9.9605e-2 -1 -4 5 u=3 imp:n=1
```

Cell 1 contains material 1, has an atom density of $9.9605e-2$, is part of universe 3, and has a neutron importance of 1.

Cell 2 is the void region above the solution. The void includes all points that have a negative sense with respect to surface 1 intersected with the positive sense of surface 4, making it infinite in height. The neutron importance is set to 1 because there is a chance that neutrons could be scattered through this void and into the solution.

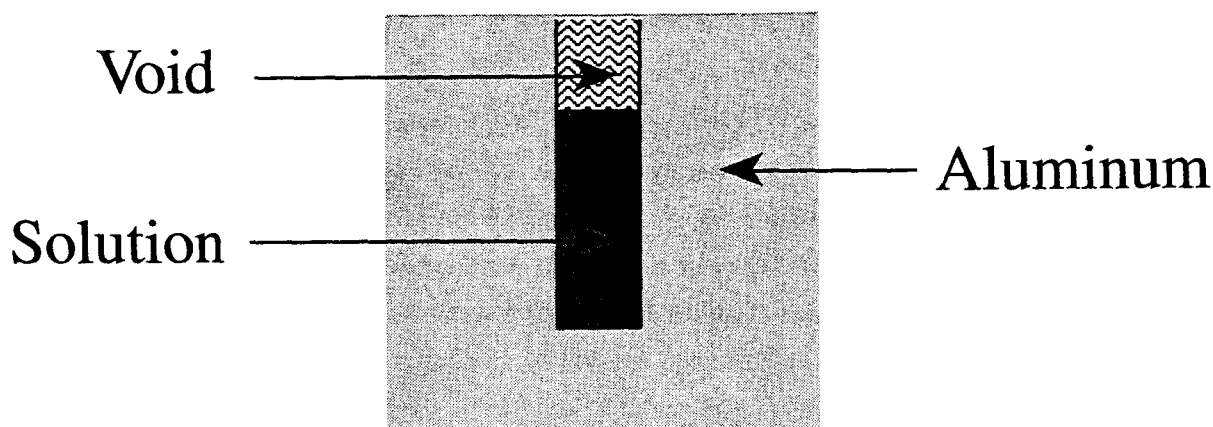
2 0 -1 4 u=3 imp:n=1

Cell 3, the aluminum container, is a union of all points that have a positive sense with respect to surface 1 or the negative sense of surface 5, thus making it infinite outside of surface 1 or below surface 5.

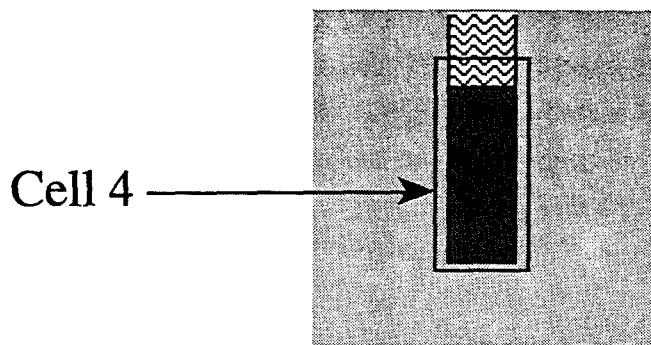
3 2 -2.7 1:-5 u=3 imp:n=1

The specification of the cells in universe 3 is complete. All of the outer cells are infinite (analogous to the sky), so we will not violate rule 1 stated earlier.

After defining these three cells, the geometry in universe 3 is as follows, with the void and aluminum extending to infinity.



We now create cell 4, the window that is filled with universe 3. Cell 4 is defined as a finite cylinder with the desired radius and height (window size).



The cell 4 material number is zero because the materials have been specified in the cells in universe 3. When cell 4 is filled by universe 3, one solution cylinder has been defined as the problem description required.

```
4 0 -2 -3 6 fill=3      imp:n=1
```

Now that we have one of the solution cylinders defined, the second one can be defined using the repeated structures capability of MCNP. A cell can be defined once and repeated many times using the `like m but construct`. This feature reduces the amount of input required from the user. In this example we will use the `like m but` feature to make the second cylinder. The format of the `like m but` card follows.

```
j like m but list
```

`j` = cell number.
`like` = keyword for cell to be repeated.
`m` = a previously defined cell number that is to be repeated.
`but` = keyword for differences between cells `m` and `j`.
`list` = specifications that define the differences between cells `m` and `j`.

Most of the data cards can be included in the `list` specification {see Chapter 3 of the MCNP manual for a complete listing of cards available}. For this example we will use the `trcl` specification that describes the relation of the origin of one cell to the origin of another.

```
trcl = 01 02 03
```

The first three entries are the `x, y, z` values of the origin of translated cell.

{See Chapter 3 of the MCNP manual.}

Simple *like m but trcl* Example

Assume we have defined cell 1 as a sphere with its origin at (0 0 0). Cell 2 is identical to cell 1 but it is located 10 cm to the left and 20 cm above cell 1 making the cell 2 origin (-10 0 20). Cell 2, using the *like m but* card, is defined as follows. The parentheses are required.

```
2 like 1 but trcl (-10 0 20)
```

Now let's continue with example 4. After defining the first solution cylinder, cell 4, using the *u* and *fill* cards, we want to create a second, identical solution cylinder with the *like m but* card, cell 5, and translate it along the x-axis with the *trcl* mnemonic so that the surface separation between the aluminum tanks is 4.0 cm.

A cell is translated relative to the coordinates of its origin. The origin of the cell being repeated is (0, 0, 0). The center-to-center spacing of the two solution cylinders is 17 cm. By simply translating the origin of cell 4, filled with universe 3, a second, identical solution cylinder is defined. The cell 5 description follows.

```
5 like 4 but trcl (17 0 0)
```

The cell cards are completed by defining the water reflector around the two solution cylinders, cell 6, and the "rest of the world" region outside the water reflector, cell 7. Your knowledge of MCNP at this point should allow you to define these two cells using surfaces 7-11 in Figure 4-3. The complete cell card section is shown in Figure 4-4, and identification of the cells is shown in Figure 4-5.

Example4, Repeated structures.

C Cell Cards

1	1	9.9605e-2	-1 -4 5	u=3	imp:n=1	\$ Solution
2	0		-1 4	u=3	imp:n=1	\$ Void region
3	2	-2.7	1:-5	u=3	imp:n=1	\$ Al container
4	0		-2 -3 6	fill=3	imp:n=1	
5	like 4 but trcl (17 0 0)				imp:n=1	
6	3	-1.0	10 -11 8 -9 7 -3	#4 #5	imp:n=1	
7	0		-10:11:-8:9:-7:3		imp:n=0	

Figure 4-4. Example 4 cell cards.

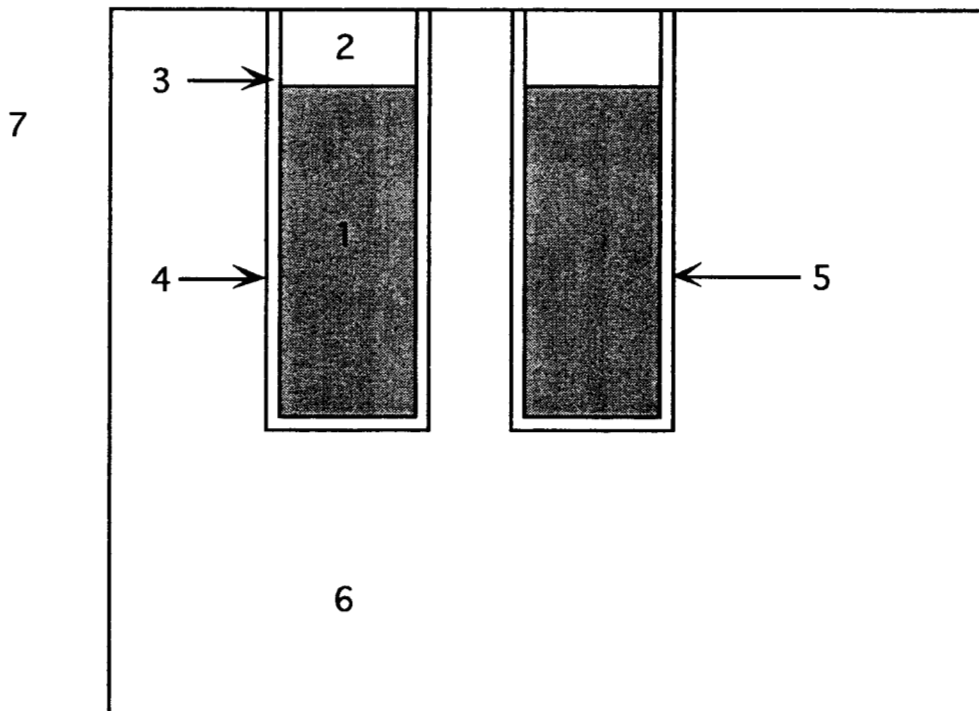


Figure 4-5. Example 4 cell diagram. (Not to scale)

4.3.B Materials

Use the information given in the problem description to define the material cards. Material 1 is the uranium solution. Material 2 is the aluminum container. Material 3 is the water for the reflector. Figure 4–6 shows the material cards for this example. The m1 card uses atom densities for the solution. The m2 and m3 cards use the number of atoms per molecule for aluminum and water, respectively. Both methods of material input are appropriate and selection of either method is generally based on the data available for the problem. A WARNING message will be printed in the output because the atom fractions on the m3 card do not add up to either the density on the cell 6 card or to 1.0. MCNP will renormalize the values given and continue executing the problem. Light water $S(\alpha,\beta)$ cross sections are used for both the uranium solution and water reflector because both contain hydrogen bound in the water molecule.

```
m1      1001  6.2210e-2  8016  3.3621e-2  9019  2.5161e-3
        92235  1.1760e-3  92238  8.2051e-5
mt1     lwtr
m2      13027  1.0
m3      1001  2      8016  1
mt3     lwtr
```

Figure 4–6. Example 4 material cards.

4.3.C MCNP Criticality Controls

The kcode specification remains the same as previous examples, but there is one change in the ksrc card. We have added a second initial source point for the additional solution cylinder. One of the reasons for this change is to ensure efficient sampling of the fissile material in the second solution cylinder. Without the added source point, the number of settling cycles chosen for the kcode card would need to be larger to ensure a converged spatial distribution of fission source points in the second cylinder. Figure 4–7 shows the control cards for this example.

```
C Control Cards
kcode 1000 1.0 15 115
ksrc 0 0 35 17 0 35
```

Figure 4–7. Example 4 control cards.

4.3.D Example 4 MCNP Input File

This completes the input requirements for this example. The completed input file should resemble the following. Do not forget the blank line delimiters.

Example4, Repeated structures.

C Cell Cards

```
1 1 9.9605e-2 -1 -4 5 u=3 imp:n=1 $ Solution
2 0 -1 4 u=3 imp:n=1 $ Void region
3 2 -2.7 1:-5 u=3 imp:n=1 $ Al container
4 0 -2 -3 6 fill=3 imp:n=1
5 like 4 but trcl (17 0 0) imp:n=1
6 3 -1.0 10 -11 8 -9 7 -3 #4 #5 imp:n=1
7 0 -10:11:-8:9:-7:3 imp:n=0
```

C Surface Cards

```
1 cz 6.35 $ Solution radius
2 cz 6.50
3 pz 80.0 $ Top of container
4 pz 70.2 $ Top of solution
5 pz 0.0
6 pz -0.15
7 pz -20.15 $ Bottom of tank
C Sides of tank
8 px -16.5
9 px 43.5
10 py -26.5
11 py 26.5
```

C Control Cards

```
kcode 1000 1.0 15 115
ksrc 0 0 35 17 0 35
m1 1001 6.2210e-2 8016 3.3621e-2 9019 2.5161e-3
92235 1.1760e-3 92238 8.2051e-5
mt1 lwtr
m2 13027 1.0
m3 1001 2 8016 1
mt3 lwtr
```

4.3.E Output

The final combined k_{eff} estimator for this problem on a SPARC 1 at the University of New Mexico was 1.0110 with an estimated standard deviation of 0.0025.

4.4 PLOTTING THE PROBLEM GEOMETRY

After creating the input file, you can generate arbitrary 2-dimensional plots of the geometry. Although the installation of this plotter may vary from machine to machine, the plot commands do not differ between platforms. It is very important to use the plotter to debug geometry problems before trying to run particles. You will save a great deal of time by doing this. Appendix E of this document shows a listing of the plotter commands. [See Appendix B of the MCNP manual for a detailed description of the plotter and plot commands.] The format for plotting follows.

```
mcnp inp=filename ip
```

where ip = initiate and plot

After receiving the plot prompt, pressing the carriage return or enter key will display a default plot. The default plot is a PX slice centered at (0, 0, 0) with an extent of -100 cm to 100 cm on the Y-axis and -100 cm to 100 cm on the Z-axis. Geometry errors are shown as red dotted lines (if using a monochrome monitor, errors are simply dotted lines). Keywords and entries can be entered after the prompt to get any 2-dimensional view desired. Only enough of the keyword has to be typed to make it unique. For example, "or" will specify the origin keyword.

We will discuss seven plot keywords. Although shown here in upper case to set them off from the rest of the text, either upper or lower case is acceptable.

ORIGIN vx vy vz – The coordinate about which the plot is centered.

Default = 0 0 0.

EXTENT eh ev – Sets the scale of the plot in cm so that eh is the horizontal distance from the origin to either side of the plot and ev is the vertical distance from the origin to the top and bottom of the plot. If one value is entered, it is duplicated for the second entry.

Default: 100 100

PX vx – Draws y-z plot plane at x=vx. Default: px 0

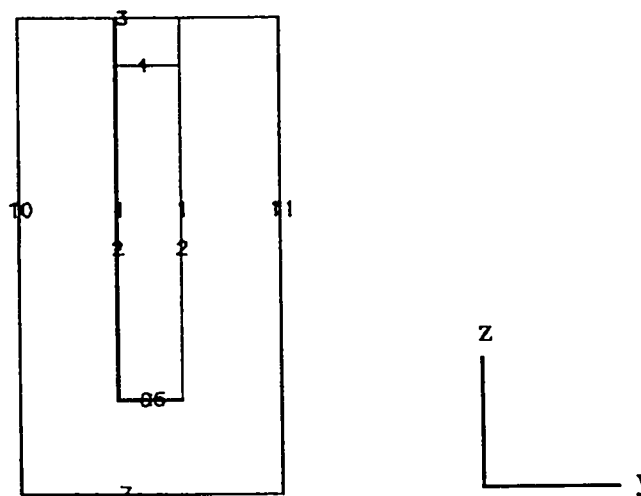
PY vy – Draws x-z plot plane at y=vy.

PZ vz – Draws x-y plot plane at z=vz.

LABEL s c – Put labels of size s on the surfaces and labels of size c on the cells. Default: 1 0 (no cell labels)

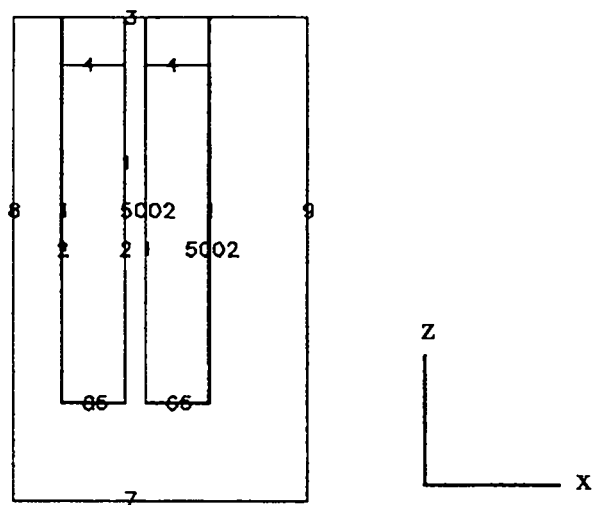
SHADE n color – Make material n the color chosen.

After a carriage return at the plotter prompt you will see a default plot showing a slice through the origin on the y-axis and z-axis with the surfaces labeled.

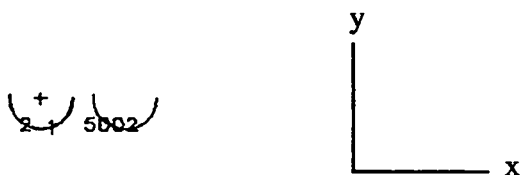


To see a vertical view of both solution cylinders with bigger surface numbers type:

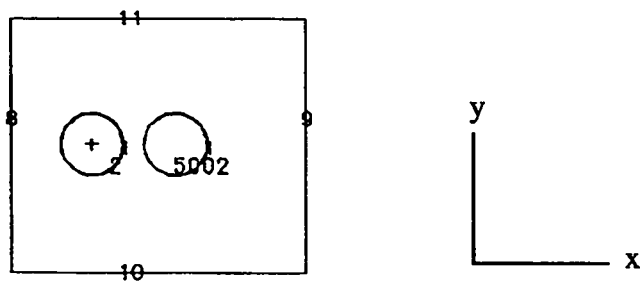
py 0 1a 1.2 0



To see a top view of the cylinders type: pz 80



This plot only draws about half of each cylinder. Plot planes should not coincide with a problem surface. Move the plot plane a small distance away from the plane pz 80 by typing: pz 79



Surfaces Generated by Repeated Structures

This view shows both solution cylinders and the water reflector. Notice that the surfaces of the left cylinder (cell 4) are numbered as defined in the input file. The cylinder on the right is the repeated structure. The outer cylinder surface number is different for cell 5. The inner cylinder is still surface 1, but the outer cylinder is 5002. When using repeated structures, MCNP will renumber the translated surfaces if needed as follows: $1000 \times \text{cell number} + \text{surface number}$. The planes for cell 5 were renumbered also, but because planes are infinite, surfaces 5003 and 5006 are identical to surfaces 3 and 6, and the code prints the WARNING message:

```
2 surfaces were deleted for being the same as others.
```

The surface numbers of the cells in a universe do not get incremented. Surfaces 1, 4, and 5 are in both cells 4 and 5.

To plot cell numbers instead of surface numbers, type:

```
label 0 1
```

To make the size of the cell numbers larger, type

```
la 1 2
```

This puts both cell and surface numbers in the plot and increases the size of the cell numbers. If you have a color terminal, materials in cells are plotted in color. To see the material numbers of cells type:

```
la 0 1 mat
```

Some other cell quantities that can be plotted are:

- den: mass density
- rho: atom density
- mas: mass
- imp:n: importances
- vol: volume
- cel: cell number (default)

To change the color of material 1 from its default color, purple, type:

```
shade 1 yellow
```

To see what colors are available, type:

```
options
```

We suggest that you experiment with the commands to get a feel for how the plotter works.

4.5 SUMMARY

This chapter introduced repeated structures, which is a very powerful capability available in MCNP. With this command you can to create geometries that involve many identical structures and still vary their characteristics. By defining one structure, you are easily able to reproduce that structure in as many places as needed.

Geometry plotting is a powerful tool. By plotting your geometry before transporting particles, geometry errors can be corrected. You can also make sure that the geometry setup is what you actually want it to be by displaying cell quantities.

Chapter 5

Hexahedral (Square) Lattices

This chapter introduces the lattice keyword (`lat`) that allows you to model virtually any square pitch or triangular pitch array. The focus in this chapter is hexahedral lattices while hexagonal (triangular) lattices are covered in Chapter 6. In this document, a hexahedral lattice will be referred to as a square lattice.

5.1 WHAT YOU WILL BE ABLE TO DO

- Use the `lat` keyword to create a square lattice.
- Understand lattice indexing.
- Create a lattice whose elements: contain different materials, are filled with different sized items, or are sometimes empty.

5.2 PROBLEM DESCRIPTION

This example is a 3x2 array of plutonium nitrate solution cylinders (PNL-TR-452). Plutonium nitrate solution is contained in six stainless steel cylinders with a 10 cm surface separation between tanks. We will assume there is no other geometry present for this example such as suspension wires for the tanks and room walls. The data for this problem is:

Plutonium Nitrate Solution

$$N_{239} = 2.7682e-4$$

$$\text{Solution height} = 39.24 \text{ cm}$$

$$N_{240} = 1.2214e-5$$

$$N_{241} = 8.3390e-7$$

$$N_{242} = 4.5800e-8$$

$$N_{\text{Hydrogen}} = 6.0070e-2$$

$$N_{\text{Oxygen}} = 3.6540e-2$$

$$N_{\text{Nitrogen}} = 2.3699e-3$$

$$N_{\text{Total}} = 9.9270e-2$$

Stainless Steel Containers

$$N_{\text{Iron}} = 6.3310\text{e-}2$$

3x2 square lattice

$$N_{\text{Chromium}} = 1.6540\text{e-}2$$

Surface separation = 10.0 cm

$$N_{\text{Nickel}} = 6.5100\text{e-}3$$

Tank i.d. = 24.98 cm

$$N_{\text{Total}} = 8.6360\text{e-}2$$

Tank wall thickness = 0.30 cm

Tank top and bottom thickness = 1.0 cm

Tank inside height = 101.7 cm

Tank pitch = 35.58 cm

5.3 EXAMPLE 5 SETUP FOR CASE I

5.3.A Geometry

Figure 5-1 shows the geometry setup for this example.

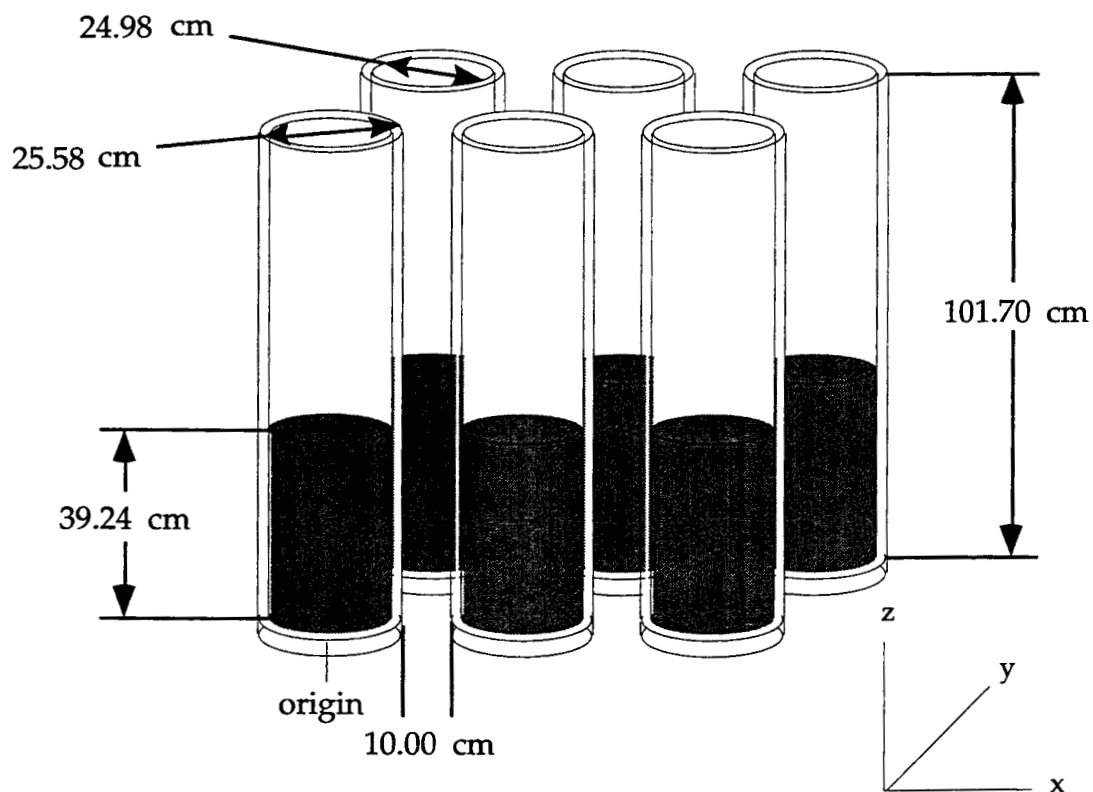


Figure 5-1. Example 5 geometry.

To model the square array we will use three steps. We start with modeling the cylindrical container. Next, a lattice cell is created and filled with the cylindrical container. Finally, we create a cell (or window) that limits the array size to 3x2 as specified in the problem description.

Cylindrical Container Surfaces

This chapter uses the lattice keyword to create a square configuration of plutonium nitrate solution cylinders. To create the cylinders we use the universe card described in the previous chapter; therefore, we need only enough surfaces to define one solution cylinder. First we define the five surfaces needed for the solution, the void above the solution, the stainless steel cylinder, and the void outside the container. Compare your surfaces with those in Figure 5-2.

```
C Solution Cylinder Surface Cards
1  cz 12.49
2  cz 12.79
5  pz 0.0
6  pz 39.24
7  pz 101.7
```

Figure 5-2. Example 5 solution cylinder surface cards.

Cylindrical Container Cells

Remember, we always begin the input file with a title card, Example5, Hexahedral Lattices.

The solution, the void region above the solution, the stainless steel container, and the void outside the container are defined as part of the same universe. That universe will then be used to fill the square lattice. The first cell, cell 1, is the plutonium nitrate solution and is assigned material 1. The material density is input in atoms/b-cm as given in the problem description. Surfaces 1, 5, and 6 with the appropriate sense create a cylinder of solution. Cell 1 is designated as part of universe 1 and the neutron importance is set to 1.

```
1  1  9.9270e-2      -1 5 -6      u=1  imp:n=1
```

A void region exists above the solution to the lid of the stainless steel container, defined as cell 2. Because it is void, it is assigned a material number of 0. Surfaces 1, 7, and 6 create the void cylinder. This cell also belongs to universe 1. Even though this region is a void, there is a chance that neutrons could be scattered through it by the stainless steel and into the solution; therefore, it is given a neutron importance of 1.

```
2  0          -1 6 -7    u=1  imp:n=1
```

Next we define the stainless steel container for the solution, cell 3. We designate the stainless steel as material 2. Once again the material density is entered in atoms/b-cm as given in the problem description. The stainless steel is defined as being inside of surface 2, not in cell 1, and not in cell 2, creating an infinitely tall cylinder of stainless steel except for the solution and void region as shown in Figure 5-3. Cell 3 is also part of universe 1 and is assigned a neutron importance of 1. (A cell 3 alternative equivalent definition is shown and allows faster particle tracking.)

```
3  2  8.6360e-2    -2 #1 #2    u=1  imp:n=1
or
3  2  8.6360e-2    -2 (1:-5:7)  u=1  imp:n=1
```

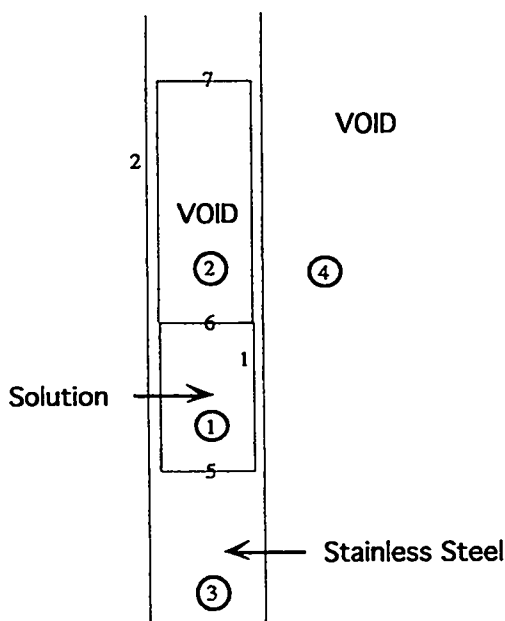


Figure 5-3. Solution container with cell numbers circled and surface numbers.

Cell 4 is the final cell belonging to universe 1. It is the void region outside the solution cylinder, defined as all space with a positive sense with respect to surface 2, in universe 1, with a neutron importance of 1.

```
4  0                                2          u=1  imp:n=1
```

Cells 1-4, all belonging to universe 1, are now complete and will be used to fill lattice elements.

Lattice Cell Surfaces

In this section we define a unit cell in the x-y plane for the lattice. Looking back at the problem description we see that the surface separation between cylinders is 10 cm. The four planes listed in Figure 5-4 are defined so that there is 5 cm between the edge of the stainless steel container and each plane. Add these lines to the surface card section.

```
C  Beginning of Lattice Surfaces
8  px 17.79
9  px -17.79
10 py 17.79
11 py -17.79
```

Figure 5-4. Example 5 lattice cell surface cards.

Lattice Cell Card

When defining a square lattice, MCNP requires that at least 4 sides be specified. Opposite sides must be identical and parallel. Two sides can be omitted, resulting in an infinite lattice in that dimension. A cell is defined to be a lattice with the `lat` keyword that is entered in the `params` section of the cell card.

```
lat = 1          square lattice
```

Cell 5 is the lattice cell and will be filled with the cells belonging to universe 1. Cell 5 is given a material number of 0 because the materials have been defined in cells 1-

4. Cell 5 is all space with a negative sense with respect to (wrt) surface 8, a positive sense wrt surface 9, a negative sense wrt surface 10, and a positive sense wrt surface 11. We have defined a unit slab, infinite in z , that is duplicated in the x and y directions by the `lat` card. The order of these surfaces on the cell card is important. It determines in which spatial directions the lattice indices increase and decrease. Each lattice element has a unique location identifier. The first index increases beyond the first surface listed and decreases beyond the second surface listed, etc., as shown in Figure 5-5. Therefore, surfaces parallel to each other must be listed as pairs. Surface 8 is parallel to surface 9. Surface 10 is parallel to surface 11. The element $[0, 0, 0]$ is the one defined on the cell card.

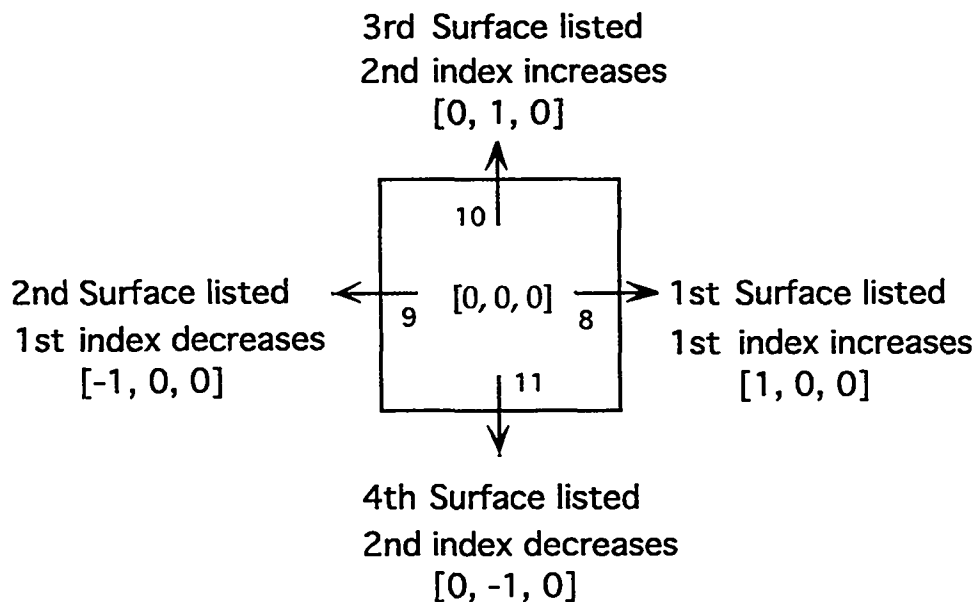


Figure 5-5. How lattice indices are determined.

Surface 8 is opposite surface 9, and surface 10 is opposite surface 11. We define the cell as a square lattice, `lat=1`, and fill the cell with universe 1, `fill=1`. This specification creates an infinite lattice in only the x and y direction. The lattice cell itself is infinite in the $\pm z$ direction. This infinite lattice is designated as universe 2. A neutron importance of 1 completes the cell.

```
5 0 -8 9 -10 11 lat=1 fill=1 u=2 imp:n=1
```

The last step for this problem is to take universe 2, cell 5, and put it in a window to limit it to a 3x2 finite array. We need to define six more surfaces for the problem. Recall an important fact about filled cells and filling universes discussed in Chapter 4.

Surface Constraints for Truncating a Lattice

The surfaces of a filled cell and of the filling universe cannot be coincident. If they are, a fatal error will result because they are in different universes. For a lattice, it is suggested that you make the surfaces of the truncating cell slightly smaller than the array. For example, if a lattice cell has a boundary of $pz = 20.00$ cm, then the window plane could be defined at $pz = 19.99$ cm. The difference is small enough that it will not affect the problem geometry.

Because cell 5 defines an infinite array we can choose a window cell that will enclose any six of the lattice cells. Figure 5-6 shows the surfaces chosen for the window cell. A px plane at 88.95 cm is at the right edge of the third lattice cell from the origin. A px plane slightly to the left, $px = 88.949$ cm, is defined so we include that third unit cell but is not coincident with the lattice cell plane at 88.95 cm ($17.79 \text{ cm} + 2 \times 35.58 \text{ cm}$). The other three planes are defined in the same manner.

```
C  Window Surfaces
3  pz -1.0
4  pz 102.7
12 px 88.949
13 px -17.789
14 py 53.369
15 py -17.789
```

Figure 5-6. Example 5 window surface cards.

Surfaces 3 and 4, the top and bottom of the problem, limit the z -extent so the array height is 103.7 cm.

We can now define cell 6. The material number is zero because the materials have already been defined in cells 1-4. The cell is then bound in the positive sense of surface 13, the negative sense of surface 12, the positive sense of surface 15, the negative sense of surface 14, the positive sense of surface 3, and the negative sense of surface 4. The cell, or window, is filled with universe 2. Remember, universe 2 is the infinite array defined by cell 5. Cell 6 data is completed by entering a neutron importance of 1.

```
6  0      13 -12 15 -14 3 -4   fill=2      imp:n=1
```

Cell 7 defines the "rest of the world", a union of space outside cell 6. It has a material number of 0 and a neutron importance of 0, so that escaping particles are terminated.

```
7  0      -13:12:-15:14:-3:4      imp:n=0
```

or

```
7  0      #6      imp:n=0
```

5.3.B Materials

Material cards should be entered as described in previous chapters using the information provided in the problem description. Because the plutonium is in a solution, light water $S(\alpha, \beta)$ cross-sections should be used for material 1. Your material cards should be similar to those in Figure 5-7.

```
C      Material cards
m1     1001  6.0070-2  8016  3.6540-2  7014  2.3699-3
       94239  2.7682-4  94240  1.2214-5  94241  8.3390-7
       94242  4.5800-8
mt1    lwtr
m2     26000  6.3310-2  24000  1.6540-2  28000  6.5100-3
```

Figure 5-7. Example 5 material cards.

Note that the code will run faster if the major components of the material are listed first. The "e" notation (e-2) used in previous examples is optional and has been omitted here.

5.3.C MCNP Criticality Controls

The kcode specification remains the same from the previous example, but there are changes in the ksrc card. For this example we have placed an initial source point in each solution cylinder to ensure sampling during the settling cycles. Figure 5-8 shows the control cards for this example.

```
C Control Cards
kcode 1000 1.0 15 115
ksrc 0 0      19.62 35.58 0      19.62 71.16 0      19.62
      0 35.58 19.62 35.58 35.58 19.62 71.16 35.58 19.62
```

Figure 5-8. Example 5 control cards.

5.3.D Example 5 Case 1 MCNP Input File

The input for this example is complete. The input file should resemble the following. Do not forget the blank line delimiters. Comments following a \$ have been used on the cell cards.

```
Example5, Hexahedral Lattices.
C Cell Cards
1 1 9.9270e-2      -1 5 -6      u=1 imp:n=1 $Pu Sol.
2 0                -1 6 -7      u=1 imp:n=1 $void
3 2 8.6360e-2      -2 #1 #2     u=1 imp:n=1 $$SS
4 0                2           u=1 imp:n=1 $void
5 0 -8 9 -10 11 lat=1 fill=1    u=2 imp:n=1 $lattice
6 0 13 -12 15 -14 3 -4 fill=2   imp:n=1 $window
7 0 -13:12:-15:14:-3:4         imp:n=0 $outside

C Solution Cylinder
1 cz 12.49
2 cz 12.79
5 pz 0.0
6 pz 39.24
7 pz 101.7
C Beginning of lattice surfaces
8 px 17.79
9 px -17.79
10 py 17.79
11 py -17.79
```

```

C   Beginning of window surfaces
3   pz -1.0
4   pz 102.7
12  px 88.949
13  px -17.789
14  py 53.369
15  py -17.789

C   Control Cards
kcode 1000 1.0 15 115
ksrc 0 0      19.62 35.58 0      19.62 71.16 0      19.62
      0 35.58 19.62 35.58 35.58 19.62 71.16 35.58 19.62

C   Material cards
m1   1001 6.0070-2 8016 3.6540-2 7014 2.3699-3
      94239 2.7682-4 94240 1.2214-5 94241 8.3390-7
      94242 4.5800-8
mt1  lwtr
m2   26000 6.3310-2 24000 1.6540-2 28000 6.5100-3

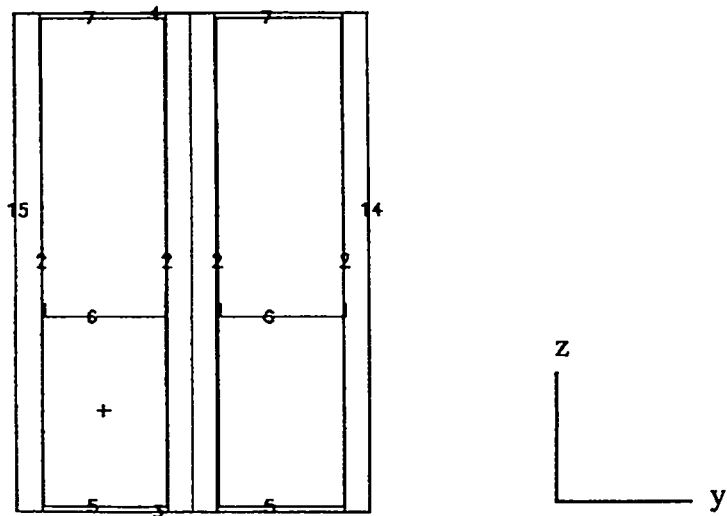
```

5.3.E Output

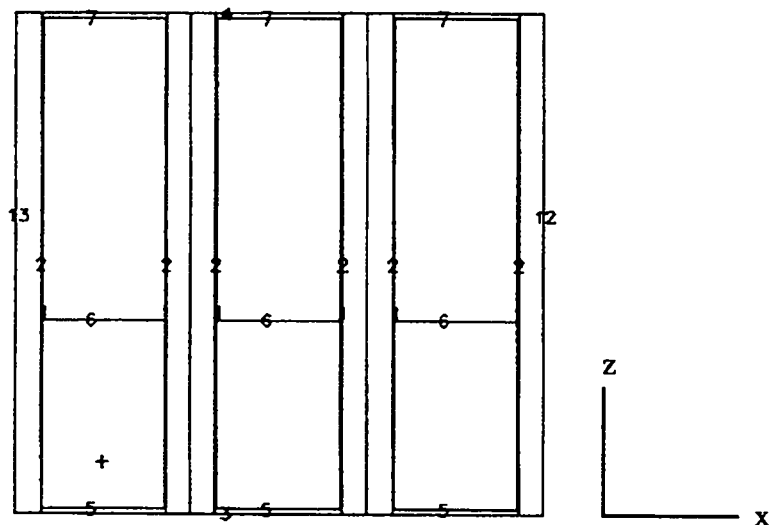
Before transporting particles, be sure to run the plotter to check for geometry errors. The plotter indicates geometry errors by dotted lines. It will only show errors for the plane you are looking at so be sure to look at the problem in the x, y, and z planes. The default plotter view may not show the entire plot. Change the origin of the plot to:

or 0 0 20

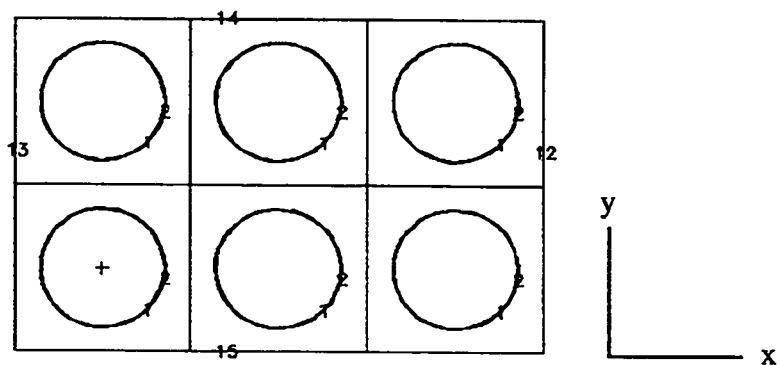
This will give the following plot:



After changing the view to $p_y=0.0$ the plot will look as follows:



A view of the pz plane at 10 cm will look as follows:



The final combined k_{eff} estimator for this problem on a SPARC 1 at the University of New Mexico was 1.0031 with an estimated standard deviation of 0.0027.

5.4 CASE II: CHANGING MATERIALS IN SELECTED ELEMENTS

The case I lattice problem was filled with six identical items. The `fill` specification was a single number that specified the universe that filled every element of the lattice. This example illustrates the expanded form of the `fill` card. Case I is modified by filling two of the containers with graphite.

Filling Lattice Elements Individually

The `fill` specification can be followed by entries that define the lattice range and fill the lattice elements individually. Each lattice element has a unique location identifier. The indices of each lattice element are determined relative to the $[0, 0, 0]$ element defined by the surfaces on the lattice cell card. These indices can be positive or negative integers or zero.

Three pairs of declarators that define the range of the three lattice indices for the x, y and z directions are followed by the universe numbers themselves. The range upper and lower bounds must be explicitly stated, separated by a colon. The range must include all elements that appear in the cell that the lattice fills. For one range pair, -5:5 or 0:10 defines a range of 11 elements, and 0:0 defines 1 element.

Recall that the order of the surfaces on the cell card identifies the ordering of the lattice elements. In this document, the first surface listed is the px plane with the largest x value, the second is the px plane with the smallest x value, the third is the py plane with the largest y value, and the fourth is the py plane with the smallest y value. The elements are incremented as follows: do all x for the first y, first z; do all x for the second y, first z; do all x for all y, first z; do all x for the first y, second z; do all x for second y, second z, etc. A void lattice cell 1 card with the `fill` card completely specified might look like







```
1 0 surface numbers u=1 lat=1 fill= -1:0 0:1 0:0 3 4 5 6
```

Four elements are defined— $[-1, 0, 0]$, $[0, 0, 0]$, $[-1, 1, 0]$, $[0, 1, 0]$ — and they are filled with different universes— 3, 4, 5, and 6, respectively.

Figure 5-9 shows the indices of the lattice elements of our problem. In this example, we want the solution cylinders in lattice elements $[2, 0, 0]$ and $[1, 1, 0]$ to be filled with material 3. The other four lattice elements will contain material 1, as before. Cell 5 is the lattice cell and therefore locates the $[0, 0, 0]$ element of the lattice. Only the elements that appear in cell 6 filled by the lattice should be included in the range.

Because 8 is the first surface number on the cell 5 card, the x range index increases beyond (to the right of) surface 8. Because 9 is the second surface number on the cell 5 card, the x index decreases beyond (to the left of) surface 9. Cell 6 encloses three elements in the plus x direction and zero elements in the minus x direction, so the first range declarator is 0:2.

Because 10 is the third surface number on the cell 5 card, the y range index increases beyond (above) surface 10. Because surface 11 is the fourth surface listed on the cell 5 card, the y range index decreases beyond (below) surface 11. Cell 6 encloses two elements in the plus y direction and zero elements in the minus y direction, so the second range declarator is 0:1. The lattice is infinite in the z direction, so there is only one element in the z direction, indicated by a range declarator of 0:0. Recall that this infinite lattice is truncated by cell 6.

$u=1$  $[0, 1, 0]$	$u=3$  $[1, 1, 0]$	$u=1$  $[2, 1, 0]$
$u=1$  $[0, 0, 0]$	$u=1$  $[1, 0, 0]$	$u=3$  $[2, 0, 0]$

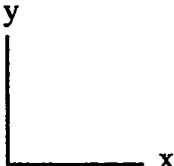


Figure 5-9. Lattice indices and universes for Case II.

Following the range declarators are the universe values themselves that fill each element of the declared lattice. Cell 6 encloses six elements, so we enter six universe numbers. Elements $[0, 0, 0]$ and $[1, 0, 0]$ are filled by universe 1, element $[2, 0, 0]$ is filled by universe 3, element $[0, 1, 0]$ is filled by universe 1, element $[1, 1, 0]$ is filled by universe 3, and element $[2, 1, 0]$ is filled by universe 1.

The complete lattice cell 5 card for Case II is:

```
5  0  -8 9 -10 11 lat=1 u=2 fill=0:2 0:1 0:0  1 1 3  1 3 1 imp:n=1
```

Now we must define the cells belonging to universe 3. Cells 1-4 belong to universe 1. The geometry for universe 3 is identical to that of universe 1. Only the material in cell 1 is different. The four cells belonging to universe 3, shown below, can be added to the cell card section after cells 1-4.

```
11  like 1 but mat=3 rho=-1.60 u=3  imp:n=1
12  like 2 but                      u=3  imp:n=1
13  like 3 but                      u=3  imp:n=1
14  like 4 but                      u=3  imp:n=1
```

We have said that cell 11 has material 3, graphite. This material is new, so an m3 card must be added to the data card section. The $S(\alpha, \beta)$ thermal neutron treatment for graphite has been included.

```
m3  6012 1
mt3 grph
```

5.5 CASE III: A LATTICE WITH ONE EMPTY ELEMENT.

A modification to Case II is to make element $[0, 0, 0]$ contain no cylinder at all. If a universe number on the fill card is the same as the universe of the lattice cell itself, that element is filled with the material specified on the lattice cell card. The material in cell 5 is zero – a void. Cell 5 belongs to universe 2. The following cell card causes element $[0, 0, 0]$ to be void as shown in Figure 5-10.

```
5  0  -8 9 -10 11 lat=1 u=2 fill=0:2 0:1 0:0  2 1 3  1 3 1 imp:n=1
```



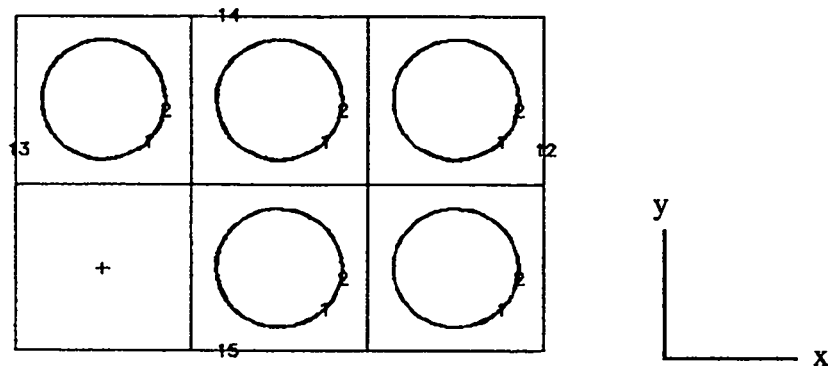


Figure 5-10. Plot of 3x2 array with empty element.

5.6 CASE IV: CHANGING SIZE OF CELLS FILLING A LATTICE.

In Case IV we want to change the radius of the solution cylinder in elements [1, 0, 0] and [2, 1, 0]. In Case I, the inner radius of the cylinder is 12.49 cm (surface 1), and the outer radius is 12.79 cm (surface 2). In Case IV, the inner cylinder radius is 5 cm, and the outer radius is 5.5 cm. The cell 5 card is similar to case II.

```
5  0  -8 9 -10 11 lat=1 u=2 fill=0:2 0:1 0:0  1 3 1  1 1 3 imp:n=1
```

The four cells belonging to universe 3 are defined differently. Two new surfaces will be used and need to be added to the surface card section:

```
21  cz  5
22  cz  5.5
```

Because the geometrical dimensions have changed, we cannot take advantage of the like m but construct. The description of cells 21-24 are very similar to cells 1-4, however. Add these cell cards to the case I input file after cells 1-4.

```
21  3 -1.60      -21  5 -6      u=3  imp:n=1
22  0           -21  6 -7      u=3  imp:n=1
23  2 8.6360e-2 -22 #21 #22    u=3  imp:n=1
24  0           22            u=3  imp:n=1
```

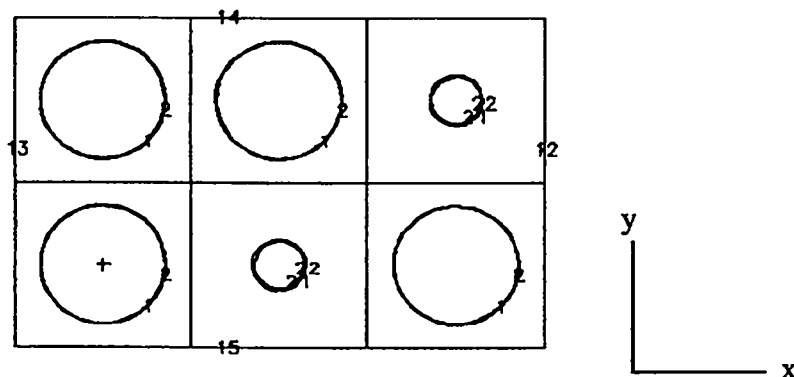
The material in cell 21 is graphite as in case III with a density of 1.60 g/cc. An m3 and an mt3 card need to be added to the data card section.

```
m3 6012 1
mt3 grph
```

If you plot this input file with the following command:

```
pz 0 or 35 20 1 ex 55
```

you see that the radial size of two cylinders is smaller.



5.7 SUMMARY

This chapter introduced the use of lattices with MCNP by modeling a 3x2 square array of solution cylinders. We modeled this system by first defining a single solution cylinder. Next, a cell was created and defined to be a lattice with the `lat` keyword. Finally, a 3x2 array was created by filling an appropriately sized box with the infinite lattice. Three other cases were presented to show how lattices can be set up to provide for elements that do not contain the same materials, or are not the same size, or lattice elements that are empty. After completing this chapter you should be able to model most 2-dimensional square lattice problems.

Three-dimensional lattices are discussed in Chapter 7.

Chapter 6

Hexagonal (Triangular) Lattices

This chapter continues discussion of the lattice keyword (`lat`) by modeling a triangular pitch array.

6.1 WHAT YOU WILL BE ABLE TO DO

- Create general planes to define a hexagonal lattice element.
- Use the `lat` keyword to create a hexagonal (triangular pitch) lattice.
- Understand hexagonal lattice indexing.

6.2 PROBLEM DESCRIPTION

Case I is a hexagonal array of seven open $U(93.2)O_2F_2$ solution cylinders (LA-10860 page 125). The uranium-fluoride solution is contained in seven aluminum cylinders with a 7.60 cm surface separation between cylinders. There is 20 cm of water reflection below and radially about the cylinders. There is no water above the aluminum containers. The data for this problem is:

Uranium-Fluoride Solution

$$N_{235} = 1.3784e-3$$

$$\text{Solution height} = 23.40 \text{ cm}$$

$$N_{238} = 9.9300e-5$$

$$N_{\text{Hydrogen}} = 6.1063e-2$$

$$N_{\text{Oxygen}} = 3.3487e-2$$

$$N_{\text{Fluorine}} = 2.9554e-3$$

$$N_{\text{Total}} = 9.8983e-2$$

Aluminum Containers

$$\rho = 2.70 \text{ g/cc}$$

7 cylinders in equilateral hexagonal
(triangular) lattice

$$\text{Surface separation} = 7.60 \text{ cm}$$

$$\text{Tank i.d.} = 15.20 \text{ cm}$$

$$\text{Tank wall thickness} = 0.15 \text{ cm}$$

Tank bottom thickness = 1.0 cm
Inside height = 40.0 cm
Pitch = 23.1 cm

6.3 EXAMPLE 6 CASE I SETUP

6.3.A Geometry

Figure 6-1 shows the geometry setup for this example.

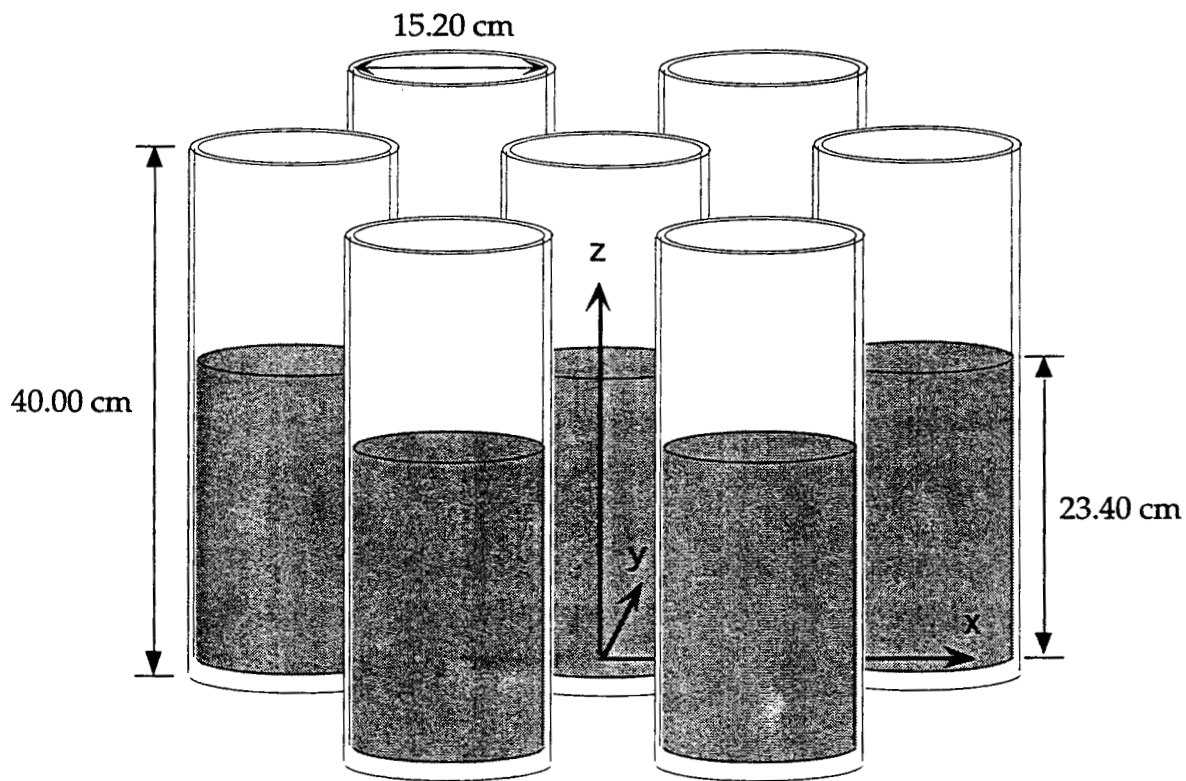


Figure 6-1. Case I geometry.

The method of modeling a hexagonal array is similar to the modeling of a hexahedral array. Three steps are involved in modeling the cylindrical container. Then a hexagonal shaped lattice cell is created for the infinite array and filled by the cylindrical container. Finally, we create a cell (window) that limits the array size to 7 elements as specified in the problem description.

Cylindrical Container Surfaces

As in chapter 5, we begin this problem by defining the surfaces for the solution, void region above the solution, the aluminum container, and the water outside the container. We want to model an open aluminum container that holds the uranium-fluoride solution. Define the surfaces for the solution and compare yours with those of Figure 6-2.

```
C Solution Cylinder Surface Cards
1  cz 7.60  $ outer radius of the solution
2  cz 7.75  $ outer radius of container
4  pz 23.4  $ top of solution
5  pz 0.0   $ bottom of solution
```

Figure 6-2. Case I solution cylinder surface cards.

Cylindrical Container Cells

The title card for this problem is:

Example6, Hexagonal Lattices.

The solution, the void region above the solution, the aluminum container, and the water outside the container are defined as part of the same universe. That universe will then be used to fill every lattice cell for the hexagonal array. This geometry is shown in Figure 6-3. Cell 1 is the uranium fluoride solution and is assigned material 1. Material density is input in atoms/b-cm as given in the problem description. Surfaces 1, 4, and 5 with the appropriate sense create a cylindrically shaped solution. Cell 1 is then designated as part of universe 1. The neutron importance is set to 1.

```
1  1  9.8983e-2      -1 5 -4    u=1  imp:n=1
```

The void region above the solution is defined as cell 2 and is assigned a material number of 0. Surfaces 1 and 4 are used to create the void cylinder. We define this cell so that the void extends to infinity above the solution. Cell 2 also belongs to universe 1 and is given a neutron importance of 1.

```
2  0                  -1 4        u=1  imp:n=1
```

Next we define the aluminum container for the solution, cell 3. We designate the aluminum as material 2. Once again the material density is entered in atoms/b-cm as

given in the problem description. The aluminum is defined as being inside of surface 2, not in cell 1, and not in cell 2. Cell 3 is also part of universe 1 and is assigned a neutron importance of 1, creating an infinitely tall cylinder of aluminum except for the solution and void region. An alternative cell 3 description that allows faster tracking is also shown.

```

3 2 -2.7      -2 #1 #2  u=1      imp:n=1
or
3 2 -2.7      -2 (1:-5) u=1      imp:n=1

```

Cell 4, the region of water outside the solution cylinder, is the final cell belonging to universe 1. This cell is defined as all space with a positive sense wrt surface 2, in universe 1, with a neutron importance of 1.

```

4 3 -1.0      2      u=1  imp:n=1

```

Cells 1-4, all belonging to universe 1, are complete and are shown in Figure 6-3. This universe will be used to fill a hexagonal lattice cell.

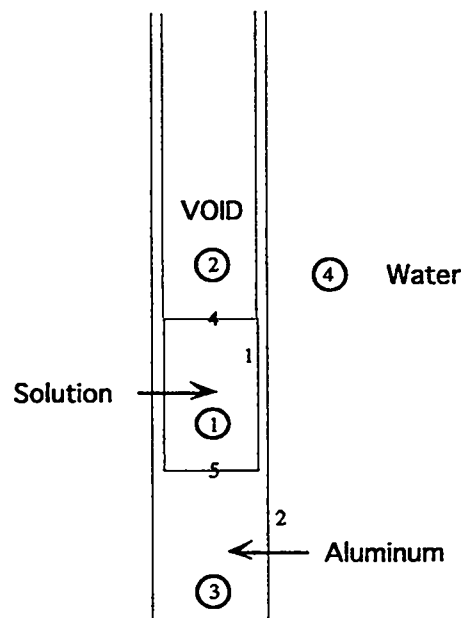


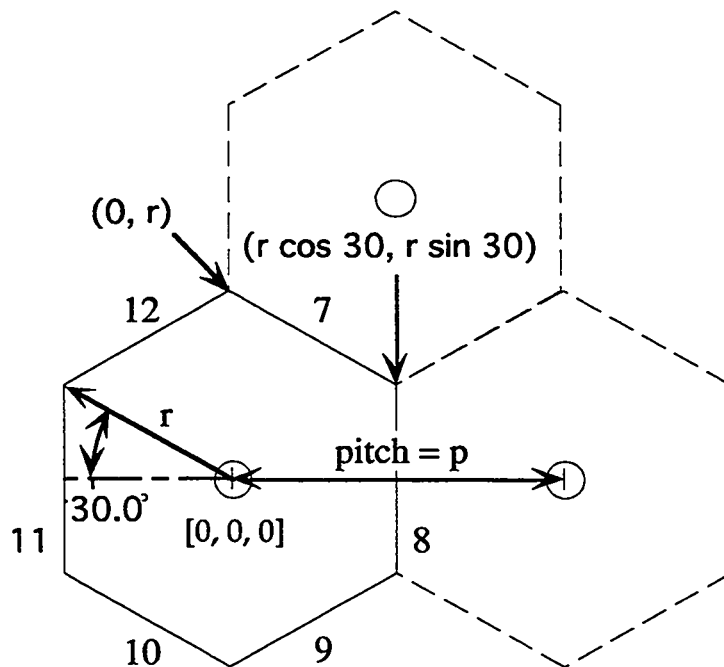
Figure 6-3. Universe 1 geometry (Cells numbers are circled).

Lattice Cell Surfaces

In this section we define the unit cell in the x-y plane for the hexagonal lattice. Opposite sides of the six-sided lattice cell must be equal in length and parallel. The dimension of concern that determines the six surfaces of the lattice cell is the pitch of the solution containers. The following "prescription" can be used to calculate the general planes for any hexagonal lattice formed from equilateral triangles.

The pitch for this example is calculated by adding the outer diameter of the aluminum container and the surface separation.

$$\begin{aligned}\text{pitch} &= \text{outer diameter} + \text{surface separation} \\ &= 15.50 \text{ cm} + 7.60 \text{ cm} \\ &= 23.10 \text{ cm}\end{aligned}$$



$$r \cos 30^\circ = p/2 \quad r = (p/2)/(\sqrt{3}/2) = p/\sqrt{3}$$

Figure 6-4. Diagram of [0, 0, 0] element.

Using Figure 6-4 we can define the six surfaces for the lattice element [0, 0, 0]. Surface numbers for these planes have been selected and need to be added to the surface card section. Surfaces 7, 9, 10, and 12 are general planes. Surfaces 8 and 11 are simple planes normal to the x-axis. {Refer to Chapter 3, Table 3.1, of the MCNP manual if you do not recall the equation of a general plane.}

Surface 7 passes through the points (0, r) and (r cos 30°, r sin 30°). The z point can have any value, so we need an equation of the form: y=mx+b. The slope m is given by:

$$m = \frac{(r - r \sin 30^\circ)}{(0 - r \cos 30^\circ)} = \frac{(r - 0.5r)}{(0 - 0.5r \sqrt{3})} = \frac{0.5r}{-0.5r \sqrt{3}} = -\frac{1}{\sqrt{3}}$$

The y-axis intercept, b, is found by choosing a point, in this case (0, r).

$$r = -\frac{1}{\sqrt{3}} * 0 + b \quad \text{or} \quad b = r$$

Therefore the equation for surface 7 is:

$$y = -\frac{1}{\sqrt{3}}x + r$$

MCNP wants this equation entered as Ax + By + Cz = D, where A = -m and D = r,

$$\text{so } \frac{1}{\sqrt{3}}x + 1y + 0z = r \quad \text{where } r \text{ has already been defined as } \frac{p}{\sqrt{3}}.$$

Therefore the coefficients of the equation for surface 7 are:

$$A = 1/\sqrt{3} \quad B = 1 \quad C = 0 \quad D = p/\sqrt{3}$$

or

$$A = 1 \quad B = \sqrt{3} \quad C = 0 \quad D = p$$

The pitch, p, has already been defined as 23.10, so the surface 7 general plane is entered as:

$$7 \quad p \quad 1 \quad 1.73205 \quad 0 \quad 23.1$$

Surface 8 passes through the x-axis at p/2. Therefore surface 8 is defined as:

$$8 \quad px \quad 11.55$$

Surface 9 is defined similarly to surface 7. This plane passes through the points (0, -r) and (r cos 30°, -r sin 30°). As with surface 7, the z-point can have any value, so we need an equation of the form y = mx + b.

$$m = \frac{(-r - (-r \sin 30^\circ))}{(0 - r \cos 30^\circ)} = \frac{(-r + 0.5r)}{(0 - 0.5r \sqrt{3})} = \frac{-0.5r}{-0.5r \sqrt{3}} = -\frac{1}{\sqrt{3}}$$

$$-r = \frac{1}{\sqrt{3}} * 0 + b \quad \text{or} \quad b = -r$$

$$y = \frac{1}{\sqrt{3}}x - r$$

The resulting MCNP format of the equation is:

$$-\frac{1}{\sqrt{3}}x + 1y + 0z = -r$$

or

$$-x + \sqrt{3}y = -p$$

The surface 9 general plane is entered as:

9 p -1 1.73205 0 -23.1

Follow the same logic for surface 10 to get the following equation of the plane.

$$\frac{1}{\sqrt{3}}x + 1y + 0z = -r$$

or

$$x + \sqrt{3}y = -p$$

The MCNP input would then appear as:

10 p 1 1.73205 0 -23.1

Surface 11 is a plane that passes through the x-axis at $-p/2$.

11 px -11.55

The final surface for the lattice cell is a plane that passes through the point $(0, r)$ and $(-r \cos 30^\circ, r \sin 30^\circ)$. Follow the same procedure as with surfaces 7, 9, and 10 to get the needed equation.

12 p -1 1.73205 0 23.1

Planes in an Equilateral Hexagonal Lattice

The equation for planar surfaces of an equilateral hexagonal lattice in the x-y plane was derived to be

$$x + \sqrt{3}y = -p$$

Recalling that the slope is the coefficient of the x term, the sign of x and p will alternate, depending on the quadrant, as shown in Figure 6-5.

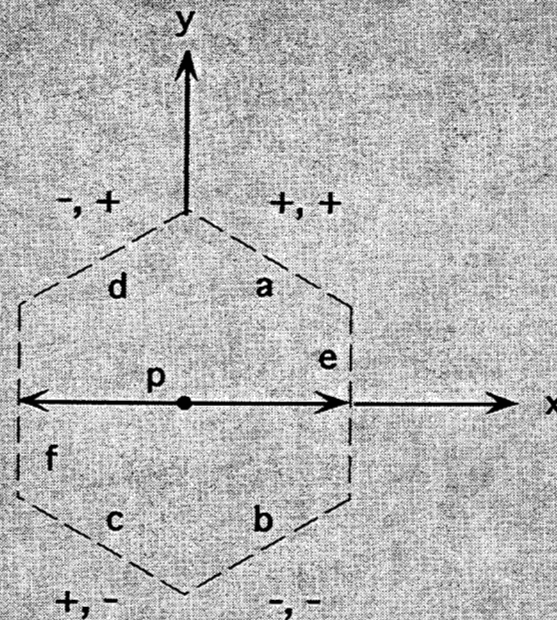


Figure 6-5. Sign of x and p by quadrant.

Thus, the equations and card specifications for surfaces a , b , c , and d are:

a:	$x + \sqrt{3}y = p$	1	$\sqrt{3}$	0	p
b:	$-x + \sqrt{3}y = -p$	-1	$\sqrt{3}$	0	$-p$
c:	$x + \sqrt{3}y = -p$	1	$\sqrt{3}$	0	$-p$
d:	$-x + \sqrt{3}y = p$	-1	$\sqrt{3}$	0	p

The px surfaces, e and f , are given by:

e:	$x = \frac{p}{2}$	$p/2$
f:	$x = -\frac{p}{2}$	$-p/2$

Returning to our problem, Figure 6-6 shows the coefficients of the equations for the hexagonal lattice cell for this problem. Once the pitch has been determined, the calculated values are used to describe the six surfaces.

```

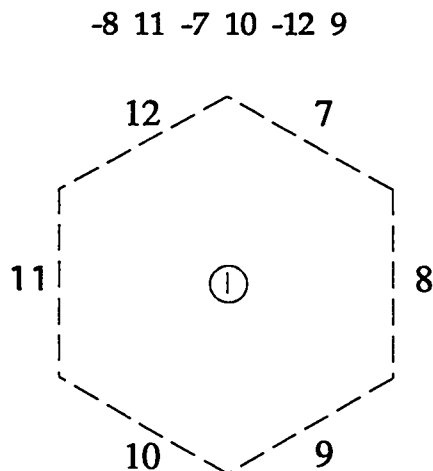
C  Surfaces 7-12 are the array lattice cell
7  p   1  1.73205  0   23.1
8  px  11.55
9  p  -1  1.73205  0  -23.1
10 p   1  1.73205  0  -23.1
11 px -11.55
12 p  -1  1.73205  0   23.1

```

Figure 6-6. Example 6 lattice cell surface cards.

Defining the Lattice Cell

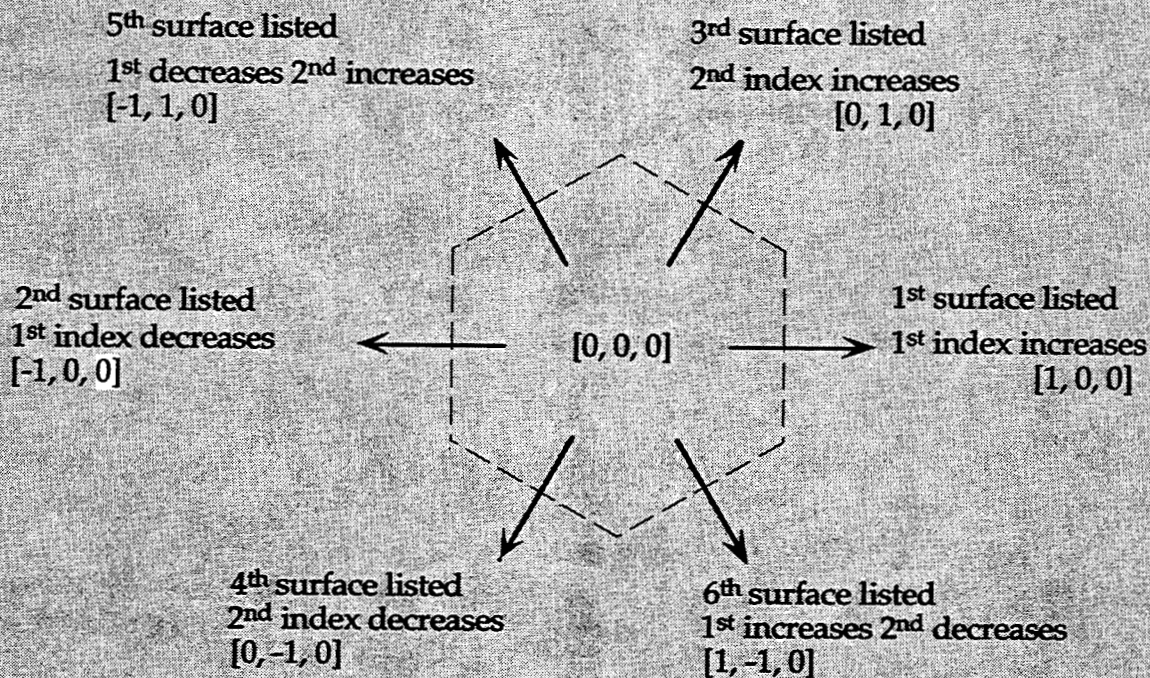
The six planes previously created will define the six-sided lattice cell, called cell 5. The material number for cell 5 is 0 because the cell is filled by universe 1. The surfaces can be listed on the card in the following manner:



The first two surfaces listed must be opposite each other. That is, surface 8 is opposite surface 11.

Ordering of Hexagonal Prism Lattice Elements

Recall from Chapter 5 that the order of the surfaces on the cell card with a lat keyword identifies the ordering of the lattice elements. For the hexagonal prism lattice cell, the indexing is shown below for element $[0, 0, 0]$.

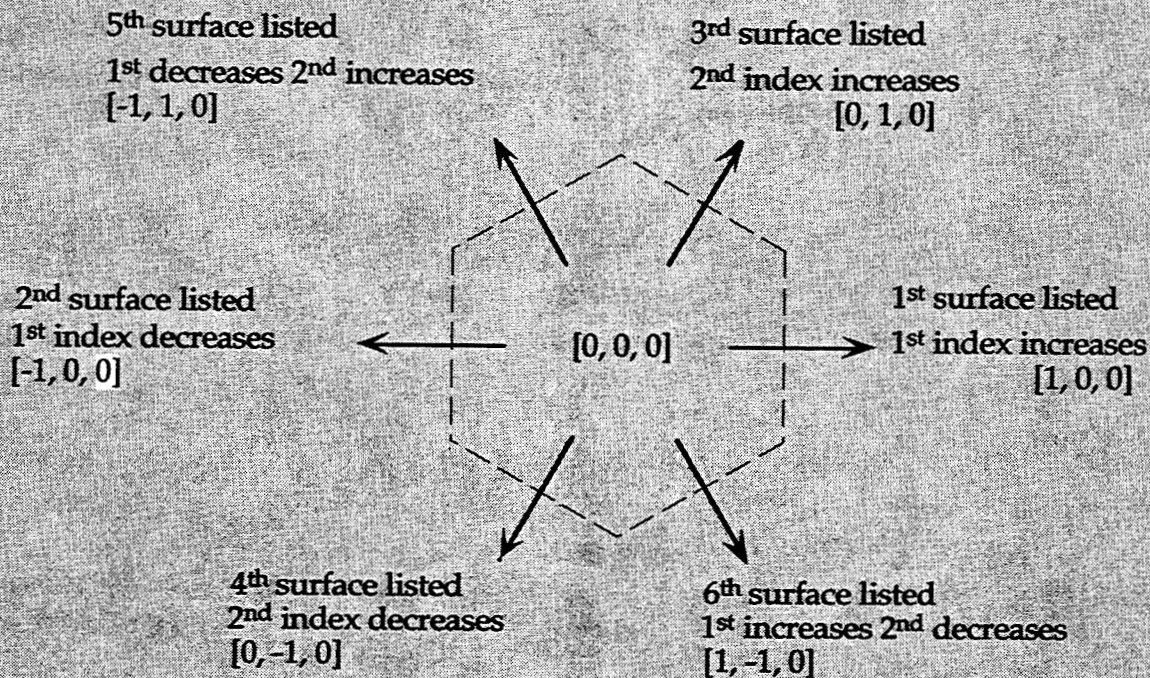


On the opposite side of the first surface listed is element $[1, 0, 0]$, opposite the second surface listed is $[-1, 0, 0]$, opposite the third is $[0, 1, 0]$, then $[0, -1, 0]$, $[-1, 1, 0]$, and $[1, -1, 0]$ opposite the fourth, fifth, and sixth surfaces, respectively. If the lattice were finite in the z-direction, opposite the seventh surface is element $[0, 0, 1]$ and opposite the eighth is $[0, 0, -1]$.

Knowing how the elements are indexed is essential when a fully specified fill card is used to fill lattice elements. In all cases, it determines how the lattice is designed.

Ordering of Hexagonal Prism Lattice Elements

Recall from Chapter 5 that the order of the surfaces on the cell card with a lat keyword identifies the ordering of the lattice elements. For the hexagonal prism lattice cell, the indexing is shown below for element $[0, 0, 0]$.



On the opposite side of the first surface listed is element $[1, 0, 0]$, opposite the second surface listed is $[-1, 0, 0]$, opposite the third is $[0, 1, 0]$, then $[0, -1, 0]$, $[-1, 1, 0]$, and $[1, -1, 0]$ opposite the fourth, fifth, and sixth surfaces, respectively. If the lattice were finite in the z-direction, opposite the seventh surface is element $[0, 0, 1]$ and opposite the eighth is $[0, 0, -1]$.

Knowing how the elements are indexed is essential when a fully specified fill card is used to fill lattice elements. In all cases, it determines how the lattice is designed.

After the cell 5 surfaces are listed, we define the cell as a hexagonal lattice (lat=2). Cell 5 is filled with universe 1 and belongs to universe 2. A neutron importance of 1 completes the infinite hexagonal lattice cell 5 description.

```
5  0  -8 11 -7 10 -12 9  lat=2  fill=1  u=2  imp:n=1
```

The third step is to place a cell (or window) around the cell 5 infinite hexagonal lattice to limit it to a seven-element array. We define two planes for the top and bottom of the solution cylinders and define a cylinder that has a radius such that only 7 lattice elements can be contained within. Remember, you cannot define the window planes at the same location as the lattice cell planes because they are in different universes. Figure 6-7 shows the surfaces chosen for this example.

```
C  Window Surfaces
3   pz  40.0  $ top of aluminum cylinder
6   pz  -1.0  $ bottom of aluminum container
13  cz  32.0  $ cylinder for array window
```

Figure 6-7. Example 6 window surface cards.

We will call the window cell 6. The material number is zero because the cell is filled by the lattice, universe 2. The cell is bound in the negative sense of surface 13, the positive sense of surface 6, and the negative sense of surface 3. Cell 6 is filled with universe 2 and has a neutron importance of 1. The infinite lattice is now limited to a system of seven solution cylinders in a hexagonal configuration.

```
6  0      -13 6 -3  fill=2      imp:n=1
```

In the problem description there is infinite water reflection except above the solution cylinders. A thickness of 20 cm of water adequately models infinite reflectors for neutrons. Two surfaces need to be added to the surface card section as shown in Figure 6-8. The cylinder is 20 cm beyond surface 13, and the plane is 20 cm below surface 6.

```

C  reflector surfaces
14  cz 52          $ outer radius of reflector
15  pz -21         $ bottom edge of reflector

```

Figure 6-8. Example 6 water reflector surfaces.

The water reflector is defined as cell 7. It is assigned material number 3, water with a density of 1 g/cc. Cell 7 is all space that is a union of the positive sense wrt surface 13 and the negative sense wrt surface 6, intersected with all space that is negative wrt surface 3, positive wrt surface 15, and negative wrt surface 14. A neutron importance of 1 completes the cell.

```

7  3 -1.0 (13:-6) -3 15 -14          imp:n=1

```

The final cell is the "rest of the world". Cell 8 is given a material number of 0. The neutron importance for this cell is 0.

```

8  0          14:3:-15          imp:n=0

```

6.3.B Materials

Material cards are constructed and entered as described previously, using the information provided in the problem description. Your material cards should resemble those in Figure 6-9. Materials 1 and 3 should use the $S(\alpha,\beta)$ thermal neutron treatment for hydrogen in light water.

```

C  Material cards
m1  1001  6.1063-2  8016  3.3487-2  9019  2.9554-3
    92235 1.3784-3  92238 9.9300-5
mt1  lwtr
m2  13027 1.0
m3  1001  2          8016  1
mt3  lwtr

```

Figure 6-9. Case I material cards.

6.3.C MCNP Criticality Controls

The kcode specification is the same as in example 5. On the ksrc card, again we will put a criticality source point in each solution cylinder. Figure 6-10 shows the control cards for this example.

```
C      Criticality Control Cards
kcode 1000 1.0 15 115
ksrc  0  0  11.7      -23.1 0 11.7      23.1 0 11.7
      -11.55 20.0 11.7      -11.55 -20.0 11.7
      11.55 20.0 11.7      11.55 -20.0 11.7
```

Figure 6-10. Case I control cards.

For large problems with fissile material at many locations, MCNP has other methods of defining the initial starting source points. Whether the problem is tightly or loosely coupled may also affect your choice of method of initial source description. It is much more important to put at least one ksrc fission source point in each fissile region for a loosely coupled problem. {Further discussion can be found in the MCNP manual.}

6.3.D Example 6 Case I MCNP Input File

The input for Case I is complete. The input file should resemble the following. Do not forget the blank line delimiters.

```
Example6, Hexagonal Lattices.
C Cell Cards
1  1  9.8983e-2      -1 5 -4      u=1  imp:n=1
2  0      -1 4      u=1  imp:n=1
3  2  -2.7      -2 #1 #2      u=1  imp:n=1
4  3  -1.0      2      u=1  imp:n=1
5  0      -8 11 -7 10 -12 9  lat=2 fill=1  u=2  imp:n=1
6  0      -13 6 -3      fill=2      imp:n=1
7  3  -1.0 (13:-6) -3 15 -14      imp:n=1
8  0      14:3:-15      imp:n=0

C Solution Cylinder Surface Cards
1  cz 7.60      $ outer radius of the solution
2  cz 7.75      $ outer radius of container
4  pz 23.4      $ top of solution
5  pz 0.0      $ bottom of solution
```

```

C  Surfaces 7-12 are for the array lattice cell
7  p   1  1.73205  0   23.1
8  px  11.55
9  p  -1  1.73205  0  -23.1
10 p   1  1.73205  0  -23.1
11 px -11.55
12 p  -1  1.73205  0   23.1
C  Window Surfaces
3  pz 40.0          $ top of aluminum cylinder
6  pz -1.0         $ bottom of aluminum container
13 cz 32.00        $ cylinder for array window
C  Reflector Surfaces
14 cz 52.00        $ outer radius of reflector
15 pz -21.00       $ bottom edge of reflector

C      Criticality Control Cards
kcode 1000 1.0 15 115
ksrc  0 0 11.7      -23.1  0 11.7      23.1  0 11.7
      -11.55 20 11.7  -11.55 -20  11.7
      11.55 20 11.7   11.55 -20  11.7
m1    1001  6.1063-2  8016  3.3487-2  9019  2.9554-3
      92235 1.3784-3  92238 9.9300-5
mt1   lwtr
m2    13027  1.0
m3    1001   2    8016  1
mt3   lwtr

```


6.4 PLOT OF GEOMETRY

Before transporting particles be sure to run the plotter to check for errors in the geometry. The default $px=0$ view will give you a message stating:

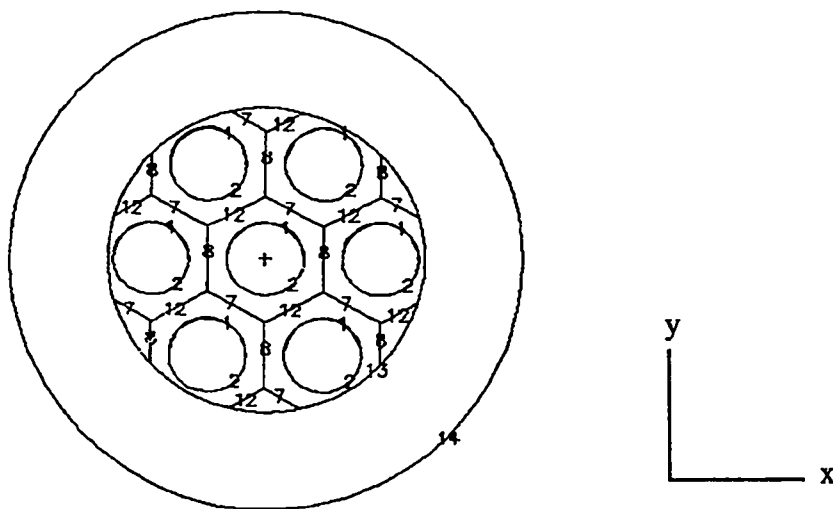
"can't yet plot parallel to axis of hexagonal prism lattice."

"no plot because it would have been empty."

The only view you can currently get is the cross-sectional view in the z-plane so enter:

`pz 10`

You will get the following plot displayed.



The final combined k_{eff} estimator for this problem on a SPARC 1 at the University of New Mexico was 1.0016 with an estimated standard deviation of 0.0032.

6.5 CASE II: EXPANDED FILL CARD IN TRIANGULAR LATTICE

The Case I problem was filled with seven identical items. As in Chapter 5, the `fill` specification was a single number. In Case II, element $[0, -1, 0]$ has a material different than the other six elements. The expanded form of the `fill` card is used.

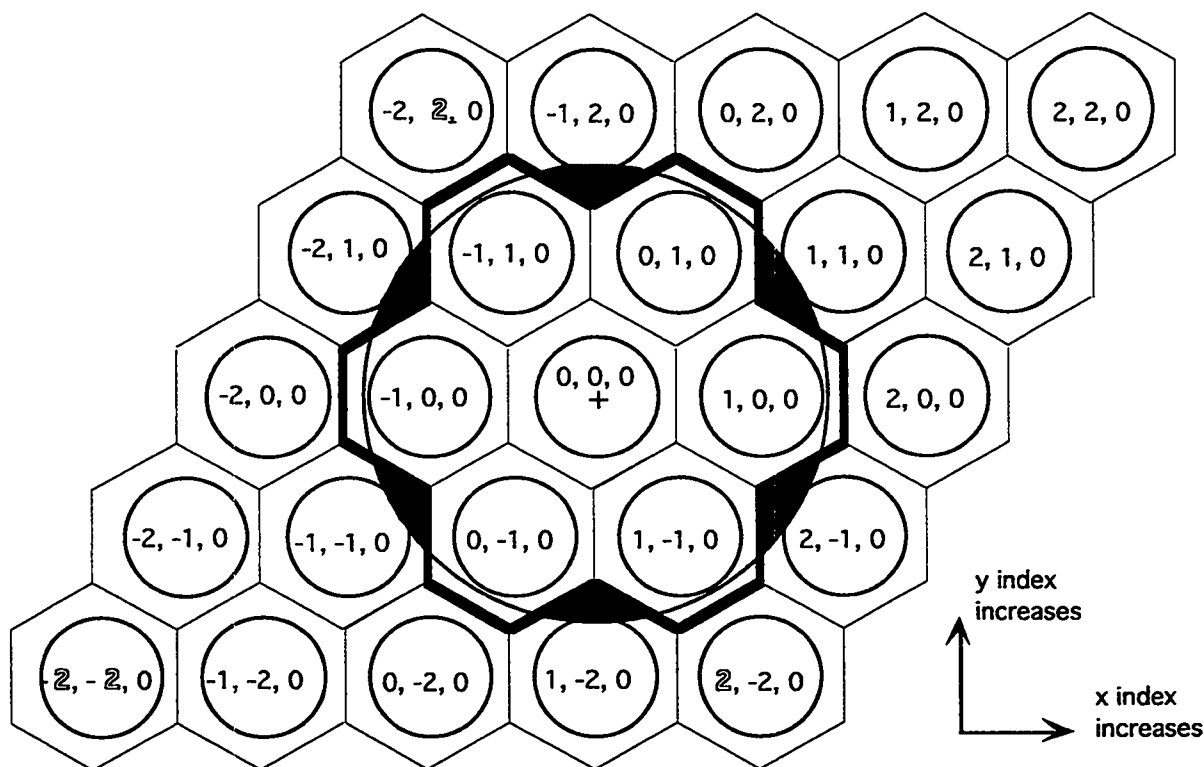


Figure 6-11. The 25 elements specified on the expanded `fill` card.

Figure 6-11 shows the range of the lattice and the individual element indices. The range of each index is the minimum and maximum of the lattice elements that are wholly or partially included in the "window" cell. The solid line outlines the seven elements of interest. The shaded regions inside the circle show the portions of the other six elements enclosed by the "window" cell. When using the explicit form of the `fill` card, at minimum, every element enclosed by the filled cell must be included in the range specification. The index numbers in an outlined font in Figure 6-11 show the lower and upper range values.

The cell card for lattice cell 5 follows.

```

5      0      -8 11 -7 10 -12 9  lat=2 u=2 fill=-2:2 -2:2 0:0
2 2 2 1 2      $ x=-2 to x=2; y=-2
2 1 3 1 1      $ "      "; y=-1
2 1 1 1 2      $ "      "; y=0
1 1 1 1 2      $ "      "; y=1
2 1 2 2 2      imp:n=1 $ "      "; y=2

```

In this problem the x range is -2 to 2 (5 elements in x), the y range is -2 to 2 (5 elements in y), and the z range is 0 to 0 (1 element in z). Twenty-five universe numbers, one for each element, must be entered. Recall the order of index incrementing: first z, first y, all x; first z, second y, all x, etc. Some of the elements are clearly not involved in the area of interest, [-2, -2, 0] for example. Those elements can be filled with the universe number of the lattice cell itself, in this case universe 2, making those elements void. A small part of element [1, -2, 0] is included in the "window", so it should be filled by universe 1.

The material in element [0, -1, 0] is changed from the uranium-fluoride solution to graphite. The universe number for the [0, -1, 0] element is 3. The following cells need to be added to the cell card section after surface 4 for universe 3.

```

9      like 1 but mat=4 rho=-1.60 u=3  imp:n=1
10     like 2 but u=3                      imp:n=1
11     like 3 but u=3                      imp:n=1
12     like 4 but u=3                      imp:n=1

```

Also, add graphite to the materials using the following:

```

m4      6012 1
mt4     grph

```

Using Figure 6-11 and the 25 entries on the `fill` card, identify which element is filled by what universe on your own. Notice that the `fill` array has 5 rows and 5 columns. Each line corresponds to a horizontal row in Figure 6-11. In a large problem, this practice helps keep track of the entries in the large array.

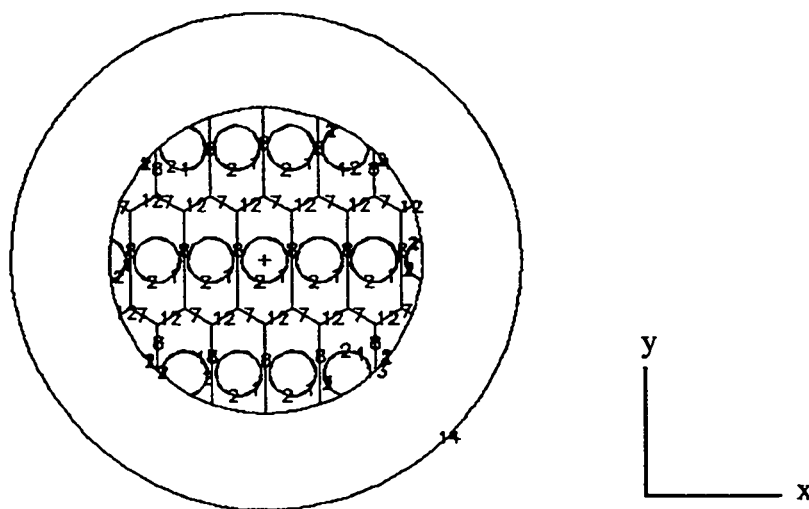
The importance of all lattice elements is set to 1. Recall that no particles ever will be tracked in some of the elements. When a particle in element [1, 0, 0] crosses the cylindrical surface, it will enter cell 6 and be tracked at that level.

6.6 NONEQUILATERAL TRIANGULAR LATTICE

It is possible to describe a lattice that is not equilateral. Using the Case I input, change the following surface cards:

OLD			NEW		
1	cz	7.6	1	cz	4.6
2	cz	7.75	2	cz	4.75
8	px	11.55	8	px	5.55
11	px	-11.55	11	px	-5.55

The following plot will be displayed using the plot command: pz 10



This section is not intended to make you an expert on describing nonequilateral hexagonal lattices. We just want to illustrate that MCNP can model many lattice shapes. The only requirements are that opposite sides must be identical and parallel and that the lattice must fill all space exactly.

6.7 SUMMARY

This chapter continued discussion of the lattice option in MCNP from the previous chapter by introducing a hexagonal array problem. The method used was very similar to that of the hexahedral array. We have shown the basics of using the `lat` keyword. {Please refer to the MCNP manual for a more detailed description of the use of lattices with MCNP.} How to model a three-dimensional hexahedral lattice is discussed in Chapter 7.

Chapter 7

3-Dimensional Square Lattices

This chapter builds on the example from Chapter 5 to create a three-dimensional square lattice of solution cylinders. Much of the example remains unchanged. If you do not understand the input in this example, refer to Chapter 5 for a more detailed description of this problem. The 3-dimensional hexagonal lattice is constructed in a similar manner, so no examples are presented in this document.

7.1 WHAT YOU WILL BE ABLE TO DO

- Create a 3-D hexahedral (square) lattice.
- Fill the lattice elements with various materials.
- Create a universe 0 lattice.

7.2 PROBLEM DESCRIPTION

This example is the hexahedral array of six plutonium nitrate solution cylinders (LA-10860, page 125) from Chapter 5. It is modified to create a second layer of six elements for a total of 12 solution cylinders. Recall that the data for this problem is:

Plutonium Nitrate Solution

$$N_{239} = 2.7682e-4$$

$$N_{240} = 1.2214e-5$$

$$N_{241} = 8.3390e-7$$

$$N_{242} = 4.5800e-8$$

$$N_{\text{Hydrogen}} = 6.0070e-2$$

$$N_{\text{Oxygen}} = 3.6540e-2$$

$$N_{\text{Nitrogen}} = 2.3699e-3$$

$$N_{\text{Total}} = 9.9270e-2$$

$$\text{Solution height} = 39.24 \text{ cm}$$

Stainless Steel Containers

$N_{\text{Iron}} = 6.3310\text{e-}2$	3x2x2 Hexahedral (square) lattice
$N_{\text{Chromium}} = 1.6540\text{e-}2$	All surface separations = 10.0 cm
$N_{\text{Nickel}} = 6.5100\text{e-}3$	Tank i.d. = 24.98 cm
$N_{\text{Total}} = 8.6360\text{e-}2$	Tank wall thickness = 0.30 cm
	Tank top and bottom thickness = 1.0 cm
	Inside height = 101.7 cm
	Tank Pitch = 35.58 cm

7.3 EXAMPLE 7 CASE I SETUP

7.3.A Solution Cylinder

In Chapter 5 cells 1-4 define the solution cylinder (see Figure 5-3). For this example cells 1 and 2 are not changed. Cells 3 and 4 will be modified. Cell 3 is the stainless steel container. In Chapter 5, the stainless steel was infinite in the z direction. Because we now want a 10 cm vertical spacing between the cylinders, a plane must be added to limit the cylinder top thickness. We will still use the lattice window cell to define the bottom thickness so cell 3 can remain infinite in -z. Cell 3 is now all space with a negative sense wrt surface 2, with a negative sense wrt surface 4, not in cell 1, and not in cell 2.

Because of the change to cell 3, the description of cell 4 has to be changed also. Cell 4, the void region between the cylinders, is now defined as all space with a positive sense wrt surface 2 unioned with all space having a positive sense wrt surface 4. Cells 1-4 belong to universe 1. Figure 7-1 shows the descriptions of cells 1-4, while Figure 7-2 shows the surface cards used in cells 1-4. Figure 7-3 shows the geometry created by cell cards 1-4.

Example7 3-D Hexahedral lattice.

C Cell Cards

1	1	9.9270e-2	-1	5	-6	u=1	imp:n=1
2	0		-1	6	-7	u=1	imp:n=1
3	2	8.6360e-2	-2	-4	#1 #2	u=1	imp:n=1
4	0		2:4			u=1	imp:n=1

Figure 7-1. Cell cards 1-4 with title card.

C	Solution Cylinder Surface Cards			
1	cz	12.49	\$	Inner cylinder
2	cz	12.79	\$	Outer SS cylinder
4	pz	102.7	\$	Top of SS tank
5	pz	0.0	\$	Bottom of solution
6	pz	39.24	\$	Top of solution
7	pz	101.7	\$	Top of void above soln.

Figure 7-2. Surface cards for cells 1-4.

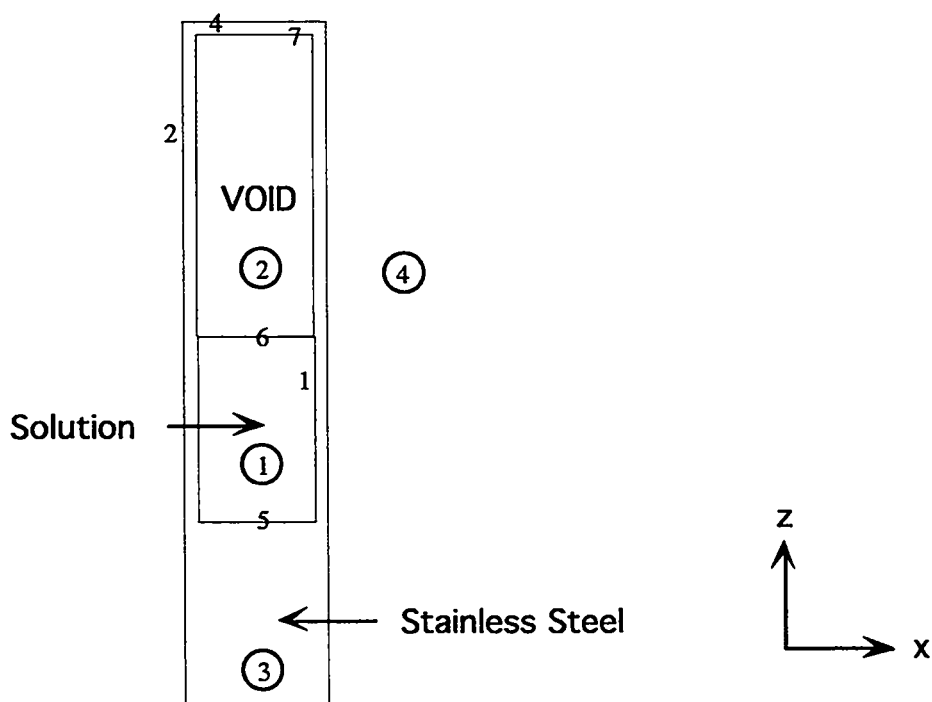


Figure 7-3. Geometry created by cell cards 1-4.

7.3.B Square Lattice Cell

In Chapter 5, the lattice cell was infinite in only the x and y directions. We will now change the lattice cell 5 description so it is finite in the x , y , and z directions by adding pz surfaces 16 and 3 to the cell description. The geometry defined by cell 5 is shown in Figure 7-4.

7.3.C Lattice Window

Next, a window cell needs to be defined, cell 6, that will limit the infinite lattice to 12 solution cylinders in a 3x2x2 configuration. On the cell 6 card, surfaces 3 and 4 are deleted and surfaces 17 and 18 are added, making two layers of solution cylinders. Surface 18 is just inside (above) the cylinder bottom, and surface 17 is just below surface 16. These surfaces limit the infinite lattice in the z direction. Notice that we have effectively made the cylinder bottom 0.999 cm thick instead of 1.0 cm for the row of cylinders adjacent to the bottom window surface. As you determine the surface values of your window cell, consider whether omitting part of your geometry will make a difference in the overall calculation. Cell 6 still is filled by universe 2. The description of cell 6 follows.

```
6  0  13 -12 15 -14 18 -17  fill=2  imp:n=1
```

Add the following two lines to the surface card section:

```
17  pz  102.69
18  pz -114.699
```

7.3.D "Rest of the World"

The final cell for this problem, cell 7, defines the "rest of the world". Cell 7 is given a material number of 0 and a neutron importance of 0.

```
7  0  -13:12:-15:14:-18:17  imp:n=0
```

7.4 MATERIALS

The material cards for this problem do not require any change from example 5 and can be copied directly as shown in Figure 7-5.

```
C      Material cards
m1     1001  6.0070-2  8016  3.6540-2  7014  2.3699-3
       94239 2.7682-4  94240 1.2214-5  94241 8.3390-7
       94242 4.5800-8
mt1    lwtr
m2     26000 6.3310-2  24000 1.6540-2  28000 6.5100-3
```

Figure 7-5. Example 7 material cards.

7.5 MCNP CRITICALITY CONTROLS

The kcode specification remains the same from the previous example. Six source points are added on the ksrc card to those defined in example 5, so each solution cylinder has a source point. Figure 7-6 shows the control cards for this example.

```
C Control Cards
kcode 1000 1.0 15 115
ksrc 0 0 19.62 35.58 0 19.62 71.16 0 19.62
      0 35.58 19.62 35.58 35.58 19.62 71.16 35.58 19.62
C These source points are placed in the added cylinders
      0 0 -94.08 35.58 0 -94.08 71.16 0 -94.08
      0 35.58 -94.08 35.58 35.58 -94.08 71.16 35.58 -94.08
```

Figure 7-6. Example 7 control cards.

7.6 EXAMPLE 7 MCNP INPUT FILE

The input requirements for this example are complete. The input file should resemble the following.

```
Example7 3-D Hexahedral lattice.
C Cell Cards
1 1 9.9270e-2 -1 5 -6 u=1 imp:n=1
2 0 -1 6 -7 u=1 imp:n=1
3 2 8.6360e-2 -2 -4 #1 #2 u=1 imp:n=1
4 0 2:4 u=1 imp:n=1
5 0 -8 9 -10 11 -16 3 lat=1 u=2 fill=1 imp:n=1
6 0 13 -12 15 -14 18 -17 fill=2 imp:n=1
7 0 -13:12:-15:14:-18:17 imp:n=0

C Solution Cylinder Surface Cards
1 cz 12.49 $ Inner cylinder
2 cz 12.79 $ Outer SS cylinder
4 pz 102.7 $ Top of SS tank
5 pz 0.0 $ Bottom of solution
6 pz 39.24 $ Top of solution
7 pz 101.7 $ Top of void above soln.
C Beginning of Lattice Surfaces
8 px 17.79
9 px -17.79
10 py 17.79
11 py -17.79
```

```

C   Window Surfaces
3   pz -1.0
12  px  88.949
13  px -17.789
14  py  53.369
15  py -17.789
16  pz 112.7          $ Top of lattice cell
C   Surfaces 17 and 18 bound the lattice in the z direction
17  pz 102.69
18  pz -114.699

C Control Cards
kcode 1000 1.0 15 115
ksrc 0 0          19.62 35.58 0          19.62 71.16 0          19.62
      0 35.58 19.62 35.58 35.58 19.62 71.16 35.58 19.62
C   These source points are placed in the added cylinders
      0 0          -94.08 35.58 0          -94.08 71.16 0          -94.08
      0 35.58 -94.08 35.58 35.58 -94.08 71.16 35.58 -94.08
C   Material cards
m1   1001 6.0070-2 8016 3.6540-2 7014 2.3699-3
      94239 2.7682-4 94240 1.2214-5 94241 8.3390-7
      94242 4.5800-8
mt1  lwtr
m2   26000 6.3310-2 24000 1.6540-2 28000 6.5100-3

```

7.7 OUTPUT

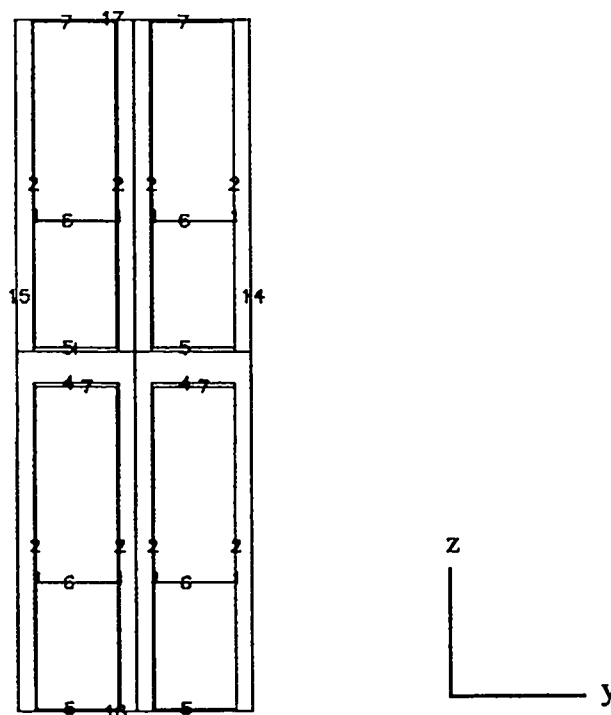
The final combined k_{eff} estimator for this problem on a SPARC 1 at the University of New Mexico was 1.0097 with an estimated standard deviation of 0.0027.

7.8 PLOT OF GEOMETRY

Before transporting particles, run the plotter to check for geometry errors in the cell descriptions. The default plot extent will show only part of the geometry. Change the extent to bring the entire geometry into view:

ex 150

The plot should appear as follows:



7.9 CASE II: CHANGING MATERIALS IN SELECTED ELEMENTS

Now we want to change the material in one of the cylinders in this system. Recalling what we learned in Chapter 5, each lattice element has a unique lattice location identifier. The $[0, 0, 0]$ element is the one described on the lattice cell card. The indices increase and decrease according to the order of the surfaces entered on the lattice cell card. The first index increases in the $+x$ direction, and the second index increases in the $+y$ direction as in Chapter 5. The fifth surface listed is the pz plane with the largest z value, and the sixth is the pz plane with the smallest z value, so the third index increases in $+z$ direction. The range of the indices for cell 6 are 0:2, 0:1, and -1:0. The elements are

incremented as follows: do all x for the first y, first z; do all x for the second y, first z; do all x for for all y, first z; do all x for the first y, second z; do all x for second y, second z, etc. With this in mind, we replace the fissile solution in element (1, 1, -1) with water.

A water-filled cylinder will be defined and belong to universe 3. The geometry for universe 3 is identical to universe 1. Only the material in cell 1 is different. The four cells belonging to universe 3, shown below, can be added to the cell cards section of example 7 after cells 1-4.

```

11  like 1 but mat=3 rho=-1.0 u=3  imp:n=1
12  like 2 but                u=3  imp:n=1
13  like 3 but                u=3  imp:n=1
14  like 4 but                u=3  imp:n=1

```

The complete lattice cell 5 card is now:

```

5 0 -8 9 -10 11 -16 3 lat=1 u=2 fill=0:2 0:1 -1:0 1 1 1 1 3 1
                                     1 1 1 1 1 1
                                     imp:n=1

```

Cell 11 is defined with material 3, so an m3 card, water, must be added to the data card section. Because we are using water, $S(\alpha, \beta)$ cross-section data for hydrogen in water are used. The new material cards are:

```

m3  1001 2  8016 1
mt3 lwtr

```

All elements except one are filled with universe 1, while the [1, 1, -1] element is filled with universe 3. An alternative way of writing cell 5 is:

```

5 0 -8 9 -10 11 -16 3 lat=1 u=2 imp:n=1 fill=0:2 0:1 -1:0
                                     1 1 1 1 3 1 1 5r

```

where 5r repeats the previous universe value 5 more times.

The final combined k_{eff} estimator for this problem on a SPARC 1 at the University of New Mexico was 0.9979 with an estimated standard deviation of 0.0035.

7.10 Universe 0 lattice

This section discusses a quick method of setting up a problem that consists only of a bare lattice, one that is not bounded by any limiting window cell. This approach is different from what has been previously described. The lattice cell itself has no universe designation; therefore, it belongs to universe 0. As always, the lattice is infinite but the elements of interest are selected by the range on a fill card. The advantages and disadvantages of this approach are discussed at the end of this section.

The Chapter 7 Case I example can be described with the cell and surface cards shown below. Notice particularly that lattice cell 5 has no universe designation and that it uses the expanded version of the fill card to select just those lattice elements desired. Cell 5 has been made finite in the z direction by the addition of surfaces 3 and 16. Cells 6 and 7 and surfaces 12-15 have been deleted because they are not needed.

Example7 level 0 lattice.

C Cell Cards

1	1	9.9270e-2	-1	5	-6	u=1	imp:n=1		
2	0		-1	6	-7	u=1	imp:n=1		
3	2	8.6360e-2	-2	-4	#1 #2	u=1	imp:n=1		
4	0			2:4		u=1	imp:n=1		
5	0	-8	9	-10	11 -16	3 lat=1	imp:n=1	fill=0:2	0:1 -1:0
								1 1 1	1 1 1
								1 1 1	1 1 1

C Surface Cards

1	cz	12.49
2	cz	12.79
3	pz	-1
4	pz	102.7
5	pz	0.0
6	pz	39.24
7	pz	101.7
8	px	17.79
9	px	-17.79
10	py	17.79
11	py	-17.79
16	pz	112.7

If a cell is not designated as belonging to a particular universe, it is part of universe 0 by default. In this example, lattice cell 5 represents an element in an infinite lattice. The fill range limits the infinite extent of the lattice by defining the elements that actually exist. In tracking, when a particle crosses from an element that exists into one that does not exist, it is terminated. Figures 7-7 and 7-8 show two views plotted using the input file above. The unfilled lattice elements do not exist in the problem. Particles that enter an undefined element are assumed to have escaped the geometry and are terminated.

```
pz=0  or= 35 20 10  ex=75
```

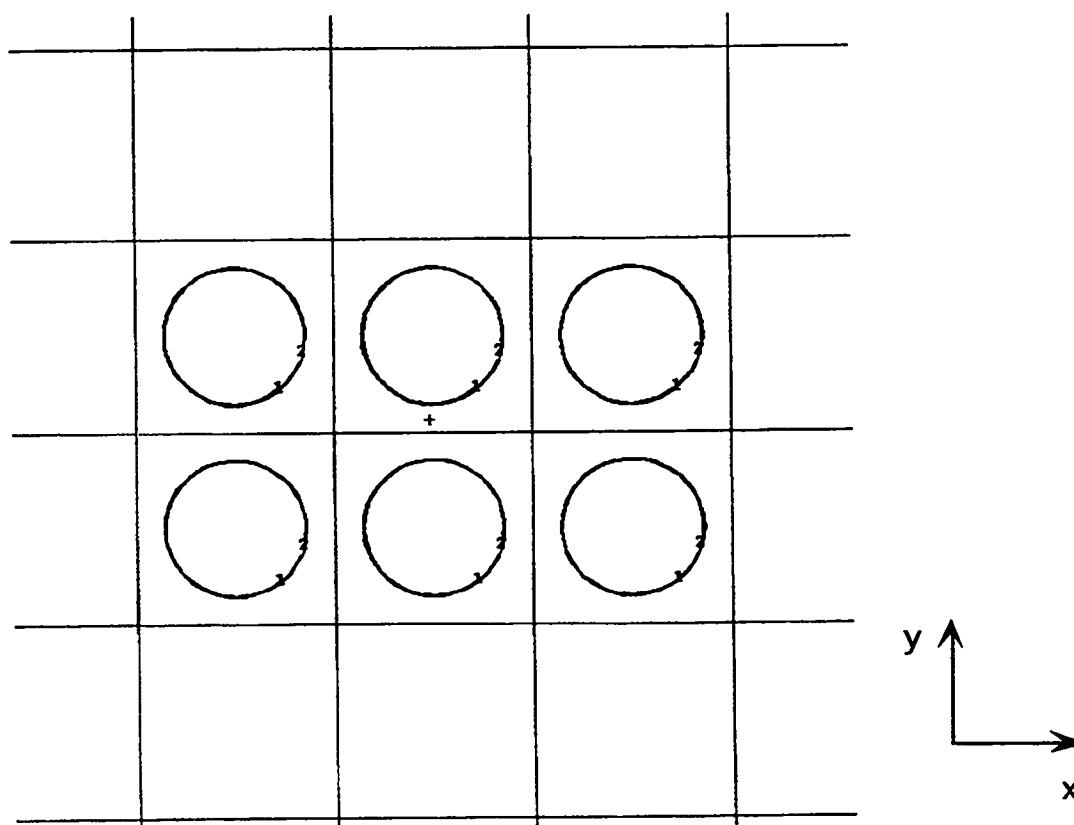


Figure 7-7. Top view of universe 0 lattice.


```
px= 0  ex=150  or= 0 0 40
```

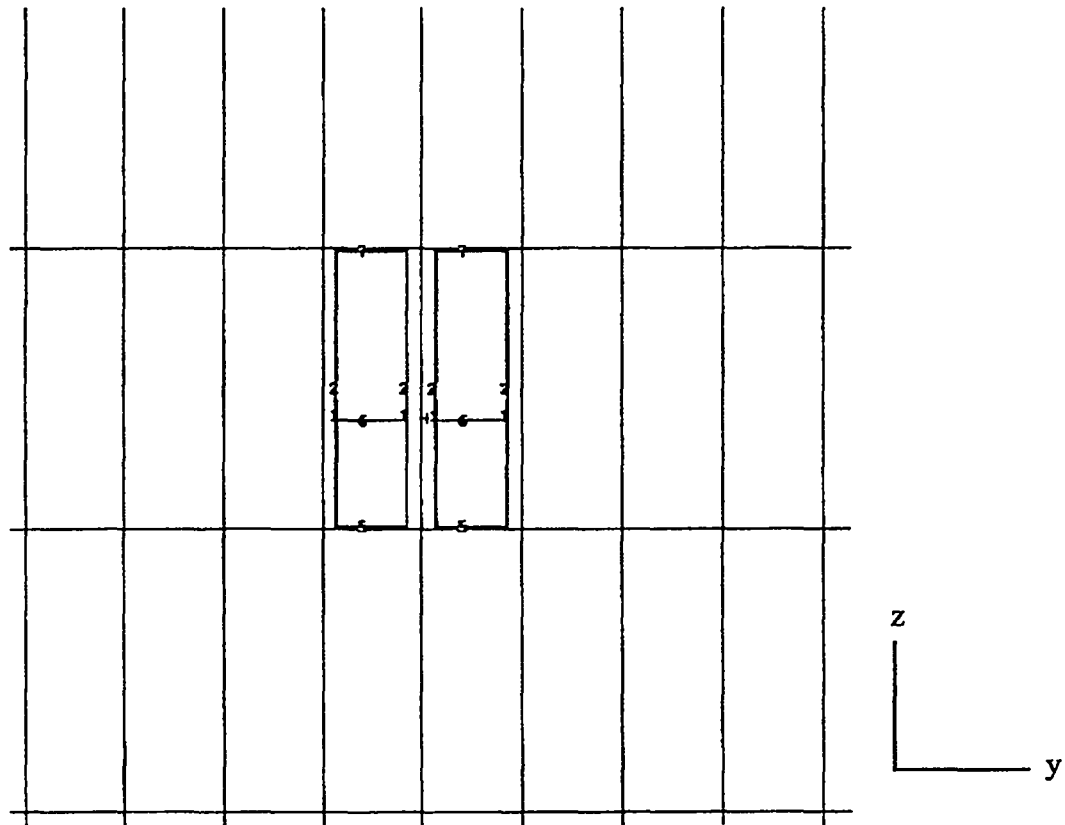


Figure 7-8. Side view of universe 0 lattice.

A zero entry in the fill array has a special meaning for a universe 0 lattice. It means that the lattice element does not exist and makes it possible to describe a rectangular array with missing elements. The following description of cell 5 produces the model shown below in Figure 7-9.

```
5  0  -8 9 -10 11 -16 3 imp:n=1 lat=1 fill=0:2 0:1 -1:0
                                1 1 1  1 1 1
                                1 1 1  1 1 0
```

pz 0 or 35 20 10 ex 100

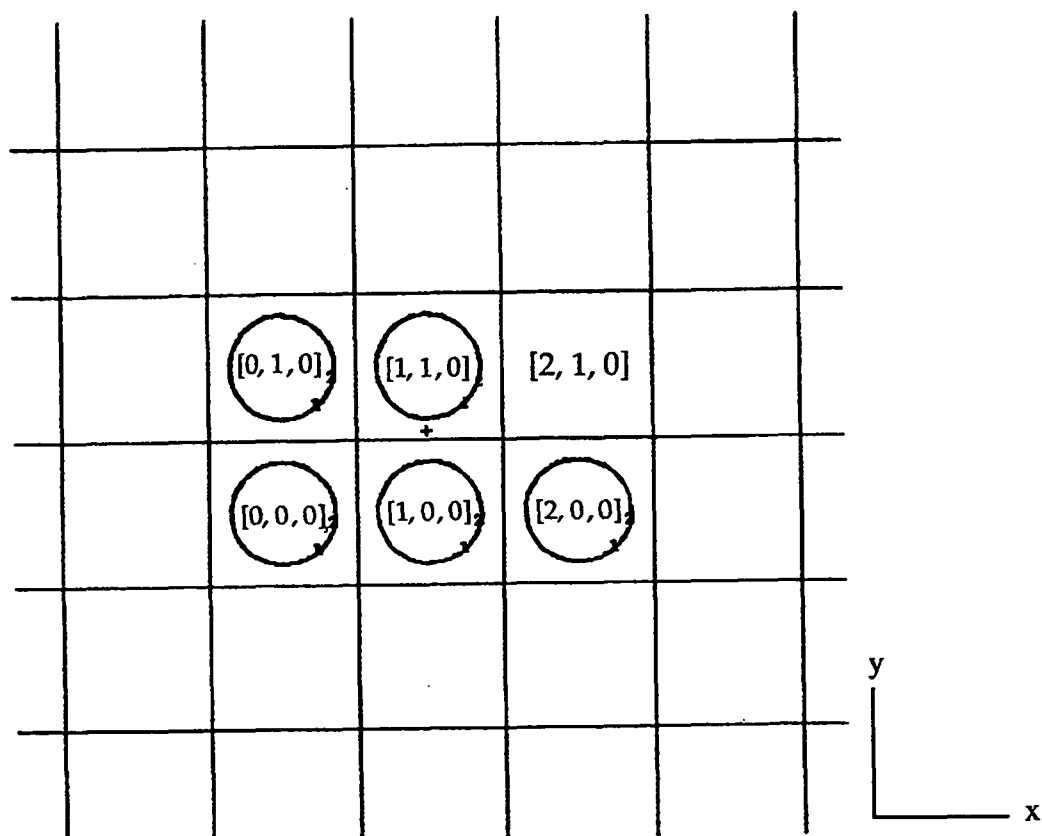


Figure 7-9. Top view of universe 0 lattice with empty element.

A source in a universe 0 lattice has some constraints. At present, the `ksrc` card can have only source points in the $[0, 0, 0]$ element in a universe 0 lattice. In this problem, the following `ksrc` card puts a starting source point at the center of the $[0, 0, 0]$ element:

`ksrc 0 0 20.62`

Source points can be put into multiple elements rather simply with the repeated structure format of the `sdef` card. The following cards illustrate that method.

```
sdef cel=d1      pos=0 0 20.62
si1  1 5(0 0 -1):1 5(1 0 -1):1      .....
sp1      1              1      .....
```

The `sdef` keyword `cel=d1` says that the source cells are given by a distribution, where `d1` points to the `si1` card. The keyword `pos` defines the xyz location of the source point. The `si1` card describes the path from the lattice cell (5) and each individual lattice element (0 0 -1) to the cell that contains the source point (1). The 1 on the `si1` card indicates that discrete values will follow. Because element 5 (2 1 0) does not exist, it is not included in the list on the `si1` card. The `sp1` card provides the probabilities of choosing a particular cell. In this case, the probabilities are equal. {To understand the cards above, see the MCNP manual, Chapter 3, Section D.}

The final combined k_{eff} estimator for this problem on a SPARC 1 at the University of New Mexico was 0.9857 with an estimated standard deviation of 0.0033.

CAUTION: Be aware that if an element does not exist, a particle cannot travel through that element to reach another element that does exist. Particles that leave element [2, 0, 0] cannot enter [1, 1, 0] because [2, 1, 0] does not exist. If you intend that [2, 1, 0] not have a solution cylinder but you want particles to be able to travel through the element to reach another, change the material in the cells that fill that element to be 0, a void, using the techniques described previously.

One limitation of this modeling method is that no geometry can exist outside the lattice elements. Because lattice elements that are not defined do not exist, and because particles are killed when they exit elements that are defined, no geometry can be described other than the universe 0 lattice. For example, a concrete wall cannot be described next to the six solution cylinders in the example. The lattice itself, filled with the appropriate cells, must be the only geometry in the problem.

The advantages of modeling a universe 0 lattice are that no "window" cell is required to limit the extent of the infinite lattice and fewer cells and surfaces are needed. Complete lattice element blocks are perhaps more intuitive. The disadvantage is that the applicability is limited by the fact that no geometry can be defined outside the lattice. Currently, when plotting, an infinite lattice appears, but only elements that exist contain other cells and surface/cell labels.

If you want to run a problem that consists of an infinite universe 0 lattice, there are two ways to do it. The first is to change the cell 5 card in the example in this chapter so that every lattice element is filled with universe 1, shown below.

```
5 0    -8 9 -10 11 -16 3 imp:n=1 lat=1 fill=1
```

The second method is to describe a geometry that is equivalent to one lattice element but that cell is not defined to be a lattice cell. The surfaces of this cell can be specified to be either reflecting surfaces or periodic surfaces. {See the MCNP manual for information about reflecting and periodic boundaries.}

7.11 SUMMARY

This chapter modified the example from Chapter 5 and made the lattice 3-dimensional by defining a lattice cell that was finite in the x, y, and z directions. We showed how to specify each element of a 3-dimensional hexahedral lattice and discussed a universe 0 lattice. {Please refer to the MCNP manual for a more detailed description of the use of lattices with MCNP.}

Primer Summary

This document was designed to help a nuclear criticality safety analyst understand and use the MCNP Monte Carlo code. It began with a simple criticality problem, the Quickstart chapter, that introduced the basic concepts of using MCNP. The chapters that followed expanded on the ideas presented in the Quickstart chapter by presenting a varying range of problems from simple cylinders to 3-dimensional lattices. Although this primer was written to stand alone, it is recommended that it be used in conjunction with the MCNP 4A manual. Many of the concepts discussed in the primer are described in greater detail in the MCNP manual.

After completing this primer, a criticality analyst should be capable of handling a majority of the situations that will arise in the field of nuclear criticality safety. The input files provided in the document can be modified by the analyst to fit a particular problem as required.

The primer provides the necessary information to create and run criticality problems; it does not attempt to teach the theory of neutron interaction. MCNP is only capable of analyzing the problem specified and will not know whether or not the problem was described correctly or if the proper materials were input. We remind you that a single calculation of k_{eff} and its associated confidence interval with MCNP or any other code is meaningless without an understanding of the context of the problem, the quality of the solution, and a reasonable idea of what the result should be.

APPENDIX A

Monte Carlo Techniques

I. INTRODUCTION

Monte Carlo methods are used in nuclear applications such as shielding, radiation transport, and neutron physics analysis. Monte Carlo refers to a statistical method wherein the expected characteristics of particles (e.g. particle flux) are estimated by sampling a large number of individual particle histories whose trajectories are simulated by a digital computer. In some cases, there are equations that adequately describe the behavior of such systems and that can be solved either analytically or numerically. Why then, if this is the case, would anyone want to use Monte Carlo techniques? The basic advantage of Monte Carlo techniques over the deterministic techniques (e.g., numerical solution of the Boltzmann transport equation) is that Monte Carlo more accurately represents the geometry and nuclear data than do deterministic techniques. Deterministic methods require reasonably simple geometries for the numerical techniques to work and use multigroup group approximations to continuous energy neutron cross section data. Monte Carlo techniques can handle complex geometries and continuous cross section data, as well as the simple geometries and multigroup data.

In many cases, the geometry of a system is more complex than a cylinder or a stack of cubes; it often includes both cylindrical and planar surfaces. For these situations, Monte Carlo is a better technique as it statistically evaluates the system with few approximations rather than trying for a numerical approximation to the analytic description. The disadvantages of Monte Carlo are that it is statistical in nature and does not provide an exact solution to the problem. All results represent estimates with associated uncertainties. Also, Monte Carlo techniques can be quite time consuming on a computer if very small uncertainties are required. The relationship between Monte Carlo and deterministic techniques can best be summarized as: deterministic techniques provide an exact solution to an approximation of the problem while Monte Carlo techniques provide an approximate solution to an exact representation of the problem.

II. MONTE CARLO APPROACH

When a neutron traverses a material, it interacts with the constituent atoms of that material. It gets scattered or absorbed depending on the process cross sections of the material. These processes occur statistically in nature with the probability of occurrence determined by a cross section. No one can predict exactly how far one particle will travel in a material before interacting; however, one can predict the distribution of flight distances that a large number of those particles will have prior to the first interaction. Using "random" numbers, the computer can generate a statistical history for the life of each particle (a random walk analysis). That is, an individual particle may experience many scattering interactions before finally being absorbed or leaking from the system. Random numbers (a set of numbers which have no pattern and are sampled uniformly between zero and one) are used at each interaction to determine which process (absorption, fission, elastic scattering, etc.) occurs, how much energy is lost, what is the new direction of the particle (for scattering), or how many neutrons are created in a fission event. The life of a particle begins at birth, either from an external neutron source or from a fission event, and ends with absorption or with a scattering event that moves the neutron outside the assembly. The events that occur during a particle's life are tabulated and become the history of that particle. Because a single particle is usually not representative of the total system, a number of histories must be evaluated to accurately describe what occurs.

III. CRITICALITY CALCULATIONS

In criticality applications, the effective multiplication factor of an assembly is of primary interest. In these calculations, a group of neutron histories is often referred to as a k_{eff} cycle (or neutron generation as defined in reactor theory) with the multiplication factor of the assembly given by the ratio of the number of neutrons generated at the end of the k_{eff} cycle (i.e., those created in fission events in this cycle) to the number of neutrons whose histories are evaluated in this cycle (i.e., the number at the start of the generation). The expected value of the multiplication factor is then estimated by averaging over the events in the k_{eff} cycle. In the same way, the expected value of the leakage probability or the fraction of events leading to capture can also be obtained.

The relative error in the estimate of the effective multiplication factor will usually decrease as the number of k_{eff} cycles increases. Thus, numerous cycles are necessary to arrive at a good estimate of k_{eff} . In addition, the first few cycles are inaccurate because the spatial neutron source has not converged. Because the distribution of source (fission) neutrons in a system is dependent on the eigenvalue of the system and on its geometry, it takes a number of inactive cycles for the Monte Carlo spatial neutron distribution to approach the converged distribution. For this reason, the first few cycles (the third number on the kcode card) are ignored in the final estimate of k_{eff} . The estimates of k_{eff} from the remaining cycles are averaged to obtain a mean value for the effective multiplication factor.

For example, let's say we evaluated G generations and discarded the first D of them. (It is recommended that $G - D > 100$ to observe any trends in the calculations.) Then the estimated effective multiplication factor of the system is given by:

$$\bar{k} = \frac{1}{(G - D)} \sum_{i=D+1}^G k_i$$

where \bar{k} is the estimated system multiplication factor and k_i is the multiplication factor determined from the i^{th} cycle. The repeatability of the estimate (i.e., if the same

calculation is performed with different random numbers, how much different will the estimate of k be?) is determined from the estimated standard deviation of the mean, σ_k . The standard deviation of the mean is calculated using the standard deviation, σ , of the distribution of k -values.

$$\sigma = \sqrt{\frac{1}{(G - D - 1)} \sum_{i=D+1}^G (k_i - kbar)^2}$$

Then the standard deviation of the mean, σ_k is:

$$\sigma_k = \frac{\sigma}{\sqrt{(G - D)}}$$

For a valid Monte Carlo calculation, the range $kbar - \sigma_k$ to $kbar + \sigma_k$ should include the precise k_{eff} result about 68% of the time. The final result of the Monte Carlo calculation would be reported as: $kbar \pm \sigma_k$ for a nominal 68% confidence interval, $kbar \pm 2\sigma_k$ for 95% and $kbar \pm 2.6\sigma_k$ for a 99% confidence interval for large N . These percentages refer to the fraction of the time the precise value of $kbar$ is included in a confidence interval.

MCNP has three different estimators for k_{eff} : collision, absorption, and track length between collisions. A statistically combined average is used as the final k_{eff} . {See Chapter 2 of the MCNP manual for a detailed discussion of the different estimators.}

Example Monte Carlo Process

The basic Monte Carlo approach can be summarized as follows: a sequence of random numbers $0 < R_i < 1$ is used to produce a random distribution of quantities that simulate the problem at hand. For example, with a *one-dimensional* slab of fissile material, it is desired to calculate the effective multiplication factor of the finite slab. The process could be done as follows:

1. For the initial k_{eff} cycle, determine the initial position of the neutron.
2. Use a random number to select the energy for the neutron (based on χ , the energy distribution of fission neutrons).
3. Use the next random number to determine the direction cosine for the neutron.
4. Determine the location of the next collision site with the next random number (the distance traveled depends on the total cross section of the material).
5. Check the new location to see if the particle has escaped (leaked) from the system. If it has, add one to the total leaked and then go back to step 1 and start another history with another neutron. Otherwise, go to step 6.
6. Determine which type of interaction occurred at the new position based on the next random number. Each type of interaction has an associated cross section that determines its probability of occurrence.
 - a. If the interaction is scattering, then determine the new energy of the neutron after scattering using the next random number. Then go to step 3 and continue following the neutron (i.e., determine the direction of the scattered neutron).
 - b. If the interaction is absorption, go to step 1 and start a new neutron in the system.

c. If the interaction is fission, use \bar{v} to determine how many neutrons are created in this fission event and tabulate the total number of new neutrons created in this k_{eff} cycle. Also store the location of the fission event with each of the new neutrons so that they can be started at this location in the next cycle (this replaces step 1 in all future k_{eff} cycles).

7. When a given set of histories has been completed (enough to provide reasonable statistics), evaluate k_{eff} by dividing the number of new neutrons created in this cycle by the number of histories evaluated in the cycle.

Repeat the process for as many cycles as required to obtain appropriate statistics.

The following is a listing of common terms used in Monte Carlo techniques.

1. Monte Carlo – A numerical analysis technique that uses random sampling to estimate the solution of a physical or mathematical problem.

2. Random Numbers – An infinite set of numbers that are uniformly distributed from 0 to 1 and are independent. We actually use pseudorandom numbers, a deterministic reproducible sequence of random numbers generated by a computer that satisfy statistical tests for randomness.

3. Monte Carlo Weight – The number of physical particles W that a Monte Carlo particle represents.

4. Random Walk – The random selection of events for a particle history.

5. History – The complete random walk of a Monte Carlo particle from its birth in the source to its death, including all progeny.

6. Monte Carlo Track – A branch, or subset, of a history that can be obtained by physical events (for example, fissions) or by variance reduction techniques (for example, geometry splitting)
7. Score – Contribution from a track to a tally.
8. History Score – Sum of all scores from one source particle's tracks.
9. Tally – Used interchangeably with score. Also, the quantity we want to estimate (average score), obtained by summing all scores from all histories.
10. Relative Error – The standard deviation of the mean of a tally divided by the mean. The error refers to the precision of the tally, not to its accuracy.
11. Importance – the expected score per unit weight of a track at phase-space point.
12. Flux Density – The product of particle density and particle speed. The flux density is often referred to simply as flux and is mathematically and physically equivalent to the sum of the lengths of all Monte Carlo tracks per unit volume per unit time. Flux density is in units of particles/cm²/shake.
13. Fluence – Integral of flux over time. If the MCNP source is in units of particles, the flux tallies are really fluence tallies. If the MCNP source is in units of particles per unit time, the flux tallies are truly fluxes. Fluence has units of particles/cm².
14. Current – The number of particles crossing a surface in a given time interval and in a given direction interval.

APPENDIX B

Calculating Atom Densities

Most Monte Carlo codes (and indeed, most neutronics codes) require that the user enter values to describe the atom densities of the materials involved in the analysis. The problem facing the user is that many times the data supplied are in the form of weight percent, volume percent, solution density, density of individual constituents, etc. These data are not always directly compatible with the input requirements of the code. This appendix is designed to cover the majority of cases for atom density calculations with a multitude of different input specifications.

I. Single material, given: mass density,

For example, calculate the atom density of uranium-238 (U-238) for a nominal mass density of 19.1 g/cc.

The basic equation for atom density is:
$$n = \frac{\rho N_a}{A} \quad (B-1)$$

where: n = atom density (atoms/cc)
 ρ = density of material (g/cc)
 N_a = Avogadro's number = 0.6022×10^{24}
 A = atomic weight of isotope (g/mole)

For this example,

$$\rho = 19.1 \frac{g}{cm^3} \quad N_a = 0.6022 \times 10^{24} \frac{atoms}{mole} \quad A = 238.05 \frac{grams}{mole}$$

$$n = 4.832 \times 10^{22} \frac{atoms}{cm^3}$$

The atom density of U-238 in the example is $4.832 \cdot 10^{22}$ atoms per cc. These units are sufficient for some codes, but others may require the entry to be in atoms per barn-cm because the cross sections are generally given in barns. Remembering that a barn is 10^{-24} cm², then you can multiply the result by this value to arrive at an atom density of U-238 of $4.832 \cdot 10^{-2}$ atoms per barn-cm. However, rather than going through this step for each calculation, Avogadro's number is often expressed as 0.6022 atoms-cm² per mole-barn. This representation of Avogadro's number incorporates the proper units and directly gives values of atom density in atoms per barn-cm.

II.a. Two materials, given: weight fractions and mixture density.

When there is a mixture of materials with a known density and individual weight fractions, the atom density equation becomes:

$$N_i = \frac{\rho_{mix} * wf_i * N_a}{A_i} \quad (B-2)$$

where: N_i = atom density of i^{th} material.
 ρ_{mix} = mass density of mixture.
 wf_i = weight fraction of i^{th} material.
 A_i = atomic weight of i^{th} material.

For example, calculate the atom densities of U-235 and U-238 in 3 weight percent enriched uranium¹, U(3). The density of the uranium is 18.9 g/cc.

$$N_{u235} := \frac{\left(18.9 \cdot \frac{g}{cm^3}\right) \cdot (0.03) \cdot 0.6022 \cdot \frac{atoms \cdot cm^2}{mol \cdot b}}{235.04 \cdot \frac{g}{mol}} \quad N_{u238} := \frac{\left(18.9 \cdot \frac{g}{cm^3}\right) \cdot (0.97) \cdot 0.6022 \cdot \frac{atoms \cdot cm^2}{mol \cdot b}}{238.05 \cdot \frac{g}{mol}}$$

$$N_{u235} = 0.0014527 \cdot \frac{atoms}{b \cdot cm}$$

$$N_{u238} = 0.0463774 \cdot \frac{atoms}{b \cdot cm}$$

¹ Note the weight percent of U-235 in uranium compounds is usually put in parentheses after the symbol for uranium, e.g. U(5) would indicate 5 weight percent U-235.

The atom fractions are then:

$$\text{Atom fraction U-235} = \frac{(1.45E-3)}{(1.45E-3) + (4.64E-2)} = 0.0303$$

$$\text{Atom fraction U-238} = \frac{(4.64E-2)}{(1.45E-3) + (4.64E-2)} = 0.9697$$

As the atomic weights of the two isotopes are within a percent of each other, there is little difference between the weight fractions and the atom fractions. However, as will be demonstrated with boron, this small difference is not always true. Note that although the example was done with only two materials, as long as the mixture density and individual weight fractions are given, the technique applies to as many materials as required.

II.b. Two materials, given: weight fractions and individual material densities.

If the individual densities and weight fractions are known, then the mixture density is determined from:

$$\frac{1}{\rho_{mix}} = \frac{wf_1}{\rho_1} + \frac{wf_2}{\rho_2} + \dots + \frac{wf_i}{\rho_i} \quad (B-3)$$

In the previous example, assume the density of U-235 is 18.6 g/cc and U-238 is 18.9 g/cc, then....

$$\frac{1}{\rho_{mix}} = \frac{0.03}{18.6} + \frac{0.97}{18.9} \quad \rho_{mix} = 18.89 \frac{g}{cm^3}$$

After obtaining the mixture density, the atom densities are calculated using equation B-2 as above.

III. Two materials given: atom fractions and atom mixture density.

Although weight fractions are generally used for enrichments, atom fractions are given in publications such as the Chart of the Nuclides or the CRC Handbook of Chemistry and Physics. To use atom fractions, an average atomic weight must be determined.

$$\bar{A} = af_1 * A_1 + af_2 * A_2 + \dots + af_i * A_i \quad (B-4)$$

The average atomic weight is used in the calculation of the mixture atom density.

$$N_{mix} = \frac{\rho_{mix} * N_a}{\bar{A}} \quad (B-5)$$

Then the individual constituent atom densities are calculated:

$$N_i = af_i * N_{mix} \quad (B-6)$$

For example, natural boron has a density of 2.34 g/cc with an atom fraction of 0.199 B-10 and 0.801 B-11.

$$\bar{A} = 0.199 * 10.01 + 0.801 * 11.01 = 10.81 g \frac{B_{nat}}{mole}$$

$$N_{mix} = N_{B_{nat}} = \frac{(2.34 g \frac{B_{nat}}{cm^3}) * (0.6022 \frac{atom - cm^2}{mole - b})}{10.81 g \frac{B_{nat}}{mole}}$$

$$= 1.304 * 10^{-1} \frac{atoms_{B_{nat}}}{b - cm}$$

Now because we know what fraction of the B_{nat} atoms are B-10 atoms, we can calculate the atom density of B-10 in natural Boron.

$$N_{B-10} = 0.199 \frac{atom_{B-10}}{atom_{B_{nat}}} * 1.304 * 10^{-1} \frac{atom_{B_{nat}}}{b - cm} = 2.59 * 10^{-2} \frac{atom_{B-10}}{b - cm}$$

Similarly for B-11

$$N_{B-11} = 0.801 \frac{atom_{B-11}}{atom_{B_{nat}}} * 1.304 * 10^{-1} \frac{atom_{B_{nat}}}{b - cm} = 1.045 * 10^{-1} \frac{atom_{B-11}}{b - cm}$$

Note that $N_{B10} + N_{B11} = N_{Bnat}$, which it should.

IV. Calculating weight fractions, atom fractions, and average atomic weight when one set of fractions is known.

In the previous section, equation B-4 showed how to calculate average average atomic weight when atom fractions are known. If, however, weight fractions are given, then a different equation is used to calculate average atomic weight.

$$\bar{A} = \left[\frac{wf_1}{A_1} + \frac{wf_2}{A_2} + \dots + \frac{wf_i}{A_i} \right]^{-1} \quad (B-7)$$

Further, you can calculate the atom fractions from the weight fractions and the average atomic weight as:

$$af_i = wf_i * \frac{\bar{A}}{A_i} \quad (B-8)$$

Or, if you have the atom fractions, calculate the weight fraction as:

$$wf_i = af_i * \frac{A_i}{A} \quad (B-9)$$

For example, continue with natural boron and calculate the weight fractions.

$$wf_{B10} = 0.199 * \frac{10.01}{10.81} = 0.184$$

$$wf_{B11} = 0.801 * \frac{11.01}{10.81} = 0.816$$

As indicated earlier there is a significant difference between weight and atom fractions for B-10 and B-11 in natural boron.

V.a. Molecules, given: chemical structure and mass density.

Determination of atom densities for constituents of a molecule is similar to the calculation when the atom fractions are known. In this case, the atom fractions are usually greater than 1 and represent the number of atoms of a particular type in the molecule.

For example, determine the atom densities of hydrogen and oxygen in water with a density of 1.0 g/cc.

$$N_{H_2O} = \frac{(1.0 \text{ g / cm}^3)(0.6022 \text{ atom-cm}^3 / \text{mole-b})}{18 \text{ g / mole}} = 3.34 * 10^{-2} \frac{\text{molecules}_{H_2O}}{\text{b-cm}}$$

In water, there are 2 atoms of H and 1 atom of O for every molecule of water.

$$N_H = 2 * N_{H_2O} = 6.68 * 10^{-2} \frac{\text{atoms}_H}{\text{b-cm}}$$

$$N_O = 1 * N_{H_2O} = 3.34 * 10^{-2} \frac{\text{atoms}_O}{\text{b-cm}}$$

V.b. Molecules with mixtures of isotopes.

In the example above, it was assumed that all hydrogen was H-1 and all oxygen was O-16. However, for many materials encountered in criticality safety, the isotopic content is very important (e.g. boron and uranium).

For example, determine the atom densities of B-10, B-11, and C in Boron Carbide (B_4C) assuming the boron is natural boron and the mixture density is 2.54 g/cc.

The molecular weight of B_4C can be found in a reference or can be calculated using equation B-4.

$$A_{B_4C} = \frac{4 \text{ moles } B_{nat}}{\text{mole } B_4C} * \frac{10.81 \text{ g}}{\text{mole } B_{nat}} + \frac{1 \text{ mole } C}{\text{mole } B_4C} * \frac{12.00 \text{ g}}{\text{mole } C} \quad A_{B_4C} = 55.24 \text{ g/mole}$$

$$N_{B_4C} = \frac{(2.54 \text{ g/cc})(.6022 \text{ molecules} - \text{cm}^2 / \text{mole} - b)}{55.24 \text{ g/mole}}$$

$$N_{B_4C} = 2.77 * 10^{-2} \frac{\text{molecules}_{B_4C}}{b - \text{cm}}$$

There are 4 atoms of B_{nat} per molecule of B_4C .

$$N_{B_{nat}} = 4 * N_{B_4C} = 1.108 * 10^{-1} \frac{\text{atoms}_{B_{nat}}}{b - \text{cm}}$$

From the earlier example, (or from the Chart of the Nuclides) the atom fractions of B-10 and B-11 in natural boron are 0.199 and 0.801, respectively.

$$N_{B_{10}} = af_{B_{10}} * N_{B_{nat}} = 0.199 * 1.108 * 10^{-1} = 2.205 * 10^{-2} \frac{\text{atoms}_{B_{10}}}{b - \text{cm}}$$

$$N_{B_{11}} = af_{B_{11}} * N_{B_{nat}} = 0.801 * 1.108 * 10^{-1} = 8.875 * 10^{-2} \frac{\text{atoms}_{B_{11}}}{b - \text{cm}}$$

These are the atom densities of B-10 and B-11 in B₄C. Now, we need to calculate the atom density of carbon in B₄C.

$$N_C = 1 * N_{B_4C} = 2.77 * 10^{-2} \frac{\text{atoms}_C}{b - cm}$$

For materials where the atom fractions are known, determination of the individual atom densities is straight forward. However, for those cases where the weight fractions are known, then the atom fractions are first calculated from equation B-8 and then used to determine atom densities, as above.

Note: in mixtures, it is important to know whether the weight or atom fractions are relative to the entire mixture or just to some constituent part of the mixture. In the example above, atom fractions for B-10 and B-11 were relative to the natural boron and not to the B₄C. As another example, in U(20)O₂, the 0.20 weight fraction of U-235 is relative to the uranium, not to the UO₂, so it can only be applied to the uranium.

Example: U(20)O₂ with a density of 10.5 g-UO₂ per cc.

First determine the average atomic weight of UO₂ with 20 weight percent U-235. Start by calculating the average atomic weight of U.

$$\bar{A}_U = \left[\frac{0.20}{235.04} + \frac{0.80}{238.05} \right]^{-1} = 237.44 \frac{gU(20)}{cm^3}$$

$$\bar{A}_{UO_2} = 237.44 + 2 * 16 = 269.44 \frac{gUO_2}{cm^3}$$

Now determine the atom density of UO₂.

$$\begin{aligned} N_{UO_2} &= \frac{(10.5 g_{UO_2} / cc)(.6022 \text{molecules} - cm^2 / mole - b)}{269.44 g / mole} \\ &= 2.35 * 10^{-2} \frac{\text{molecules}_{UO_2}}{b - cm} \end{aligned}$$

There is 1 atom of U and 2 atoms of O for each molecule of UO_2 .

$$N_O = 2 * N_{\text{UO}_2} = 4.70 * 10^{-2} \frac{\text{atoms}_O}{b - \text{cm}}$$

$$N_U = 1 * N_{\text{UO}_2} = 2.35 * 10^{-2} \frac{\text{atoms}_U}{b - \text{cm}}$$

But twenty weight percent of the uranium is U-235 while eighty weight percent is U-238. Use the weight fractions to calculate uranium atom fractions from equation B-8.

$$af_{U235} = wf_{U235} * \frac{\bar{A}}{A_{235}} = 0.20 * \frac{237.44}{235.04} = 0.202$$

$$af_{U238} = wf_{U238} * \frac{\bar{A}}{A_{238}} = 0.80 * \frac{237.44}{238.05} = 0.798$$

Then calculate the atom densities.

$$N_{U235} = f_{U235} * N_U = 0.202 * 2.35 * 10^{-2} = 4.75 * 10^{-3} \frac{\text{atoms}_{U235}}{b - \text{cm}}$$

$$N_{U238} = f_{U238} * N_U = 0.798 * 2.35 * 10^{-2} = 1.875 * 10^{-2} \frac{\text{atoms}_{U238}}{b - \text{cm}}$$

VI. Solution Systems.

Because solution systems have a number of parameters (solution density, molality, normality, single constituent density, H/U ratio, H/Pu ratio, H/X ratio) that can be used to characterize them, calculation of atom densities in solution is usually more complex than for solids. If the solution density is given, then the atom densities are calculated using the technique given in Section V.a. (where water is used as the example).

VI.a. H/X ratio, fissile component density, and with chemical formula.

The H/X ratio (ratio of hydrogen atoms to fissile atoms) is often used in criticality studies to indicate amount of moderation in the system. When the fissile mass density is provided along with H/X, all of the atom densities can be determined.

Using the example from Chapter 3 of the Primer, we have U(4.89)O₂F₂ in solution with water; H/X = 524 and the U-235 density is 0.0425 gU235/cc.

First calculate the fissile atom density.

$$N_{U235} = \frac{\rho_{U235} * N_{AV}}{A_{235}} = \frac{(0.0425 \text{ gU235 / cc})(0.6022 \text{ atoms} - \text{cm}^3 / \text{mole} - b)}{235.04 \frac{\text{g}}{\text{mole}}}$$

$$N_{U235} = 1.0889 * 10^{-4} \frac{\text{atoms}_{U235}}{\text{b} - \text{cm}}$$

We know the weight fractions of U-235 and U-238, but we want the atom fractions. To get these values we need to use equation B-7 to calculate the average atomic weight of the (U-235,U-238) mixture.

$$wf_{U235} = 0.0489 \quad wf_{U238} = (1 - 0.0489) = 0.9511$$

$$\bar{A} = \left[\frac{0.0489}{235.04} + \frac{0.9511}{238.05} \right]^{-1} = 237.90 \frac{\text{gU}(4.89)}{\text{cm}^3}$$

Use equation B-8 to calculate the atom fractions.

$$af_{235} = wf_{235} * \frac{\bar{A}}{A_{235}} = 0.0489 * \frac{237.90}{235.04} = 0.0495 \frac{\text{atoms}_{U235}}{\text{atoms}_U}$$

$$af_{238} = wf_{238} * \frac{\bar{A}}{A_{238}} = 0.9511 * \frac{237.90}{238.05} = 0.9505 \frac{\text{atoms}_{U238}}{\text{atoms}_U}$$

The uranium atom density is determined by dividing the U-235 atom density by the U-235 atom fraction.

$$N_U = \frac{N_{235}}{af_{235}} = \frac{1.0889 * 10^{-4} \frac{atoms_{U235}}{b - cm}}{0.0495 \frac{atoms_{U235}}{atoms_U}} = 2.1998 * 10^{-3} \frac{atoms_U}{b - cm}$$

$$N_{U238} = af_{238} * N_U = 0.9505 \frac{atoms_{U238}}{atoms_U} * 2.1998 * 10^{-3} \frac{atoms_U}{b - cm} = 2.0909 * 10^{-3} \frac{atoms_{U238}}{b - cm}$$

Now calculate the O₂ and F₂ densities from the uranium atom density.

$$N_O = 2 * N_U = 4.3996 * 10^{-3} \frac{atoms_O}{b - cm} \quad (\text{in } UO_2F_2)$$

$$N_F = 2 * N_U = 4.3996 * 10^{-3} \frac{atoms_F}{b - cm}$$

With UO₂F₂ solutions, there is a substantial amount of water for which the atom densities of H and O can be determined from the H/X ratio.

$$N_H = H / X * N_{U235} = 524 * 1.0889 * 10^{-4} = 5.7058 * 10^{-2} \frac{atoms_H}{b - cm}$$

$$N_O = N_H * \frac{1atom_O}{2atoms_H} = 2.8529 * 10^{-2} \frac{atoms_O}{b - cm} \quad (\text{in } H_2O)$$

The total atom density for oxygen is the sum of its atom density in UO₂F₂ and its atom density in H₂O.

$$N_O = 2.8529 * 10^{-2} \frac{atoms_O}{b - cm} + 4.3996 * 10^{-3} \frac{atoms_O}{b - cm} = 3.2929 * 10^{-2} \frac{atoms_O}{b - cm}$$

The final values, in atoms/b-cm, that were used in Chapter 3 are:

$$N_{235} = 1.0889 \cdot 10^{-4}$$

$$N_{238} = 2.0909 \cdot 10^{-3}$$

$$N_H = 5.7058 \cdot 10^{-2}$$

$$N_O = 3.2929 \cdot 10^{-2}$$

$$N_F = 4.3996 \cdot 10^{-3}$$

$$N_{total} = 9.6586 \cdot 10^{-2}$$

APPENDIX C

Specifications & Atom Densities Of Selected Materials

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Criticality Safety Group
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April 1994

The following material compositions, specifications, and atom densities have been compiled by the above author from various sources. They are provided for the convenience of users of computer codes for nuclear analysis. No warranty is made nor is any legal liability or responsibility assumed for the accuracy, completeness, or usefulness of the following information. Reference to any specific commercial product by trade name or registered trademark does not necessarily constitute or imply its endorsement.

Atomic weights used in the following were taken from "Nuclides and Isotopes, Fourteenth Edition," General Electric Company, San Jose, California.

Atom densities are given in units of atoms/barn-cm.

BISCO® modified NS-4 with 4.5% Boron

Los Alamos National Laboratory Analysis

Density = 1.119 g/cc

Nuclide	Wt. Frac.	Atom Dens.
C	0.4771	0.02677
N	0.0356	0.00171
H	0.0787	0.05262
Si	0.0018	0.00004
Na	0.0494	0.00145
B(nat)	0.0455	0.00284
O	0.3119	0.01314

BORON CARBIDE (Natural Boron): B₄C

Density = 2.51 g/cc

A = 55.2570

Nuclide	Wt. Frac.	Atom Dens.
natB	0.7826	0.10941
C	0.2174	0.027359

CELOTEX® (Lignocellulosic Fiberboard)*

Normal density = 16 ± 2 lb/ft³

Celotex ~ C₆H₁₀O₅ (cellulose)

$$A = 162.143$$

Atom Densities as Function of Celotex Density

Density (g/cc)	Density (lb/ft ³)	C	H	O
0.31	19.34	6.908-3	1.1514-2	5.757-3
0.30	18.71	6.685-3	1.1142-2	5.571-3
0.29	18.09	6.463-3	1.0771-2	5.385-3
0.2886	18.0	6.431-3	1.0719-2	5.359-3
0.28	17.46	6.240-3	1.0400-2	5.200-3
0.27	16.84	6.017-3	1.0028-2	5.014-3
0.26	16.22	5.794-3	9.657-3	4.828-3
0.2565	16.0	5.716-3	9.527-3	4.763-3
0.25	15.59	5.571-3	9.285-3	4.643-3
0.24	14.97	5.348-3	8.914-3	4.457-3
0.23	14.35	5.125-3	8.542-3	4.271-3
0.2245	14.0	5.003-3	8.338-3	4.169-3
0.22	13.72	4.903-3	8.171-3	4.086-3
0.21	13.10	4.680-3	7.800-3	3.900-3
0.20	12.47	4.457-3	7.428-3	3.714-3
0.19	11.85	4.234-3	7.057-3	3.528-3
0.18	11.23	4.011-3	6.685-3	3.343-3

Ref: ASTM C-208, "Standard Specification for Insulating Board (Cellulosic Fiber),
Structural and Decorative"

CONCRETE (KENO Regular Concrete Standard Mix)

Density = 2.3 g/cc

Nuclide	Wt. Frac.	Atom Dens.
H	0.010	0.01374
O	0.532	0.04606
Si	0.337	0.01662
Al	0.034	0.00175
Na	0.029	0.00175
Ca	0.044	0.00152
Fe	0.014	0.00035

CONCRETE [LOS ALAMOS (MCNP) Mix]

Density = 2.25 g/cc

Nuclide	Wt. Frac.	Atom Dens.
H	0.00453	0.006094
O	0.51260	0.043421
Si	0.36036	0.017390
Al	0.03555	0.001786
Na	0.01527	0.000900
Ca	0.05791	0.001958
Fe	0.01378	0.000334

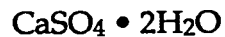
CONCRETE (NBS Ordinary)

Density = 2.35 g/cc

Nuclide	NBS Wt. Frac	Adj.* Wt. Frac.	Adj. Atom Dens.
H	0.0056	0.006	0.00842
O	0.4956	0.500	0.04423
Si	0.3135	0.315	0.01587
Al	0.0456	0.048	0.00252
Na	0.0171	0.017	0.00105
Ca	0.0826	0.083	0.00293
Fe	0.0122	0.012	0.00030
K	0.0192	0.019	0.00069
Mg	0.0024	-	
S	0.0012	-	

* adjusted to sum to unity without minor trace elements

GYPSUM (Calcium Sulfate)



Density = 2.32 g/cc

A = 172.17

Nuclide	Atom Density
Ca	0.008115
S	0.008115
O	0.048689
H	0.032460

INCONEL (KENO Standard Mix)

Density = 8.3 g/cc

Nuclide	Wt. Frac.	Atom Dens.
Si	0.025	0.00445
Ti	0.025	0.00261
Cr	0.15	0.01442
Fe	0.07	0.00626
Ni	0.73	0.06217

INCONEL X (Simplified)

Density = 8.5 g/cc

Nuclide	Wt. Frac.	Atom Dens.
Ni	0.78	0.0680
Cr	0.15	0.0148
Fe	0.07	0.0064

KYNAR®: C₂H₂F₂,

Density = 1.76 g/cc

A = 64.0347

Nuclide	Wt. Frac.	Atom Dens.
C	0.3751	0.0331
H	0.0315	0.0331
F	0.5934	0.0331

LEXAN®: C₁₆H₁₄O₃

Los Alamos National Laboratory Analysis

Density = 1.20 g/cc

A = 254.2855

Nuclide	Wt. Frac.	Atom Dens.
C	0.755749	0.045471
H	0.055494	0.039787
O	0.188757	0.008527

MAGNESIUM OXIDE: MgO

Density = 3.22 g/cc

A = 40.3044

Nuclide	Wt. Frac.	Atom Dens.
Mg	0.6030	0.04811
O	0.3970	0.04811

NYLON®: C₁₂H₂₂N₂O₂,

Density = 1.14 g/cc

A = 226.319

Nuclide	Wt. Frac.	Atom Dens.
C	0.63685	0.036401
H	0.09798	0.066737
N	0.12378	0.006067
O	0.14139	0.006067

PARAFFIN: C₂₅H₅₂

Density = 0.93 g/cc

A = 352.688

Nuclide	Wt. Frac.	Atom Dens.
C	0.8514	0.03970
H	0.1486	0.08257

PLEXIGLAS® & LUCITE®: C₅H₈O₂

Density = 1.18 g/cc

A = 100.117

Nuclide	Wt. Frac.	Atom Dens.
C	0.59985	0.03549
H	0.08054	0.05678
O	0.31961	0.01420

POLYETHYLENE: CH₂

Density = 0.92 g/cc

A = 14.0269

Nuclide	Wt. Frac.	Atom Dens.
C	0.85628	0.03950
H	0.14372	0.07899

POLYURETHANE FOAM

Los Alamos National Laboratory Analysis

Density = 0.021 g/cc

Nuclide	Wt. Frac.	Atom Dens.
H	0.041	5.144E-4
C	0.544	5.728E-4
N	0.121	10.925E-4
O	0.294	2.324E-4

POLYVINYL CHLORIDE (PVC): C₂H₃Cl

Density = 1.65 g/cc

Nuclide	Wt. Frac.	Atom Dens.
C	0.3844	0.03180
H	0.0484	0.04771
N	0.5672	0.01590

PYREX[®] [Borated Glass], (KENO Standard Mix)

Density = 2.23 g/cc

Nuclide	Wt. Frac.	Atom Dens.
natB	0.037	0.00460
Al	0.010	0.0005
Na	0.041	0.00240
O	0.535	0.04491
Si	0.377	0.01803

SILICON RUBBER (G.E. RTV12A)

(Weight fractions below provided by G.E. Silicone Products Div.)

Density = 1.0185 g/cc

Nuclide	Wt. Frac.	Atom Dens.
C	0.3211	0.01640
Si	0.3745	0.00818
O	0.2235	0.00857
H	0.0807	0.04911

STEEL, CARBON

Density = 7.82 g/cc

Nuclide	Wt. Frac.	Atom Dens.
C	0.005	0.00196
Fe	0.995	0.08390

STAINLESS STEEL 304

Density = 7.92 g/cc

Nuclide	Wt. Frac.	Atom Dens.
Fe	0.695	0.05936
Cr	0.190	0.01743
Ni	0.095	0.00772
Mn	0.020	0.00174

STAINLESS STEEL 316

Density = 7.92 g/cc

Nuclide	Wt. Frac.	Atom Dens.
Fe	0.655	0.05594
Cr	0.170	0.01559
Ni	0.120	0.00975
Mo	0.025	0.00124
Mn	0.020	0.00174
Si	0.010	0.00170

STAINLESS STEEL 347

Density = 7.92 g/cc

Nuclide	Wt. Frac.	Atom Dens.
Fe	0.685	0.05850
Cr	0.180	0.01651
Ni	0.105	0.00853
Mn	0.020	0.00174
Si	0.010	0.00170

TEFLON®: CF₂

Los Alamos National Laboratory Analysis

Density = 2.15 - 2.20 g/cc

A = 50.0078

Nuclide	Wt. Frac.	Atom Dens.
C	0.2402	0.02650
F	0.7598	0.05298

APPENDIX D

Listing of Available Default Cross-Sections

These cross sections are what Los Alamos believes to be the best for criticality calculations. The sources of this data base are ENDF/B-V and Los Alamos evaluations. {More information is available in Appendix G of the MCNP manual.}

<u>Isotope</u>	<u>ZAID</u>
H-1	1001
H-2	1002
H-3	1003
He-3	2003
He-4	2004
Li-6	3006
Li-7	3007
Be-7	4007
Be-9	4009
B-10	5010
B-11	5011
C-nat	6000
C-12	6012
C-13	6013
N-14	7014
N-15	7015
O-16	8016
F-19	9019
Na-23	11023
Mg-nat	12000
Al-27	13027
Si-nat	14000
P-31	15031
S-32	16032
Cl-nat	17000

Ar-nat	18000
K-nat	19000
Ca-nat	20000
Sc-21	21045
Ti-nat	22000
V-nat	23000
Cr-nat	24000
Mn-55	25055
Fe-nat	26000
Co-59	27059
Ni-nat	28000
Cu-nat	29000
Ga-nat	31000
As-74	33074
As-75	33075
Br-79	35079
Br-81	35081
Kr-78	36078
Kr-80	36080
Kr-82	36082
Kr-83	36083
Kr-84	36084
Kr-86	36086
Rb-85	37085
Rb-87	37087
Y-88	39088
Y-89	39089
Zr-nat	40000
Zr-93	40093
Nb-93	41093
Mo-nat	42000
Mo-95	42095
Tc-99	43099
Ru-101	44101
Ru-103	44103

Rh-103	45103
Rh-105	45105
Average fission product from U-235	45117
Pd-105	46105
Pd-108	46108
Average fission product from Pu-239	46119
Ag-nat	47000
Ag-107	47107
Ag-109	47109
Cd-nat	48000
Sn-nat.....	50000
Fission products	50120
I-127	53127
I-135.....	53135
Xe-nat	54000
Xe-131	54131
Xe-134	54134
Xe-135	54135
Ce-133	55133
Ce-135	55135
Ba-138	56138
Pr-141	59141
Nd-143	60143
Nd-145	60145
Nd-147	60147
Nd-148	60148
Pm-147	61147
Pm-148	61148
Pm-149	61149
Sm-147	62147
Sm-149	62149
Sm-151	62151
Sm-152	62152
Eu-nat	63000
Eu-151	63151

Eu-152	63152
Eu-153	62153
Eu-154	62154
Eu-155	62155
Gd-nat	64000
Gd-152	64152
Gd-154	64154
Gd-155	64155
Gd-156	64156
Gd-157	64157
Gd-158	64158
Gd-160	64160
Ho-165	67165
Th-169	69169
Hf-nat	72000
Ta-181	73181
W-nat	74000
W-182	74182
W-183	74183
W-184	74184
W-186	74186
Re-185	75185
Ir-nat	77000
Pt-nat	78000
Au-197	79197
Pb-nat	82000
Bi-209	83209
Th-231	90231
Th-232	90232
Th-233	91233
U-233	92233
U-234	92234
U-235	92235
U-236	92236
U-237	92237

U-238	92238
U-239	92239
U-240	92240
Np-235	93235
Np-236	93236
Np-237	93237
Np-238	93238
Pu-237	94237
Pu-238	94238
Pu-239	94239
Pu-240	94240
Pu-241	94241
Pu-242	94242
Pu-243	94243
Am-241	95241
Am-242m	95242
Am-243	95243
Cm-242	96242
Cm-243	96243
Cm-244	96244
Cm-245	96245
Cm-246	96246
Cm-247	96247
Cm-248	96248
Bk-249	97249
Cf-249	98249
Cf-250	98250
Cf-251	98251
Cf-252	98252

S(α,β) IDENTIFIERS FOR THE MTm CARD

The cross sections shown here are at 300 Kelvin. {Appendix G of the MCNP manual gives a complete listing of the S(α,β) cross sections.}

<u>ZAID</u>	<u>Description</u>	<u>Isotopes</u>
LWTR	Light water	1001
POLY	Polyethylene	1001
H/ZR	^1H in ZrH_x	1001
BENZ	Benzene	1001,6000,6012
HWTR	Heavy Water	1002
BE	Beryllium metal	4009
GRPH	Graphite	6000,6012
ZR/H	Zr in ZrH_x	40000

APPENDIX E

Geometry PLOT and Tally MCPLLOT Commands

This appendix contains only a summary of the available commands for the geometry and tally plotting capabilities included in MCNP. All commands can be shortened to the fewest letters that unambiguously identify the command. {Please refer to Appendix B of the MCNP manual for a complete listing of commands.}

PLOT

Used to plot two-dimensional slices of a problem geometry specified in the input file. This feature is invaluable when debugging geometries. Commands are shown in upper case but can be input in lower case. PLOT examples have been shown in several of the Primer chapters.

I. General Commands

& Continue reading commands for the current plot from the next input line. The & must be the last thing on the line.

RETURN If **PLOT** was called by **MCPLLOT**, control returns to **MCPLLOT**. Otherwise RETURN has no effect.

MCPLLOT Call or return to MCPLLOT.

END Terminate execution of **PLOT**.

II. Inquiry Commands

When one of these commands is encountered, the requested display is made and then PLOT waits for the user to enter another line, which can be just a carriage return, before resuming. The same thing will happen if PLOT sends any kind of warning or comment to the user as it prepares the data for a plot.

OPTIONS Display a list of the **PLOT** command keywords and available colors.

STATUS Display the current values of the plotting parameters.

III. Plot Commands

Plot commands define the values of the parameters used in drawing the next plot. Parameters entered for one plot remain in effect for subsequent plots until they are overridden, either by the same command with new values or by a conflicting command.

BASIS X1 Y1 Z1 X2 Y2 Z2

Orients the plot so that the direction (X1 Y1 Z1) points to the right and the direction (X2 Y2 Z2) points up. The default values are 0 1 0 0 1, causing the Y-axis to point to the right and the Z-axis to point up.

ORIGIN VX VY VZ

Positions the plot so that the origin, which is in the middle of the plot, is at the point (VX, VY, VZ). The default values are 0 0 0.

EXTENT EH EV

Sets the scale of the plot so that the horizontal distance from the origin to other side of the plot is EH and the vertical distance from the origin to the top or bottom is EV. If EV is omitted, it will be set equal to EH. If EV is not equal to EH, the plot will be distorted. The default values are 100 and 100.

PX VX

Plots a cross section of the geometry in a plane perpendicular to the X-axis at a distance VX from the origin. This command is a shortcut equivalent of BASIS 0 1 0 0 0 1 ORIGIN VX vy vz, where vy and vz are the current values of VY and VZ.

PY VY

Plots a cross section of the geometry in a plane perpendicular to

the Y-axis at a distance VY from the origin.

PZ VZ

Plots a cross section of the geometry in a plane perpendicular to the Z-axis at a distance VZ from the origin.

LABEL S C DES

Puts labels of size S on the surfaces and labels of size C in the cells.

Uses the quantity indicated by DES and labels each cell by the value of the parameter indicated by DES. C and DES are optional parameters. The sizes are relative to 0.01 times the height of the view surface, which is the size of the smallest size of hardware characters on the Tektronix 4014. If S or C is zero, then that kind of label will be omitted. If S or C is not zero, it must be in the range from 0.2 to 100. The defaults are S=1, C=0 and DES = CEL.

CEL	cell names
VOL	volume
MAS	mass
MAT	material number
U	universe
LAT	lattice type
FILL	filling universe

SCALES n Put scales and a grid on the plot. Scales and grids are incompatible with VIEWPORT SQUARE. The following values are available for n:

- 0 neither scales nor a grid. (default)
- 1 scales on the edges.
- 2 scales on the edges and a grid on the plot.

COLOR n	Turn color on or off and set the resolution. n can have the following values: on turn color on. off turn color off
50 < n < 1000	set the color resolution to n. A larger value increases resolution and drawing time.
SHADE	M1 = parameter M2 = parameter ... Make the cells containing problem material number M; a particular color. Use the LABEL command to display material numbers. Parameter designates the desired color (e.g., green, blue, etc.). OPTIONS will list available colors if your display is a color monitor.

IV. Zoom Commands

Zoom commands redefine the origin, basis and extent relative to the current origin, basis and extent. The new origin, basis and extent will be used for all subsequent plots until they are again redefined, either by zoom commands or by plot commands. The zoom commands are usually used to zoom in on some feature of the plot.

CENTER DH DV	Changes the origin of the plot by the amount DH in the horizontal direction and by the amount DV in the vertical direction. This command is usually used to define the center of a portion of the current plot that the user wants to enlarge.
FACTOR F	Enlarges the plot by the factor 1/F. F must be greater than 10E-6.
THETA TH	Rotates the plot counterclockwise by the angle TH, in degrees.

MC PLOT

MCNP can plot tally results from your criticality calculation so you can graphically view your results. These plots are very informative and their use is strongly encouraged. It can draw ordinary two-dimensional x-y plots, contour plots, and three-dimensional surface plots, and supports a wide variety of plot options. More than one curve can be plotted on a single x-y plot. This section covers these general topics in the following order: execute line options, plot conventions and command syntax, plot commands grouped by function, and MCTAL files. **MC PLOT** options and keywords are shown in upper case but are usually typed by the user in lower case.

Tally results can be plotted after particle transport has finished, displaying the final tally results, or during the run, displaying the temporary status of one or more tallies as transport is ongoing. After transport is finished, **MC PLOT** is invoked by typing a "z" on the MCNP execute line, either as a separate procedure using existing RUNTPE or MCTAL files or as part of a regular uninterrupted MCNP run. There are two ways to request that a plot be produced periodically during the run: use a MPLOT card in the INP file or use the TTY interrupt feature. (See Chapter 3 of the MCNP manual for an explanation of the MPLOT card.) A TTY interrupt <ctrl-c> causes MCNP to pause at the end of the history that is running when the interrupt occurs and allows plots to be made by calling **MC PLOT**, which takes plot requests from the terminal. No output is sent to the COMOUT file. The following commands can not be used: RMCTAL, RUNTPE, DUMP and END. **MC PLOT** can be used to make plots on a machine different from the one on which the problem was run. If the INP file has a PRDMP card with a nonzero third entry, MCNP writes a MCTAL file at the end of the run. The MCTAL file contains all the tally data in the last RUNTPE dump. The MCTAL file is a coded ASCII file that can be converted and moved from one kind of machine to another. The name of the output MCTAL file can be specified by including mctal=filename in the execute line message. The default name is a unique name based on MCTAL.

Some examples of **MC PLOT** commands are provided in Section X after the description of **MC PLOT** commands.

V. Input for MCNPLOT and Execution Line Options

To run only the **MCNPLOT** tally plotter after termination of MCNP, enter the following command:

```
mcnp z options
```

where 'z' invokes **MCNPLOT**. "Options" is explained in the next paragraph.

```
mcnp inp=filename ixrz options
```

causes MCNP to run the problem specified in filename and then the prompt `mcplot>` appears for MCNPLOT commands.

The following options can be entered on the execution line:

NOTEK Suppress plotting at the terminal and send all plots to the graphics metafile, **PLOTM**. **NOTEK** is for production and batch situations and for when the user's terminal has no graphics capability.

COM=aaaa Use file **aaaa** as the source of plot requests. When an EOF is read, control is transferred to the terminal. In a production or batch situation, end a file with an **END** command to prevent transfer of control. Never end the **COM** file with a blank line. If **COM** is absent, the terminal is used as the source of plot requests.

RUNTPE=aaaa Read file **aaaa** as the source of MCNP tally data. The default is **RUNTPE**, if it exists. If the default **RUNTPE** file does not exist, the user will be prompted for an **RMCTAL** or **RUNTPE** command.

PLOTM=aaaa Name the graphics metafile **aaaa**. The default name is **PLOTM**. When **CGS** is being used, there can be no more than 6 characters in **aaaa**. At **FORTLIB** sites, **PLOTM=aaaa** is ignored and the graphics file is named according to the rules of **GRAFLIB**.

COMOUT=aaaa Write all plot requests to the file aaaa. The default name is COMOUT. MCPLLOT writes the COMOUT file in order to give the user the opportunity to do the same plotting at some later time, using all or part of the old COMOUT file as the COM file in the second run.

VI. Inquiry Commands

When one of these commands is encountered, the requested display is made and then **MCPLLOT** waits for the user to enter another line, which can be just a carriage return, before resuming. The same thing will happen if **MCPLLOT** sends any kind of warning or comment to the user as it prepares the data for a plot.

OPTIONS Display a list of the MCPLLOT keywords.

STATUS Display the current values of the plotting parameters.

VII. File Manipulation Commands

These commands tell MCNP where to find the data that it will display.

RUNTPE aa n Read dump n from RUNTPE file aa. If the parameter n is omitted, the last dump in the file is read.

DUMP n Read dump n of the current RUNTPE file.

WMCTAL aa Write the tally data in the current RUNTPE dump to MCTAL file a.

RMCTAL aa Read MCTAL file aa.

VIII. MCPLOT Plotting Commands

&	MUST be entered at the end of a line of input that will be continued.
CO PLOT	Make plot of data so far and keep plot open for more plots (must be used to plot two or more curves on the same plot).
END	Terminate tally plotting.
FREQ	Specifies the interval between calls to produce an interactive plot on the M PLOT card. N N > 0 Make a plot every N histories = 0 Make no plots < 0 Make a plot every N minutes
KCODE	Plot individual or average k_{eff} or removal lifetimes by cycle number. I I=1 for collision estimator for k_{eff} =2 for absorption estimator for k_{eff} =3 for track-length estimator for k_{eff} =4 for collision estimator for removal lifetime =5 for absorption estimator for removal lifetime =11-15 for quantity I-10 averaged over the active cycles =16 for average combined col/abs/trk-len k_{eff} =17 for average combined col/abs/trk-len k_{eff} by k_{eff} cycles skipped =18 for average combined col/abs/trk-len k_{eff} figure of merit =19 for average combined col/abs/trk-len k_{eff} relative error

MPLOT Produce plots of k_{eff} while the problem is running (in the INP file only).

MC PLOT FREQ N Keyword1=PARAMETER1 Keyword2=PARAMETER2

Keywordi= all tally plot Keywords except END, RMCTAL, RUNTPE, and DUMP N= k_{eff} cycles between automatic plots (default is 5 k_{eff} cycles).

NOERRBAR Do not display statistical error bars.

PRINTPTS Display the x-y coordinates of points in the current plot.

RESET A Reset parameters of command A to default (A="ALL" resets all commands).

RETURN Concludes the interactive plotting when running histories.

SCALES Select the type of scales to put on the plot.

N

N=0 for no scales on the top edges and no grid on the plot.

N=1 for scales on the edges and no grid on the plot (default).

N=2 for scales and grid on the plot.

XLIMS Optional definition of lower and upper limits of x variable.

MIN MAX NSTEPS

MIN and MAX = lower and upper limits for the x variable.

NSTEPS = number of subdivisions on the linear x axis.

YLIMS Optional definition of lower and upper limits of y variable.

MIN MAX NSTEPS

MIN and MAX = lower and upper limits for the y variable.

NSTEPS = number of subdivisions on the linear y axis.

IX. Labelling Commands

- LABEL "A"** Use A (up to 8 characters) as a label for current curve that is printed in the legend.
- SUBTITLE** Write a subtitle anywhere on the plot (margins, between axes, etc.)
X Y "A"
X Y is the location to put the subtitle.
A in quotations is text for subtitle line (up to 40 characters)
- TITLE** Create a one or two line title for the plot.
N "A" (default is name of current RUNTPE or MCTAL and title)
N=1 or 2 to put "A" on the first or second main title line.
A in quotation marks is text for main title line (up to 40 characters).
- XTITLE "A"** Use A as the title for the x-axis (default is name of x-axis variable).
- YTITLE "A"** Use A as the title for the y-axis (default is name of y-axis variable).

X. Examples for Plotting k_{eff} as a Function of k_{eff} Cycle Number.

Some examples of commands for useful MCNP k_{eff} plots are given in this section. Note that the shortened form for the commands is illustrated.

Example of commands to plot all three AVERAGE k_{eff} estimators and the combined AVERAGE k_{eff} as a function of cycle number.

```
kcode 11 cop kc 12 cop kc 13 cop kc 16
```

To reproduce the above example but to plot the estimated one sigma error bars for only the combined average k_{eff} , use:

```
noe kc 11 cop kc 12 cop kc 13 cop reset noe kc 16
```

Example of commands to generate a plot of all three individual cycle k_{eff} estimators and the combined AVERAGE k_{eff} as a function of cycle number with custom labels. The & is required to continue the first line.

```
kc 1 label "k(col)" coplot kc 2 la "k(abs)" cop kc 3 &  
la "k(trk)" cop kc 16 la "k(c/a/t)"
```

To reproduce the above example but to not plot the first 10 cycles from a 110 k_{eff} cycle run, add:

```
xlims 10 110
```

```
kc 1 xlims 10 110 label "k(col)" coplot kc 2 la "k(abs)"&  
cop kc 3 la "k(trk)" cop kc 16 la "k(c/a/t)"
```

An example of the use of automatic MCNP plotting is to put the following mplot card into an INP input file:

```
mplot noe kc 11 cop kc 12 cop kc 13 cop reset noe kc 16
```

APPENDIX F

MCNP Surface Cards

Mnemonic	Type	Description	Equation	Card Entries
P	Plane	General	$Ax + By + Cz - D = 0$	<i>ABCD</i>
PX	"	Normal to X-axis	$x - D = 0$	<i>D</i>
PY	"	Normal to Y-axis	$y - D = 0$	<i>D</i>
PZ	"	Normal to Z-axis	$z - D = 0$	<i>D</i>
SO	Sphere	Centered at Origin	$x^2 + y^2 + z^2 - R^2 = 0$	<i>R</i>
S	"	General	$(x - \bar{x})^2 + (y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	<i>xyzR</i>
SX	"	Centered on X-axis	$(x - \bar{x})^2 + y^2 + z^2 - R^2 = 0$	<i>xR</i>
SY	"	Centered on Y-axis	$x^2 + (y - \bar{y})^2 + z^2 - R^2 = 0$	<i>yR</i>
SZ	"	Centered on Z-axis	$x^2 + y^2 + (z - \bar{z})^2 - R^2 = 0$	<i>zR</i>
C/X	Cylinder	Parallel to X-axis	$(y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	<i>yzR</i>
C/Y	"	Parallel to Y-axis	$(x - \bar{x})^2 + (z - \bar{z})^2 - R^2 = 0$	<i>xzR</i>
C/Z	"	Parallel to Z-axis	$(x - \bar{x})^2 + (y - \bar{y})^2 - R^2 = 0$	<i>xyR</i>
CX	"	On X-axis	$y^2 + z^2 - R^2 = 0$	<i>R</i>
CY	"	On Y-axis	$x^2 + z^2 - R^2 = 0$	<i>R</i>
CZ	"	On Z-axis	$x^2 + y^2 - R^2 = 0$	<i>R</i>
K/X	Cone	Parallel to X-axis	$\sqrt{(y - \bar{y})^2 + (z - \bar{z})^2} - t(x - \bar{x}) = 0$	<i>xyz t² ± 1</i>
K/Y	"	Parallel to Y-axis	$\sqrt{(x - \bar{x})^2 + (z - \bar{z})^2} - t(y - \bar{y}) = 0$	<i>xyz t² ± 1</i>
K/Z	"	Parallel to Z-axis	$\sqrt{(x - \bar{x})^2 + (y - \bar{y})^2} - t(z - \bar{z}) = 0$	<i>xyz t² ± 1</i>
KX	"	On X-axis	$\sqrt{y^2 + z^2} - t(x - \bar{x}) = 0$	<i>x t² ± 1</i>
KY	"	On Y-axis	$\sqrt{x^2 + z^2} - t(y - \bar{y}) = 0$	<i>y t² ± 1</i>

KZ	"	On Z-axis	$\sqrt{x^2 + y^2} - t(z - \bar{z}) = 0$	$\bar{z}t^2 \pm 1$ ± 1 used only for sheet cone
SQ	Ellipsoid Hyperboloid Paraboloid	Axes Parallel to X-, Y-, or Z-axis	$A(x - \bar{x})^2 + B(y - \bar{y})^2 + C(z - \bar{z})^2$ $+ 2D(x - \bar{x}) + 2E(y - \bar{y})$ $+ 2F(z - \bar{z}) + G$	$ABCDE$ $FG\bar{x}\bar{y}\bar{z}$
GQ	Cylinder Cone Ellipsoid Hyperboloid Paraboloid	Axes Not Parallel to X-, Y-, Z-axis	$Ax^2 + By^2 + Cz^2 + Dxy + Eyz$ $+ Fxz + Gx + Hy + Jz + K = 0$	$ABCDE$ $FGHJK$
TX	Elliptical or Circular Torus. Axis is Parallel to the X-, Y-, or Z-axis		$\frac{(x - \bar{x})^2}{B^2} + \frac{(\sqrt{(y - \bar{y})^2 + (z - \bar{z})^2} - A)^2}{C^2} - 1 = 0$	$\bar{x}\bar{y}\bar{z}AB$
TY			$\frac{(y - \bar{y})^2}{B^2} + \frac{(\sqrt{(x - \bar{x})^2 + (z - \bar{z})^2} - A)^2}{C^2} - 1 = 0$	$\bar{x}\bar{y}\bar{z}AB$
TZ			$\frac{(z - \bar{z})^2}{B^2} + \frac{(\sqrt{(x - \bar{x})^2 + (y - \bar{y})^2} - A)^2}{C^2} - 1 = 0$	$\bar{x}\bar{y}\bar{z}AB$

X Y Z P Surfaces defined by points

{See Chapter 3 of the MCNP manual for examples using the surface cards listed here.}

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