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# **KENO V.a Primer: A Primer for Criticality Calculations with SCALE/KENO V.a Using GeeWiz**

**December 2005**

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Nuclear Science and Technology Division (94)

**KENO V.a Primer: A Primer for Criticality Calculations with  
SCALE/KENO V.a Using GeeWiz**

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## ACRONYMS AND ABBREVIATIONS

1-D	one-dimensional
238GROUPNDF5	ENDF/B-V 238-group library
2-D	two-dimensional
27GROUPNDF4	27-group ENDF/B-IV library
3-D	three-dimensional
44GROUPNDF5	ENDF/B-V 44-group library
AEC	U.S. Atomic Energy Commission
CSAS	Criticality Safety Analysis Sequences
CSEWG	Cross-Section Evaluation Working Group
EALF	energy of the average lethargy causing fission
GeeWiz	Graphically Enhanced Editing Wizard
GEN	number of generations
HANSEN-ROACH	Hansen-Roach 16-group library
HEU	high-enriched uranium
ICSBEP	International Criticality Safety Benchmark Experiments Project
IEU	intermediate-enriched uranium
INFHOMMEDIUM	infinite homogeneous medium
$k_{\text{eff}}$	effective multiplication factor
KMART	KENO Module for Activity-Reaction Rate Tabulation
LAW	Library to Analyze Radioactive Waste
LEU	low-enriched uranium
LWR	light-water-reactor
MIPLIB	Material Information Processor Library
MOX	mixed oxide
NRC	U.S. Nuclear Regulatory Commission
NPG	neutrons per generation
MSRE	Molten Salt Reactor Experiment
NITAWL	Nordheim Integral Treatment And Workline Library Production
ORNL	Oak Ridge National Laboratory
PCTR	Physical Constant Test Reactor
PFE	Programmer's File Editor
PMC	Produce Multigroup Cross sections
PWR	pressurized water reactor
RSICC	Radiation Safety Information Computational Center
SCALE	Standardized Computer Analyses for Licensing Evaluations
V6 238GROUP	ENDF/B-VI 238-group library



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## **ABSTRACT**

The SCALE (Standardized Computer Analyses for Licensing Evaluation) computer software system developed at Oak Ridge National Laboratory (ORNL) is widely used and accepted around the world for criticality safety analyses. The well-known KENO V.a three-dimensional Monte Carlo criticality computer code is the primary criticality safety analysis tool in SCALE. The KENO V.a primer is designed to help a new user understand and use the SCALE/KENO V.a Monte Carlo code for nuclear criticality safety analyses. It assumes that the user has a college education in a technical field. There is no assumption of familiarity with Monte Carlo codes in general or with SCALE/KENO V.a in particular. The primer is designed to teach by example, with each example illustrating two or three features of SCALE/KENO V.a that are useful in criticality analyses.

The primer is based on SCALE 5, which includes the Graphically Enhanced Editing Wizard (GeeWiz) Windows user interface. Each example uses GeeWiz to provide the framework for preparing input data and viewing output results. Starting with a *Quickstart* section, the primer gives an overview of the basic requirements for SCALE/KENO V.a input and allows the user to quickly run a simple criticality problem with SCALE/KENO V.a. The sections that follow *Quickstart* include a list of basic objectives at the beginning that identifies the goal of the section and the individual SCALE/KENO V.a features that are covered in detail in the example problems in that section. Upon completion of the primer, a new user should be comfortable using GeeWiz to set up criticality problems in SCALE/KENO V.a.

The primer provides a starting point for the criticality safety analyst using SCALE/KENO V.a. Complete descriptions are provided in the SCALE/KENO V.a manual. Although the primer is self-contained, it is intended as a companion volume to the

SCALE/KENO V.a documentation. (The SCALE manual is provided on the SCALE installation CD.) The primer provides specific examples of using SCALE/KENO V.a for criticality analyses; the SCALE/KENO V.a manual provides information on the use of SCALE/KENO V.a and all its modules. The primer also contains a number of appendices that give the user additional information about available cross-section libraries in SCALE/KENO V.a, example input files, and other reference data. This information is provided in appendices so as not to obscure the basic information illustrated in each example.

# 1. INTRODUCTION

This primer is designed to help you understand and use the KENO V.a three-dimensional (3-D) Monte Carlo code for nuclear criticality safety analyses. KENO V.a is part of the SCALE (Standardized Computer Analyses for Licensing Evaluation) code system.<sup>1</sup> 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 SCALE and KENO V.a in particular. The primer is designed to teach by example, with each example illustrating two or three features of KENO V.a that are useful in criticality safety analyses.

The primer is based on SCALE 5, which includes the SCALE Graphically Enhanced Editting Wizard (**GeeWiz**), a Windows program to assist criticality safety analysts in creating and executing SCALE input files for KENO V.a. GeeWiz version 5.01a (March 3, 2005) and KENO V.a version 5.02 (April 11, 2005) were used for all SCALE 5 examples. Some examples are also provided for SCALE 5.1, where they differ significantly from SCALE 5. Each of the examples will use GeeWiz to provide the framework for data input. Starting with a *Quickstart* section, the primer gives an overview of the basic requirements for SCALE/KENO V.a input and allows you to quickly run a simple criticality problem with SCALE/KENO V.a. This section is not designed to explain GeeWiz, the input, or the SCALE/KENO V.a options in detail; rather, it introduces the GeeWiz user interface and some basic concepts that are further explained in following sections. Each following section has a list of basic objectives at the beginning that identifies the goal of the section and the individual SCALE/KENO V.a features that are then covered in detail in the example problems in that section. It is expected that on completion of the primer, you will be comfortable using GeeWiz to set up criticality problems in SCALE/KENO V.a. You will be able to utilize SCALE/KENO V.a in criticality calculations and will be capable of handling most situations that normally arise in a facility. The primer provides a set of basic input files that can be selectively modified by you to fit the particular problem at hand.

Although much of the information to perform an analysis is provided in the primer, there is no substitute for understanding your problem and the theory of neutron interactions. The SCALE/KENO V.a code is only capable 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. However, the two-dimensional (2-D) color geometry plots and the external KENO3D visualization package are quite useful for identifying geometry errors. Remember that a single calculation of  $k_{\text{eff}}$  and its associated confidence interval with SCALE/KENO V.a 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 safety analyst using SCALE/KENO V.a. Complete descriptions are provided in the SCALE manual.<sup>1</sup> Although the primer is self-contained, it is intended as a companion volume to the SCALE manual. (The SCALE manual is provided on the SCALE installation CD.) The primer provides specific examples using SCALE/KENO V.a for criticality safety analyses while the documentation provides information on

the use of SCALE and all its modules. The primer also contains appendices that give the user additional information about available cross-section libraries in SCALE and example input files. 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 Times New Roman font. Information that you type into an input file (or provide to GeeWiz) is set in Courier font. Characters in the Courier font represent commands, keywords, or data that would be used as computer input. References to items displayed on the screen by GeeWiz are highlighted in **bold font**. Because the primer often references the SCALE manual, these references will be set in square brackets; e.g., [see SCALE Manual Section x].

It is hoped that you find the primer useful and easy to read. You will get the most from this tutorial if you start with **Section 2: SCALE/KENO V.a Quickstart** and proceed through the rest of the sections in order. Each section assumes that you know and are comfortable with the concepts discussed in the previous sections. Although it may be tempting to pick up the primer and immediately go to an example problem that is similar to your analysis requirement, this approach will not provide you with the background or confidence in your analysis that is necessary for accurate and effective implementation of procedures and limits. There is no substitute for a thorough understanding of the techniques used in a SCALE/KENO V.a analysis. A little extra time spent going through the primer and doing the examples will save many hours of possible confusion and frustration later.

## 1.1 OVERVIEW OF SCALE

The SCALE code system dates back to 1969, when the current Nuclear Science and Technology Division at Oak Ridge National Laboratory (ORNL) began providing computational support in the use of the new KENO code to staff at the U.S. Atomic Energy Commission (AEC). From 1969 to 1976 the AEC certification staff relied on the ORNL staff to assist them in the correct use of codes and data for criticality, shielding, and heat transfer analyses of transportation packages. Shortly after creation of the U.S. Nuclear Regulatory Commission (NRC), the NRC staff proposed the development of an easy-to-use analysis system that would provide the technical capabilities of the individual modules with which they were familiar. With this proposal, the concept of the SCALE code system was born.

The NRC staff provided ORNL with some general development criteria for SCALE: (1) focus on applications related to nuclear fuel facilities and package designs, (2) use well-established computer codes and data libraries, (3) design an input format for the occasional or novice user, (4) prepare “standard” analysis sequences (control modules) that will automate the use of multiple codes (functional modules) and data to perform a system analysis, and (5) provide complete documentation and public availability. The initial version of SCALE was released by the Radiation Safety Information Computational Center (RSICC) at ORNL in 1980. Since that time, the system has been considerably enhanced, and the release used in this primer is Version 5. SCALE runs on Unix, Windows, and Linux computer platforms.

The concept of SCALE was to provide “standardized” sequences. Input for the control modules has been designed to be free-form with extensive use of keywords and engineering-type input requirements. The most important feature of the SCALE system is the capability to simplify the user knowledge and effort required to prepare material mixtures and to perform adequate problem-dependent cross-section processing.

At the center of the Criticality Safety Analysis Sequences (CSAS) is the library of subroutines referred to as the Material Information Processor Library or MIPLIB. The purpose of MIPLIB is to allow users to specify problem materials using easily remembered and easily recognizable keywords that are associated with mixtures, elements, and nuclides provided in the Standard Composition Library. MIPLIB also uses other keywords and simple geometry input specifications to prepare input for the modules that perform the problem-dependent cross-section processing: BONAMI, NITAWL, CENTRM, PMC, and XSDRNPM. A keyword supplied by the user selects the cross-section library from a standard set provided in SCALE or designates the reference to a user-supplied library.

The modular structure of SCALE allows back-to-back execution of the functional modules to perform a system analysis. However, a variety of control modules such as CSAS have been developed that automate and standardize various analytic sequences. The control module input format has been designed to help minimize input errors. Upon processing the user-specified input, the SCALE system control modules immediately print an input checklist in which the user (or reviewer) can easily establish that the input describes the system to be analyzed.

The CSAS control module is the primary criticality safety control module for the calculation of the neutron multiplication factor of a system. Multiple sequences within the CSAS module provide capabilities for a number of analyses, such as modeling a one-dimensional (1-D) or a 3-D system, searching on geometry spacing or material concentrations, and processing cross sections.

BONAMI performs resonance shielding through the application of the Bondarenko shielding factor method. BONAMI is typically used to process data in the unresolved resonance energy range. As input, BONAMI requires the presence of shielding factor data on the AMPX master library interface. As output, BONAMI produces a problem-dependent master library.

NITAWL uses the Nordheim Integral Treatment to perform neutron cross-section processing in the resolved resonance energy range. This involves a fine energy group calculation of the slowing-down flux across each resonance with subsequent flux weighting of the resonance cross sections. NITAWL also assembles group-to-group transfer arrays from the elastic and inelastic scattering components and performs other tasks in producing the problem-dependent working library.

CENTRM computes continuous-energy neutron spectra using 1-D discrete ordinates or infinite media geometry. CENTRM determines the problem-specific fluxes for processing

resonance-shielded multigroup data using a 1-D unit cell, and then utilizing the spectrum as a problem-dependent weight function for multigroup averaging. The multigroup data processing is done by the PMC code, which reads the CENTRM continuous-energy flux spectra and cross-section data; calculates problem-dependent, group-averaged cross sections over some specified energy range; and then replaces the corresponding data in an input AMPX master library.

XSDRNPM is a 1-D discrete ordinates transport code for performing neutron or coupled-neutron-gamma calculations. The code has a variety of uses within SCALE. In the CSAS sequences, it is used for preparation of cell-averaged cross sections for subsequent system analysis in KENO V.a and for 1-D criticality safety analysis.

KENO V.a is a 3-D multigroup Monte Carlo code employed to determine effective multiplication factors ( $k_{\text{eff}}$ ) for multidimensional systems. The basic geometrical bodies allowed for defining the model are cuboids, spheres, cylinders, hemispheres, and arrays. Color 2-D plots of the geometry model can be generated in KENO V.a, or the model may be viewed using the 3-D visualization tool KENO3D.

Although the control modules are typically designated by their principal analytic sequence, note that more than one sequence may exist within a control module. The sequences available in CSAS are discussed in Section 3.

Note that SCALE includes another version of KENO known as KENO-VI. As the geometry package for KENO-VI is different from that for KENO V.a, a different control module, CSAS6, provides an automated criticality safety sequence using KENO-VI for performing 3-D Monte Carlo analyses of very complex geometries (e.g., hexagonal lattices or nonorthogonal geometry).

The SCALE code system includes several problem-independent multigroup cross-section libraries for criticality analyses. The generally recommended libraries are 238- and 44-group ENDF/B-V neutron libraries.<sup>2</sup> A 238-group ENDF/B-VI library is available in SCALE 5.1.

The SCALE modules used for preparing problem-dependent cross-section libraries and performing criticality safety analyses are well established and in routine use by much of the U.S. and international criticality safety communities as the primary computational tool or as a backup/review tool.

## 2. SCALE/KENO V.A *QUICKSTART*

### 2.1 WHAT YOU WILL BE ABLE TO DO

- Describe the structure of SCALE/KENO V.a input files.
- Use the GeeWiz user interface to create a SCALE/KENO V.a input file.
- Set up and run a simple criticality problem using SCALE/KENO V.a.
- Find and interpret  $k_{\text{eff}}$  information from SCALE/KENO V.a output.

### 2.2 SCALE/KENO V.a INPUT FILE

The SCALE/KENO V.a input file describes the problem geometry, specifies the materials and the neutron source, and defines the control parameters for analyzing the problem. The geometry is constructed by defining objects and their relationship with other objects in a system. Each object can be filled with a material or a void.

A SCALE/KENO V.a input file consists of some or all of the above data, depending on the type of problem being analyzed and the amount and type of output desired. The most user-friendly method for entering the data is to use the GeeWiz user interface.

### 2.3 EXAMPLE PROBLEM

This section should provide enough information to run a simple example problem. It is our intent that you gain confidence in using GeeWiz to enter SCALE/KENO V.a input data right away, so we walk through this example problem step-by-step, explaining each input step. For the present, it is important that you enter this problem exactly as we describe it. As you gain more experience with GeeWiz and SCALE/KENO V.a, you may find other ways to set up input files that are more logical to you. For example, you may find alternate methods for the geometry setup.

### 2.3.1 Problem Description

This problem is a bare sphere of delta-phase plutonium metal (density of 15.61 g/cc) 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  $^{239}\text{Pu}$  = 3.7047E-2 atoms/b-cm

$N_{240}$  = Atom density of  $^{240}\text{Pu}$  = 1.751E-3 atoms/b-cm

$N_{241}$  = Atom density of  $^{241}\text{Pu}$  = 1.17E-4 atoms/b-cm

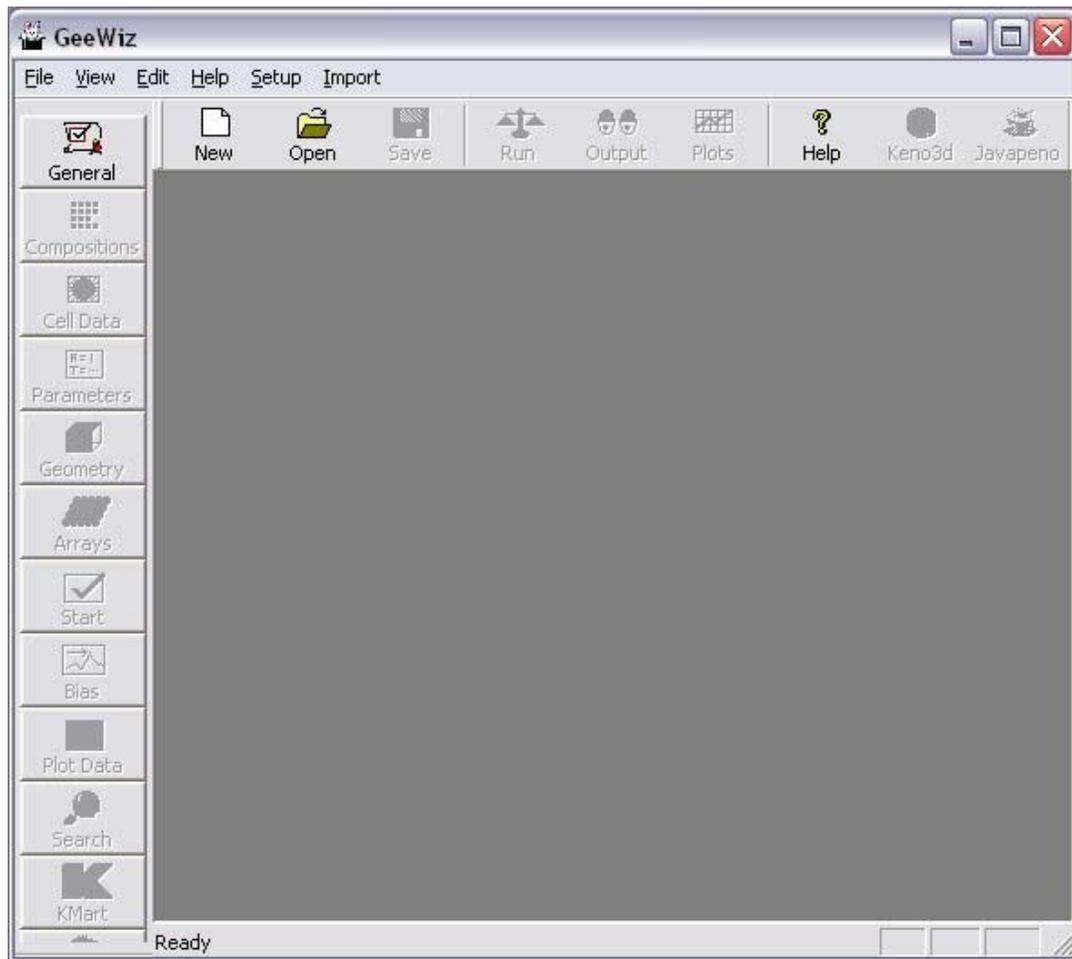
$N_{\text{Ga}}$  = Atom density of Ga = 1.375E-3 atoms/b-cm

Spherical nickel coating: thickness = 0.0127 cm

$N_{\text{Ni}}$  = Atom density of Ni = 9.1322E-2 atoms/b-cm

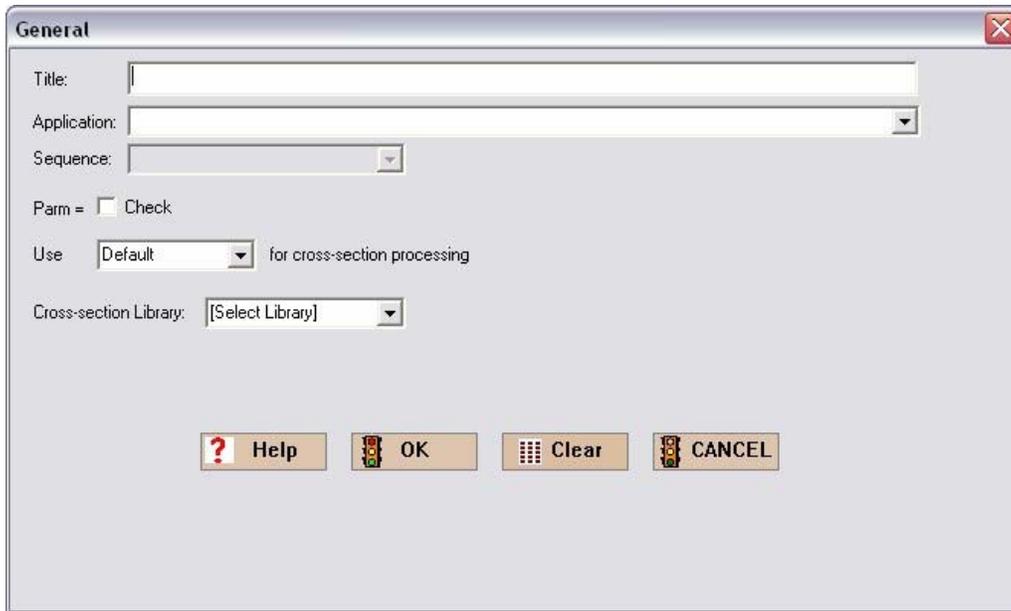
### 2.3.2 GeeWiz Input – General Information

Now you are ready to begin entering the example problem. First start the GeeWiz user interface. You should see a screen that looks like Fig. 1.



**Fig. 1. GeeWiz start screen.**

Clicking on the **General** button on the left-hand side toolbar will bring up a window as shown in Fig. 2. In this window, you enter the **Title**, the **SCALE Application and Sequence**, and the **Cross-section Library** information. You can also enter a program for processing cross-section data, but we will leave that as **Default** in this primer.

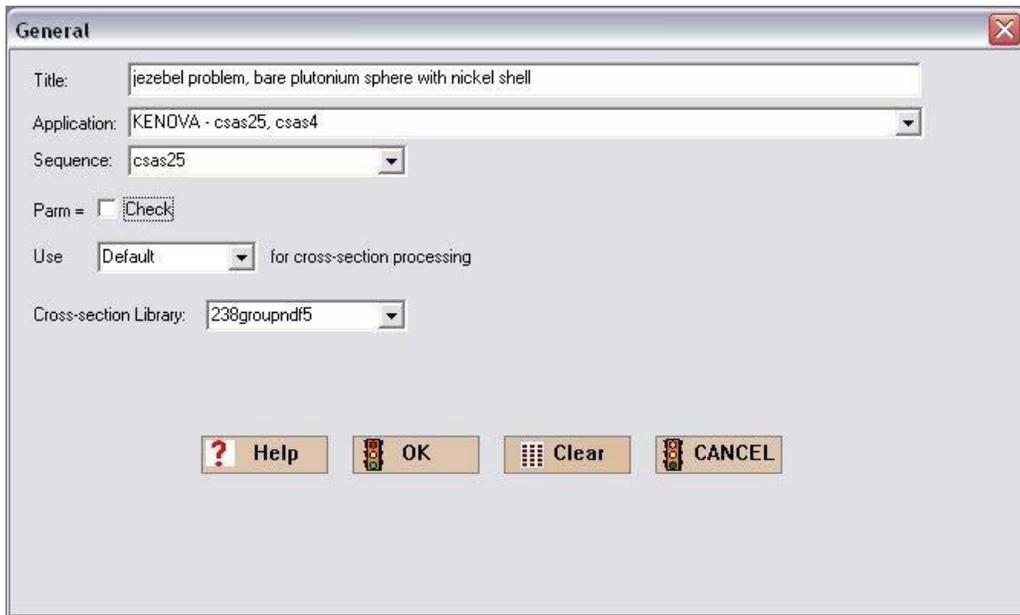


**Fig. 2. General form.**

Enter the **Title** as follows:

jezebel problem, bare plutonium sphere with nickel shell

Again note that information to be entered into GeeWiz will appear in the Courier font. For **Application** click on the down arrow and select KENOVA - csas25, csas4. Then select csas25 as the **Sequence**. For **Cross-section Library**, select 238groupndf5. The **General** screen should look like that in Fig. 3.

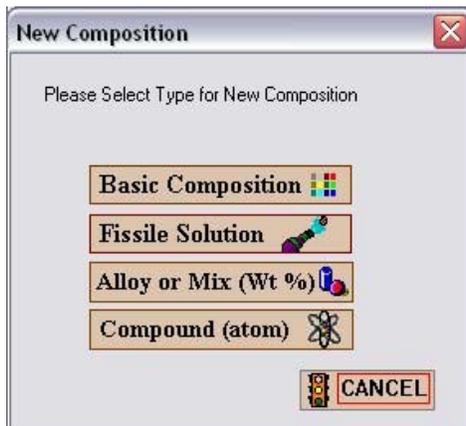


**Fig. 3. General information for example problem.**

Now select **OK** to save this information in a temporary file. Later you will save all of the input information under a file name.

### 2.3.3 Materials

The next section of GeeWiz input provides information on the materials in the problem. For the example problem, there are four materials in the core region and then the nickel shell in the outer region. To enter these, select **Compositions** from the menu on the left-hand side of GeeWiz. This button opens the form for specifying new materials in the model, as shown in Fig. 4. In SCALE 5.1, the user must click the **Create** button to open the form in Fig. 4.



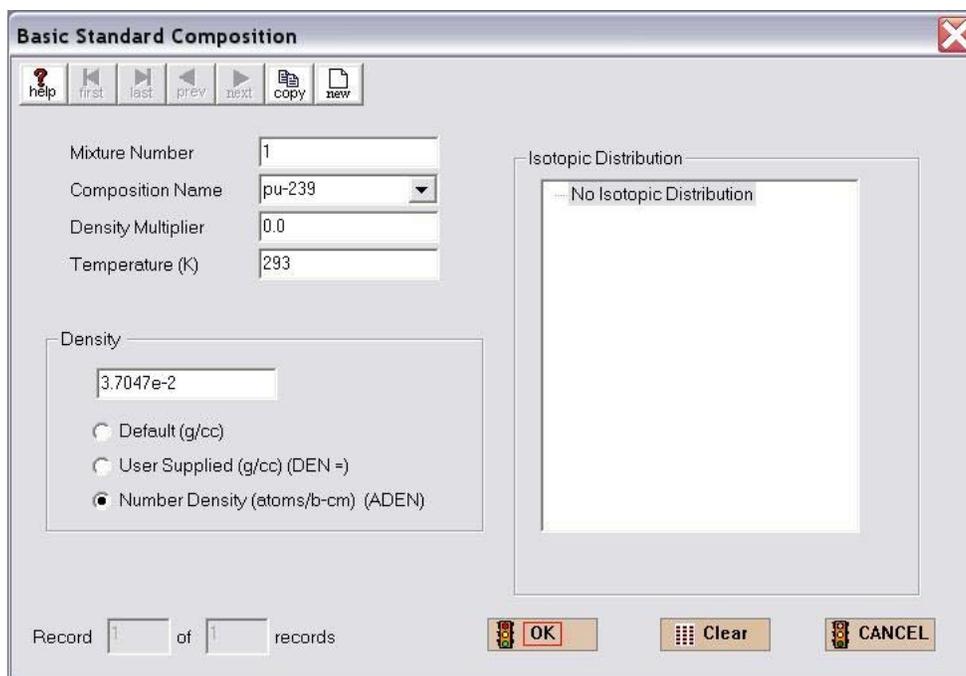
**Fig. 4. New compositions window.**

You will be entering data for  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{241}\text{Pu}$ , gallium, and nickel, all of which are in the Standard Compositions Library and are Basic Compositions. Selecting the **Basic Composition** button will bring up the **Basic Standard Composition** form shown in Fig. 5.

The screenshot shows a software window titled "Basic Standard Composition". At the top, there is a toolbar with icons for help, first, last, prev, next, copy, and new. Below the toolbar, there are several input fields: "Mixture Number" with the value "1", "Composition Name" with a dropdown arrow, "Density Multiplier" with the value "1", and "Temperature (K)" with the value "300". Below these fields is a "Density" section containing a text input field and three radio buttons: "Default (g/cc)" (which is selected), "User Supplied (g/cc) (DEN =)", and "Number Density (atoms/b-cm) (ADEN)". At the bottom of the window, it displays "Record 1 of 1 records" and three buttons: "OK", "Clear", and "CANCEL".

**Fig. 5. Basic standard composition window.**

As the first four materials are mixed together, they will be part of mixture number 1. You will enter four compositions for mixture 1. The entry for the first material, pu-239, should look like that in Fig. 6. The **Mixture Number** should already be set to 1. Select pu-239 as the **Composition Name** from the list of materials in the library. Set the **Temperature** to 293. To enter the atom densities that are given in the example problem description, you need to select **Number Density** in the **Density** section and then enter the appropriate value. In this case, enter  $3.7047e-2$ .



**Fig. 6. Data for  $^{239}\text{Pu}$  in mixture 1.**

To enter the data for the rest of the materials, select **copy** from the toolbar. Then modify the **Composition Name** and **Number Density**. The mixture number should remain the same for each of the four materials. The entries for the next three materials (pu240, pu-241, and ga) should look like those shown in Figs. 7 through 9.

**Basic Standard Composition**

help first last prev next copy new

Mixture Number: 1  
 Composition Name: pu-240  
 Density Multiplier: 0.0  
 Temperature (K): 293

Density: 1.751e-3  
 Default (g/cc)  
 User Supplied (g/cc) (DEN =)  
 Number Density (atoms/b-cm) (ADEN)

Isotopic Distribution: No Isotopic Distribution

Record 2 of 2 records

OK Clear CANCEL

**Fig. 7. Data for  $^{240}\text{Pu}$  in mixture 1.**

**Basic Standard Composition**

help first last prev next copy new

Mixture Number: 1  
 Composition Name: pu-241  
 Density Multiplier: 0.0  
 Temperature (K): 293

Density: 1.17e-4  
 Default (g/cc)  
 User Supplied (g/cc) (DEN =)  
 Number Density (atoms/b-cm) (ADEN)

Isotopic Distribution: No Isotopic Distribution

Record 3 of 3 records

OK Clear CANCEL

**Fig. 8. Data for  $^{241}\text{Pu}$  in mixture 1.**

The last mixture 1 material is gallium; enter its data as shown in Fig. 9. Note that the notation in the lower left-hand corner indicates that it is Record 4 of 4 Records, so there are four materials that have been entered to this point. After entering the data for gallium, select **OK** to save all the material information for mixture 1.

The screenshot shows a software window titled "Basic Standard Composition" with a standard Windows-style title bar (minimize, maximize, close). The window contains several input fields and controls:

- Toolbar:** Includes icons for help, first, last, prev, next, copy, and new.
- Mixture Number:** A text box containing the value "1".
- Composition Name:** A dropdown menu showing "ga".
- Density Multiplier:** A text box containing "0.0".
- Temperature (K):** A text box containing "293".
- Density Section:** A text box containing "1.375e-3" and three radio buttons:
  - Default (g/cc)
  - User Supplied (g/cc) (DEN =)
  - Number Density (atoms/b-cm) (ADEN)
- Isotopic Distribution:** A large empty rectangular area with the text "No Isotopic Distribution" at the top.
- Status Bar:** Shows "Record 4 of 4 records".
- Buttons:** "OK", "Clear", and "CANCEL" buttons are located at the bottom right.

**Fig. 9. Data for gallium in mixture 1.**

After clicking on **OK**, GeeWiz will bring up a summary screen as shown in Fig. 10. On this screen is the information for each of the four materials, the mixture number, and the atom densities. Now to enter the information for the second mixture, which has only one material, nickel, select **Create** from the summary screen toolbar. This will bring up the New Composition window. Again select **Basic Composition** to bring up the **Basic Standard Composition** form. Note that GeeWiz has already updated the **Mixture Number** to 2. Select **ni**, then select **Number Density** to allow you to enter  $9.1322e-2$ . Set the **Temperature** to 293. The completed screen for nickel should look like that shown in Fig. 11.

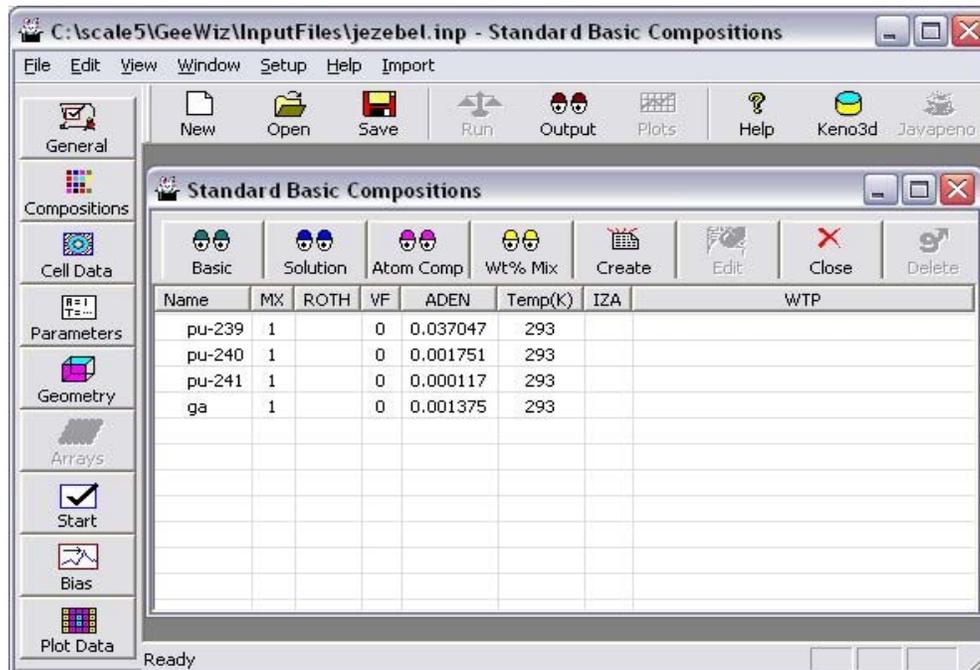


Fig. 10. Standard basic composition summary.

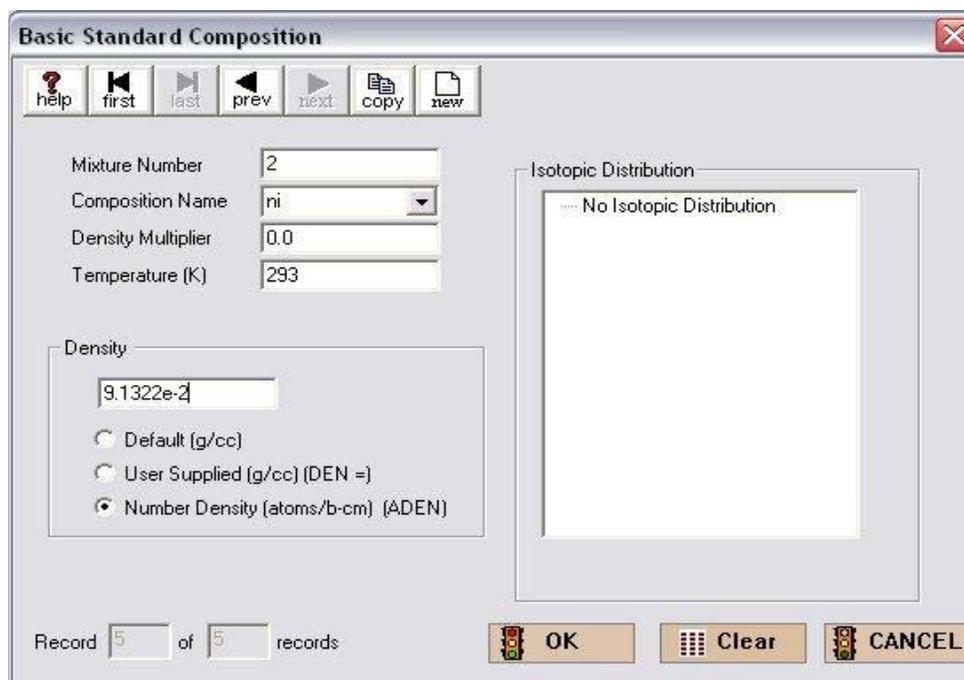
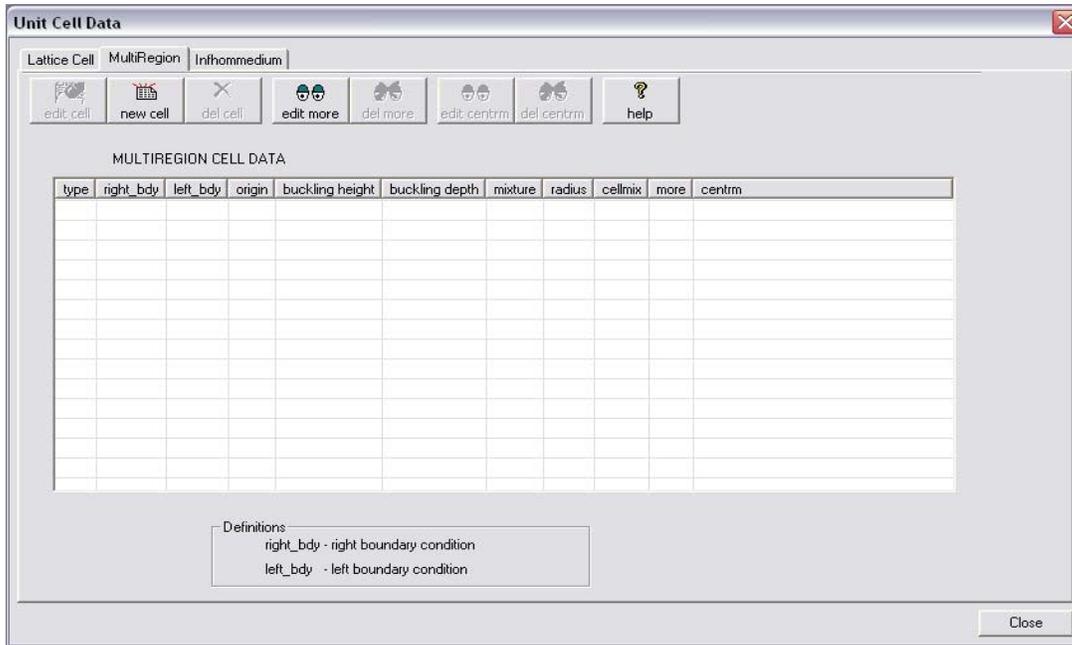


Fig. 11. Data for nickel in mixture 2.

After entering the data for nickel, select **OK** to save all the material information for mixture 2. This brings you back to the composition summary screen with the five materials listed. As we have no more material data, select **Close** on the summary screen. The next information to be entered is for the unit cell. To enter this information, select **Cell Data** from the toolbar on the left-hand side of GeeWiz. This button opens the form for specifying unit cell information. Now select the **MultiRegion** tab to get the summary form shown in Fig. 12.



**Fig. 12. Multiregion cell data summary.**

To enter the cell data, select **new cell** from the toolbar. This brings up the **Multiregion Cell Data** form. The **Geometry Type** should be `Spherical`, the **Inner Boundary** defaults to `reflected`, and the **Outer Boundary** defaults to `vacuum`. The information should look like that in Fig. 13.



Now repeat the process for the second zone with a **Radius** of 6.39763 cm and **Mixture 2** ni. Click **OK** to retain this information and return to the **Multiregion Cell Data** form, which should now look like Fig. 15.

Multiregion Cell Data

Geometry Type: Spherical

Left (Inner) Boundary Condition: Reflected

Right (Outer) Boundary Condition: Vacuum

CELLMIX =  \*

\* CELLMIX value should not be an existing mixture number.

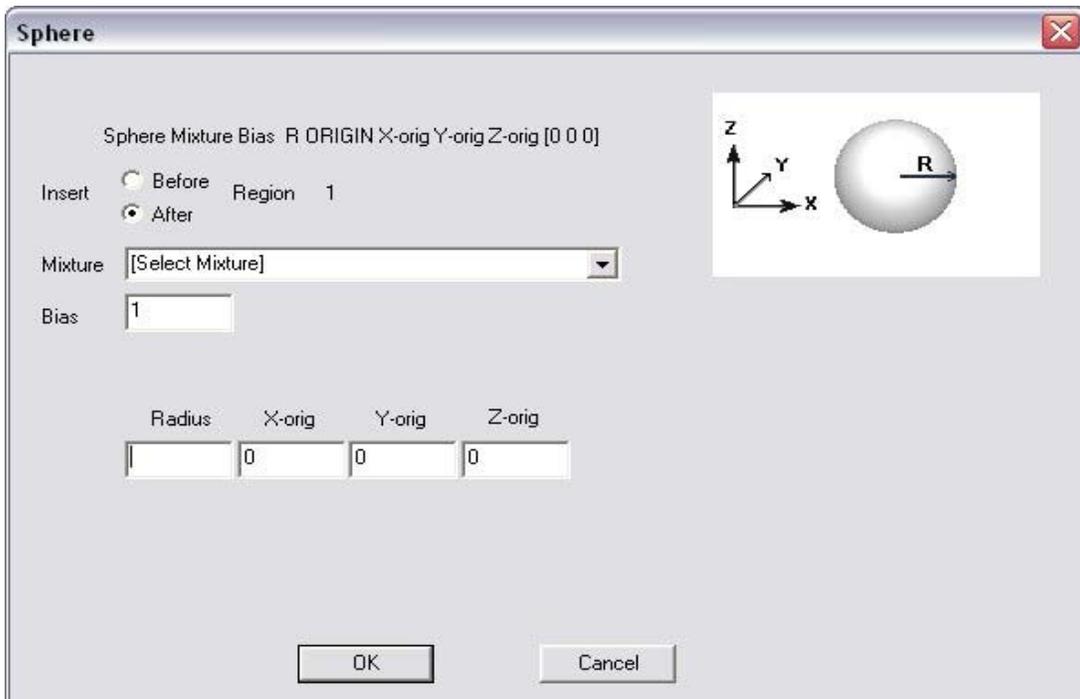
Zone	Mixture	Radius(cm)
1	1	6.38493
2	2	6.39763

? Help    OK    CANCEL

**Fig. 15. Unit cell summary data with zone information.**

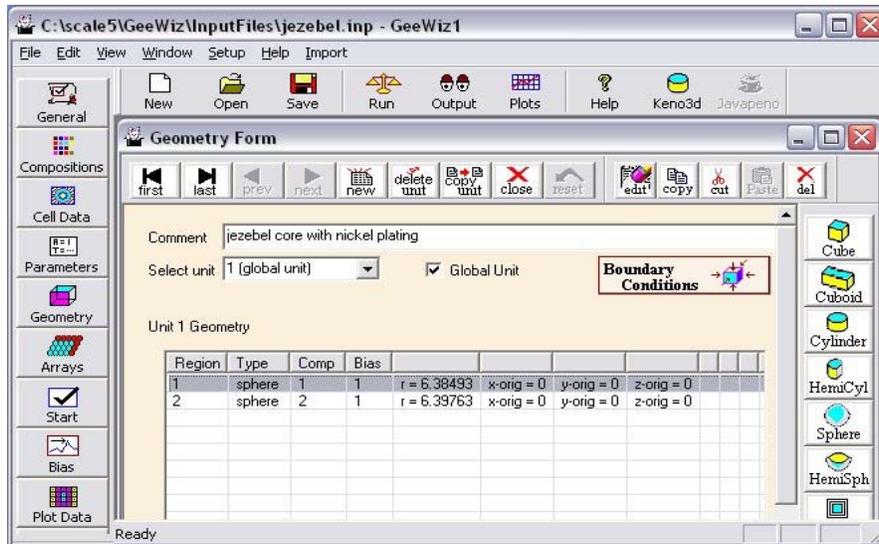
Click **OK** and GeeWiz will display a summary of the multiregion unit cell information as shown in Fig. 16. Click **Close** to close the **Unit Cell Data** form.





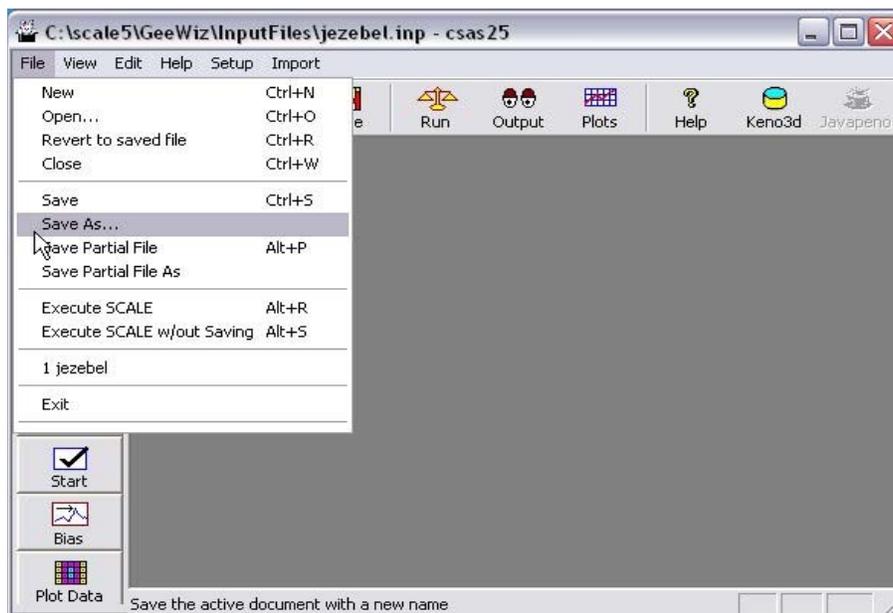
**Fig. 17. Sphere form.**

Select the appropriate mixture, 1 pu-239, pu-240, pu-241, ga, enter the radius of 6.38493, and then select **OK**. To enter the information for the second zone, again select the appropriate geometry from the right toolbar, **sphere**. This opens a new **Sphere** form. Select mixture 2 ni, enter the radius of 6.39763, and then select **OK**. Now you need to check the box beside **Global Unit** by clicking on the box. The global unit in KENO V.a is the final unit that defines the entire system to be analyzed. Then enter a comment next to **Comment**. The comment for this problem should read, jezebel core with nickel plating. The Geometry Summary form should look like Fig. 18. Selecting **Close** from the toolbar will save this information and will return you to the main GeeWiz screen.



**Fig. 18. Geometry summary screen.**

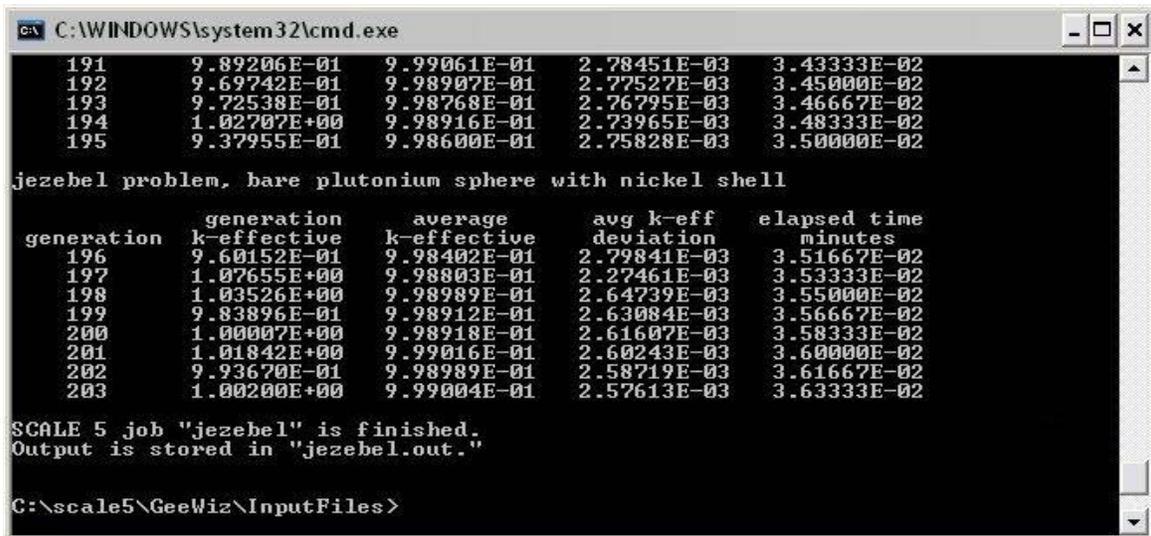
This completes the information necessary to run the example problem. The next step is to save all data in an input file. To do this, select **File** from the top of the GeeWiz screen. This will bring up the pulldown menu as shown in Fig. 19. From the pulldown menu, select **Save As...** and then enter the file name, such as `jezebel`. You can view the SCALE input file created by GeeWiz by clicking on **Edit**, then **Edit File Ctrl+E**, or by using the shortcut keys **Ctrl+E**. Example input files for all cases can be found in Appendix B.



**Fig. 19. Pulldown menu for saving input file.**

## 2.4 RUNNING SCALE/KENO V.A

To run SCALE/KENO V.a, click the **Run** button on the toolbar. This will run SCALE/KENO V.a in a DOS window. At the completion of the run, the screen should look like that in Fig. 20.



```
C:\WINDOWS\system32\cmd.exe
191 9.89206E-01 9.99061E-01 2.78451E-03 3.43333E-02
192 9.69742E-01 9.98907E-01 2.77527E-03 3.45000E-02
193 9.72538E-01 9.98768E-01 2.76795E-03 3.46667E-02
194 1.02707E+00 9.98916E-01 2.73965E-03 3.48333E-02
195 9.37955E-01 9.98600E-01 2.75828E-03 3.50000E-02

jezebel problem, bare plutonium sphere with nickel shell

generation      generation      average      avg k-eff      elapsed time
generation      k-effective    k-effective  deviation      minutes
196 9.60152E-01 9.98402E-01 2.79841E-03 3.51667E-02
197 1.07655E+00 9.98803E-01 2.27461E-03 3.53333E-02
198 1.03526E+00 9.98989E-01 2.64739E-03 3.55000E-02
199 9.83896E-01 9.98912E-01 2.63084E-03 3.56667E-02
200 1.00007E+00 9.98918E-01 2.61607E-03 3.58333E-02
201 1.01842E+00 9.99016E-01 2.60243E-03 3.60000E-02
202 9.93670E-01 9.98989E-01 2.58719E-03 3.61667E-02
203 1.00200E+00 9.99004E-01 2.57613E-03 3.63333E-02

SCALE 5 job "jezebel" is finished.
Output is stored in "jezebel.out."

C:\scale5\GeeWiz\InputFiles>
```

Fig. 20. DOS window showing completed run.

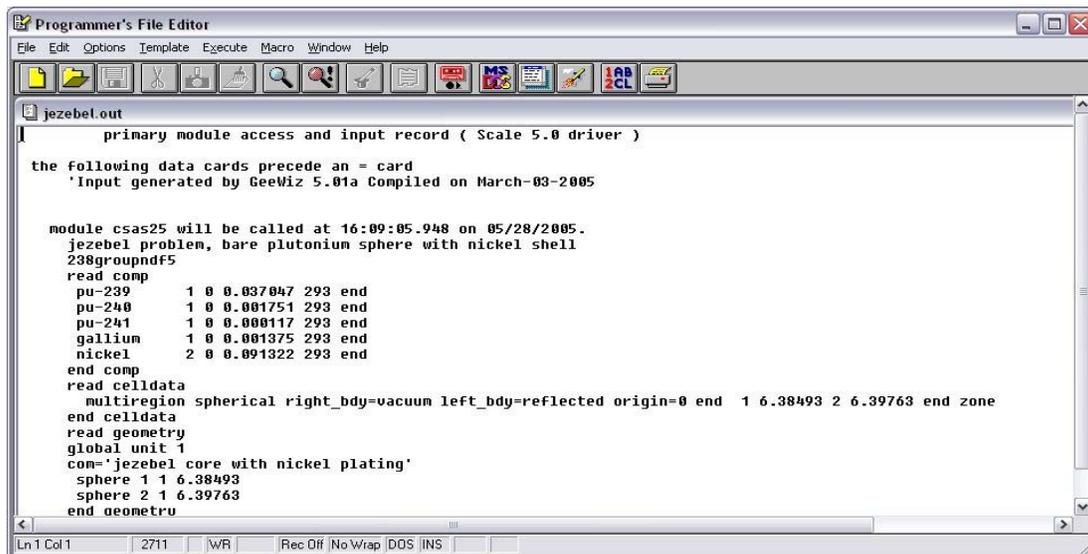
Note that it indicates **SCALE 5 job jezebel is finished**. It also indicates that the **Output is stored in jezebel.out**. If you had a different name for your input file, then the output will be stored in a file of that name with the **.out** extension. The elapsed time in the DOS window may not match that shown in Fig. 20 as each computer has different clock speeds.

## 2.5 SCALE OUTPUT

To view the output, click on the **Output** button. The text editor selected by the user in Setup [default is Programmer's File Editor (PFE)] automatically loads the output file. The output for this problem consists of the following sections:

- echo of input,
- CSAS information and brief review of input values,
- BONAMI data from cross-section processing,
- NITAWL data from cross-section processing, and
- KENO V.a information.

The initial display of the output file shows the input echo as in Fig. 21.



```
Programmer's File Editor
File Edit Options Template Execute Macro Window Help
jezebel.out
primary module access and input record ( Scale 5.0 driver )
the following data cards precede an = card
'Input generated by GeeWiz 5.01a Compiled on March-03-2005

module csas25 will be called at 16:09:05.948 on 05/28/2005.
jezebel problem, bare plutonium sphere with nickel shell
238groupndf5
read comp
pu-239      1 0 0.037047 293 end
pu-240      1 0 0.001751 293 end
pu-241      1 0 0.000117 293 end
gallium     1 0 0.001375 293 end
nickel      2 0 0.091322 293 end
end comp
read celldata
  multiregion spherical right_bdy=vacuum left_bdy=reflected origin=0 end 1 6.38493 2 6.39763 end zone
end celldata
read geometry
global unit 1
com='jezebel core with nickel plating'
  sphere 1 1 6.38493
  sphere 2 1 6.39763
end neonetru
```

Fig. 21. Input echo at top of output file.

For this *Quickstart* section, we will look at a few items in the KENO V.a information section. The first will be the information following the line **keno message number k5-123**. Press the F2 key in PFE to find k5-123. This message states that execution of KENO was terminated due to completion of the specified number of generations. This means that the problem ran to completion based on the generations specified by the user (in this case the default

value). Below the message are lines with information on the neutron lifetime, generation time,  $\bar{\nu}$ , average fission group, and energy of the average lethargy causing fission. These parameters will be discussed in later sections. For the example problem, this information should appear as shown in Fig. 22.

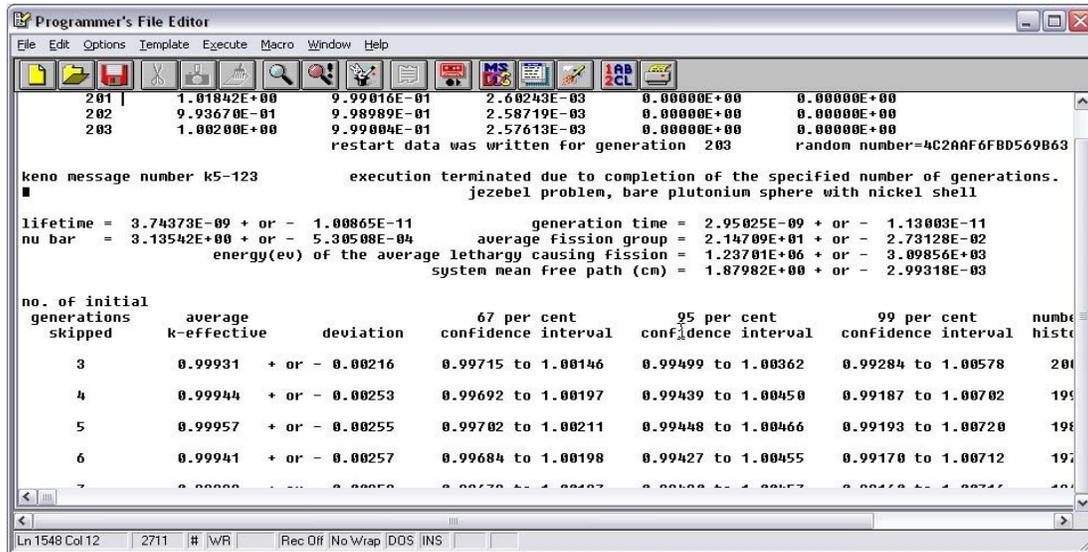
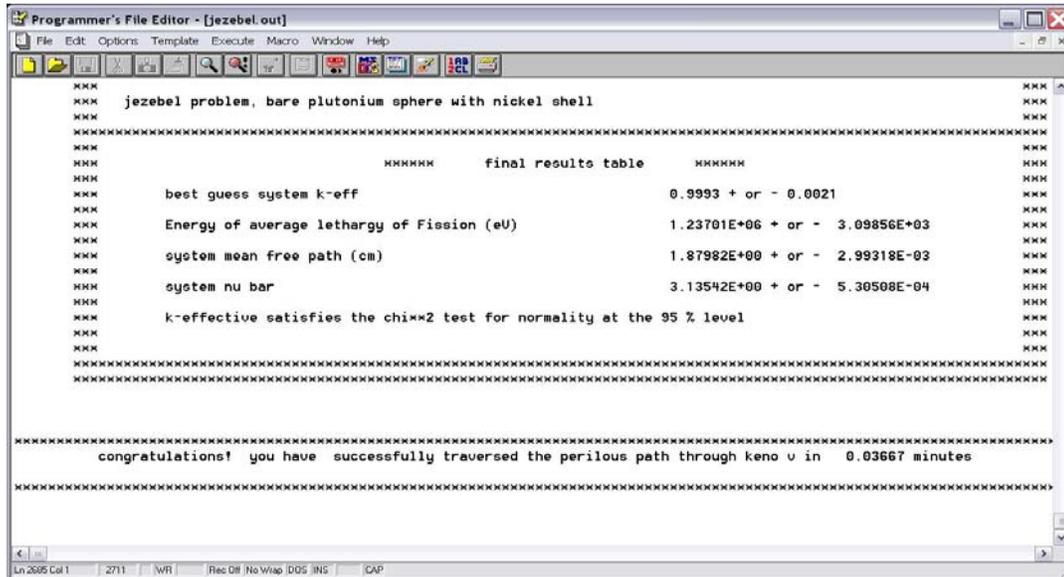


Fig. 22. KENO output for Jezebel problem.

Following the neutron parameters table is a table providing the calculated  $k_{\text{eff}}$  of the problem versus number of initial generations skipped. For the example problem, the calculated  $k_{\text{eff}}$  after skipping three initial generations is  $0.99931 \pm 0.00216$ , as shown in Fig. 22. Also note that the smallest standard deviation for the example problem occurs after skipping three initial generations. This  $k_{\text{eff}}$  is printed as the best estimate  $k_{\text{eff}}$  in the final results table at the end of the output file (Fig. 23).

If your input did not run successfully, the error messages will be listed on the screen during execution or in the output file. In most cases, the errors are related to input data problems. Check to make sure your input file has the same data as the one listed in this section. The output echo of the input file for the example problem is shown in Fig. 24.



**Fig. 23. KENO final results table.**

primary module access and input record ( Scale 5.0 driver )

the following data cards precede an = card

'Input generated by GeeWiz 5.01a Compiled on March-03-2005

```

module csas25 will be called at 22:53:32.626 on 06/14/2005.
jezebel problem, bare plutonium sphere with nickel shell
238groupndf5
read comp
  pu-239      1 0 0.037047 293 end
  pu-240      1 0 0.001751 293 end
  pu-241      1 0 0.000117 293 end
  gallium     1 0 0.001375 293 end
  nickel      2 0 0.091322 293 end
end comp
read celldata
  multiregion spherical right_bdy=vacuum left_bdy=reflected origin=0 end
1 6.38493 2 6.39763 end zone
end celldata
read geometry
global unit 1
com='jezebel core with nickel plating'
  sphere 1 1 6.38493
  sphere 2 1 6.39763
end geometry
end data

```

**Fig. 24. Example problem input echo.**

## 2.6 SUMMARY

This section has helped you to:

- Describe the structure of SCALE/KENO V.a input files and know that there are parts describing the sequence, the materials, and the KENO information.
- Use the GeeWiz user interface to create a SCALE/KENO V.a input file.
- Set up and run a simple criticality problem using SCALE/KENO V.a.
- Find and interpret  $k_{\text{eff}}$  information from your output.

Now that you have successfully run SCALE/KENO V.a, you are ready to learn in detail the options available in each input segment and how to set up more complex problems. The sections that follow present these details in a similar format to that used in this *Quickstart* section.



## 3. MATERIAL INFORMATION INPUT

In the *Quickstart* section (Sect. 2), you ran a simple problem with SCALE using the GeeWiz User Interface. From this you gained confidence in using the code and some experience with GeeWiz. This section and subsequent sections provide a more detailed explanation of the commands used in the *Quickstart* section.

### 3.1 WHAT YOU WILL BE ABLE TO DO

- Define the different criticality sequences used in SCALE.
- Describe the cross-section libraries available for criticality safety analyses.
- Use the GeeWiz user interface to provide data on elements, isotopes, compounds, and solutions.
- Interpret basic output information from a SCALE/KENO V.a analysis.

### 3.2 CSAS SEQUENCES

To minimize human error, the SCALE data handling and program flow are automated as much as possible through the use of control modules. These control modules are incorporated into sequences that select the modules required for a particular analysis. For criticality safety work, these CSAS sequences (Table 1) provide automated, problem-dependent, cross-section processing followed by calculation of the neutron multiplication factor for the system being modeled. These control sequences use the cross-section processing codes BONAMI (for the unresolved resonance energy range) and NITAWL or CENTRM/PMC (for the resolved resonance range) to provide resonance-corrected cross sections. CENTRM and PMC provide a more rigorous method than NITAWL for generating resonance-corrected cross sections using continuous energy data. Note that NITAWL was the default used in SCALE 5, while CENTRM/PMC are used by default in SCALE 5.1.

The CSAS1 sequence uses XSDRNPM to calculate the neutron multiplication factor ( $k_{\text{eff}}$ ) for a 1-D system model. XSDRNPM can be used by all CSAS sequences to generate cell-weighted cross sections based on unit cell geometry. ICE is used by CSAS1 to provide a Monte Carlo-formatted mixed (i.e., macroscopic) cross-section library. KENO V.a uses the processed cross sections and calculates the  $k_{\text{eff}}$  of 3-D system models. The geometric modeling capabilities available in KENO V.a, coupled with the automated cross-section processing within the control sequences, allow complex 3-D systems to be easily analyzed. The CSAS25 sequence is used most often for KENO V.a criticality calculations. A search capability is achieved in the CSAS4 sequences by repeatedly activating the control module MODIFY to alter the dimensions

or the nuclide concentrations and the functional module KENO V.a to calculate the  $k_{\text{eff}}$  for the new dimensions or concentrations.

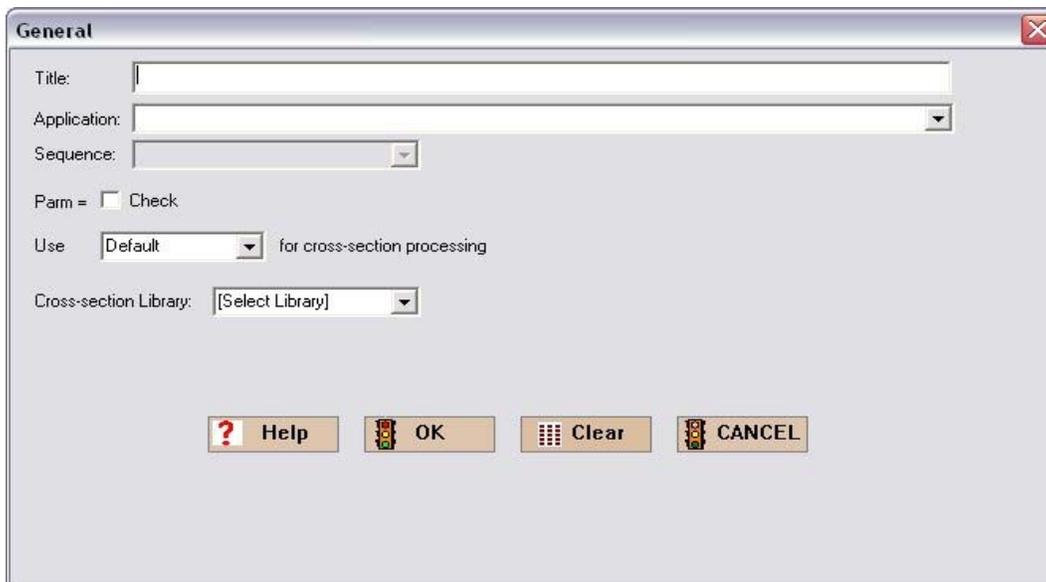
**Table 1. CSAS sequences for criticality safety**

Control sequence	Function	Functional modules executed by the control sequence			
CSASI	Macroscopic cross sections	BONAMI	CENTRM/PMC <sup>a</sup>	ICE	
CSASN	Microscopic cross sections	BONAMI	CENTRM/PMC <sup>a</sup>		
CSAS1	k-eff (1-D)	BONAMI	CENTRM/PMC <sup>a</sup>	XSDRNPM	
CSAS25	k-eff (3-D)	BONAMI	CENTRM/PMC <sup>a</sup>	KENO V.a	
CSAS4	k-eff (3-D) search	BONAMI	CENTRM/PMC <sup>a</sup>	KENO V.a	MODIFY <sup>b</sup>

<sup>a</sup> NITAWL is used if PARM=NITAWL is specified. NITAWL is default in SCALE 5.

<sup>b</sup> MODIFY is a control module.

The selection of a sequence is done through the **General Information** window (Fig. 25) of GeeWiz. Click on the **General** button to open this window. Information in this window includes the version of SCALE you are using as determined by GeeWiz, a **Title** for the problem, the **Application**, and the **Sequence** that you want to execute. The available sequences are listed on a pulldown menu as shown in Fig. 26. Select the application and the sequence you want by clicking on them.



**Fig. 25. General information window in GeeWiz.**

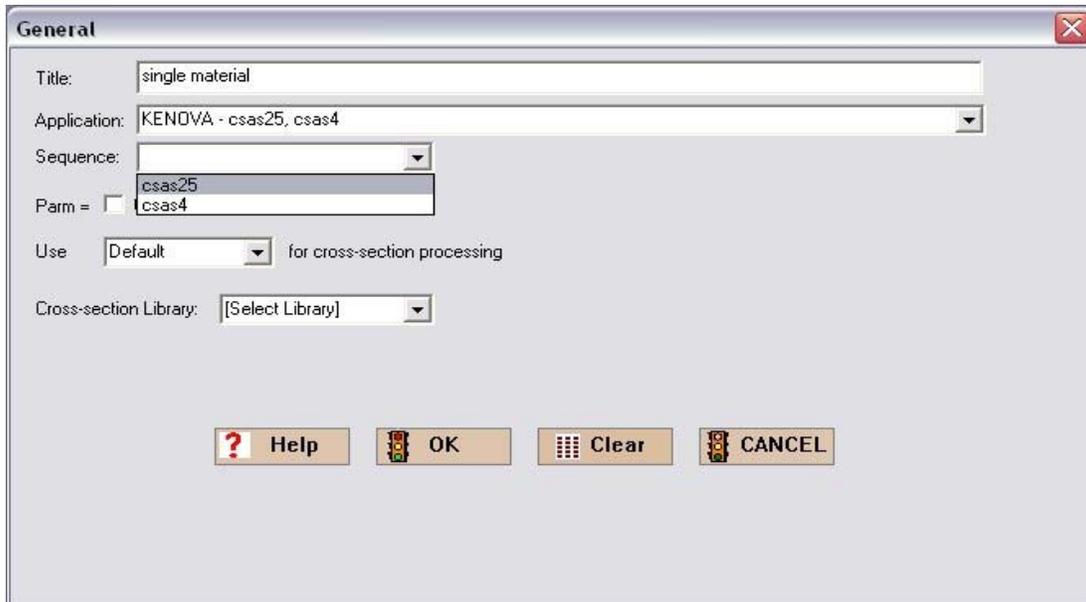


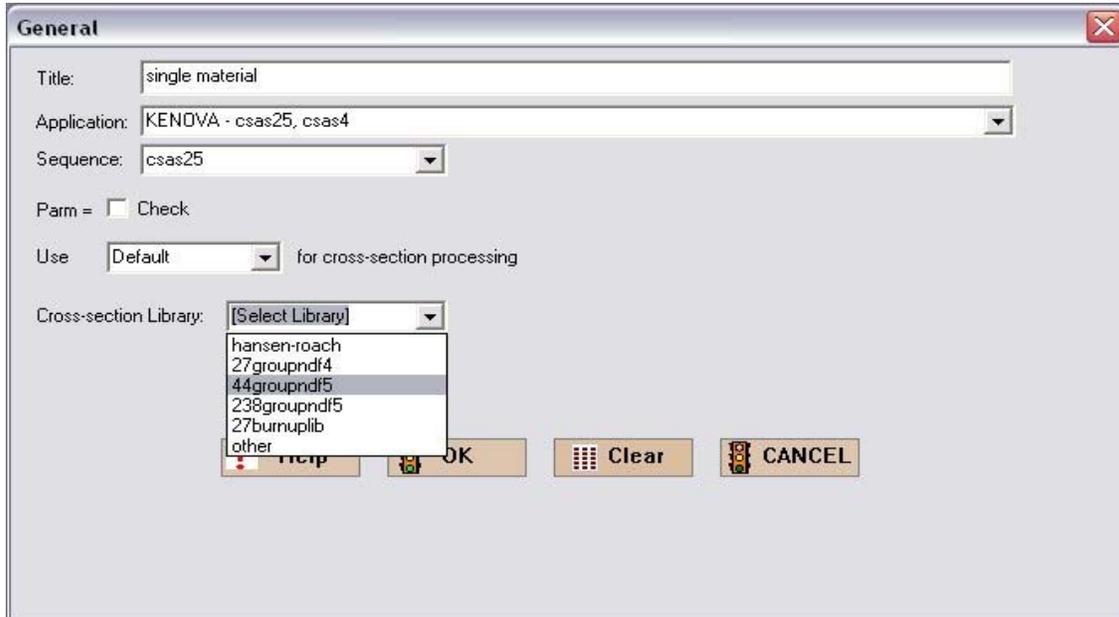
Fig. 26. Criticality safety sequence pulldown menu.

### 3.3 CROSS-SECTION LIBRARIES

Each CSAS sequence (1) uses the Standard Composition Library (described later in this section) for specifying the materials and mixtures used in a calculation and (2) provides automatic problem-dependent cross-section preparation prior to the criticality calculation. This section describes the cross-section libraries most useful for criticality calculations in the SCALE system. There are several multigroup cross-section libraries distributed with SCALE for criticality safety analyses. The Hansen-Roach 16-group library (HANSEN-ROACH) is based on the original Hansen and Roach data. Important nuclides not available in the library were added by collapsing the 218-group ENDF/B-IV library to the 16-group structure. Although not recommended, it is included in SCALE for historical purposes. The 238-group ENDF/B-V library (238GROUPNDF5) is the most complete library in SCALE 5. This library contains data for all ENDF/B-V nuclides and has 148 fast and 90 thermal groups. Most resonance nuclides in the 238-group library have resonance data in the resolved resonance region and Bondarenko factors in the unresolved resonance region. The 44-group ENDF/B-V library (44GROUPNDF5) is a broad-group version of 238GROUPNDF5 designed for analysis of light-water-reactor (LWR) fresh and spent fuel systems and has been extensively validated against LWR critical experiments.

**The 238- and 44-group libraries are the preferred criticality safety analysis libraries in SCALE. The 44-group library is recommended for LWR systems, and the 238-group library is recommended for all other types of systems.** Note that a 238-group ENDF/B-VI library is available in SCALE 5.1. See Appendix A for a more detailed discussion of the cross-section libraries.

A library is selected in GeeWiz from the pulldown menu for Cross-section Library (See Fig. 27). Table 2 lists the standard SCALE cross-section libraries, along with the alphanumeric name and the main source of data for each library.



**Fig. 27. Cross-section library pulldown menu.**

**Table 2. SCALE cross-section libraries for criticality analyses**

Alphanumeric name	Description	Primary source of data
HANSEN-ROACH	Hansen-Roach 16-group library	Hansen and Roach data
44GROUPNDF5	ENDF/B-V 44-group library	Collapsed from 238-group ENDF/B-V library
238GROUPNDF5	ENDF/B-V 238-group library	ENDF/B-V data
V6-238GROUP*	ENDF/B-VI 238-group library	ENDF/B-VI data

\*Available in SCALE 5.1.

The criticality sequences access BONAMI first to process nuclides with Bondarenko data. The master library output from BONAMI is input to NITAWL, where resonance data are processed via the Nordheim integral treatment or to CENTRM, which performs a 1-D continuous energy calculation that is subsequently collapsed to multigroup cross sections by PMC. In either case, the result is an AMPX working-format library that is used by KENO V.a. **Note that CENTRM must be used to process ENDF/B-VI cross-section libraries.**

### 3.4 MATERIAL INPUT

Information on materials in a system is entered into GeeWiz, which puts that information in the format required by MIPLIB in CSAS. CSAS utilizes this data along with standardized procedures to provide data to create problem-dependent cross-section libraries. Input data to GeeWiz identify the materials from the Standard Composition Library and associated physical densities to calculate the number densities (atoms/b-cm) of each material specified in the problem, to develop data used by the resonance processors, and to utilize the automatic mesh-generator to calculate the mesh intervals used in the optional XSDRNPM cell-weighting calculation. These input data include (1) the Standard Composition data that are used in the standardized number density calculations (a standardized alphanumeric name, mixture number, and other data to define materials, including volume fraction or percent theoretical density, temperature, and isotopic distribution), and (2) the unit cell description defining the materials, dimensions, and boundary conditions of the geometry that will be used in the Dancoff factor calculations, the resonance self-shielding calculations, and the flux-weighting cell calculations necessary for cross-section processing.

The Standard Composition Library describes the various predefined isotopes, elements (both symbols and full names), compounds, alloys, and other materials that can be used to define the material mixtures for a given problem. A complete description of the materials in the library is found in the SCALE manual [Vol. 3, Sect. M8]. The library contains over 600 compounds, alloys, elements, and isotopes that one may use in defining the material mixtures for a given problem. Additionally, there are four fissile solutions available for which the user can specify the heavy metal, acid, and water components [ $\text{UO}_2\text{F}_2$ ,  $\text{UO}_2(\text{NO}_3)_2$ ,  $\text{Pu}(\text{NO}_3)_4$ , and  $\text{Th}(\text{NO}_3)_4$ ].

When formulating a mixture, it is often necessary to know the density (g/cc) of the mixture and the weight fractions of the various constituent materials. Note that default densities should not be used for materials containing enriched isotopes, especially light elements with strong absorbers such as boron,  $\text{B}_4\text{C}$ , or lithium. The temperature of a given material can be entered (the default is 300 K, i.e., room temperature). The temperature is used to correctly process resonance data, Bondarenko data, and/or thermal-scattering data.

### 3.5 EXAMPLE PROBLEMS

Four example problems will be used to illustrate how to enter material information into GeeWiz. These problems examine uranium in a bare (unreflected) finite cylinder with four different material compositions: pure  $^{235}\text{U}$  metal, U(93.7) metal, U(93.7) $\text{O}_2$ , and U(30.3) $\text{O}_2\text{F}_2$

solution. These examples are from LA-10860,<sup>3</sup> p. 98 and p. 26, and from the International Criticality Safety Benchmark Experiments Project (ICSBEP) CD.<sup>4</sup>

### 3.5.1 Bare <sup>235</sup>U Metal Cylinder

The bare metal cylinder problems have an effective radius of 7.82 cm with an estimated critical height of 15.64 cm (H/D=1). A cylinder containing pure <sup>235</sup>U is modeled first to demonstrate using GeeWiz to enter a single isotope (see Fig. 28). The dimensions are derived using buckling conversion from the critical radius of the Godiva sphere (8.741 cm). For Godiva, the uranium density is 18.742 g/cc.

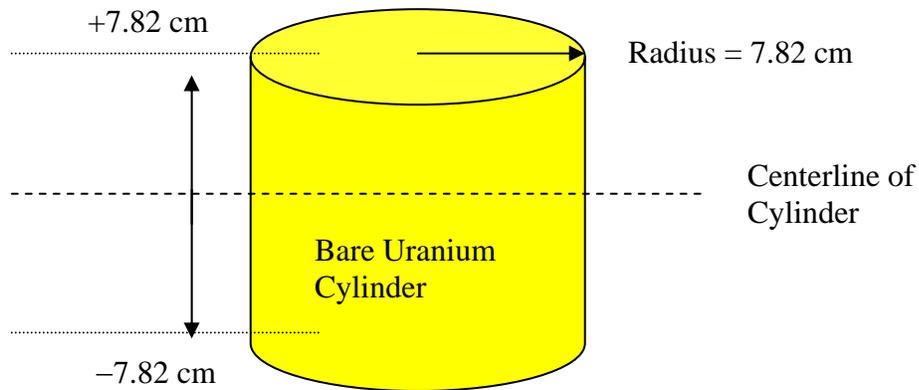
*Core Material ( $\rho_{mix} = 18.742$  g/cc-mixture)*

U metal (100 percent <sup>235</sup>U)

Configuration 1. *Bare Uranium Cylinder*

Radius = 7.82 cm

Height =  $\pm 7.82$  cm

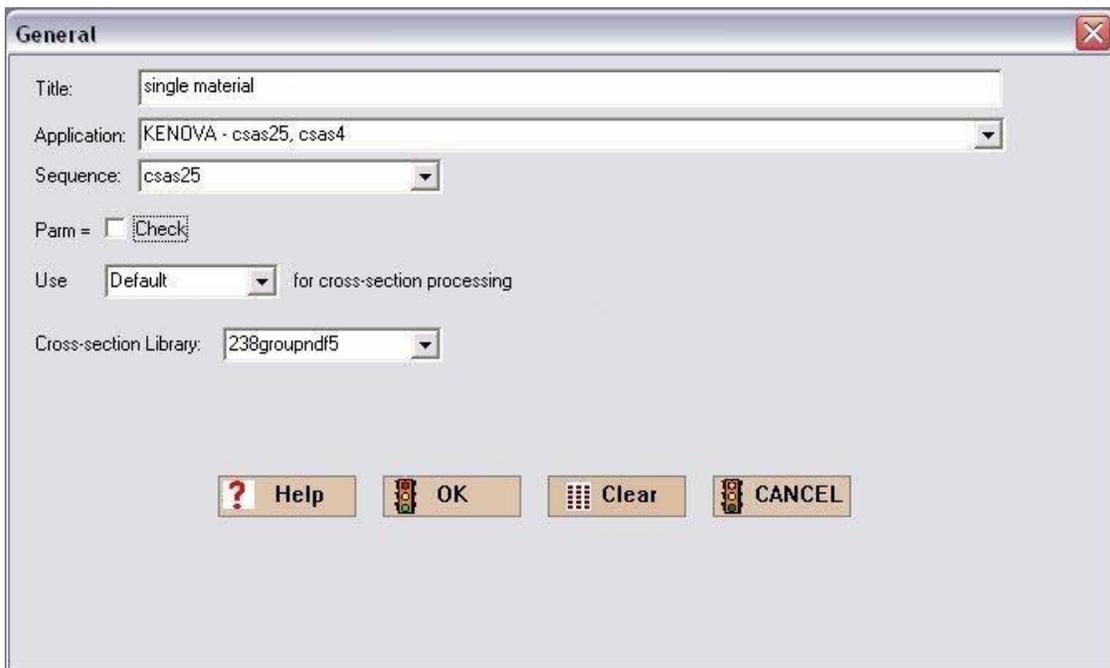


**Fig. 28. Configuration 1 geometry.**

The initial data entry for this example is the same as that described in the *Quickstart* section. Start the GeeWiz user interface and then select **File** and **New Problem**. Selecting the **General** button on the left-hand side menu will bring up the screen where you enter the problem title, the SCALE sequence, the cross-section library, and the unit cell type information. Other parameter information can be entered if desired. Now enter the title as follows:

EXAMPLE PROBLEM 1

Again note that information to be entered into GeeWiz will appear in the Courier font. Now select `csas25` as the sequence. For **Cross-section Library**, select `238groupndf5`. The general information screen should look like that in Fig. 29.



The screenshot shows a dialog box titled "General" with a close button (X) in the top right corner. The dialog contains the following fields and controls:

- Title:** A text input field containing "single material".
- Application:** A dropdown menu showing "KENDVA - csas25, csas4".
- Sequence:** A dropdown menu showing "csas25".
- Parm =** A checkbox labeled "Check" which is checked.
- Use:** A dropdown menu showing "Default" followed by the text "for cross-section processing".
- Cross-section Library:** A dropdown menu showing "238groupndf5".
- Buttons:** Four buttons at the bottom: "Help" (with a question mark icon), "OK" (with a green checkmark icon), "Clear" (with a grid icon), and "CANCEL" (with a red X icon).

**Fig. 29. Example 1 general information form.**

When completed, select **OK/Save** to save this information in a temporary file. Later you will save all of the input information under a file name.

### 3.5.1.1 Material Input

The Material Input is entered using GeeWiz's Materials windows. Clicking on the **Compositions** button on the left opens the **New Composition** form for specifying new materials in the model, as shown in Fig. 30. In SCALE 5.1, the **Standard Basic Compositions** form (Fig. 31) is opened, and the user must click **Create** to open the **New Composition** form.

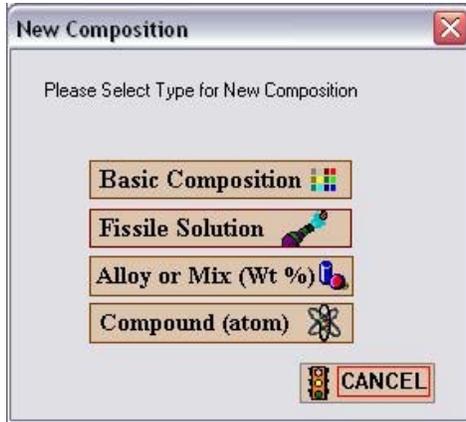


Fig. 30. New composition form.

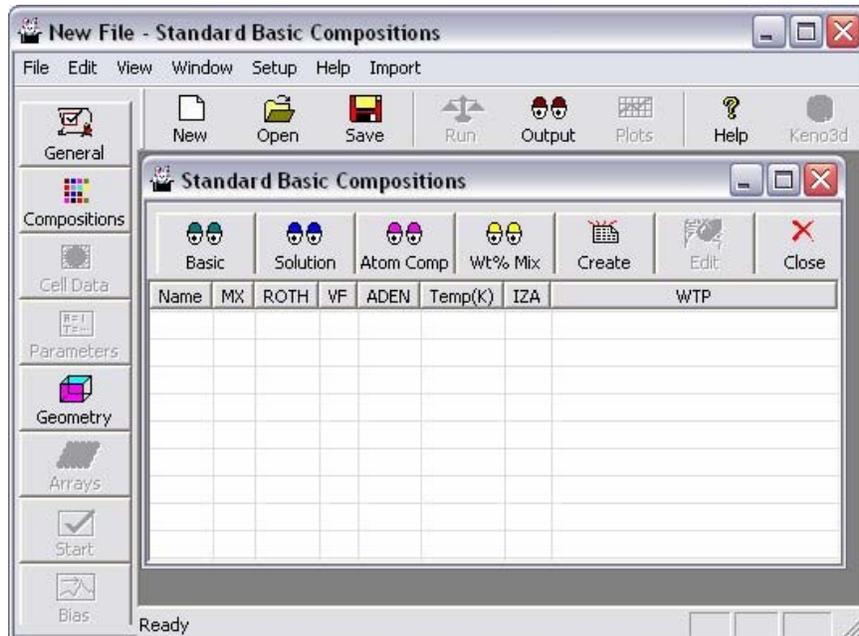


Fig. 31. Standard basic compositions input form.

You will be entering data for  $^{235}\text{U}$ , which is in the Standard Composition Library and is a Basic Composition. For this example problem, we will select **Basic Compositions**, which brings up the screen shown in Fig. 32. The **Mixture Number** starts with 1. Under **Composition Name** scroll down the menu and select u-235. This brings up the default values of **Density Multiplier** (1) and **Temperature (K)** (300). Now we need to enter the density by selecting **User Supplied (g/cc)** and then entering the value 18.742 in the data entry box. The completed screen should look like Fig. 33.

The screenshot shows a software window titled "Basic Standard Composition". At the top, there is a toolbar with icons for help, first, last, prev, next, copy, and new. Below the toolbar, there are four input fields: "Mixture Number" (value: 1), "Composition Name" (dropdown menu), "Density Multiplier" (value: 1), and "Temperature (K)" (value: 300). A "Density" section contains a text input box and three radio buttons: "Default (g/cc)" (selected), "User Supplied (g/cc) (DEN =)", and "Number Density (atoms/b-cm) (ADEN)". At the bottom left, it displays "Record 6 of 6 records". At the bottom right, there are three buttons: "OK", "Clear", and "CANCEL".

**Fig. 32. Basic standard composition input form.**

**Basic Standard Composition**

help first last prev next copy new

Mixture Number: 1  
Composition Name: u-235  
Density Multiplier: 1  
Temperature (K): 300

Density: 18.742  
 Default (g/cc)  
 User Supplied (g/cc) (DEN =)  
 Number Density (atoms/b-cm) (ADEN)

Isotopic Distribution: --- No Isotopic Distribution

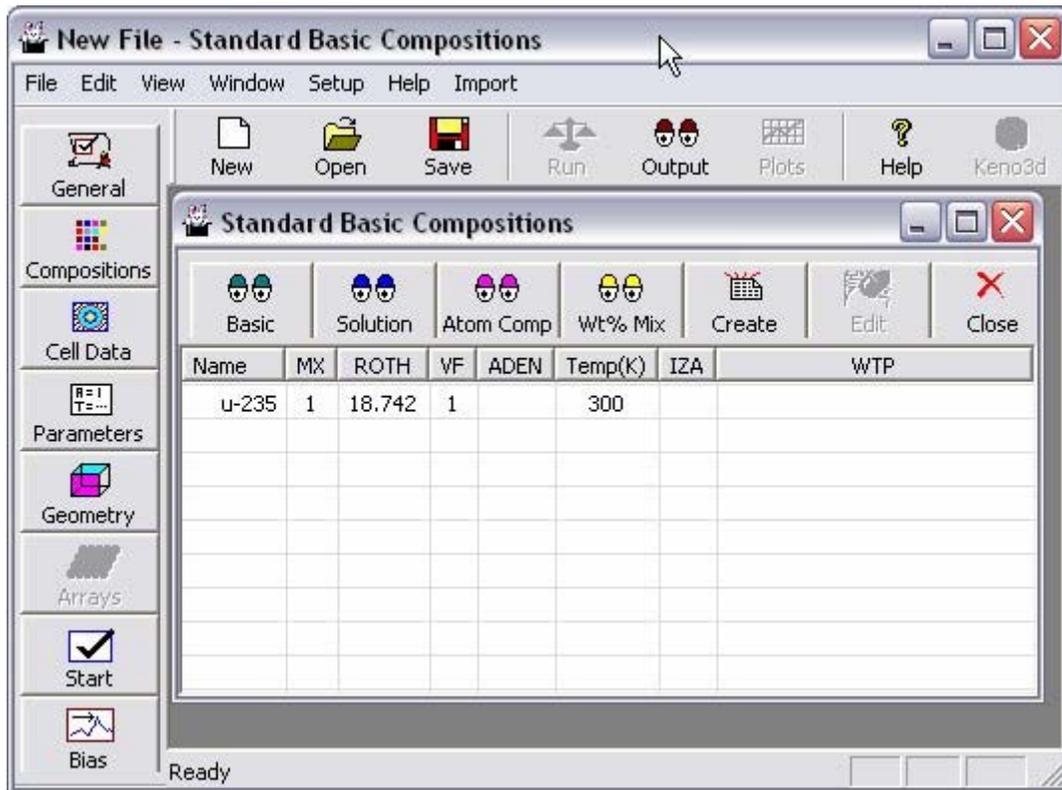
Record 1 of 1 records

OK Clear CANCEL

**Fig. 33. Example 1 material input.**

For this example,  $^{235}\text{U}$  is the only material, so select **OK** to bring up the summary form for Standard Basic Compositions as shown in Fig. 34. As this is all the material information for this problem, select **Close** to get back to the basic GeeWiz screen.

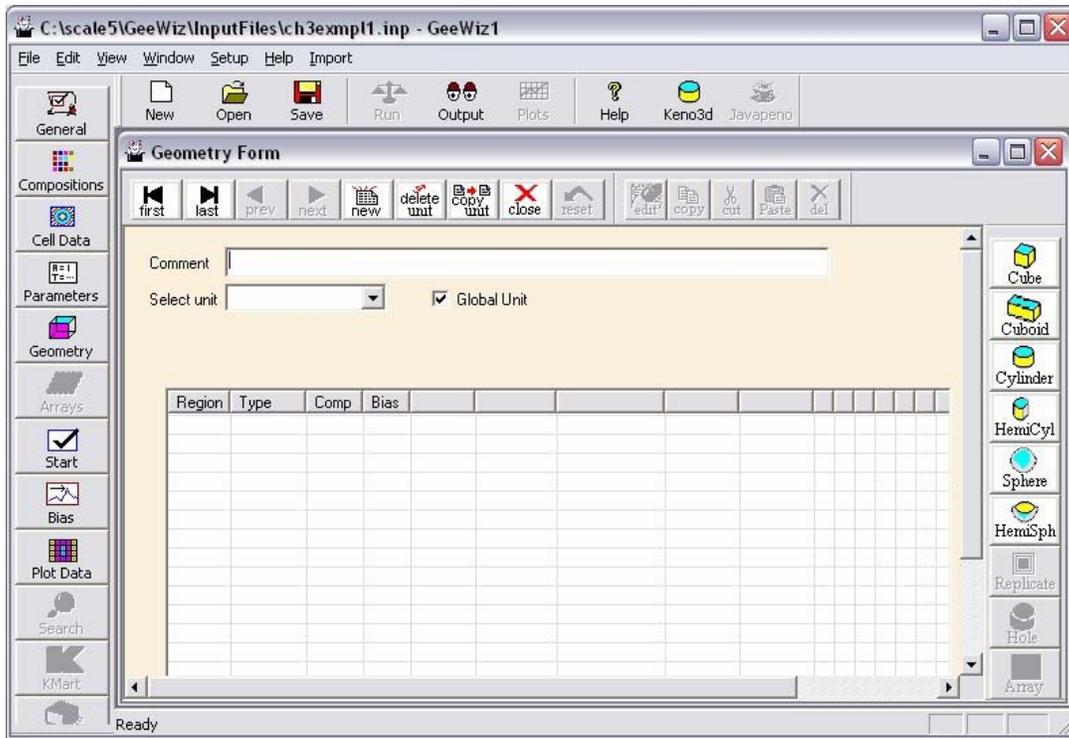
Because we want to use the infinite homogeneous medium unit cell type, the unit **Cell Data** are not required.



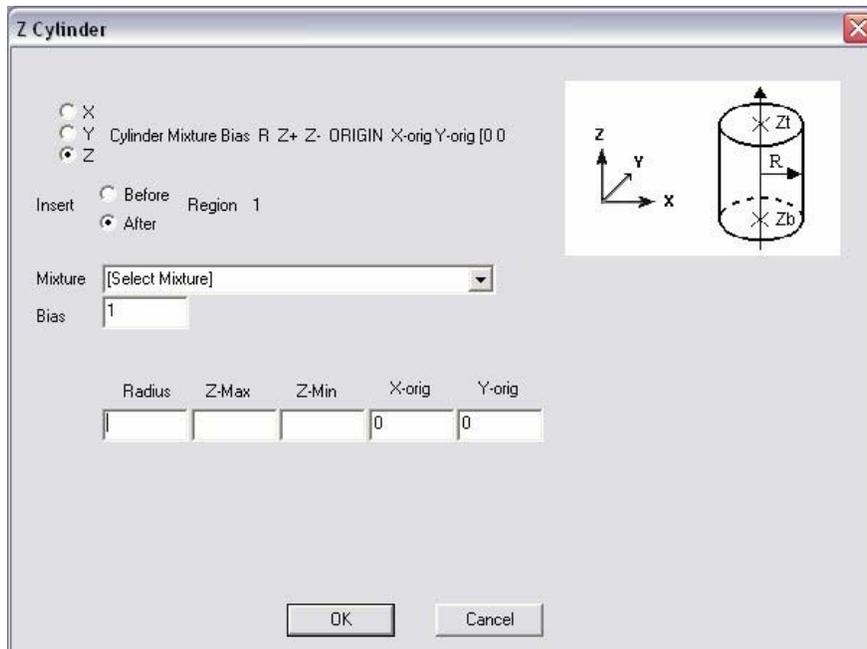
**Fig. 34. Summary of material input.**

### 3.5.1.2 KENO V.a Input

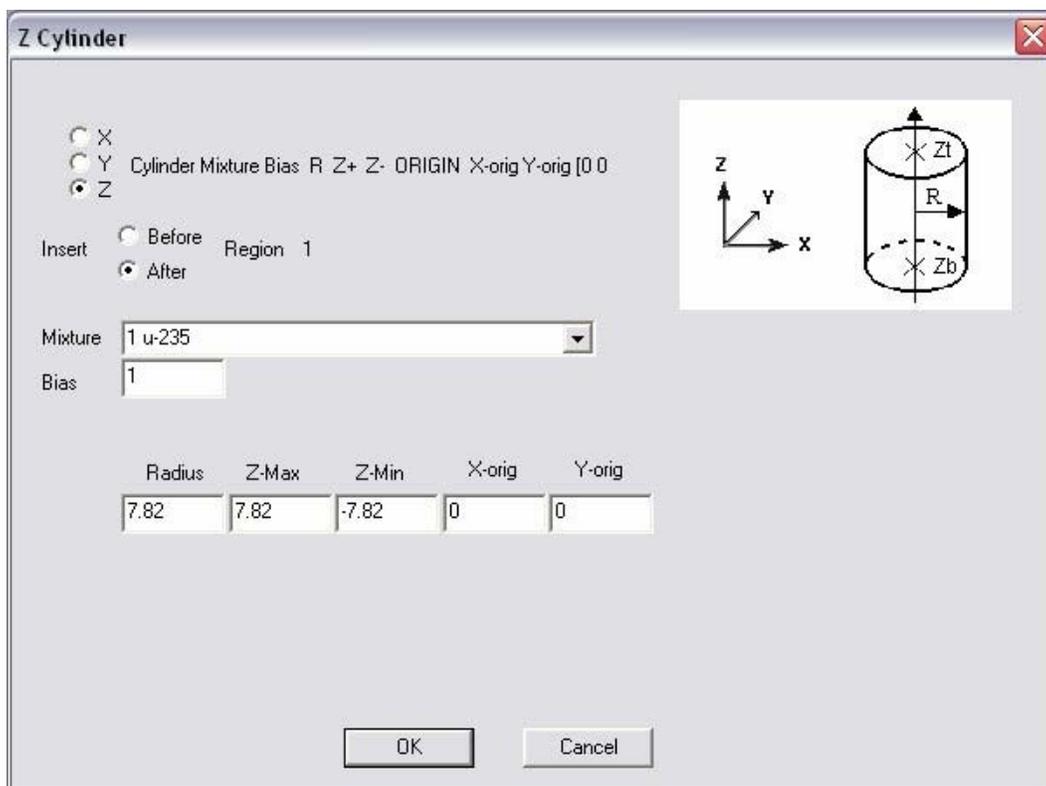
With this simple geometry, only a few entries are needed to complete the KENO input form. The only KENO V.a input required for this problem is the geometry. Select **Geometry** from the left-hand toolbar to bring up the geometry summary form shown in Fig. 35. To enter geometry information, select the appropriate geometry from the right toolbar. For this problem, that would be **cylinder**. This brings up the **Z-cylinder** input form shown in Fig. 36. For **Mixture** select 1 u-235 from the pulldown menu. Then enter 7.82 for the **Radius**, 7.82 for the **Top**, and -7.82 for the **Bottom**. This completes the **Geometry** window information and it should look like Fig. 37.



**Fig. 35. Geometry summary form.**



**Fig. 36. Z cylinder input form.**



**Fig. 37. Example 1 Z-cylinder geometry information.**

Click on **OK**, and that brings you back to the geometry summary form. Enter a comment in the **COM=** box such as, `bare cylinder`, and check the box beside **Global Unit** by clicking on the box. The global unit in KENO is the final unit that defines the entire system to be analyzed. The geometry summary screen should look like Fig. 38. Selecting **Close** from the menu bar will save this information and will take you back to the main GeeWiz screen. This completes the information required for the first example. Click on the **Run** button, and GeeWiz will prompt you to save the input file. GeeWiz opens a DOS window to execute SCALE. The user can observe the progress of the calculation. The beginning of the job should look like Fig. 39. The screen will show the input and output file names and then will indicate which programs are being executed. When KENO V.a is started, the title is displayed and then the calculated  $k_{\text{eff}}$  values from each generation are shown.

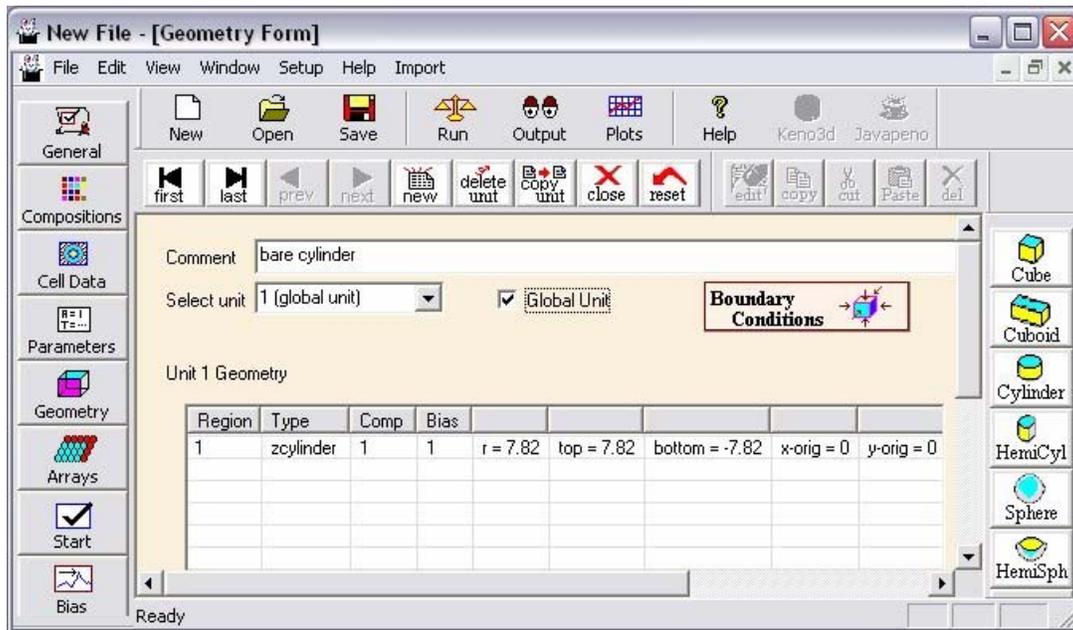


Fig. 38. Geometry summary form for example 1.

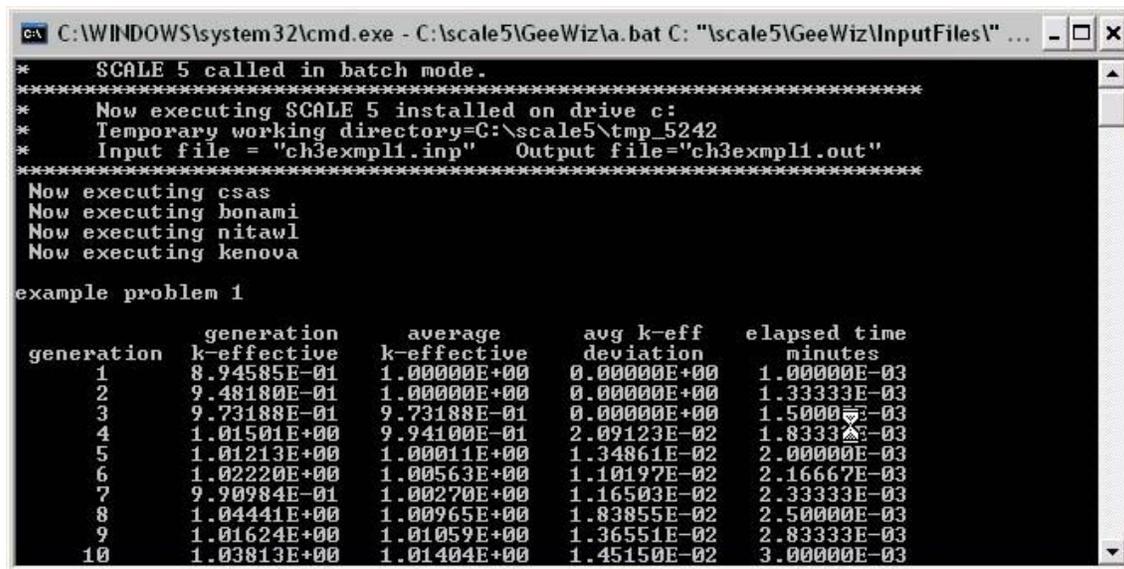


Fig. 39. SCALE output in DOS window at job initiation.

When the run is completed, the DOS window should look like that in Fig. 40, which indicates that the job is finished. If the job does not run successfully, try checking the error message with those given in the SCALE manual [Vol. 2, Sect. F11.7] to determine how to fix the problem.

```

C:\WINDOWS\system32\cmd.exe
190 1.03947E+00 1.02326E+00 1.98524E-03 4.61667E-02
191 1.00166E+00 1.02315E+00 1.97884E-03 4.63333E-02
192 1.03028E+00 1.02319E+00 1.96798E-03 4.66667E-02
193 9.97450E-01 1.02305E+00 1.96786E-03 4.68333E-02
194 9.68739E-01 1.02277E+00 1.99315E-03 4.71667E-02
195 9.94640E-01 1.02262E+00 2.01965E-03 4.73333E-02

example problem 1

generation      generation      average      avg k-eff      elapsed time
generation      k-effective     k-effective     deviation      minutes
196 9.92372E-01 1.02247E+00 2.04932E-03 4.75000E-02
197 1.01755E+00 1.02244E+00 2.04265E-03 4.78333E-02
198 9.78890E-01 1.02222E+00 2.06495E-03 4.80000E-02
199 1.05522E+00 1.02239E+00 2.04024E-03 4.83333E-02
200 1.03205E+00 1.02244E+00 2.02895E-03 4.85000E-02
201 1.00443E+00 1.02235E+00 2.01081E-03 4.88333E-02
202 1.01783E+00 1.02232E+00 2.00122E-03 4.90000E-02
203 1.04269E+00 1.02242E+00 1.98769E-03 4.91667E-02

SCALE 5 job "ch3exmpl1" is finished.
Output is stored in "ch3exmpl1.out."

C:\scale5\GeeWiz\InputFiles>

```

Fig. 40. SCALE output in DOS window at job completion.

### 3.5.1.3 Basic Output

To view the output, click the **Output** toolbar button. The output file will be opened in the text editor. There are many pages in the output file. Each module has a section of output, starting with the CSAS control module, which is then followed by the functional modules BONAMI, NITAWL, and KENO V.a. For the moment, we will look only at parts of the KENO V.a output. After the KENO V.a banner page, there is information on run parameters, materials, and geometry. Next, there is a table of calculated  $k_{\text{eff}}$  values by generation along with elapsed time and average  $k_{\text{eff}}$ . These are the same data that appear in the DOS window during execution. At the end of this table, there should be a message:

```

keno message number k5-123
execution terminated due to completion of the
specified number of generations.

```

This indicates normal termination of the run. A table of system parameters such as lifetime, average fission group, and energy of the average lethargy causing fission follows. This information allows you to check the spectrum of the modeled system. In this example, the spectrum should be quite hard as there is only fissile material in the system. This is indicated by the short lifetime of 5.488 nanoseconds and the relatively high energy, 0.957 MeV, of neutrons causing fission. The **lifetime** is the average lifespan of a neutron (in seconds) from the time

it is born until it is absorbed or leaks from the system. The **generation time** is the average time (in seconds) between successive neutron generations. The average number of neutrons per fission, **nu bar**, and its associated deviation are printed and the **average fission group** (the average energy group at which fission occurs) and its associated deviation are printed. Then, the **energy(ev) of the average lethargy causing fission (EALF)** and its associated deviation are printed. The EALF value is frequently used as a gauge of the average neutron energy of the system (i.e., how fast or thermal the spectrum is).

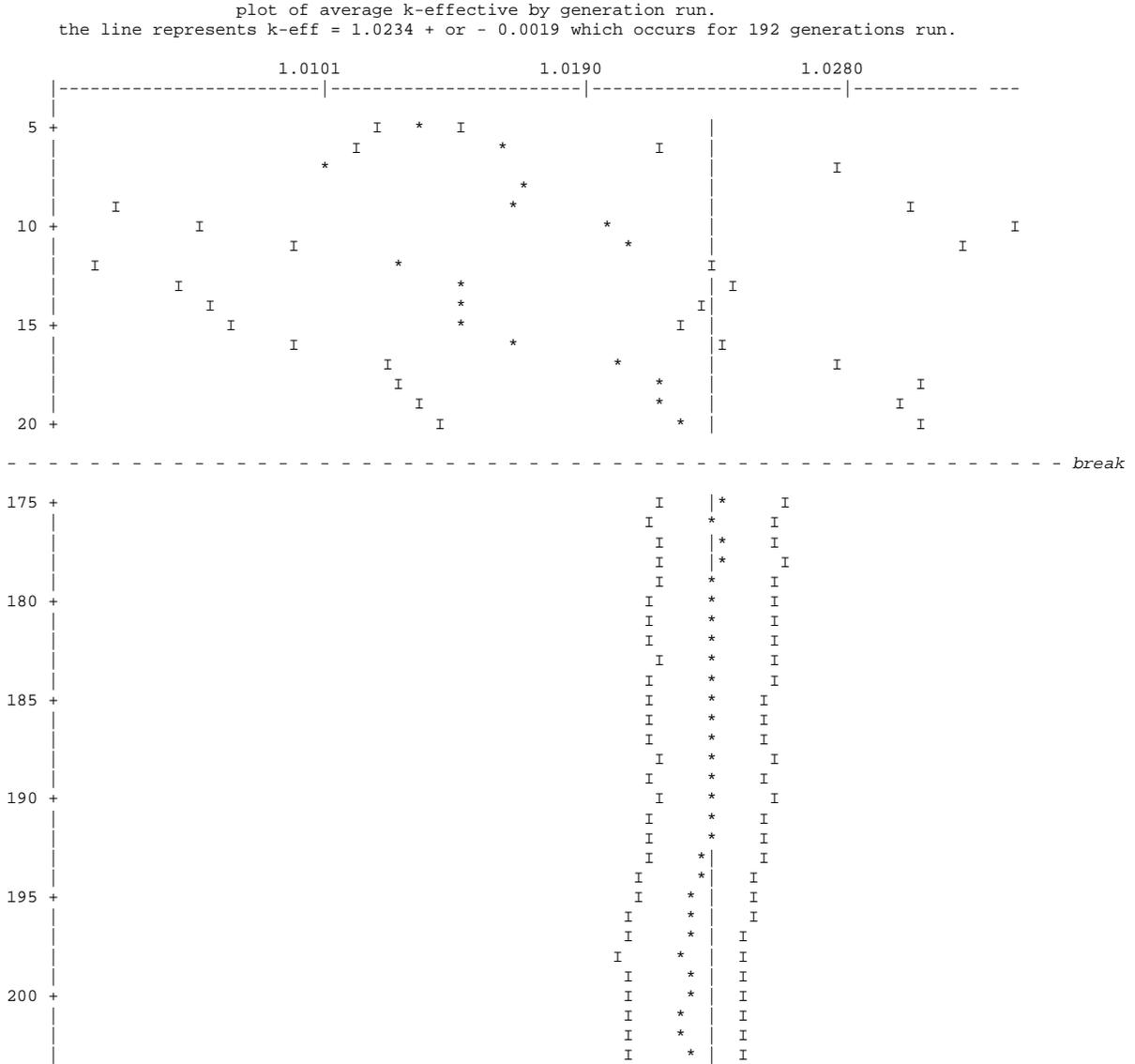
The final  $k_{\text{eff}}$  edit prints the average  $k_{\text{eff}}$  and its associated deviation and the limits of  $k_{\text{eff}}$  for the 67, 95, and 99% confidence intervals. The number of histories used in calculating the average  $k_{\text{eff}}$  is also printed. These results are based on skipping increasing numbers of the initial generations. Fig. 41 shows an abbreviated version of the table without the 95 and 99% confidence intervals. The user should carefully examine the final  $k_{\text{eff}}$  edit to determine if the average  $k_{\text{eff}}$  is relatively stable. If a noticeable drift is apparent as the number of initial generations skipped increases, it may indicate a problem in source convergence. If this appears to be the case, the problem should be rerun with a better initial source distribution (i.e., increase the number of neutrons per generation, NPG) and should be run for a sufficient number of generations (GEN) that the average  $k_{\text{eff}}$  becomes stable.

no. of initial generations skipped	average k-effective	deviation	67 per cent confidence interval	number of histories
3	1.02267	+ or - 0.00197	1.02070 to 1.02464	200000
4	1.02271	+ or - 0.00198	1.02073 to 1.02469	199000
5	1.02276	+ or - 0.00198	1.02078 to 1.02475	198000
6	1.02276	+ or - 0.00199	1.02077 to 1.02476	197000
7	1.02293	+ or - 0.00200	1.02092 to 1.02493	196000

**Fig. 41. Example of the final  $k_{\text{eff}}$  edit.**

Following the final  $k_{\text{eff}}$  edit are two plots of average  $k_{\text{eff}}$ : (1) versus the number of generations run and (2) versus the number of generations skipped. The limits of one standard deviation are plotted on either side of each average  $k_{\text{eff}}$ . In the first plot (Fig. 42), KENO omits the calculated  $k_{\text{eff}}$ s of the first NSK generations (number of generations skipped) in the calculation of the average  $k_{\text{eff}}$ s. The dotted line represents the value of the average  $k_{\text{eff}}$  corresponding to the smallest deviation when the average  $k_{\text{eff}}$  and its deviation are computed for each generation over the range from NSK +1 through the total number of generations (NGEN). Figure 42 is an example of this type of plot with the middle section removed for illustrative purposes. This plot is a graphical representation of the first table of calculated  $k_{\text{eff}}$ s in the output. The primary use for this plot is to determine if the

problem has source convergence difficulties. For this example, the source appears to be well-converged, as is indicated by the stability of the average  $k_{\text{eff}}$  and by the minimum variance in  $k_{\text{eff}}$  near the end of the problem.



**Fig. 42. Plot of average  $k_{\text{eff}}$  by generation run (excerpts).**

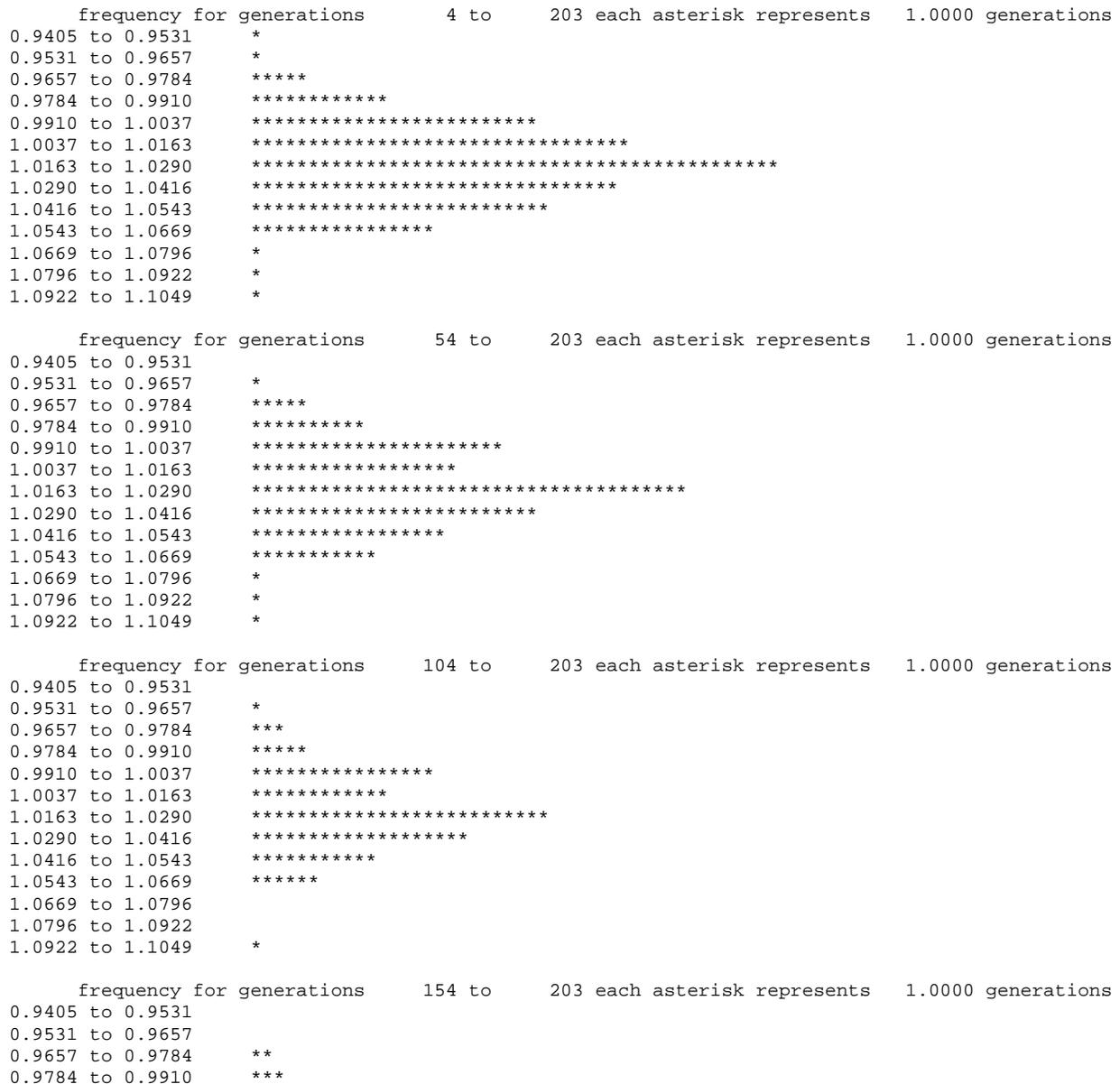
The second output plot graphically depicts the average  $k_{\text{eff}}$ s by generation skipped from the final  $k_{\text{eff}}$  edit in Fig. 41 for all generations from NSK+1 to NGEN. The dotted line represents the value of the average  $k_{\text{eff}}$  corresponding to the smallest deviation in the plot. An easy way to conceptualize the data in this plot is to think of each average  $k_{\text{eff}}$  as the average when the data for all previous generations are discarded. Because it typically takes somewhere between 3 and 100 generations to obtain a converged source distribution, this plot can help the analyst determine how many initial generations should be removed from the average  $k_{\text{eff}}$  calculation.

After the plots, there is a final edit of fissions, absorptions, and leakage by energy group. The fission fraction for each group and the fission production, absorptions, and leakage with their associated percent deviation are printed as shown in Fig. 43. (**NOTE:** No leakage is associated with faces having specular, mirror image, or periodic reflection. Thus, there is no leakage associated with an infinite problem.) Totals are printed at the end of the table, and the sum of the leakage and absorptions printed for the system total should be approximately 1. For this example, 43.4% of the neutrons were absorbed while 56.8% leaked from the system. The number of fissions printed for the system total, in this case **1.02267**, should be and is the same as the first  $k_{\text{eff}}$  printed in the final  $k_{\text{eff}}$  edit. The total elapsed time, **0.04950 minutes**, and final random number, **03851D84B8A2E548**, are printed at the end of this edit.

group	fission fraction	fissions	percent deviation	absorptions	percent deviation	leakage	percent deviation
1	0.0000	1.39299E-05	100.0000	2.75566E-06	100.0000	0.00000E+00	0.0000
2	0.0000	1.60203E-05	70.5328	3.37408E-06	70.5328	3.56005E-06	100.0000
3	0.0001	5.98034E-05	52.0123	1.31382E-05	52.0123	1.88996E-05	44.6937
4	0.0000	7.85000E-06	100.0000	1.77549E-06	100.0000	0.00000E+00	0.0000
5	0.0001	8.68129E-05	36.1534	2.01912E-05	36.1534	2.41573E-05	41.9379
6	0.0016	1.61920E-03	8.8659	4.03005E-04	8.8659	4.57544E-04	9.1226
7	0.0057	5.80397E-03	4.1479	1.58611E-03	4.1479	1.84936E-03	5.0326
8	0.0160	1.63367E-02	2.4215	4.80097E-03	2.4215	6.19887E-03	2.6623
9	0.0298	3.04518E-02	1.3241	9.84601E-03	1.3241	1.84039E-02	1.4698
10	0.0169	1.72335E-02	1.5596	5.88363E-03	1.5596	1.02871E-02	2.0057
11	0.0872	8.91990E-02	0.7376	3.20956E-02	0.7376	5.23536E-02	0.8642
12	0.0627	6.41040E-02	0.8787	2.42039E-02	0.8787	3.65096E-02	1.1055
13	0.0186	1.90438E-02	1.6283	7.33280E-03	1.6283	1.07268E-02	1.8772
14	0.0925	9.45621E-02	0.6621	3.72423E-02	0.6621	5.23551E-02	0.9204
15	0.0818	8.36632E-02	0.7182	3.38977E-02	0.7182	4.81399E-02	0.8998
16	0.0262	2.68063E-02	1.2796	1.10556E-02	1.2796	1.60479E-02	1.7521
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
238	0.0000	0.00000E+00	0.0000	0.00000E+00	0.0000	0.00000E+00	0.0000
system total =		1.02267E+00	0.1662	4.33643E-01	0.1752	5.67786E-01	0.1303
elapsed time		0.04950 minutes					
random number=		03851D84B8A2E548					

**Fig. 43. Final edit of fissions, absorptions, and leakage.**

The last section of the output contains the frequency distributions that indicate the number of generations whose  $k_{\text{eff}}$  is within a specified interval. The intervals are determined by the code based on the upper and lower limits of the calculated  $k_{\text{eff}}$ s for all generations. One asterisk is printed for each generation  $k_{\text{eff}}$ . The distributions should be reasonably symmetrical and bell-shaped for a good statistical analysis of  $k_{\text{eff}}$  (Fig. 44).



**Fig. 44. Calculated  $k_{\text{eff}}$  by generation frequency plot.**

At the very end of the run is a summary table as shown in Fig. 45.

```

*****
***
***   example problem 1
***
*****
***
***           *****   final results table   *****
***
***   best guess system k-eff                   1.0226 + or - 0.0019
***
***   Energy of average lethargy of Fission (eV) 9.57289E+05 + or - 2.58267E+03
***
***   system mean free path (cm)                1.98340E+00 + or - 2.43286E-03
***
***   system nu bar                             2.60534E+00 + or - 4.54386E-04
***
***   k-effective satisfies the chi**2 test for normality at the 95 % level
***
***
*****
*****

```

**Fig. 45. KENO V.a final results table.**

For this example,  $k_{\text{eff}}$  is calculated as  $1.0226 \pm 0.0019$ , which is slightly above critical due to the use of 100%  $^{235}\text{U}$  instead of 93.7% as in Godiva.

### 3.5.2 Bare U(93.71) Cylinder

This example changes the material from pure  $^{235}\text{U}$  to uranium metal enriched to 93.71%  $^{235}\text{U}$ . Again the effective radius is 7.82 cm with an estimated critical height of 15.64 cm ( $H/D=1$ ). The geometry is unchanged from that shown in Fig. 28. The dimensions are derived using buckling conversion from the critical radius of the Godiva sphere (8.741 cm). For this problem, the uranium density is 18.742 g/cc.

*Core Material ( $\rho_{\text{mix}} = 18.742$  g/cc-mixture)*

U metal (93.71 percent  $^{235}\text{U}$  and 6.29 percent  $^{238}\text{U}$ )

The data entry is the same as for the first problem. The only change is in the materials. You can either create a new file or edit the one from before, saving it under a different name.

The following discussion assumes that you are editing the input from the previous case.

### 3.5.2.1 Material Input

For this example problem, we will again select **Compositions**. Select mixture 1 on the summary form and click **Edit**. This opens the **Basic Standard Composition** form with the data for mixture 1, U-235. Under **Composition Name** scroll down the menu and select **u**. This brings up a window to the right-labeled **Isotopic Distribution** that displays the default isotopic distribution of uranium (Fig. 46). Clicking on **Edit Selection** opens another window with the seven isotopes of uranium listed. We need to enter the isotopic distribution of the uranium (in weight percent) for the problem, which is 93.71 for **92235** ( $^{235}\text{U}$ ) and 6.29 for **92238** ( $^{238}\text{U}$ ) (see Fig. 47).

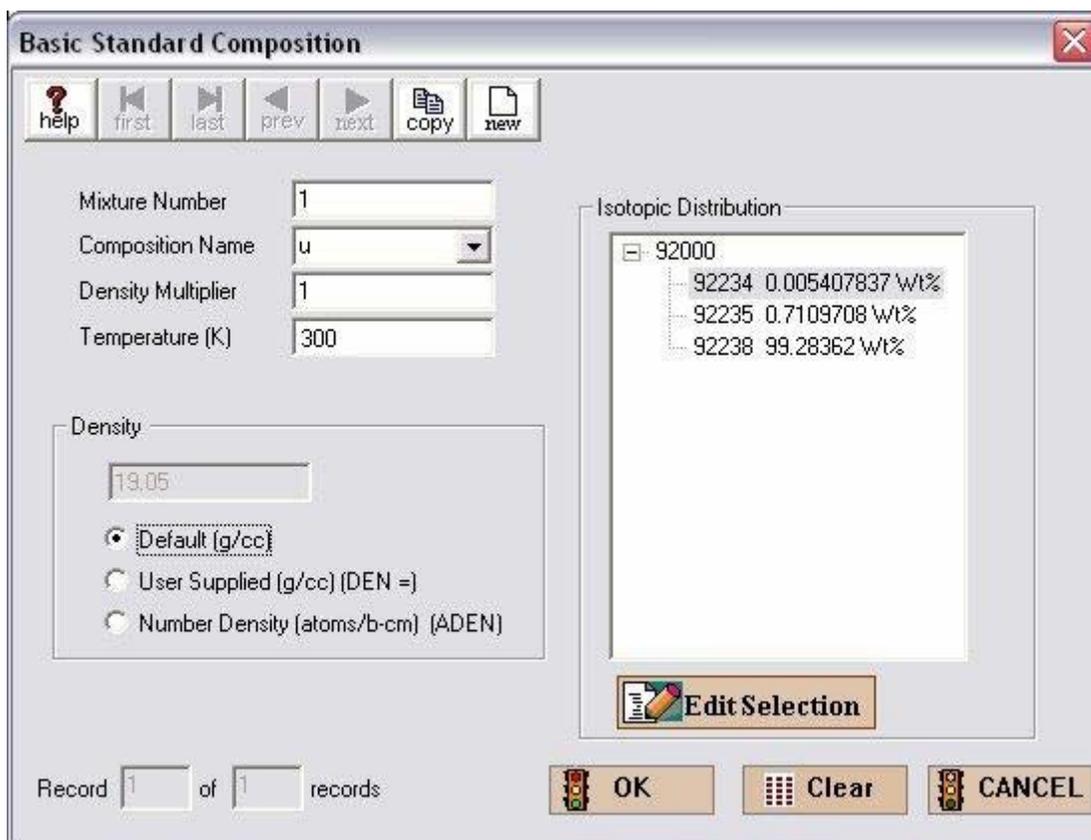
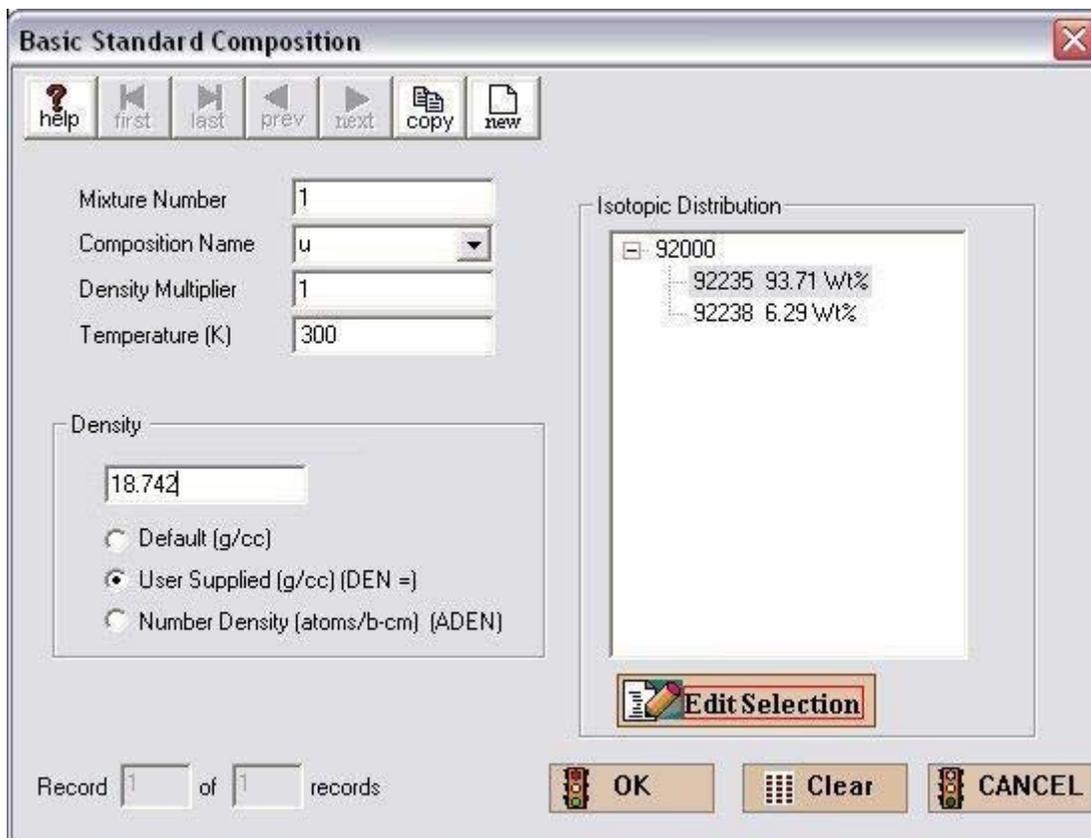


Fig. 46. Standard composition screen for isotopic distribution.



**Fig. 47. Isotopic distribution window.**

After you select **OK**, the composition box disappears and you can enter the density by selecting **User Supplied (g/cc)** and then entering the value 18.742 in the data entry box. The information should look like Fig. 48.



**Fig. 48. Material information for example 2.**

For this example,  $u$  is the only material, so select **OK** and then **Close**.

### 3.5.2.2 KENO V.a Input

This completes the information required for the second example. Select **File**, then **Save As**. For the filename, you need to use a different name than before, such as `bare_u_cyl`. After saving, click **Run**. Note that if the DOS window from the previous case is still open, the **Run** button will be deactivated. A DOS window will open and show the progress of the calculation. For this example,  $k_{\text{eff}}$  is calculated as  $0.9917 \pm 0.0020$ , which is close to critical as expected.

### 3.5.3 Bare U(93.71)O<sub>2</sub> Cylinder

This example changes the material from uranium metal to uranium dioxide while keeping the enrichment at 93.71% <sup>235</sup>U. The material change affects the geometry, so the new estimated critical radius is 12.8 cm with an estimated critical height of 25.6 cm (H/D=1). The core material has a density of 95% of the theoretical density of UO<sub>2</sub>; theoretical density is 10.96 g/cc.

*Core Material ( $\rho_{mix} = 95\%$  of theoretical density – 10.96 g/cc-mixture)*

U (93.71 percent <sup>235</sup>U and 6.29 percent <sup>238</sup>U)

The data entry is the same as for the first problem. Both the Materials and the Geometry will change. It is suggested that you create a new file for this problem. Enter the **General** information as for the previous two examples.

#### 3.5.3.1 Material Input

Select **Composition** and **Basic Composition**. The **Mixture Number** starts with 1. Under **Composition Name** scroll down the menu and select uo2. This displays a window to the right labeled **Isotopic Distribution**. Click on **Edit Selection** and enter the isotopic composition of the uranium (in weight percent) for the problem, which is 93.71 for 92235 and 6.29 for 92238. Then select **OK** and enter a density multiplier of 0.95. The theoretical density of UO<sub>2</sub> is listed in the density box as 10.96 g/cc, so the density multiplier will modify that to 0.95\*10.96 or 10.412 g/cc. The data for this problem should look like Fig. 49.

For this example, uo2 is the only material, so select **OK** and then **Close** the **Standard Basic Compositions** summary form. This completes the materials input data required for this example.

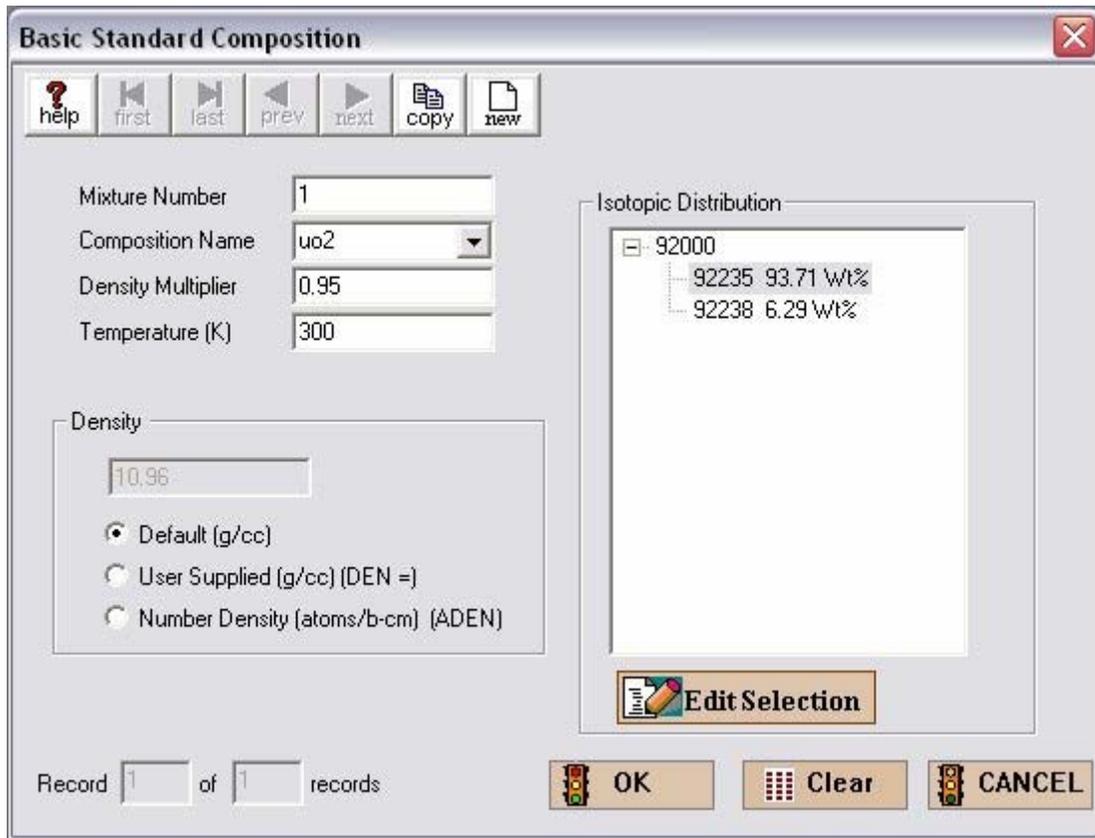


Fig. 49. Standard composition input for U(93.71)O<sub>2</sub>.

### 3.5.3.2 KENO V.a Input

Open the **Geometry** window. Enter a comment in the **COM=** box. Then click on the **Cylinder** button. For **Mixture** select 1 u from the pulldown menu. Then enter 12.8 for the **Radius**, 12.8 for **Top**, and -12.8 for **Bottom**. Click **OK** to close the Z cylinder form. Then click the **Global Unit** check box. This completes the information required for this example. **Close** the Geometry window and click **Run**. A DOS window opens and displays the progress of the calculation. For this example,  $k_{\text{eff}}$  is calculated as  $0.9874 \pm 0.0018$ , which is close to critical as expected.

### 3.5.4 Bare U(30.3)O<sub>2</sub>F<sub>2</sub> Cylinder

This example demonstrates one way of entering information for a fissile solution. The data are from p. 35 in LA-10860 for U(30.3)O<sub>2</sub>F<sub>2</sub> solution with H/<sup>235</sup>U ratio of 106 and a fissile density of 0.220 g-<sup>235</sup>U/cc. The information is given for an unreflected sphere with a critical volume of 20.0 liters. Using buckling conversion, a critical cylinder with H/D=1 has a critical radius of 15.225 cm with a critical height of 30.45 cm. GeeWiz has a special entry screen for fissile solutions, but you need the fuel density, the excess acid molarity, and the specific gravity of the solution. Because these parameters are not part of the data in LA-10860, we will use calculated atom densities for H, O, F, <sup>235</sup>U, and <sup>238</sup>U for entry in GeeWiz:

$$N_H = 5.97522 \times 10^{-2} \text{ atoms-H / b-cm}$$

$$N_O = 3.35605 \times 10^{-2} \text{ atoms-O / b-cm}$$

$$N_F = 3.6844 \times 10^{-3} \text{ atoms-F / b-cm}$$

$$N_{U235} = 5.637 \times 10^{-4} \text{ atoms-}^{235}\text{U / b-cm}$$

$$N_{U238} = 1.2802 \times 10^{-3} \text{ atoms-}^{238}\text{U / b-cm}$$

The data entry is the same as for the previous problems. We will concentrate on the Materials entries. Create a new file for this problem and enter the **General** information as previously.

#### 3.5.4.1 Material Input

For this problem, again select **Basic Composition**. As the materials are mixed together and you are entering atom densities, they will all be part of mixture number 1. You will enter five materials (u-235, u-238, h, o, and f) for mixture 1. The **Mixture Number** starts with 1. Under **Composition Name** scroll down the menu and select u-235. In the density boxes below, select **Number Density (atoms/b-cm)**. Enter the <sup>235</sup>U atom density of  $5.637 \times 10^{-4}$  as 5.637e-4. (You can also enter the density as 0.0005637.). The form should look like Fig. 50.

Note that GeeWiz automatically updates the **Mixture Number** when you go to a new composition, so you will need to reset it back to 1 for the u-238, h, o, and f entries. For each of these materials, enter the atom density as given above. Then select **OK**. This completes the materials input data required for this example. The **Standard Basic Compositions** summary form should look like Fig. 51.



### 3.5.4.2 KENO V.a Input

Open the **Geometry** screen. Enter a comment in the **COM=** field. Then click on the **cylinder** button. For **Mixture** select 1 u-235, u-238, f, o, h from the pulldown menu. Then enter 15.225 for the **Radius**, 15.225 for **Top**, and -15.225 for **Bottom**. Click **OK** and then click the **Global Unit** check box. This completes the **Geometry** information. This completes the information required for the third example. Click **Run**, a DOS window opens and shows the progress of the analysis. For this example,  $k_{\text{eff}}$  (skipping three generations) is calculated as  $0.9958 \pm 0.0024$ , which is quite close to critical as expected.

## 3.6 SUMMARY

This section has helped you to:

- Define the different criticality sequences used in SCALE.
- Describe the cross-section libraries available for criticality analyses.
- Use the GeeWiz user interface to provide data on elements, isotopes, compounds, and solutions.
- Interpret basic output information from a SCALE / KENO V.a analysis.

Now that you have spent time with the Material Input, we will proceed to more complicated geometries, such as reflected systems and lattices.

## 4. GEOMETRY INPUT

In the previous section you modeled a number of simple geometries with various material compositions. You used the GeeWiz user interface to provide data on elements, isotopes, compounds, and solutions. This section presents an explanation of the commands used for simple geometries such as cylinders and spheres and for more complicated geometries such as reflected systems and lattices.

### 4.1 WHAT YOU WILL BE ABLE TO DO

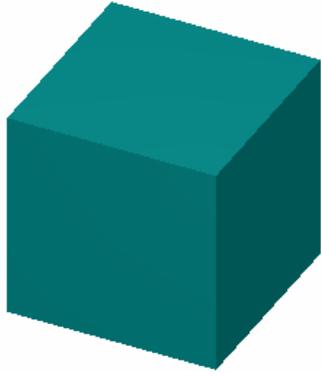
- Use GeeWiz to describe the basic shapes (sphere, cylinder, cube, cuboid).
- Understand how units are created (including nesting of shapes).
- Locate and change the location of the origin for shapes and units.
- Create simple arrays consisting of a single unit.
- Create arrays with multiple units of nominally different sizes.

### 4.2 BASIC GEOMETRY SHAPES

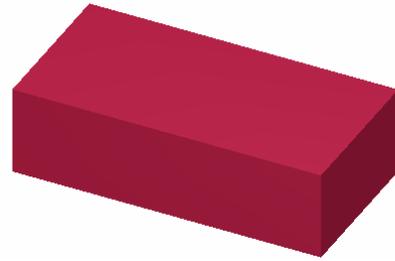
SCALE/KENO V.a uses a set of basic shapes to build the geometry models. You have used GeeWiz to enter data on cylinders in Sect. 3. This and the other basic shapes are described in Table 3 and illustrated in Fig. 52.

**Table 3. Basic shapes**

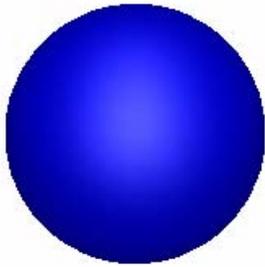
Keyword	Description
CUBE	Box with equal X, Y, and Z dimensions
CUBOID	Box or rectangular parallelepiped; X, Y, and Z dimensions are not necessarily equal
SPHERE	Sphere
CYLINDER	Cylinder that has its length along the X, Y, or Z axis
HEMISPHERE	Partial sphere with a flat surface parallel to the X, Y, or Z axis
HEMICYL	Cylindrical segment whose axis is in the X, Y, or Z direction with a flat surface parallel to the cylinder axis



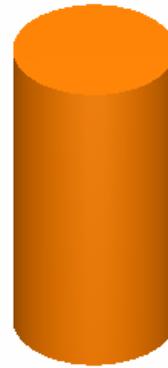
Cube



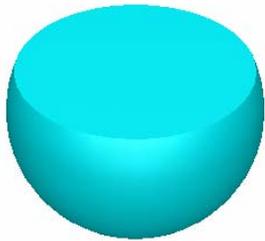
Cuboid



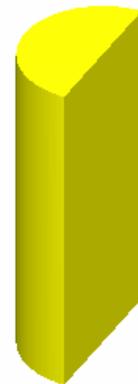
Sphere



Cylinder



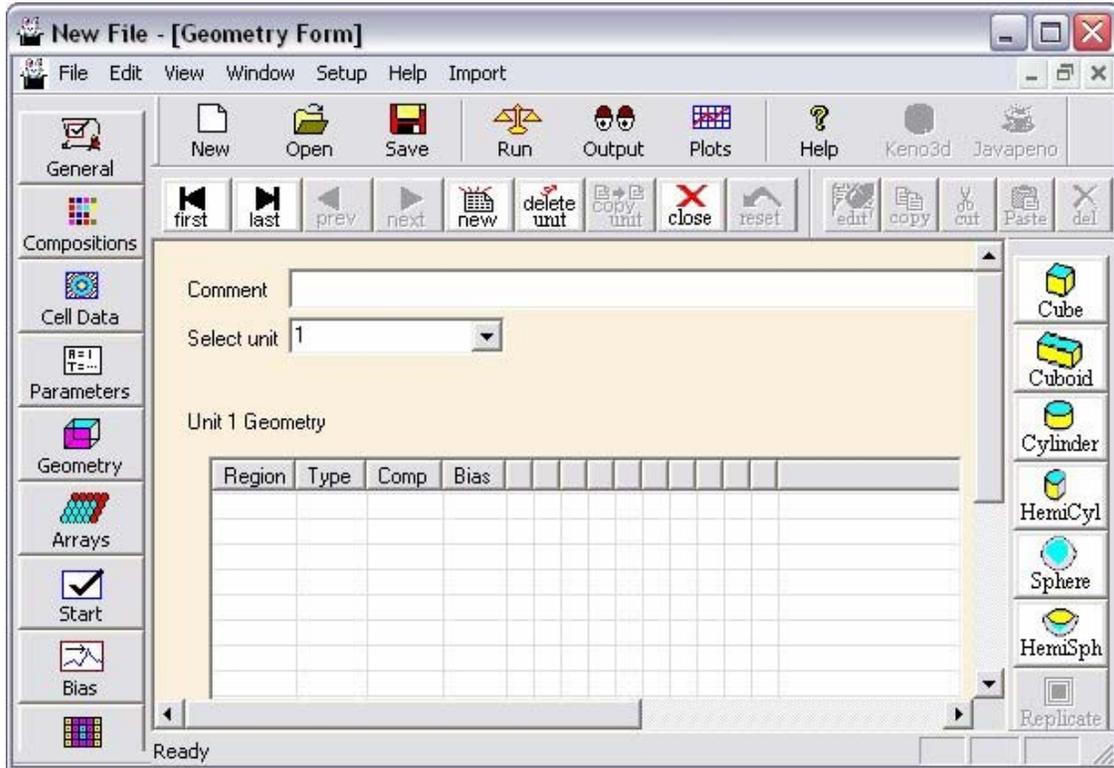
Hemisphere



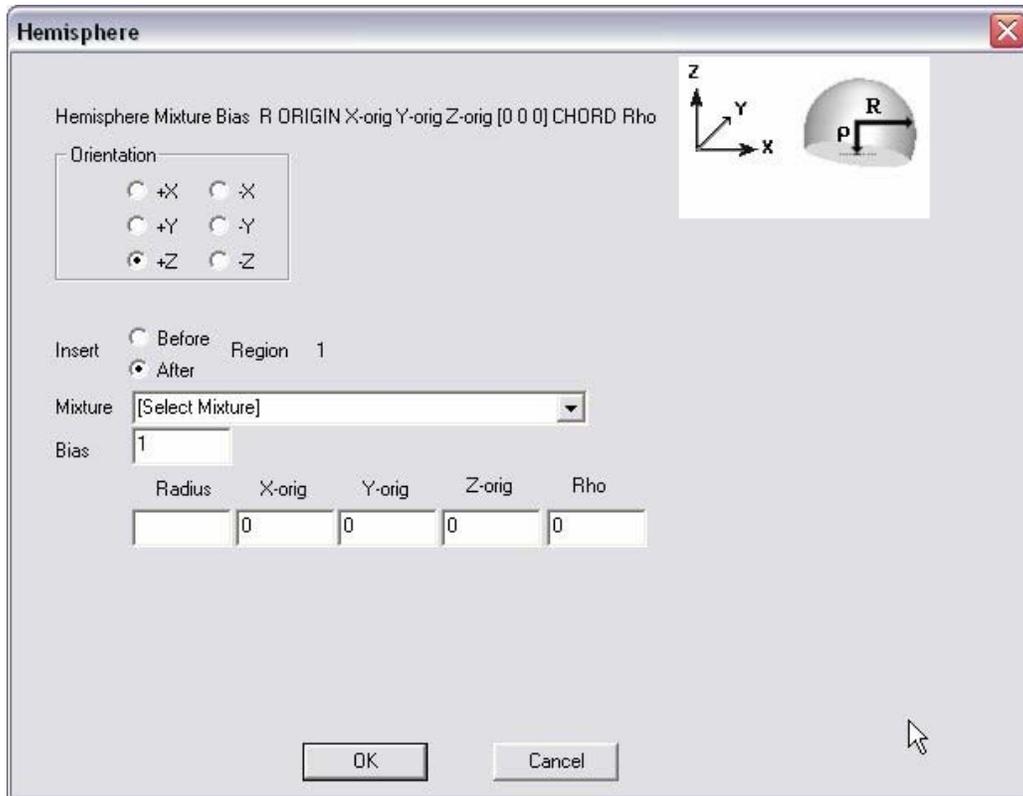
Hemicylinder

**Fig. 52. KENO V.a basic geometry shapes.**

These six shapes are the basic geometry options in KENO V.a and are shown on the right side of the **Geometry** input form (Fig. 53). Each shape has a set of quantitative information needed to describe its size and location. Selection of a geometry option will bring up the associated shape input form where the appropriate information is entered. Fig. 54 shows the input form for a hemisphere; the other input forms ask for similar information. A description of the options for each basic shape can be found in the SCALE manual [Vol. 2, Sect. F11.4.4].



**Fig. 53. Geometry form.**



**Fig. 54. Hemisphere input form.**

The description of a cylinder requires the **Radius**, **Top** coordinate and **Bottom** coordinate data as a minimum. For a cuboid, the **+X**, **-X**, **+Y**, **-Y**, **+Z**, and **-Z** data are necessary to specify the shape. Because a cube is a cuboid with equal sides, only **+X** and **-X** need to be specified for this shape. Finally, for a sphere, only the **Radius** is required. For most of these shapes, additional information may be entered to locate the origin or to describe the plane surface in a hemicylinder or hemisphere shape.

#### **4.2.1 Simple Cylinder Examples**

To understand how shape parameters are entered using GeeWiz, some example problems will be used. These problems are based on the bare metal cylinder example from Sect. 3. Various cylindrical configurations will be examined.

## 4.2.2 Bare Metal Cylinder Along Z-Axis

Locating the bare metal cylinder centered on the Z-axis (Fig. 55) is identical to the first example problem in Sect. 3. A summary of the input information follows.

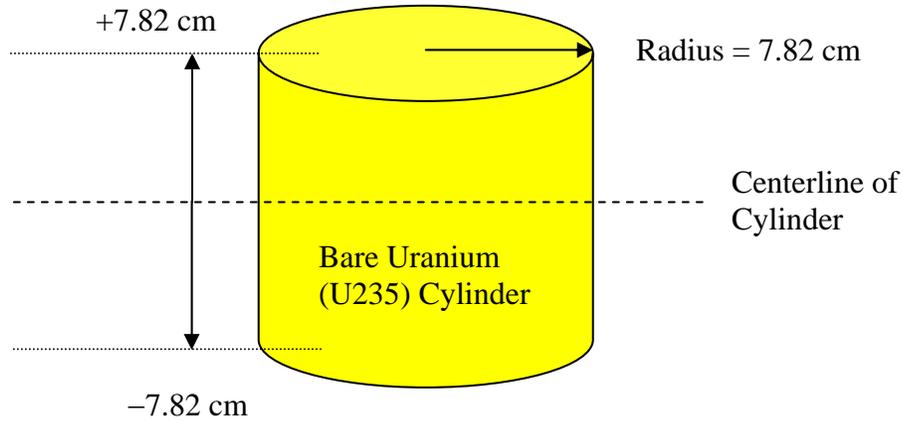
*Core Material* ( $\rho_{mix} = 18.742$  g/cc-mixture)

U metal (100 percent  $^{235}\text{U}$ )

Configuration 1.     *Bare Uranium Cylinder along Z-axis*

Radius            = 7.82 cm

Height            =  $\pm 7.82$  cm



**Fig. 55. Configuration 1 geometry.**

Based on the knowledge gained from completing Sect. 3 of the primer, you should be able to open a new file and enter the title, cross section, and material information. Note that all problems in this chapter use the 238-group ENDF/B-V library.

#### 4.2.2.1 KENO V.a Input

With this simple geometry, only a few entries are needed to complete the KENO geometry input form. Select **Geometry** from the left toolbar to bring up the geometry summary form shown in Fig. 53. To enter geometry information, select the appropriate geometry from the right toolbar. For this problem, that would be **cylinder**. This brings up the **Z-cylinder** input form.

For **Mixture** select 1 u-235 from the pulldown menu. Then enter 7.82 for the **Radius**, 7.82 for the **Top**, and -7.82 for the **Bottom**. This completes the **Z-Cylinder** information; it should look like Fig. 56.

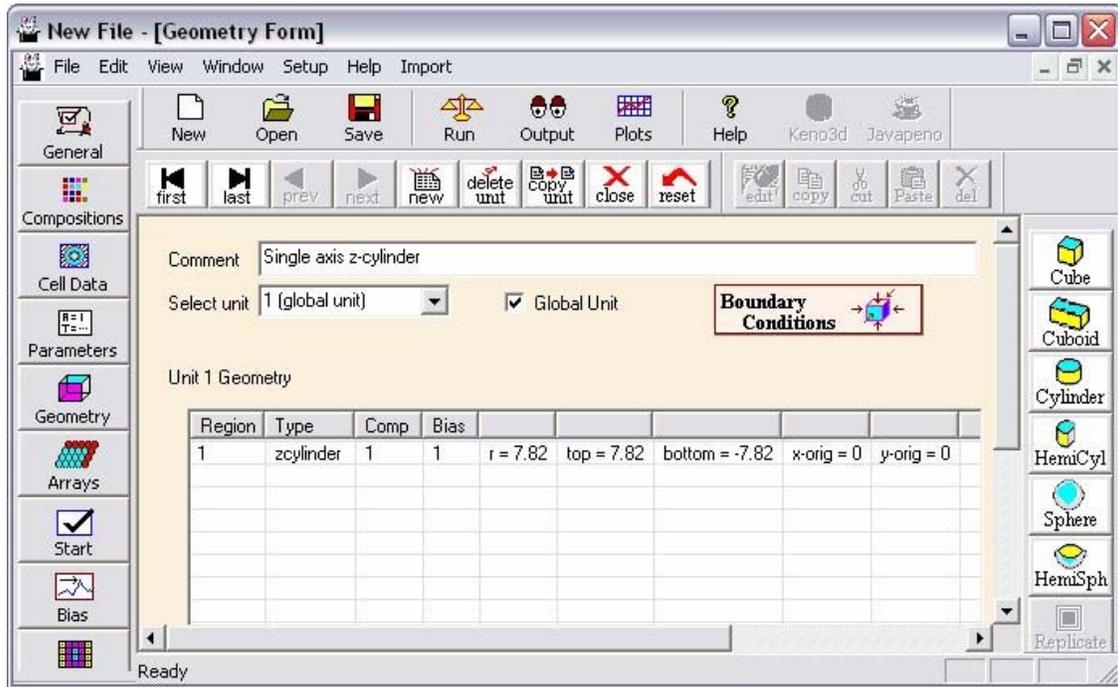
The screenshot shows the 'Z Cylinder' dialog box with the following settings:

- Orientation:** Z (selected)
- Insert:** After (selected), Region 1
- Mixture:** 1 u-235
- Bias:** 1
- Radius:** 7.82
- Z-Max:** 7.82
- Z-Min:** -7.82
- X-orig:** 0
- Y-orig:** 0

The diagram on the right illustrates a cylinder in a 3D coordinate system (x, y, z). The cylinder's top is at Zt, its bottom is at Zb, and its radius is R.

Fig. 56. Z-cylinder data for example 1.

Click on **OK**, and that brings you back to the Geometry Summary form. Enter a comment in the **COM=** box, such as `single z-axis cylinder`, and check the box beside **Global Unit** by clicking on the box. As stated earlier, the global unit in KENO is the final unit that defines the entire system to be analyzed. The geometry summary form should look like Fig. 57.



**Fig. 57. Geometry for Z-axis cylinder.**

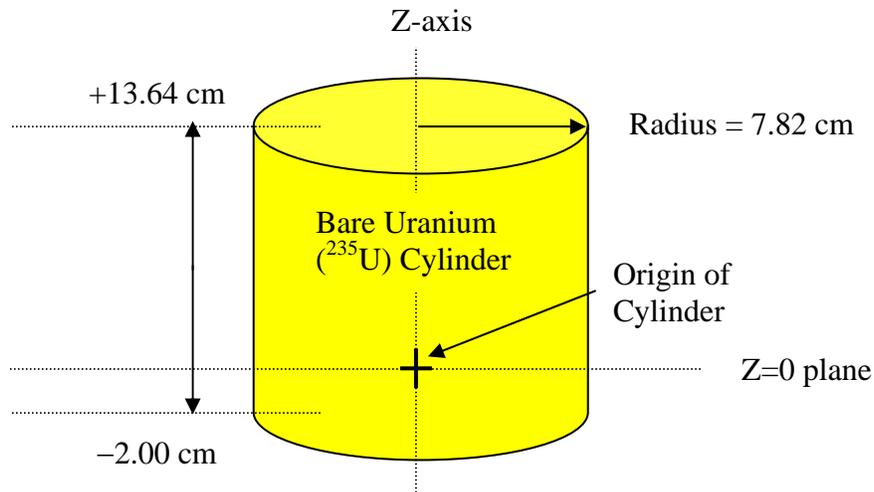
Selecting **Close** from the menu bar saves this information and takes you back to the main GeeWiz screen. This completes the information required for this example. Select **Run**. GeeWiz opens a DOS window that shows the progress of the calculation.

#### 4.2.2.2 Basic Output

To make sure the input is correct, check the value of  $k_{\text{eff}}$ . As in the first example of the previous section, it should be approximately  $1.0226 \pm 0.0019$ . Once again, the  $k_{\text{eff}}$  is above critical, as we modeled a pure  $^{235}\text{U}$  system rather than the critical Godiva, which was a U(93.7) system.

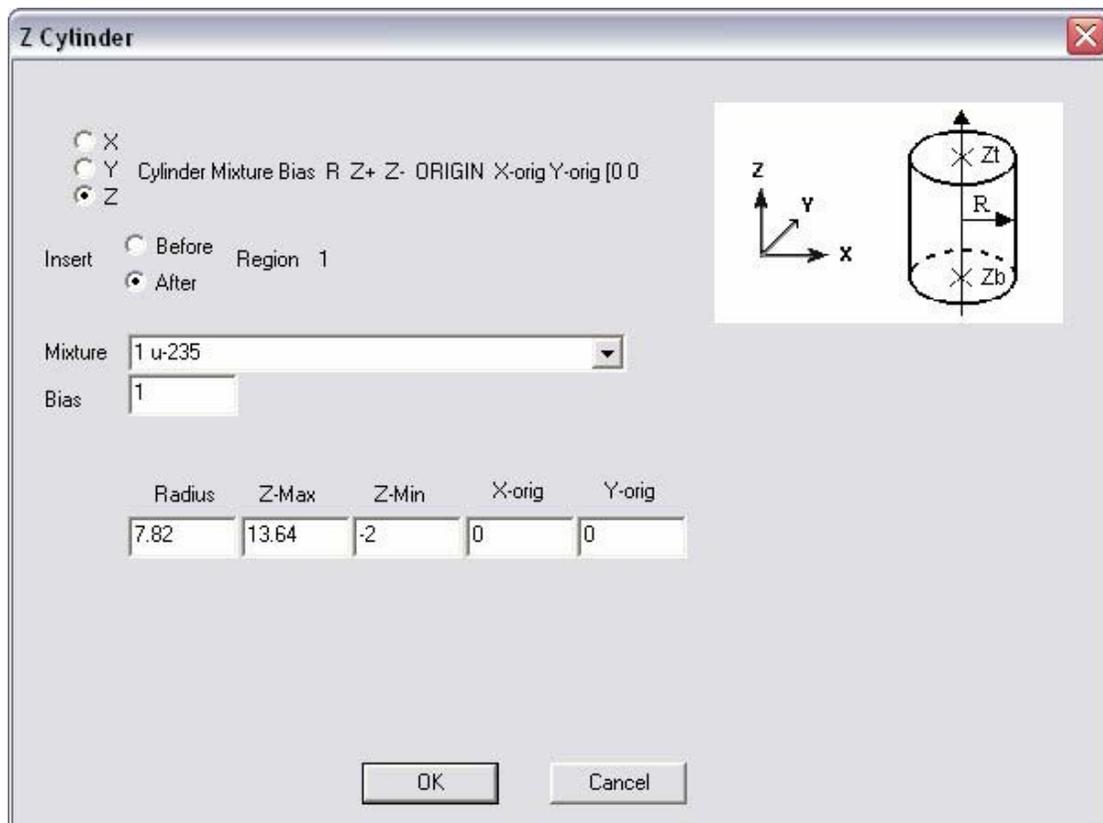
### 4.2.3 Bare Metal Cylinder Along Z-Axis With Origin Located 2 cm Above Cylinder Base

There are some fissile systems you will encounter where you want to locate the cylinder origin at a point other than the center of the cylinder. Moving the origin up and down along the Z-axis is done by changing the values of **Top** and **Bottom**. For example, suppose we want to locate the origin at a point 2 cm above the base of the cylinder (see Fig. 58).



**Fig. 58. Configuration 2 geometry.**

Using the input file from configuration 1, you would only need to change the height parameters on the **Geometry** form. To do this select **Geometry**, which brings up the geometry summary form. This has one region. Click on the region and then select **Edit**. This brings up the Z cylinder input form with the data for configuration 1. Change the **Top** to 13.64 and the **Bottom** to -2 so the screen looks like Fig. 59.

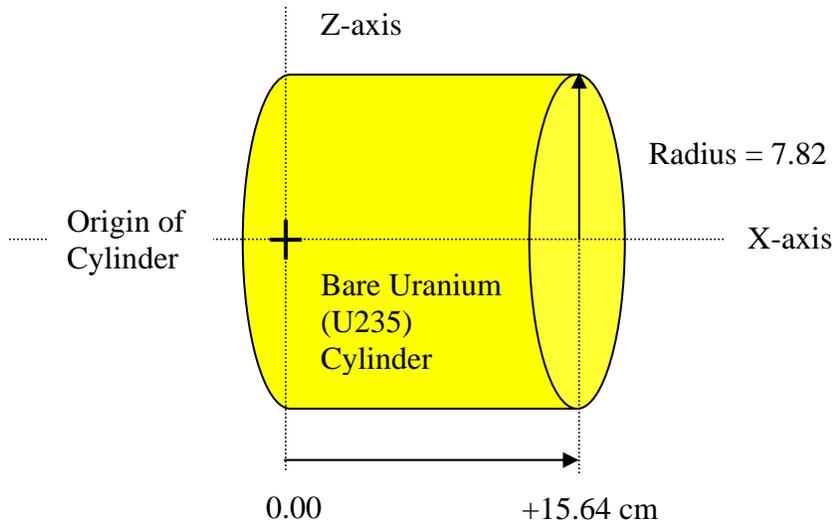


**Fig. 59. Geometry input for configuration 2.**

Save the changes in a new input file and execute SCALE. As no changes were made to the physical system, the  $k_{\text{eff}}$  value for this run should be within two standard deviations of that from the previous run. The  $k_{\text{eff}}$  calculated is  $1.0226 \pm 0.0019$ , which meets this criterion.

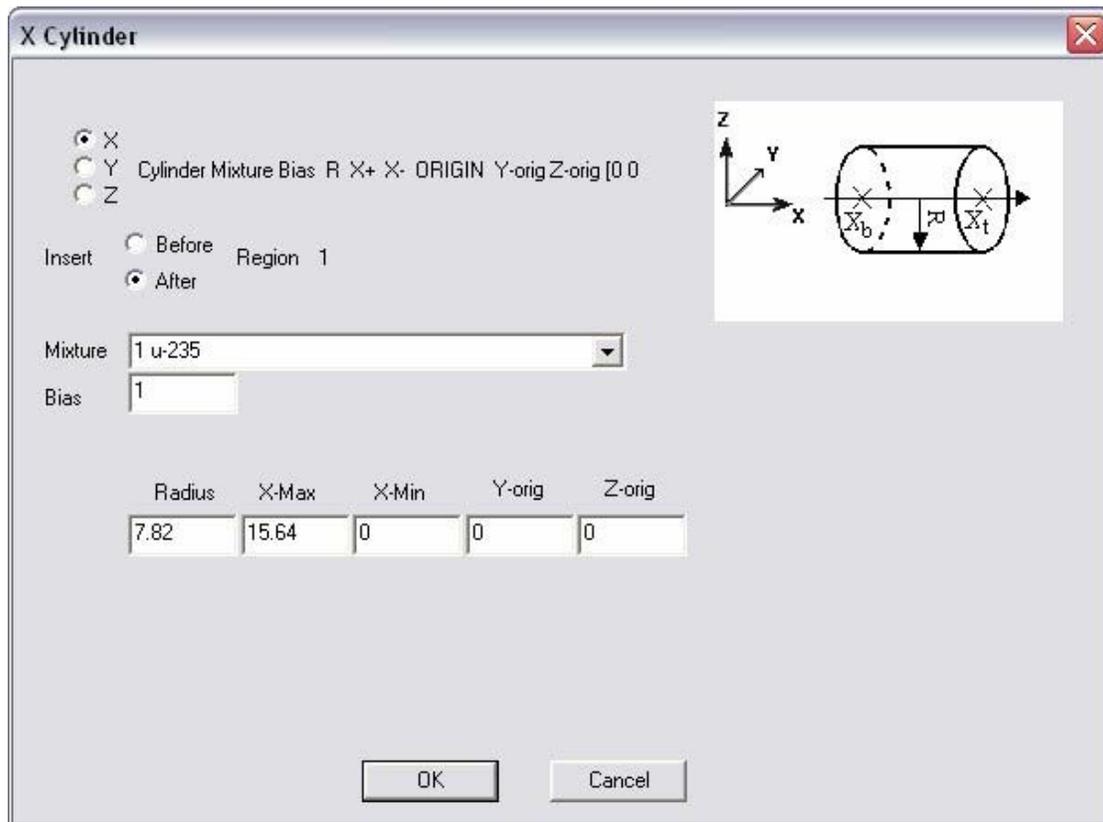
#### 4.2.4 Bare Metal Cylinder Along X-Axis With Origin Located at Cylinder Base

The next problem is for a horizontal cylinder with the origin located at the base as in Fig. 60. We need to change to an X-cylinder and alter the values of **Top** and **Bottom** to locate the origin at the desired point. (**NOTE:** When entering **Top** and **Bottom** values, the **Bottom** value can be positive, negative, or zero, but it must be less than the **Top** value.)



**Fig. 60. Configuration 3 geometry.**

Using the configuration 1 input file, you need to change the cylinder orientation and height parameters. From the geometry summary screen, select the first region of Unit 1 and click **Edit**. The **Z-cylinder** input form appears. Select **X** to change to an X-cylinder. Change Top to 15.64 and a Bottom to 0.00 as shown in Fig. 61.



**Fig. 61. KENO geometry input for configuration 3 geometry.**

Save the changes in a new input file and execute SCALE. Again, as no changes were made to the physical system, the  $k_{\text{eff}}$  value for this run should be within two standard deviations of those from the previous runs. The  $k_{\text{eff}}$  calculated is  $1.0184 \pm 0.0020$ , which is within approximately two standard deviations of the previous results.

The same approach applies to locating the origin of cubes and cuboids. You enter values of the maximum and minimum parameters to locate the origin on each axis. For spheres and cylinders, the concept is the same, but you enter the coordinates of the origin of the sphere or cylinder.

### 4.3 KENO V.A GEOMETRY RULES

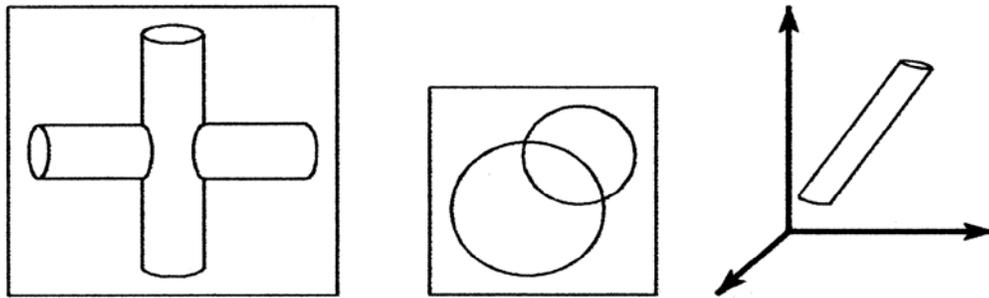
There are seven basic rules that guide the geometry input to SCALE/KENO V.a.

1. *Volumes are built in sections called units.* Each unit is independent of all other units and has its own coordinate system.
2. Units are built from the inside out using regions. Regions are made using the basic KENO geometry types. Within a unit, a region must fully enclose all previously defined regions.
3. Regions may share boundaries but may not intersect.
4. All volumes are oriented along a major axis. Volumes may not be rotated.
5. *A hole is used to place a unit within a region in a different unit.* The hole must be completely contained within the region. As many holes as required may be placed in a unit as long as they do not intersect other holes or regions.
6. *An ARRAY is an ordered stack of units.* The touching faces of adjacent units in an ARRAY must be the same size. Only one ARRAY may be placed directly in a unit. Additional ARRAYS may be placed in units using holes.
7. A GLOBAL unit or array, which defines the outermost boundary of the problem, should be specified for each problem. If a GLOBAL unit or array is not specified, the code will specify one that may not be what the user intends.

### 4.4 GEOMETRIC ARRANGEMENTS

Geometric arrangements in KENO V.a are achieved in a manner similar to using a child's building blocks. Each building block is called a unit. Units are constructed of combinations of basic shapes (i.e., cubes, cuboids, cylinders, spheres, hemispheres, and hemicylinders). These shapes can be placed anywhere within a unit as long as they are oriented along the coordinate system of the unit and do not intersect other regions (i.e., shapes). This means, for example, that a cylinder must have its axis parallel to one of the coordinate axes, while a rectangular parallelepiped (cuboid) must have its faces perpendicular to the three coordinate axes. The most stringent KENO V.a geometry restriction is that none of the options allow geometry regions to intersect. Fig. 62 shows some situations that are not allowed.

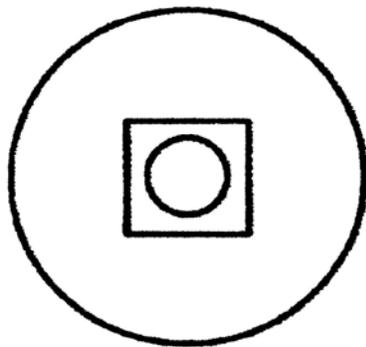
Unless special options (e.g., holes — discussed in Sect. 5) are invoked, each geometric region in a unit must completely enclose each interior region. However, regions can touch at points of tangency and share faces. See Fig. 63 for examples of allowable situations.



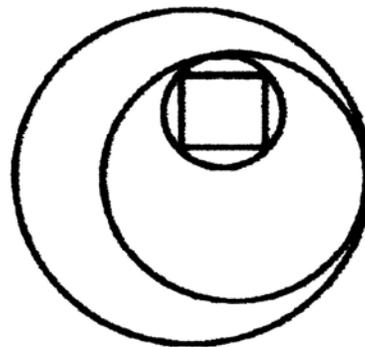
**INTERSECTING REGIONS    INTERSECTING REGIONS    ROTATED REGION**

**Fig. 62. Examples of geometry not allowed in KENO V.a.**

**ORNL-DWG 83-14791**



**REGIONS ENCOMPASSING  
INTERIOR REGIONS**



**REGIONS ENCOMPASSING  
REGIONS AND TOUCHING**

**Fig. 63. Examples of correct KENO V.a units.**

A unit can be thought of as a container that encloses a number of shapes. In its simplest form, a unit encloses one or more basic shapes with the smallest shape completely enclosed by the next smallest and so on. This is the way to model reflected single units or containers with fissile solutions. It is important to note that the origin of a unit is set by the origin of the first, innermost shape. Also, note that the shapes must be entered on the geometry screen from smallest to largest.

## 4.5 NESTED REGIONS IN A UNIT

To illustrate how to enter KENO geometry information for nested regions in a unit via GeeWiz, two example problems will be used. The first is a reflected cylinder of Pu metal, and the second is a sphere inside a cylinder inside a cube.

### 4.5.1 Reflected Pu Metal Cylinder

The reflected Pu metal cylinder problem comes from LA-10860, pg. 102. The fissile material is Pu metal (density = 15.44 g/cc) with a maximum of 5.0 wt %  $^{240}\text{Pu}$ . The core has a diameter of 5.72 cm with an H/D = 7.16, or a critical height of 40.96 cm. Surrounding the core is a graphite reflector (density = 1.60 g/cc) with a thickness of 17.78 cm in both the radial and axial directions (see Fig. 64).

*Core Material ( $\rho_{mix} = 15.44$  g/cc-mixture)*

Pu metal (95 wt %  $^{239}\text{Pu}$ , 5 wt %  $^{240}\text{Pu}$ )

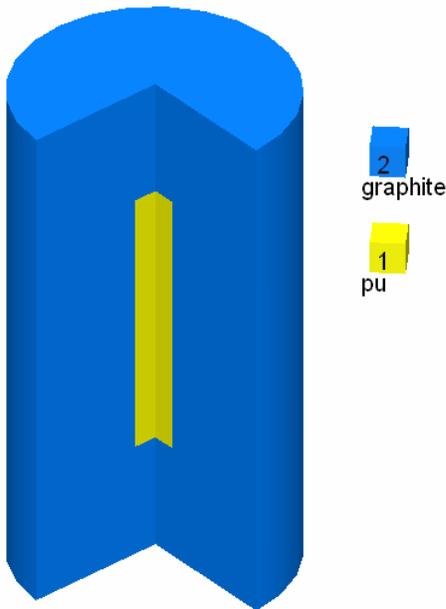
Core Radius = 2.86 cm

Core Height =  $\pm$  20.48 cm

*Reflector Material ( $\rho = 1.60$  g/cc-mixture)*

Graphite

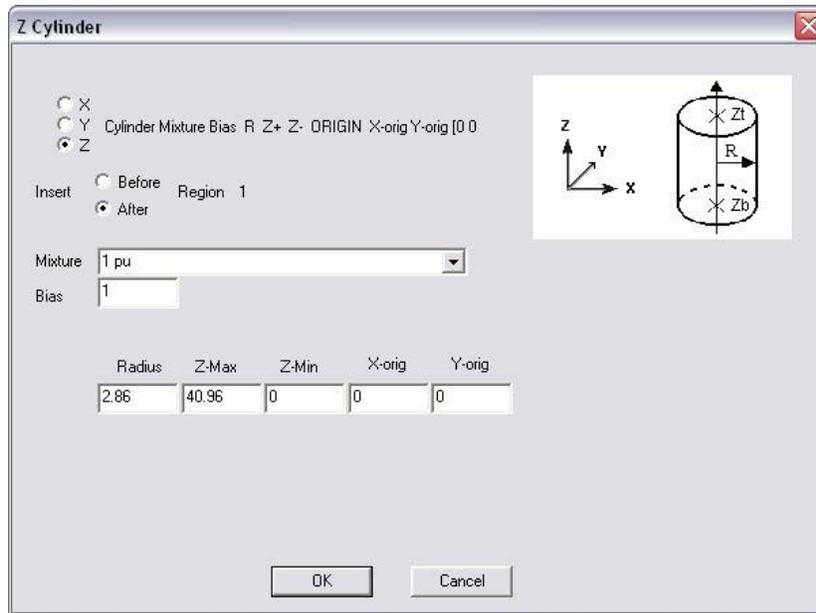
Reflector Thickness = 17.78 cm



**Fig. 64. Reflected Pu metal cylinder geometry.**

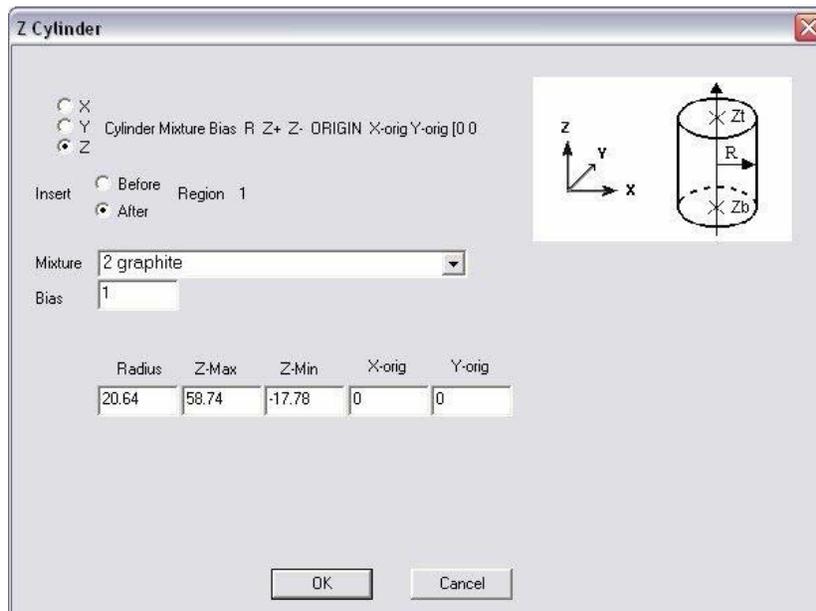
Based on the knowledge gained from completing Sect. 3 of the primer, you should be able to open a new file, enter the title, cross section, and material information. Remember to specify the isotopic composition for material 1 with 95 wt %  $^{239}\text{Pu}$  and 5 wt %  $^{240}\text{Pu}$  and a plutonium density of 15.44 g/cc.

For this geometry, there will be two shapes (or regions) in one unit, and that unit will be the Global Unit for the problem. First, we will describe the inner cylinder containing the plutonium and then the outer cylinder containing graphite. These are nested regions, so they obey KENO V.a geometry rules 1 and 2. Open the **Geometry** input form. Enter a comment in the **COM=** box and then select **Cylinder** from the geometry buttons on the right. This brings up the Z-Cylinder input form with a default orientation along the Z-axis. For **Mixture** select 1 pu from the pulldown menu. Then enter 2.86 for the **Radius**, 40.96 for **Top**, and 0.0 for **Bottom**. This puts the origin at the bottom center of the core cylinder. This is now the origin for the unit and for all other shapes in the unit. This geometry screen for the core should look like Fig. 65. Then click **OK**. Notice that after entering the first region, the geometry screen now has a box for global unit. Check this box to make this the global unit for this analysis.



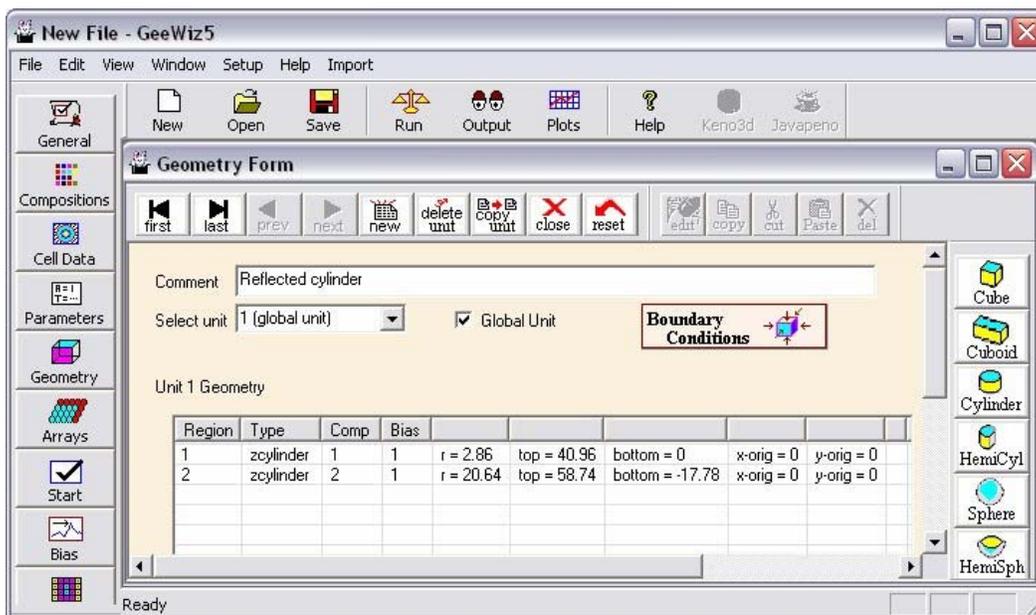
**Fig. 65. Geometry description for region 1.**

To enter the data for the reflector (Region 2), select the **Cylinder** button on the right. (**NOTE:** Each geometry shape is a new region in the unit.) On the Z-Cylinder input form, select 2 c-graphite from the **Mixture** pulldown menu. Then enter 20.64 ( $= 2.86 + 17.78$ ) for the **Radius**, 58.74 ( $= 40.96 + 17.78$ ) for **Top**, and -17.78 ( $= 0.00 - 17.78$ ) for **Bottom**. The **Geometry** input form should look like Fig. 66. Then click **OK**.



**Fig. 66. Geometry description for region 2.**

This completes the geometry input (see Fig. 67).

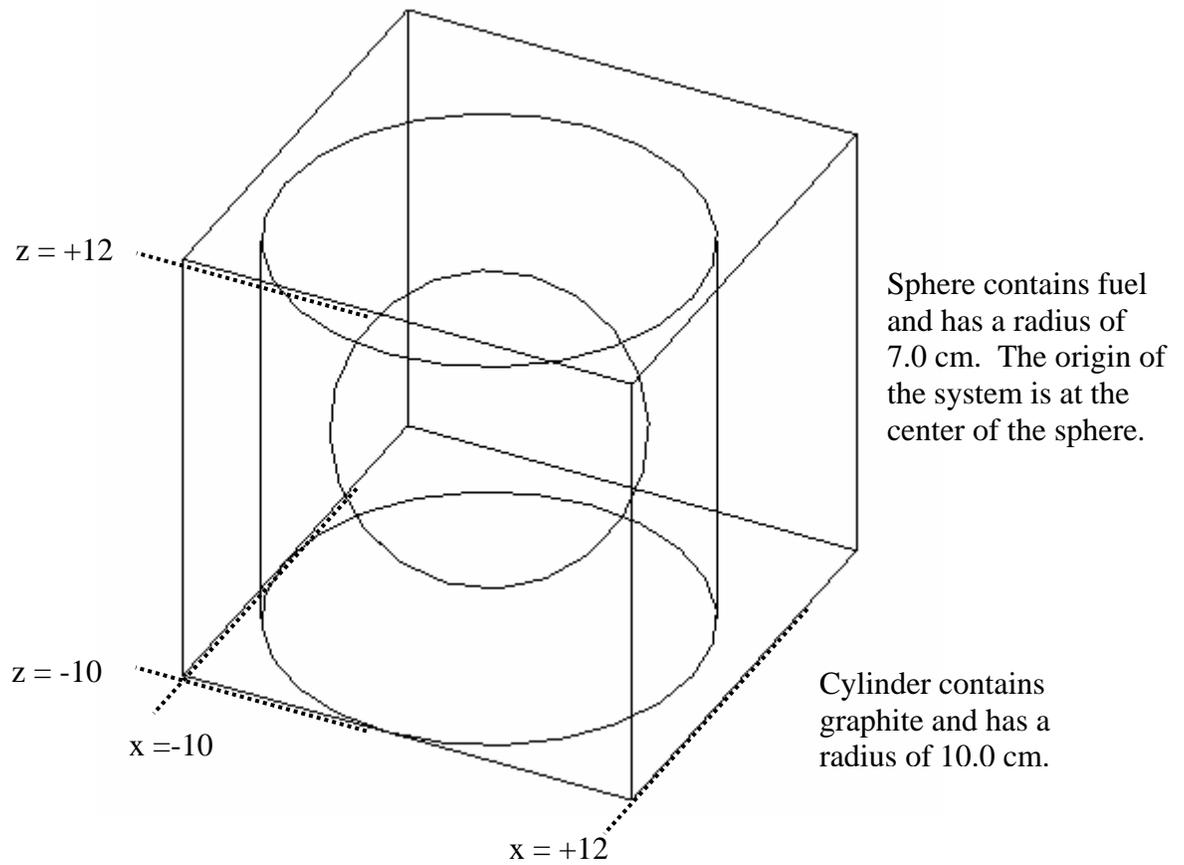


**Fig. 67. KENO geometry input for reflected Pu cylinder.**

Save the changes in a new input file and execute SCALE. As this is a critical experiment, the calculated  $k_{\text{eff}}$  value for this run would be expected to be close to 1.0. However, the calculated  $k_{\text{eff}}$  value is  $0.9736 \pm 0.0019$ , which is more than 2% low. These experiments all seem to calculate low, which may be why they are not included in the ICSBEP benchmark set.

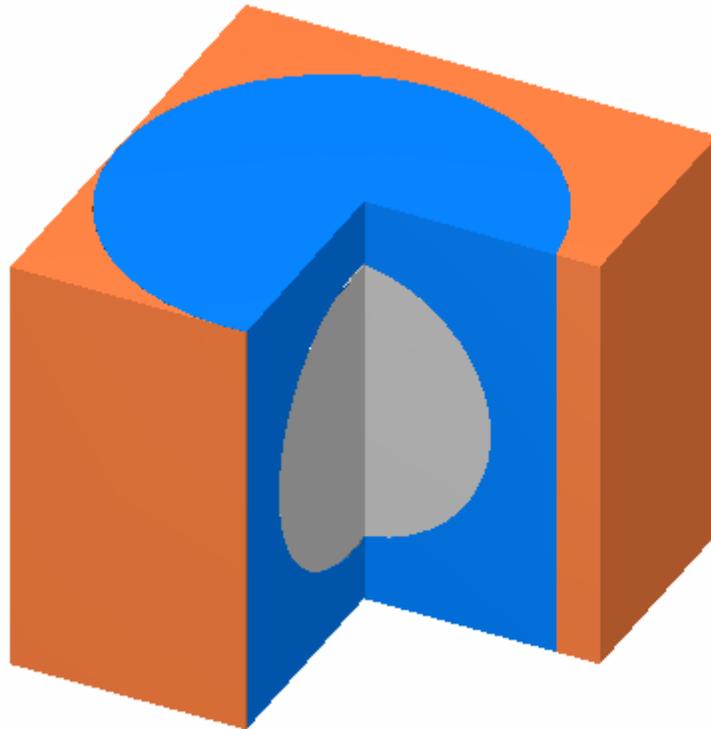
#### 4.5.2 $^{235}\text{U}$ Sphere With Graphite and Water Reflectors

This problem consists of a metal  $^{235}\text{U}$  sphere inside a graphite cylinder inside a cube of water. The centers of the sphere and cylinder are offset such that the outside edge of the cylinder touches two of the outside edges of the cube (see Fig. 68). This is consistent with KENO V.a geometry rule 3, which indicates regions may share boundaries but may not intersect. The materials are  $^{235}\text{U}$  metal (density = 18.74 g/cc), graphite (density = 1.65 g/cc) and water (default density of 0.9982 g/cc). The  $^{235}\text{U}$  sphere radius is 7.0 cm; the graphite cylinder has a radius of 10 cm and a height of 20 cm. The water cube surrounding the cylinder is 22 cm on a side. The bottom of the cylinder is coincident with the bottom of the cube.



**Fig. 68.**  $^{235}\text{U}$  sphere surrounded by graphite and water.

A cutaway view of the geometry is shown in Fig. 69. The top 3 cm have been removed from the view to be able to see the cylinder inside the box. Note that the graphite cylinder touches the water cube along the front edge and along the left edge. Also note that the bottom of the cylinder is coincident with the bottom of the cube.

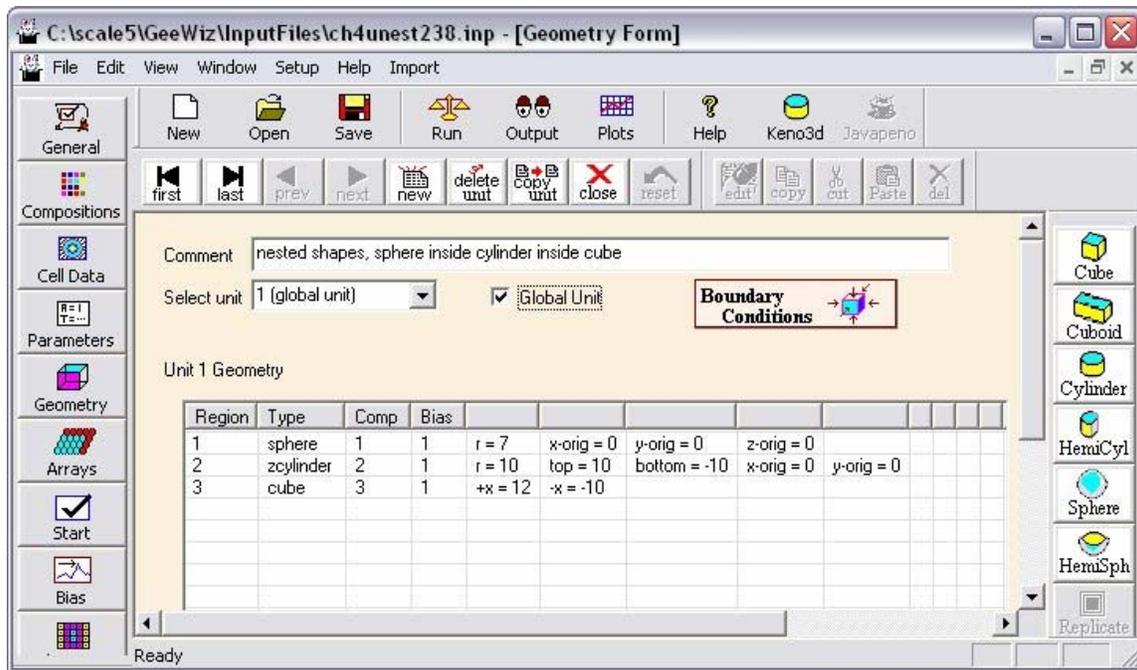


**Fig. 69. Cutaway view of  $^{235}\text{U}$  sphere inside graphite and water.**

Using your knowledge from previous sections, you should be able to open a new file and enter the title, cross section, and material information for the three materials.

For this geometry, there will be three regions in one unit, and that unit will be the global unit for the problem. First, we will describe the sphere containing the uranium, then the cylinder containing the graphite, and finally the outer cube containing water. These are nested regions and are entered like those in the previous example. Select the **Geometry** button on the left, and enter a comment in the **COM=** box. Then select the **sphere** button from the right. For **Mixture** select 1 u-235 from the pulldown menu, and then enter 7.0 for **Radius**. This puts the origin at the sphere center; this is now the origin for the unit and for all other shapes in the unit. Then select **OK**, which takes you back to the geometry summary screen. Now check the **Global Unit** box. To enter the data for the graphite reflector, select the cylinder button from the right. For **Mixture** select 2 c-graphite from the pulldown menu. Then enter 10 for the **Radius**, 10 for **Top**, and -10 for the **Bottom**. This creates a cylinder centered around the sphere. When you are done entering the information, select **OK**. To enter the data for the outside water reflector, select the cube button and for **Mixture** select 3 h2o from the pulldown menu. The cube is slightly off center from the cylinder and sphere, so entering 12 for the **+X**, and -10 for the **-X** will create a cube with three sides touching the cylinder and

with the other three sides 2 cm beyond the cylinder. Because the cube data are entered as a single set of positions, which are then replicated for all three axes, the touching sides will either be  $-X$  and  $-Y$ , or  $+X$  and  $+Y$ . If you need to change this and have  $-X$  and  $+Y$ , (or some other combination), then you would need to choose **Cuboid** instead of **Cube**. All six parameters are entered for a **Cuboid**, so you can position it in any location. This completes the geometry input (see Fig. 70). Save the changes in a new input file. You can view the geometry by clicking on the **KENO3D** toolbar button. For more information on how to use KENO3D, refer to Sect. 8.3.



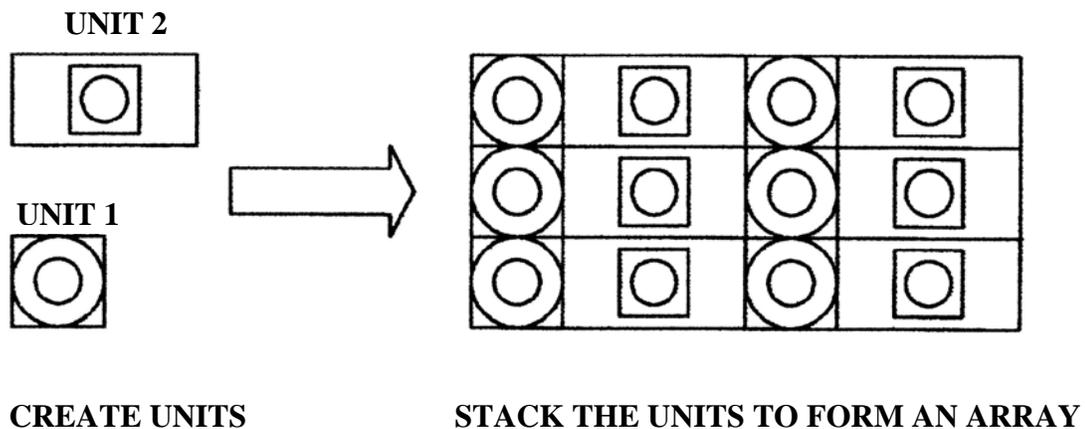
**Fig. 70. KENO geometry input for  $^{235}\text{U}$  sphere in graphite and water.**

Click **Run** to execute SCALE. The calculated  $k_{\text{eff}}$  is  $0.9992 \pm 0.0018$ .

## 4.6 ARRAYS

An array or lattice is constructed by stacking the units. Each unit in an array or lattice has its own coordinate system; however, all coordinate systems in all units must have the same orientation. All geometry data used in a problem are correlated to the absolute coordinate system by specifying a global unit or a global array.

Lattices or arrays are created by stacking units that have a rectangular parallelepiped (CUBE or CUBOID shape) outer region. The dimensions of adjacent faces of adjacent units stacked in this manner must match exactly. See Fig. 71 for a typical example.



**Fig. 71. Example of array construction.**

The ARRAY option is provided to allow placing an array or lattice within a unit. Only one array can be placed directly in a unit. However, multiple arrays can be placed within a unit by using holes as described in Sect. 5. Arrays of dissimilar arrays can be created by stacking units that contain arrays (a.k.a., “arrays of arrays”). See Fig. 72 for an example of an array composed of units containing holes and arrays.

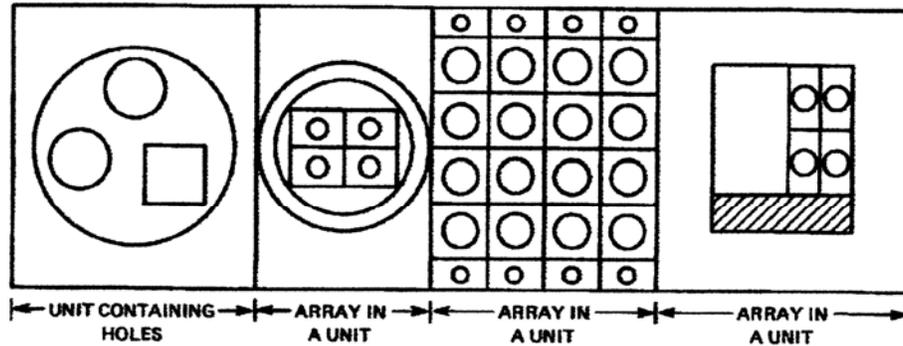


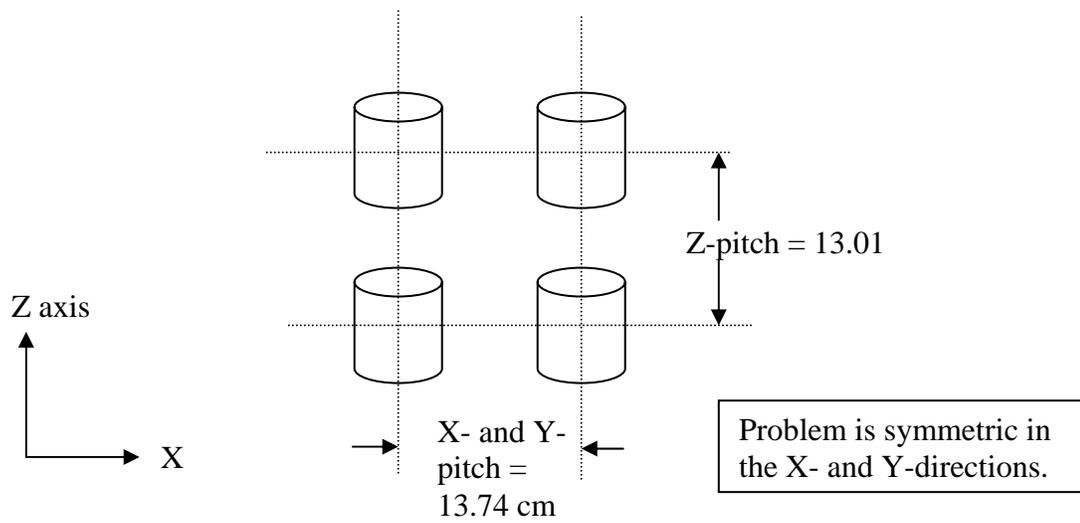
Fig. 72. Example of an array composed of units containing arrays and holes.

The focus of this section will be on simple arrays; i.e., arrays containing a single unit or arrays with multiple units of nominally different sizes.

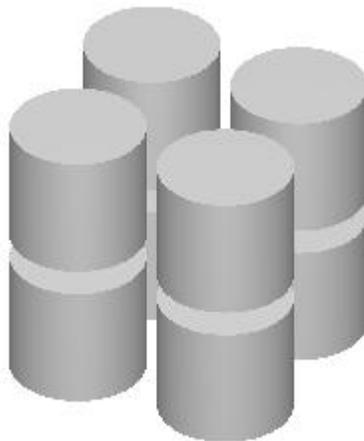
#### 4.6.1 Arrays With Single Units

This problem consists of a  $2 \times 2 \times 2$  array of bare metal U(93.2) cylinders. Each cylinder has a diameter of 11.496 cm and an outside height of 10.765 cm. The uranium has a density of 18.76 g/cc with 1 wt %  $^{234}\text{U}$ , 93.2 wt %  $^{235}\text{U}$ , 0.2 wt %  $^{236}\text{U}$ , and 5.6 wt %  $^{238}\text{U}$ . The pitch in the X and Y directions is 13.74 cm and 13.01 in the Z-direction. There are no external reflectors or other materials in the array. The geometry is shown in Fig. 73 and Fig. 74.

One of the requirements for a unit to be placed in an array is that the outside shape of the unit must be either a cube or a cuboid. As the constituents of the array are cylinders, they will need to be enclosed by cuboids to become part of the array. The dimensions of the cuboid are usually determined by the X-, Y-, and Z-pitch dimensions. For an array of single elements, the cuboid will have an X-dimension equal to the pitch in the X-direction, a Y-dimension equal to the pitch in the Y-direction, and a Z-dimension equal to the pitch in the Z-direction.



**Fig. 73.  $2 \times 2 \times 2$  array geometry.**

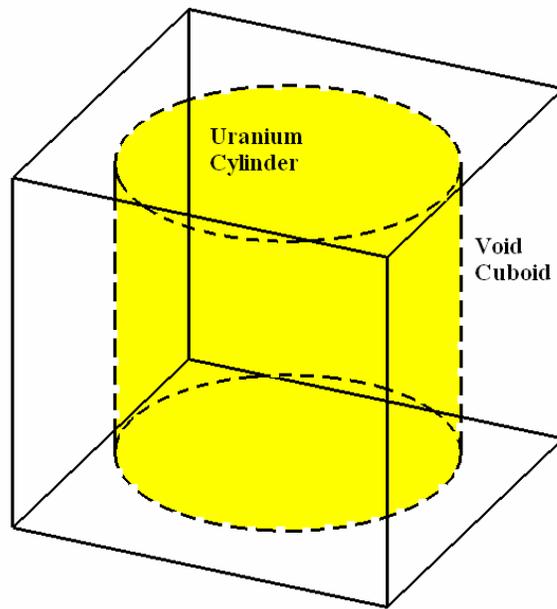


**Fig. 74. 3-D view of array.**

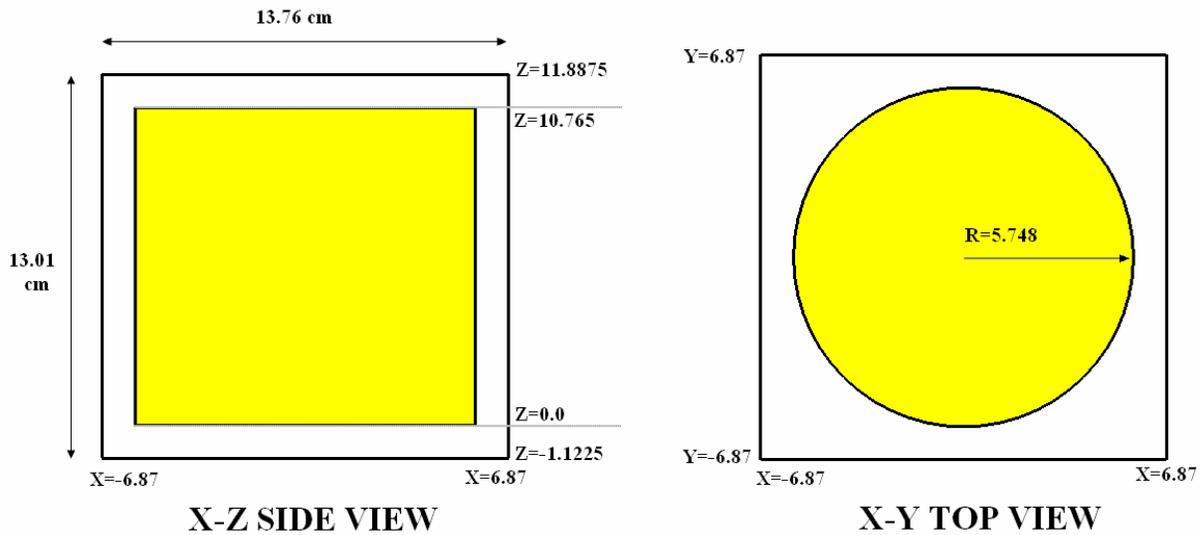
Using your knowledge from previous sections, you should be able to open a new file, and to enter the title, cross section, and material information for the uranium, including the isotopic composition weight percentages.

For this geometry, there will be two regions in one unit, but that unit is not the Global Unit for the problem. The Global Unit for this problem will be the array containing the eight units. First, we will describe the cylinder containing the uranium, then the cuboid enclosing the cylinder, to create an element of the array. These are nested shapes and are entered in the same manner as for the previous example. However, we must be careful when entering the Z data for both the cylinder and the cuboid. Once we have entered the Z or height information for the cylinder, we will have fixed the coordinate system and its origin. There are three easy choices for the location of the origin: at the bottom center of the cylinder, at the middle of the cylinder, or at the top center of the cylinder. In this particular problem, any of these origins will work. However, in other problems, one origin location may make data input for other shapes in a unit easier than the other origin locations.

For this problem, let's choose the origin to be located at the bottom center of the cylinder. Then the **Top** for the cylinder will be 10.765 and the **Bottom** will be 0.0 (see Fig. 75). For the cuboid, the origin is located in the middle in the X- and Y-directions so the +X and +Y will be 6.87 while the -X and -Y will be -6.87. Because the origin is located at the bottom of the cylinder, the Z-coordinates of the cuboid will be offset. The length of the cuboid in the Z-direction is the pitch, and there should be an equal amount of the cuboid above the cylinder and below the cylinder. The additional distance in the Z-direction outside the cuboid is  $(13.01 - 10.765 = 2.245 \text{ cm})$ . This 2.245 cm is equally split top and bottom, making the top Z-coordinate  $+Z = 10.765 + 1.1225 = 11.8875$  and the bottom Z-coordinate  $-Z = 0.0 - 1.1225 = -1.1225$ . These parameters are sufficient for describing the single array element as shown in Fig. 75.



**3-D ISOMETRIC VIEW**



**Fig. 75. Single array element (cuboid enclosing a cylinder).**

Describe the geometry by opening the **Geometry** window. Although this is not the global unit, we still need to enter a comment in the **COM=** box. Then select the **Cylinder** button on the right. For **Mixture** select 1 u from the pulldown menu, and then enter 5.748 for the **Radius**, 10.765 for **Top**, and 0.0 for **Bottom**. This puts the origin at the bottom

center of the cylinder; this is now the origin for the unit and for all other regions in the unit. To enter the data for the enclosing cuboid, select the cuboid button and for **Mixture** select 0 void from the pulldown menu. Then enter 6.87 for +**X** and +**Y**, -6.87 for -**X** and -**Y**, 11.8875 for +**Z**, and -1.1225 for -**Z**. This creates a cuboid around the cylinder with the proper spacing. Note that GeeWiz uses two shortcut keys to reduce the effort for the user. The “P” key alternates positive and negative repeating values in consecutive fields, while the “R” key repeats the value in the current field. For example, you can enter 6.87 for +**X** and then press the “P” key three times to fill the -**X**, +**Y**, and -**Y** fields for this cuboid. This completes the geometry input (see Fig. 76), but we still need to enter the **Array** data.

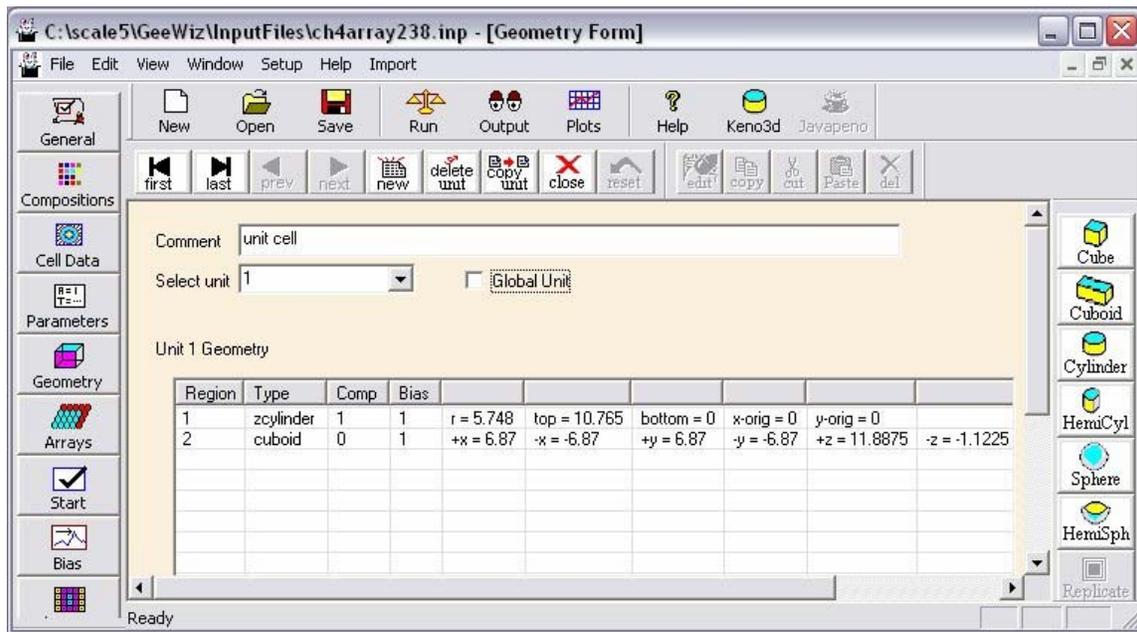
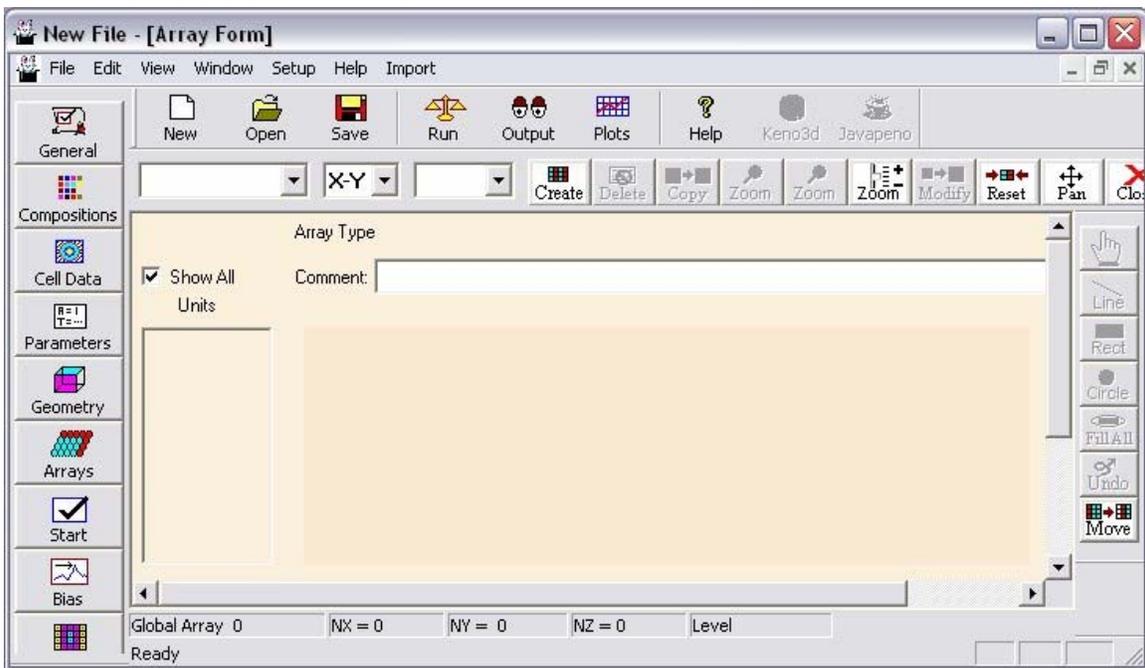
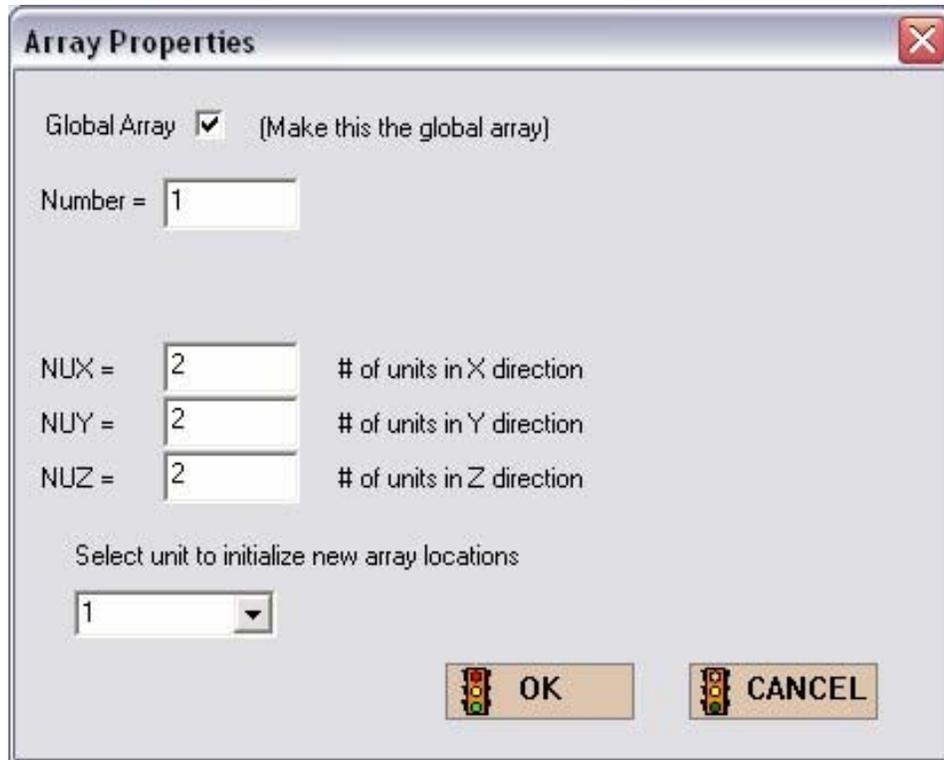


Fig. 76. Single unit geometry for array.

Now describe the array by opening the **Arrays** window (Fig. 77). To enter the array data, first click on **Create** on the array toolbar. This will open a window where you will enter the dimensions of the array. For this problem, the array is the global unit, so check the **Global Array** box. Now the array is 2 units in the X-direction, 2 units in the Y-direction, and 2 units in the Z-direction, so enter 2 for **NUX**, 2 for **NUY** and 2 for **NUZ**. Notice that it has already identified the array as number 1. At the bottom there is a box that allows you to fill the array with a given unit. When you only have one unit, as is the case here, then that unit number will be in the box. With more than one unit, you will want to enter the unit number for the unit with largest number of items in the array. This is the starting arrangement, which you can modify as desired. The screen should look like Fig. 78.



**Fig. 77. Array screen in GeeWiz.**



**Fig. 78. Array properties for  $2 \times 2 \times 2$  array.**

Then click **OK**. This will display an X-Y grid of the  $Z=1$  plane on the screen. The grid shows a  $2 \times 2$  arrangement filled with unit 1 for the X-Y plane, as indicated on the screen. As there are two X-Y planes, both levels,  $Z=1$  and  $Z=2$ , are filled with unit 1. The completed screen should look like Fig. 79. After you have checked your input, click on the **Close** button on the array toolbar. This will save the array information.

Save the changes in a new input file and execute SCALE. The calculated  $k_{\text{eff}}$  for this critical experiment is  $0.9971 \pm 0.0016$ .

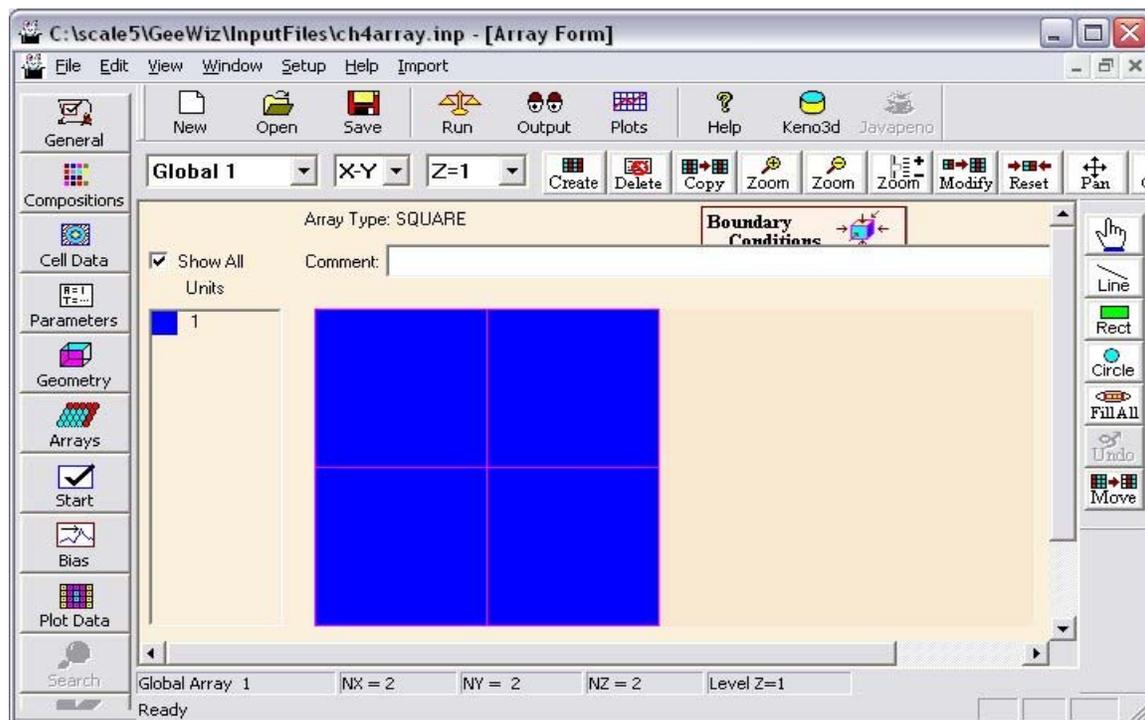
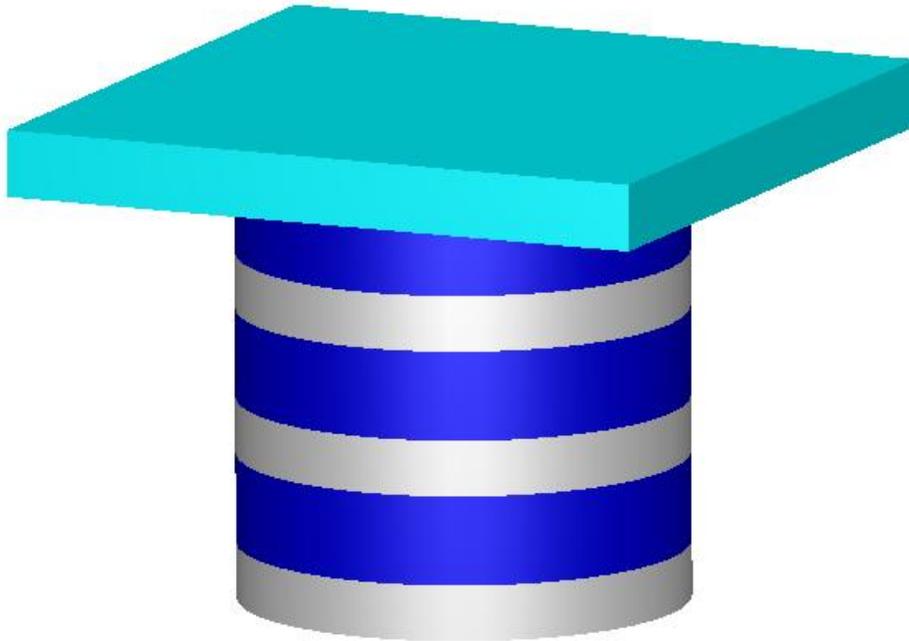


Fig. 79. Array form for  $2 \times 2 \times 2$  array.

#### 4.6.2 Arrays With Multiple Units of Different Nominal Sizes

This problem consists of a stack of six cylindrical disks covered by a square plate on the top (Fig. 80). There are two types of disks. One contains graphite (density = 1.65 g/cc), and is 10 cm in radius and 2.5 cm thick. The second one contains U(93.2) and is 10 cm in radius and 4 cm thick. The uranium has a density of 18.74 g/cc with 1 wt %  $^{234}\text{U}$ , 93.2 wt %  $^{235}\text{U}$ , 0.2 wt %  $^{236}\text{U}$ , and 5.6 wt %  $^{238}\text{U}$ . The bottom disk, which is graphite, is followed by uranium, graphite, uranium, graphite, and uranium. The top plate is aluminum of nominal density,  $30 \times 30$  cm square, and 3 cm thick. There are no external reflectors or other materials in the array.

One of the requirements for a unit to be placed in an array is that the touching faces of adjacent units must be the same size. This means that the enclosing cuboid for both cylinder types must be the same size as the top plate. Thus, the length of the X and Y sides of the cuboid must be 30 cm. Notice that there is no constraint on the Z-dimension of the cuboid as there are no adjacent faces in that direction.



**Fig. 80. Geometry of stack.**

Using your knowledge from previous sections, you should be able to open a new file, enter the title, cross section, and material information for the graphite, uranium (including the isotopic composition weight percentages), and aluminum.

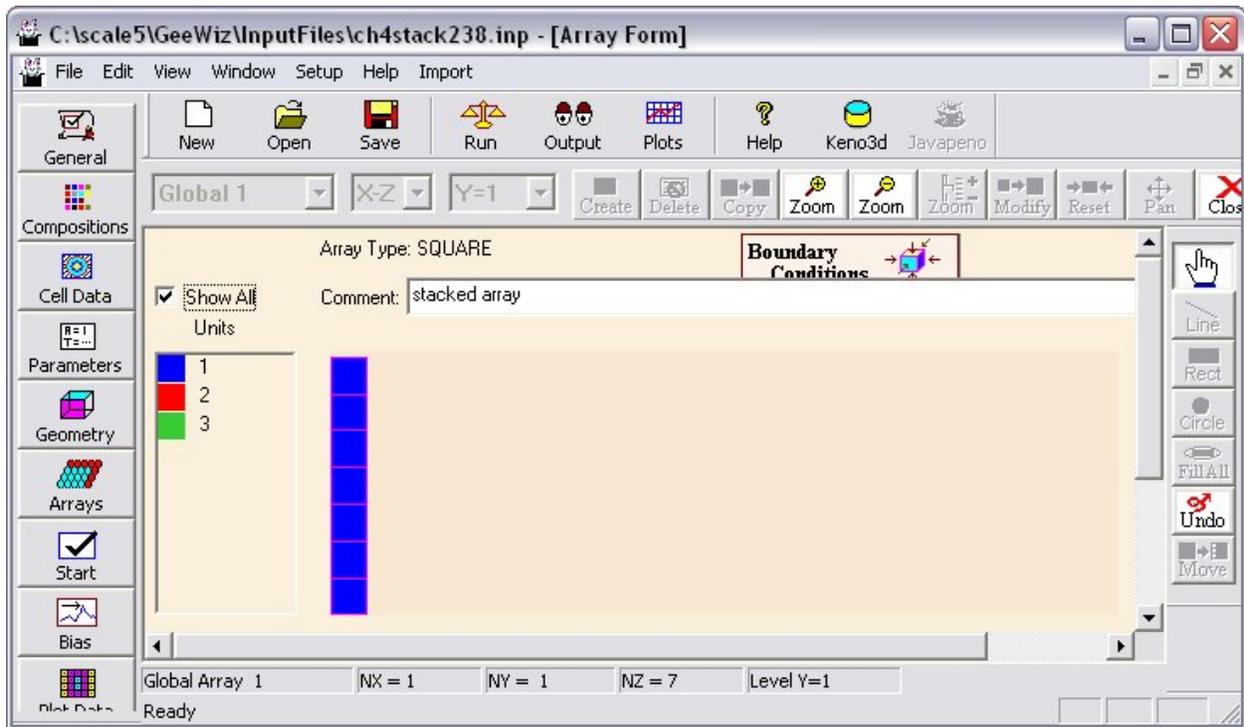
Describe the geometry by opening the **Geometry** screen. Enter a comment in the **COM=** box and then select the **Cylinder** button. For **Mixture** select 1 c-graphite from the pulldown menu, then enter 10 for the **Radius**, 1.25 for **Top**, and -1.25 for **Bottom**. This puts the origin for the unit and for all other shapes in the unit at the center of the cylinder. With the origin at the center of the cylinder, the Z-coordinates for the enclosing cuboid become symmetric. To enter the data for the enclosing cuboid, select the **Cuboid** button and for **Mixture** select 0 void from the pulldown menu. Then enter 15 for +**X** and +**Y**, -15 for -**X** and -**Y**, 1.25 for +**Z**, and -1.25 for -**Z**. This creates a cuboid around the cylinder with the proper spacing. As this is not the global unit, we will leave the **Global Unit** box blank.

Now describe the uranium cylinder by clicking the **New** button on the geometry toolbar. Again, enter a comment in the **COM =** box and then select the **Cylinder** button. For **Mixture** select 2 u from the pulldown menu, then enter 10 for the **Radius**, 2 for the **Top**, and -2 for the **Bottom**. With the origin at the center of the cylinder, the Z-coordinates for this enclosing cuboid become symmetric. To enter the data for the enclosing cuboid, select the **Cuboid** button and for **Mixture** select 0 void from the pulldown menu. Then enter 15 for +**X** and +**Y**,

-15 for **-X** and **-Y**, 2 for **+Z**, and -2 for **-Z**. This creates a cuboid around the cylinder with the proper spacing. As this is not the global unit, we will leave the **Global Unit** box blank.

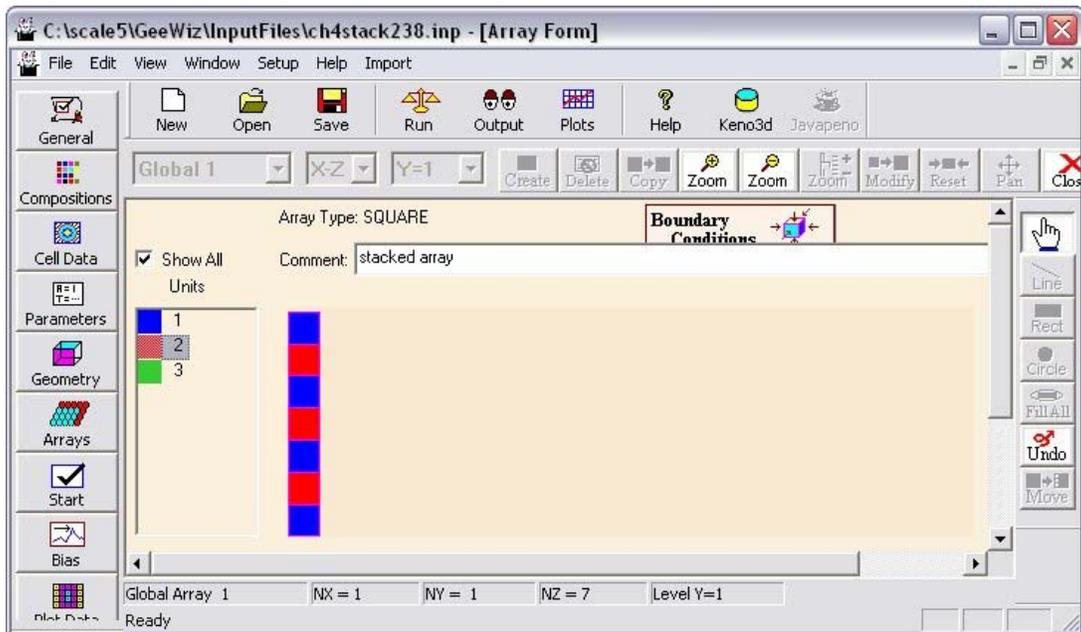
Now describe the aluminum plate by clicking the **New** button on the geometry toolbar. Enter a comment in the **COM =** box, then select the **Cuboid** button, and for **Mixture** select 3 a1 from the pulldown menu. Then enter 15 for **+X** and **+Y**, -15 for **-X** and **-Y**, 1.5 for **+Z**, and -1.5 for **-Z**. When the geometry input values alternate sign as they do here, remember that you can use the “P” shortcut key in GeeWiz to repeat the first value entered with alternating plus/minus signs. For example, enter 15 for **+X** and then press “P” three times. GeeWiz will fill the **-X**, **+Y**, and **-Y** fields with values of -15, 15, and -15, respectively. Likewise, enter 1.5 for **+Z** and press “P” for GeeWiz to add -1.5 for **-Z**. This completes the geometry input, but we still need to enter the array data.

To enter the array data, click **Arrays** on the left toolbar, and then click on **Create** on the array toolbar. This will open a window where you will enter the dimensions of the array. For this problem, the array is the global unit, so check the **Global Array** box. Now the array is 1 unit in the X-direction, 1 unit in the Y-direction, and 7 units in the Z-direction, so enter 1 for **NUX**, 1 for **NUY** and 7 for **NUZ**. Notice that it has already identified the array as number 1. In the bottom box to select the unit to initialize new array positions, select either 1 or 2 as there are three units of each in the array. The starting arrangement, which you will later modify, will be a  $1 \times 1 \times 7$  array filled with either unit 1 or 2, as indicated in the bottom box. Then click **OK**. This will display a grid of the first plane on the screen in the left-hand corner. However, it only shows as a  $1 \times 1$  array as you are looking at the X-Y plane. Click on **X-Z** plane to display the  $1 \times 7$  array as shown in Fig. 81. Notice that the **Show All** box has been checked to display all the units previously described in the geometry section. Also, depending on the array size, the entire array may not fit on the screen. You can use the **Zoom +** (fewer units on screen) or **Zoom -** (more units on screen) buttons located on the array toolbar to adjust the display as desired.



**Fig. 81. Initial array screen for stacked disks problem.**

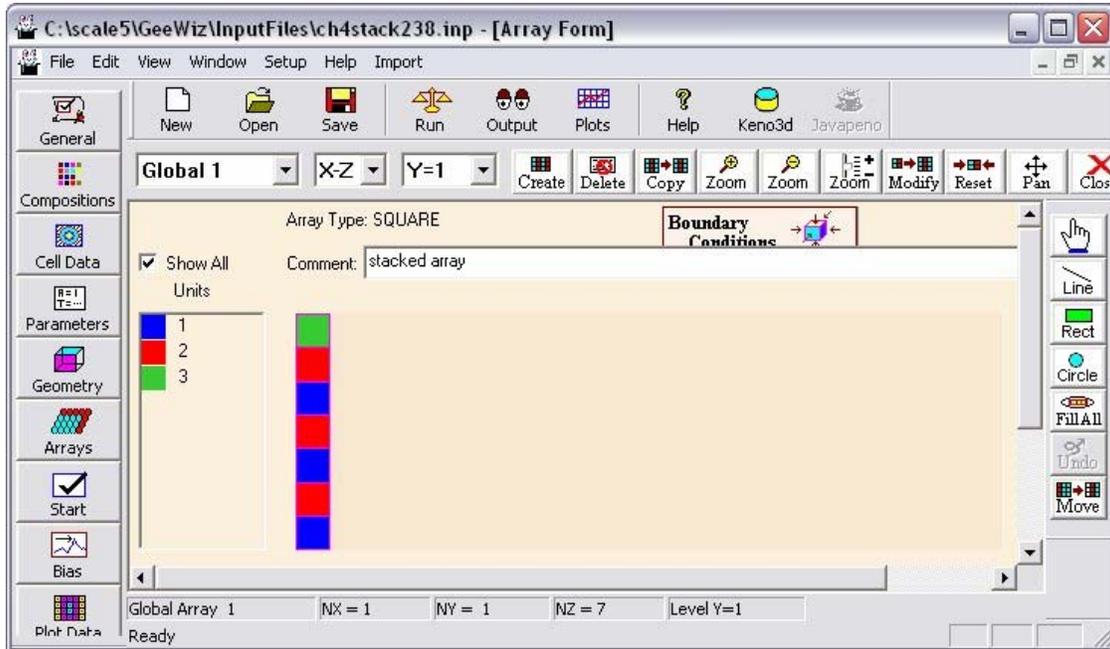
Because we have three different units, we need to tell GeeWiz which unit to put in each array position. First, click on the Unit No. you want to put in the array. In Fig. 81 the array is initially filled with unit 1 so we will select unit 2 to place it in its proper positions. Then select the pointer button on the right. Then click on the second location from the bottom, then the fourth location from the bottom, and lastly, the sixth location from the bottom. This puts unit 2 in these locations in the array as shown in Fig. 82.



**Fig. 82. Placing unit 2 in the array.**

Now repeat the process with unit 3, placing it in the top position (or the seventh from the bottom). When finished, click again on the pointer button to toggle off unit placement. When completed, the array screen should look like Fig. 83. After you have checked your input, then click on the **Close** button on the array toolbar. This will save the array information.

Save the changes in a new input file and execute SCALE. The calculated  $k_{\text{eff}}$  is  $0.9479 \pm 0.0018$ .



**Fig. 83. Completed array screen for stacked disks problem.**

## 4.7 SUMMARY

This section has helped you to:

- Use GeeWiz to describe the basic shapes (sphere, cylinders, cube, cuboid).
- Understand how units are created (including nesting of shapes).
- Locate and change the location of the origin for shapes and units.
- Create simple arrays consisting of a single unit.
- Create arrays with multiple units of nominally different sizes.

Now that you have spent time with the material and simple geometry input, we will proceed to more complicated geometries such as hemispheres, hemicylinders, and holes.

## **5. ADVANCED GEOMETRY INPUT**

In the last section you ran some nested geometry problems and some simple array problems. This section provides an explanation of the more complex hemicylinder shapes and the keyword hole to create non-nested units.

### **5.1 WHAT YOU WILL BE ABLE TO DO**

- Use GeeWiz to describe hemispheres and hemicylinders.
- Define units for partially filled shapes such as tanks or spheres.
- Understand how holes are used to include multiple non-nested shapes in a unit.
- Create arrays containing basic shapes and holes.

### **5.2 HEMISPHERES AND HEMICYLINDERS**

In addition to the basic shapes discussed in Sect. 4, KENO V.a has two additional shapes used to describe parts of a cylinder or sphere. These “hemi” shapes are described in Table 4.

**Table 4. “Hemi” shapes**

<b>HEMISPHERE</b>	is used to specify a spherical segment with a flat base whose spherical surface exists in the positive Z direction. The base or flat portion of the spherical segment is centered about a point that may be specified in the optional region origin data. By default, the center of the spherical surface is the origin and the distance to the base from the center of the spherical surface is zero (i.e., a true hemisphere). See Fig. 84.
<b>HEMISPHE<math>bc</math></b>	is used to specify a spherical segment with a flat base whose spherical surface exists in the $bc$ direction ( $b = +$ or $-$ , $c = X, Y,$ or $Z$ ). The base or flat portion of the spherical segment is located a distance $\rho$ from the center of the spherical surface, and the center may be specified in the optional region origin data. <b>HEMISPHE+Z</b> is the same as the previously described <b>HEMISPHERE</b> and <b>HEMISPHE-Z</b> is the mirror image of <b>HEMISPHE+Z</b> , therefore existing only in the negative Z direction. By default the center of the spherical surface is the origin and the distance of the base from the center of the spherical surface is zero (i.e., a true hemisphere).
<b><math>b</math>HEMICYL<math>cd</math></b>	is used to specify a cylindrical segment whose axis is in the $b$ direction ( $b = X, Y,$ or $Z$ ) and whose cylindrical surface exists only in the $c$ direction from a plane perpendicular to the $d$ -axis ( $c = +$ or $-$ , $d = X, Y,$ or $Z$ ). The position of the plane (cut surface) can be specified in the optional region chord data. This plane cuts the cylinder parallel to the axis at some distance, $\rho$ , from the axis. By default, the axis passes through the origin and $\rho$ is zero. (Examples: <b>ZHEMICYL+X</b> , <b>YHEMICYL-Z</b> , <b>XHEMICYL+Y</b> ) See Fig. 85.

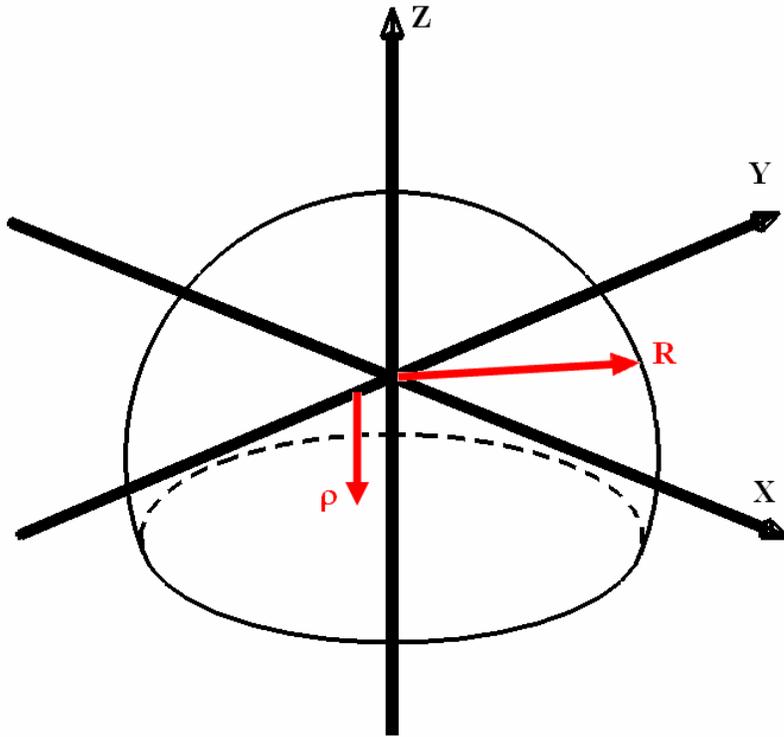


Fig. 84. Parameters for a hemisphere.

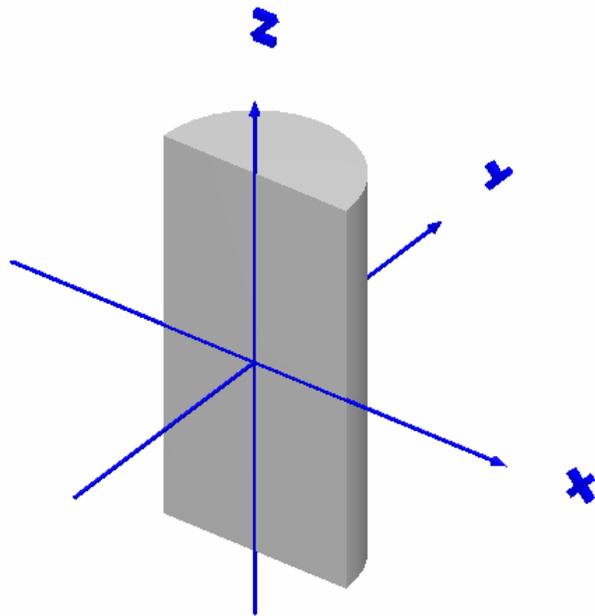
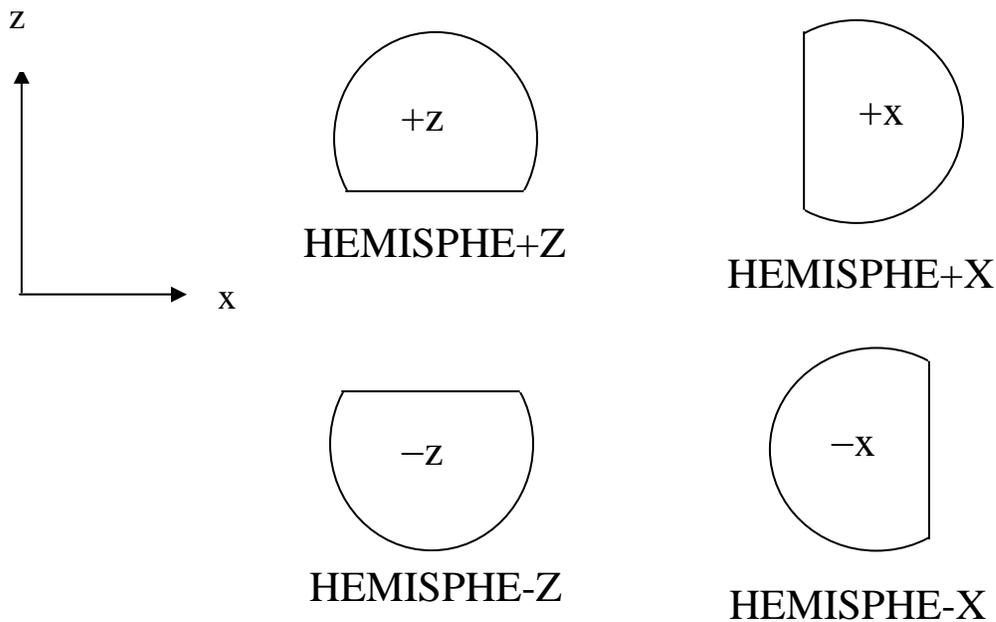


Fig. 85. ZHEMICYL+Y example.

### 5.2.1 Description of a Hemisphere or Hemicylinder

Two parameters are needed to describe the location of the flat surface of the hemisphere or hemicylinder: the axis and the distance from the center of the shape. For example, Fig. 86 shows a flat surface perpendicular to the Z-axis or to the X-axis. The sign is determined by the curved surface. If the curved surface is in the positive direction, then the sign is +; if it is in the negative direction, the sign is -.



**Fig. 86. Direction of curvature.**

The location of the flat surface is defined by  $\rho$ , the chord, as the distance from the origin to the flat surface. The sign of  $\rho$  indicates whether the flat surface is between the origin and the curved surface (sign is -) or whether it is on the other side of the origin from the curved surface (sign is +). See Fig. 87 for examples.

## HEMISPHE-Z or XHEMICYL-Z or YHEMICYL-Z

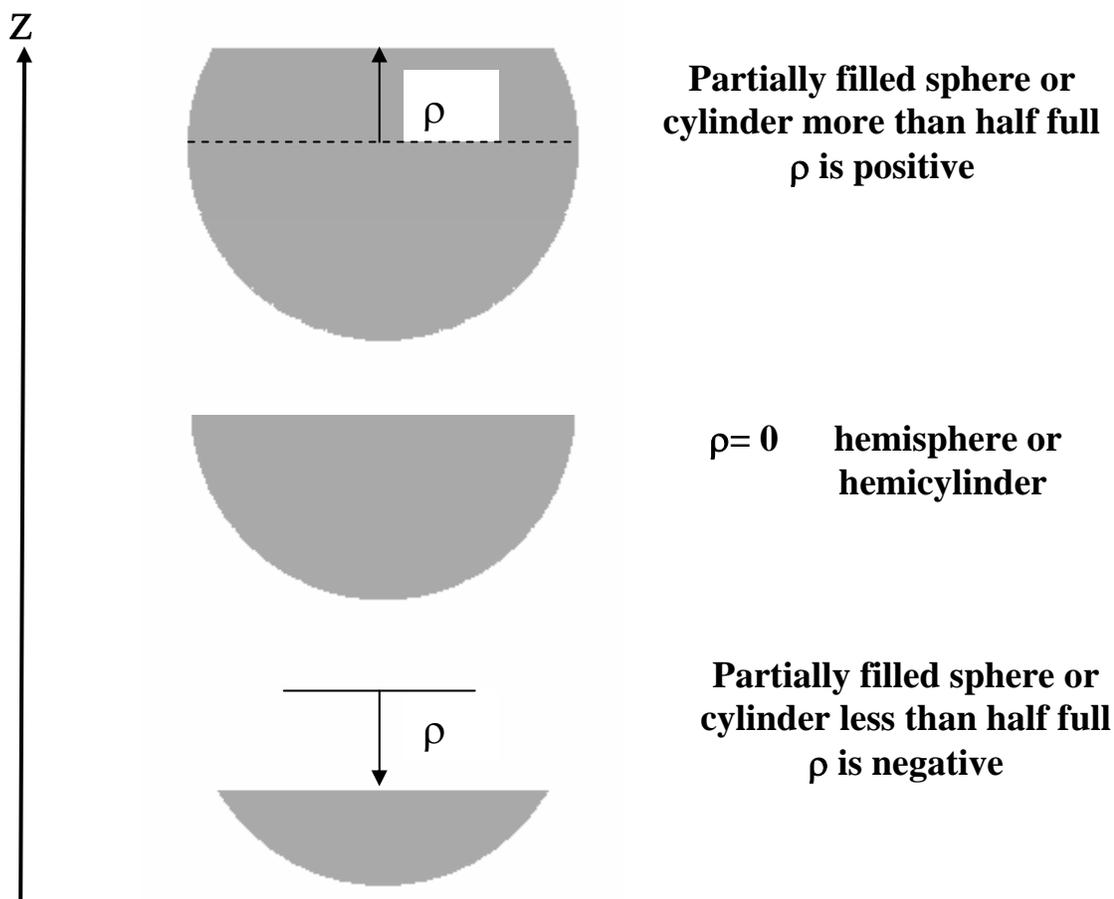
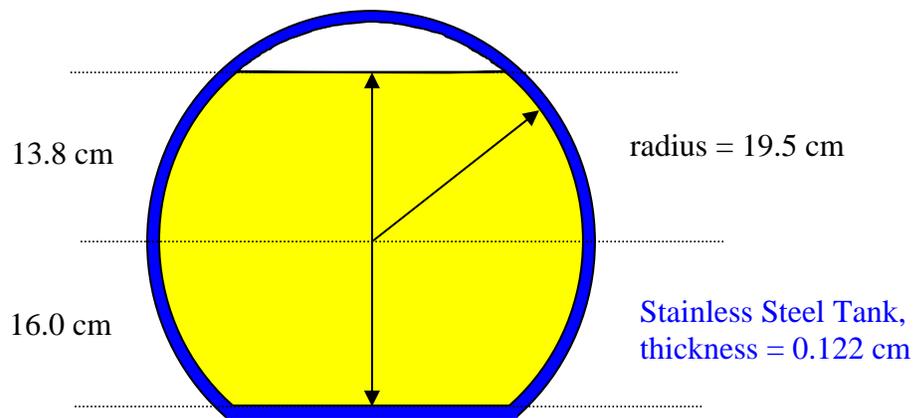


Fig. 87. Use of  $\rho$  to characterize flat surface.

### 5.2.2 Flat-Bottomed Spherical Tank

To understand how a hemisphere might be used to describe a partially filled, flat-bottomed spherical tank, an example problem is given. For this problem, the flat portion of the sphere is located 16 cm from the center, the sphere is filled 13.8 cm above the center, and it is a 19.5-cm-radius sphere. The material in the sphere is  $\text{Pu}(\text{NO}_3)_4$  with 4.6%  $^{240}\text{Pu}$ . The sphere is stainless steel with a 0.122 cm thick wall. The experimental arrangement is shown in Fig. 88. The solution characteristics are 39 g Pu/liter, acid molarity of 0.4 moles/liter, and a specific gravity of 1.103.



**Fig. 88. Flat-bottom sphere.**

By now, you should be comfortable using GeeWiz to enter the **General** information with the title, sequence, unit cell type, and cross-section library. Because this is the first example we have done where the fissile material is in solution, we will walk through that process. For this problem, we again select **Compositions** from the menu on the left. If you are running SCALE 5, select **Fissile Solution**. Under **Composition Name** there are only four choices provided on the menu: `solnuo2f2`, `solnuo2(no3)2`, `solnpu(no3)4`, and `solnth(no3)4`. For this problem, select `solnpu(no3)4`. Under **Isotopic Distribution**, click **Edit Selection** and then enter 4.6 for **94240** ( $^{240}\text{Pu}$ ). Then click on **94239** ( $^{239}\text{Pu}$ ) data entry area and select the **Fill to 100%** box. GeeWiz should enter 95.4 for the weight percent of **94239** ( $^{239}\text{Pu}$ ). Now we need to enter the solution information. For **Fuel Density (g/l)** enter 39.0; for **Acid Molarity (moles/l)** enter 0.4; and for **Specific Gravity** enter 1.103. The completed form should look like Fig. 89. Click **OK**.

If you are running SCALE 5.1, select **Solution**. Then click **Create** to open the **Solution** form. Note that the solution input changed significantly in SCALE 5.1. Enter the **Solution Density** of 1.103. Set **Number of Components** = 1. The **Acid** is `hno3` with **Amount** 0.4 moles/liter (MOLAR). Component 1 (**Comp 1**) is `pu(no3)4` with **Amount** 39 grams/liter (RHO). Under **Isotopic Distribution**, click **Edit Selection** and then enter 4.6 for **94240** ( $^{240}\text{Pu}$ ). Then click on **94239** ( $^{239}\text{Pu}$ ) data entry area and select the **Fill to 100%** box. The completed form should look like Fig. 90.

Then for Composition 2, click on **Create** from the **Standard Solution Compositions** screen, and then select **Basic Composition**. From the pulldown menu, select `ss316` (i.e., stainless steel type 316) as the composition name, and accept the default values by clicking on **OK**. This completes the material input for this example.

**Fissile Solution**

help first last prev next copy new

Mixture Number: 1

Composition Name: solnpu(no3)4

Volume Fraction: 1

Temperature (K): 300

Fuel Density (g/l): 39

Acid Molarity (moles/l): 0.4

Specific Gravity: 1.103 (optional)

Isotopic Distribution

- 94000
  - 94239 95.4 Wt%
  - 94240 4.6 Wt%

Edit Selection

Record 1 of 2 records

OK Clear CANCEL

**Fig. 89. Material input for fissile solution in SCALE 5.**

**Solution**

help first last prev next copy new

Mixture: 1 Solution Density: 1.103 Temperature (K): 300 Volume Fraction: 1

Number Of Components = 1 (e.g. Fuels, Metals, or salts)

	Name	Amount	Units
Acid	hno3	0.4	moles/liter (MOLAR)
Comp 1	pu(no3)4	39	grams/liter (RHO)

pu(no3)4 Isotopic Distribution

- 94000
  - 94239 95.4 Wt%
  - 94240 4.6 Wt%

Edit Selection

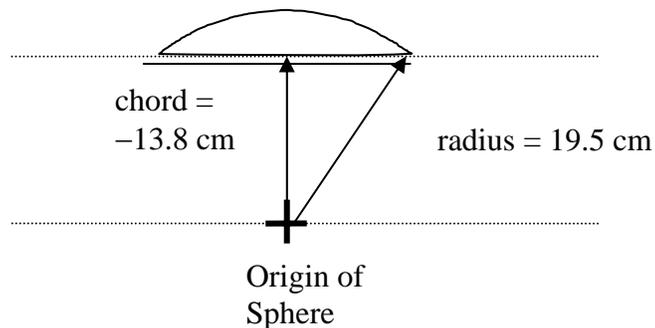
Record 1 of 2 records

OK CANCEL

**Fig. 90. Material input for fissile solution in SCALE 5.1.**

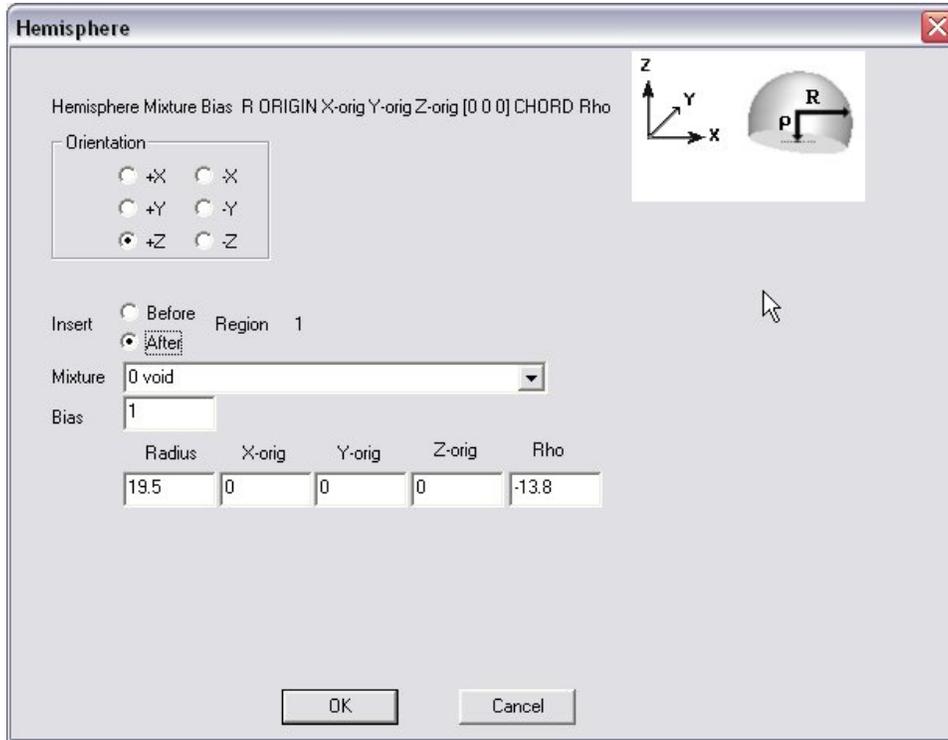
For this geometry, there will be three hemispheres in one unit, and that unit will be the global unit for the problem. Remember that nested shapes must not intersect, so the first shape listed in the geometry must be completely contained within the second shape, which must be completely contained in the third shape, etc. There are three shapes needed: the hemisphere containing the void; the hemisphere containing the solution and the void; and the hemisphere representing the stainless steel container, which contains the void, the solution, and the stainless steel. So for the first shape, we will select the smallest, which is the hemisphere containing the void. For a hemisphere, we need to specify the axis perpendicular to the flat surface, the radius, and the chord.

Select **Geometry** from the left toolbar to bring up the geometry summary form. To enter geometry information, select the appropriate geometry from the right toolbar. For this problem, that would be **HemiSph**. This brings up the hemisphere input form. The default value is a +z hemisphere, which is what we want for this problem. A +z hemisphere has the flat surface perpendicular to the Z-axis and the curved part in the positive Z-direction. For **Mixture** select 0 void from the pulldown menu. Then enter 19.5 for the **Radius**, and -13.8 for **Rho** (the chord). Remember that a negative chord length indicates that the hemisphere is less than half full. This puts the origin at the center of the sphere, and indicates that the flat surface is 13.8 cm above the origin, between the origin and the curved sphere surface. This creates a region like that in Fig. 91.



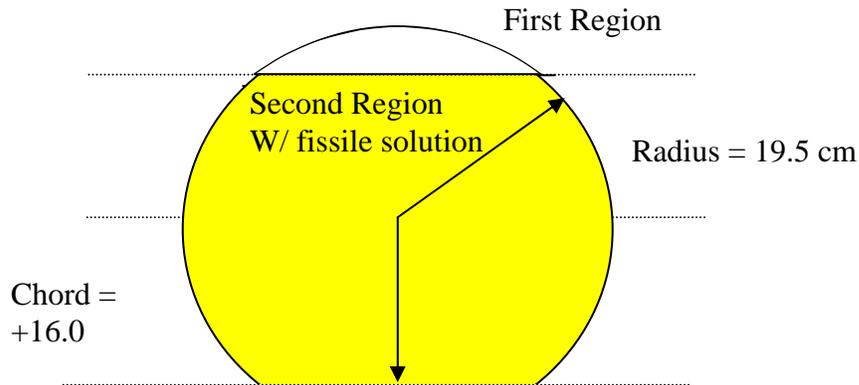
**Fig. 91. Hemisphere containing void.**

Now the hemisphere geometry form should look like Fig. 92. Click on **OK**. That brings you back to the main geometry form, where we can enter the information for the next hemisphere.



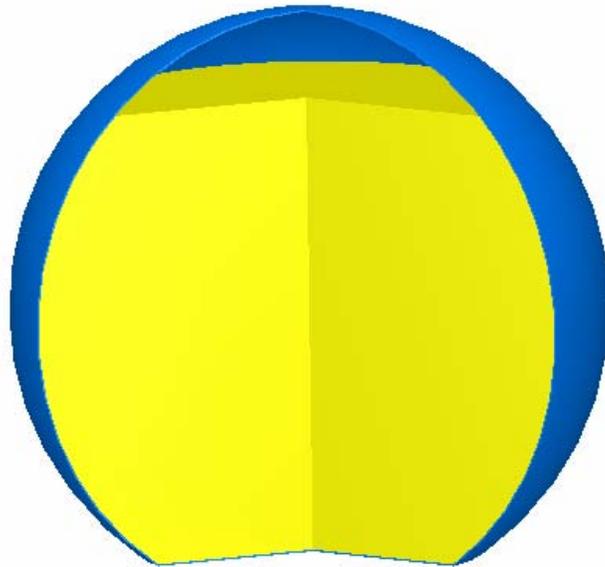
**Fig. 92. Hemisphere geometry input for flat-bottom sphere example.**

Remember as we enter a second shape that it only fills that region not already filled by the first shape. Thus, we can enter another hemisphere with the same origin containing the fissile solution. This will not cover the void, but will fill the hemisphere from its bottom to the bottom of the void. Again, select the **HemiSph** geometry from the right toolbar. This brings up the hemisphere input form. The second shape is also a +z hemisphere, so the default is appropriate. For **Mixture** select 1 solnpu(no3)4 from the pulldown menu. Then enter 19.5 for the **Radius**, and 16.0 for **Rho**. Recall that a positive chord length indicates that the hemisphere is more than half full. This entry indicates that the flat surface is 16.0 cm below the origin, on the other side of the origin from the curved sphere surface as shown in Fig. 93. Notice that nested shapes are not necessarily the same shape. In the example, the first region is a small arc wholly contained in the second region, a hemisphere. Remember, the second region contains the first region but does not cover that region. Thus, region 1 is a void in region 2.



**Fig. 93. First and second regions.**

Again, as we enter the third shape it only fills that region not already filled by the previous regions. Thus, we will enter another hemisphere with the same origin but a slightly larger radius and chord ( $\rho$ ). This will fill the thin outer edge of the hemisphere with stainless steel. So, select the **HemiSph** geometry from the right toolbar. The third shape is also a +z hemisphere, so the default is appropriate. For **Mixture** select 2 SS316 from the pulldown menu. Then enter 19.622 ( $= 19.5 + 0.122$ ) for the **Radius**, and 16.122 ( $= 16.0 + 0.122$ ) for **Rho**. This puts the origin at the center of the sphere, and indicates that the flat surface is 16.122 cm below the origin, on the other side of the origin from the curved sphere surface. A cutaway view of the final geometry is shown in Fig. 94. The complete geometry input is shown in Fig. 95.



**Fig. 94. 3-D view of nested hemispheres.**

C:\scale5\GeeWiz\InputFiles\ch5flatsphere.inp - [Geometry Form]

File Edit View Window Setup Help Import

New Open Save Run Output Plots Help Keno3d Javapeno

first last prev next new delete unit copy unit close reset edit copy cut Paste del

Comment flat bottom sphere

Select unit 1 (global unit)  Global Unit **Boundary Conditions**

Unit 1 Geometry

Region	Type	Comp	Bias					
1	hemisphere+z	0	1	r = 19.5	x-orig = 0	y-orig = 0	z-orig = 0	chord = -13.8
2	hemisphere+z	1	1	r = 19.5	x-orig = 0	y-orig = 0	z-orig = 0	chord = 16
3	hemisphere+z	2	1	r = 19.622	x-orig = 0	y-orig = 0	z-orig = 0	chord = 16.122

Hemi-Cylinder

Cube  
Cuboid  
Cylinder  
HemiCyl  
SphereHem  
HemiSph

**Fig. 95. Geometry summary for flat sphere example.**

Notice that we have added a comment, `flat bottom sphere`, in the Comment box and selected the **Global Unit** box for the unit containing the three hemispheres. After checking that the input data match, **Close** the geometry form and then click **Run**. The calculated  $k_{\text{eff}}$  is  $1.0004 \pm 0.0024$ .

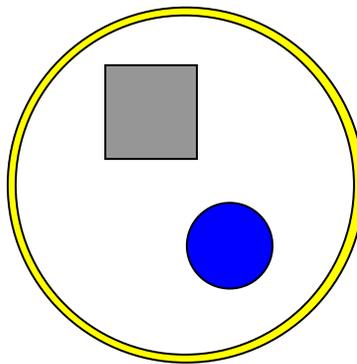
## 5.3 HOLES

For many problems, the requirement of nested shapes does not interfere with creating an accurate model. However, there will be times when a unit contains more than one shape and the shapes are not nested. For those situations, KENO V.a. uses a shape called a hole. There are four basic rules for holes.

1. A hole contains a single unit.
2. Holes may not intersect.
3. Holes may be nested.
4. As many holes as needed may be placed in a region as long as they don't intersect.

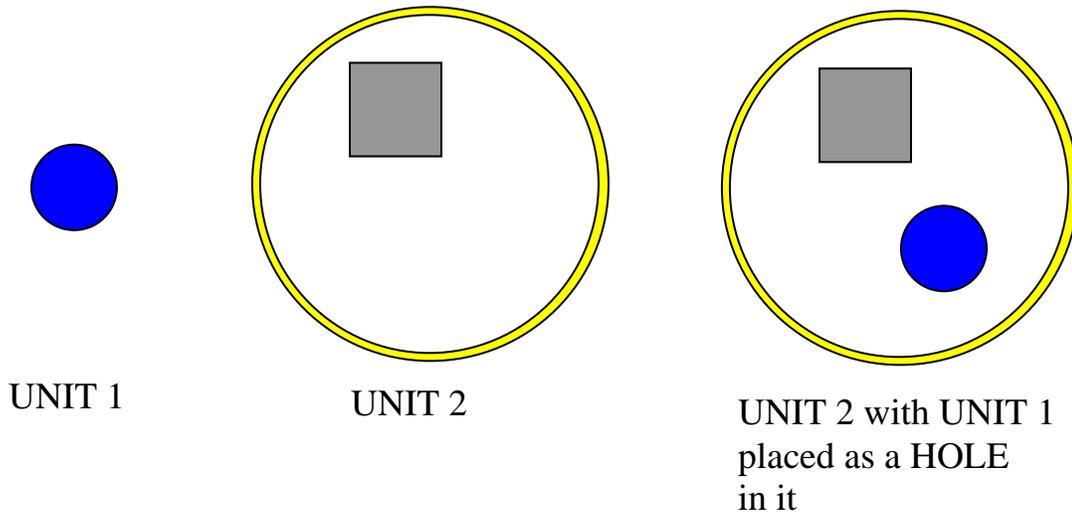
### 5.3.1 Simple Hole Example

As a simple example of the use of holes, assume that you want to model a steel cylinder containing a box of graphite and a cylinder of uranium. The geometric arrangement might look like that in Fig. 96.



**Fig. 96. Hole example problem.**

Because the graphite box and the uranium cylinder are not nested, they cannot be entered in the normal manner. What we need to do is create two units: a uranium cylinder unit and a unit with the graphite box inside the steel cylinder. (Note: We could just as easily have selected the graphite box as a single unit and put the uranium cylinder inside the steel cylinder as the second unit.) The process looks something like Fig. 97.

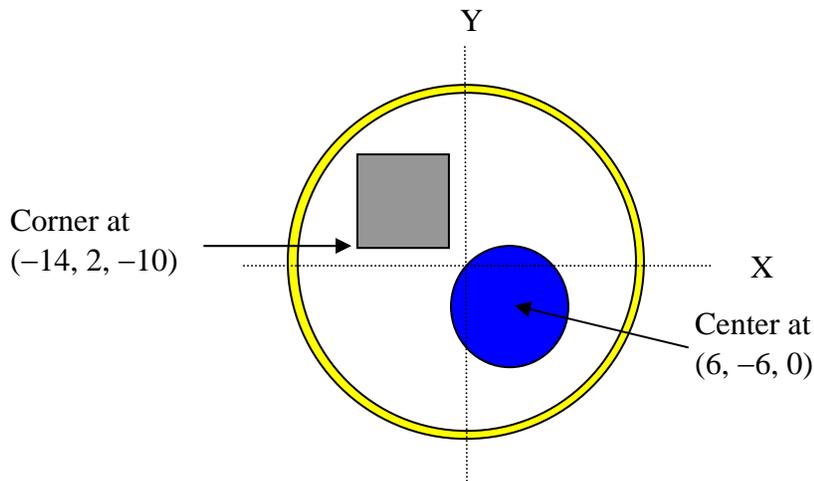


**Fig. 97. Using a hole to place one unit inside another.**

The input for the process would be as follows. First, unit 1 will be the uranium cylinder. Then create unit 2 in four steps as follows:

1. The first shape in unit 2 will be the box with the placement of its origin relative to the center of the steel cylinder.
2. The second shape in unit 2 will be the inside of the steel cylinder and will contain void as its material.
3. The third step is to place unit 1 as a hole inside unit 2. Because the hole is being placed in region 2 (the void), it must appear immediately after that region in the geometry description.
4. The third shape in unit 2 is the outside of the steel cylinder, which will contain steel. This forms the combination of unit 2 and unit 1 as shown in Fig. 97.

For this problem, we have a pure  $^{235}\text{U}$  metal cylinder (density = 18.7 g/cc) with a radius of 6.85 cm and a height of 20 cm. There is a box of graphite (default density) with length and width of 12 cm and a height of 20 cm. These are placed in a stainless steel 316 (SS316) cylinder (default density) with an inside diameter of 40 cm and a wall thickness of 0.2 cm. The inside height of the SS316 cylinder is 20 cm. With the origin located at the center of the SS316 cylinder, the lower left corner of the graphite box is located at  $(-14, 2, -10)$ . The center of the uranium cylinder is located at  $(6, -6, 0)$ . The arrangement is shown in Fig. 98.



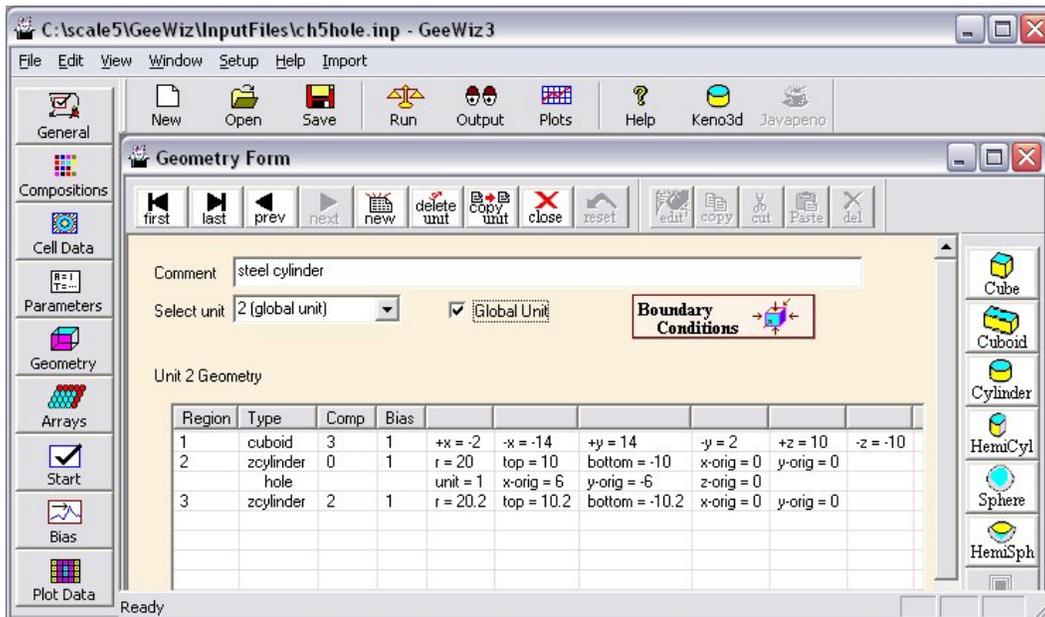
**Fig. 98. Plan view of holes example problem.**

Create a new file with appropriate **General** and **Material** information. For this geometry, we will follow the steps listed on the previous page. After selecting the **Geometry** form, select **Cylinder** from the right toolbar. Unit 1 is a z cylinder, which is the default. For **Mixture** select  $u-235$  from the pulldown menu. Then enter  $6.85$  for the **Radius**,  $10.0$  for **Top**, and  $-10.0$  for **Bottom**, leaving the defaults for **X-orig** and **Y-orig** at zero. This puts the origin at the center of the cylinder. Select **OK** and then enter a comment in the **COM=** box. This is all that is needed for unit 1. When we place it as a hole in unit 2, we will refer to it by its unit number. Click on the **new** button at the top of the main geometry form to save this information and go to the next unit.

The first region in unit 2 will be the graphite box. To locate it properly with respect to the origin of the SS316 cylinder, we will adjust the **+X**, **-X**, **+Y**, **-Y**, **+Z**, and **-Z** values. As the coordinates of the lower left-hand corner are  $(-14, 2, 0)$ , then **-X** will be  $-14$ , **-Y** will be  $2$ , and **-Z** will be  $-10$ . The maximum values are calculated by adding the appropriate dimension to the minimum values. Thus for **+X**, it will be  $(-14+12 = -2)$ , etc.

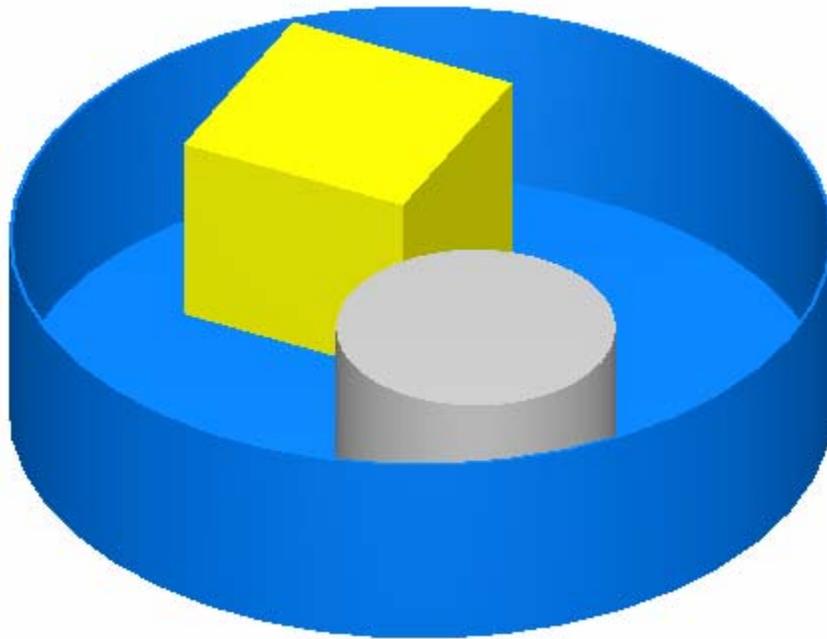
The second region in unit 2 will be the inside of the SS316 cylinder and will contain void as its material. So enter the data on the region 2 cylinder as before with 0 void for the **Mixture**, a **Top** of 10, a **Bottom** of -10, and the origin at (0,0). The next entry is the hole. Because the hole is being placed in region 2 (the void), it must appear immediately after that region in the geometry description. If the hole is placed last in this problem, you will get an error message indicating hole 1 intersects with region 3. This type of message usually indicates that the hole doesn't follow the region in which it is located or that the placement of the origin of the hole is incorrect.

To enter data on the hole, select **Hole** from the right-hand toolbar. Note that the **Hole** button is only active if the region where it is to be inserted (region 2 in this case) is highlighted. There is no entry for **Mixture**, but it does ask for **Hole Unit Number**; select 1 from the pulldown menu. If there were other units, then you would select the number of the appropriate unit. The last three entries specify the location of the hole's origin with respect to the origin of the unit in which it is placed. For this problem, the hole origin is located at (6, -6, 0) with respect to the SS316 cylinder origin. Enter 6 for **X**, -6 for **Y**, and 0.0 for **Z**. The last region in unit 2 is the outside of the SS316 cylinder. After entering the appropriate data for this cylinder, check the **Global Unit** box because unit 2 is the global unit for this example. After entering an appropriate comment, the geometry form for unit 2 should look like Fig. 99.



**Fig. 99. Unit 2 geometry input for hole example.**

The completed geometry for this problem should look like Fig. 100. (The top half of the system has been removed for viewing.)



**Fig. 100. 3-D view of geometry for hole example problem.**

After checking that the input data match, select **Close** on the geometry form and then **Run** to execute SCALE. The calculated  $k_{\text{eff}}$  is  $0.9934 \pm 0.0019$ .

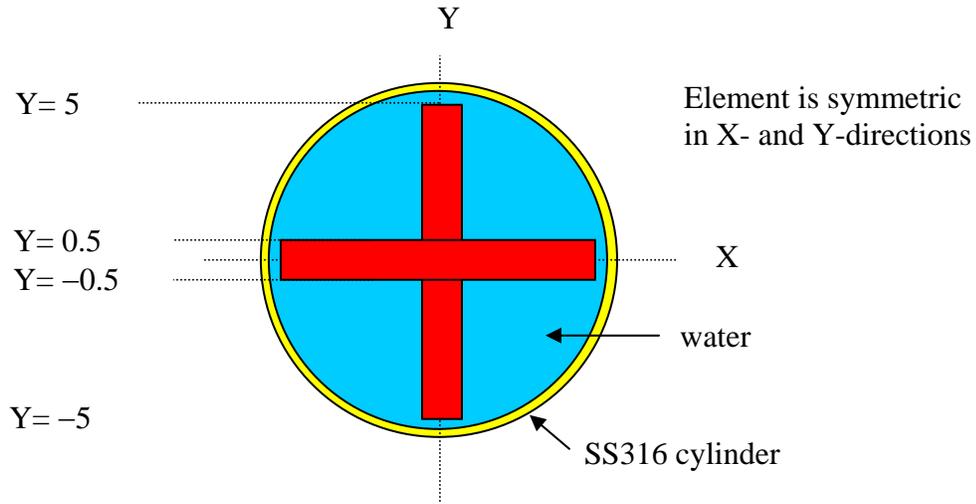
## **5.4 USING HOLES AND ARRAYS**

Many problems involve an array of items such as fuel pins. This example problem demonstrates how to enter data for a unit containing a hole and then use that unit in an ARRAY.

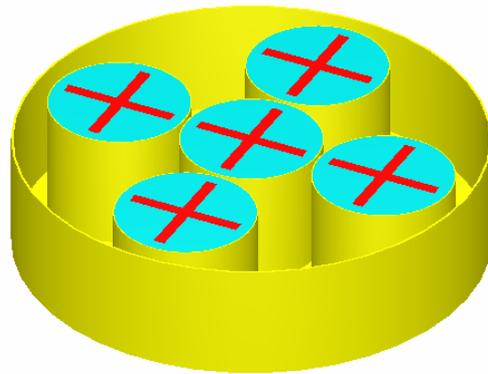
### **5.4.1 Shipping Container With Five Cylinders of Cruciform U(93.2)C Ceramic Elements**

This problem is a cruciform-shaped U(93.2)C ceramic element in water inside a SS316 cylinder (see Fig. 101). Five of these cylinders are then placed inside a larger SS316 cylinder. The cruciform element is 10 cm on a side with a width of 1 cm and a height of 20 cm. Each element is contained in a SS316 cylinder with an inner diameter of 12 cm and a

height of 20 cm. The SS316 is 0.1 cm thick. These cylinders are packed in a cruciform-shaped array with a pitch of 12.4 cm. The five containers are then placed inside a SS316 cylinder with an inside diameter of 40 cm, height of 20.4 cm, and thickness of 0.2 cm. The problem geometry is shown in Fig. 102.

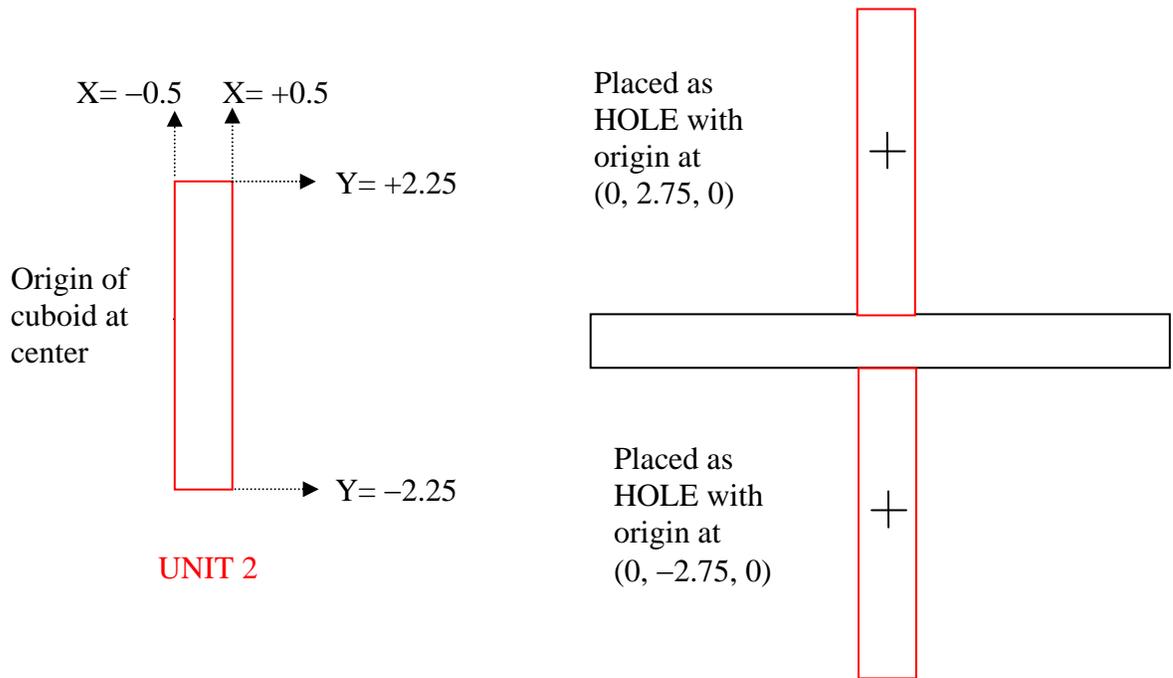


**Fig. 101. SS316 cylinder with U(93.2)C cruciform element.**



**Fig. 102. Five cruciform cylinders in shipping container.**

By now, you should be quite comfortable entering the **General** information and **Material** descriptions. We will proceed to the **Geometry** for this problem. As the cruciform elements are not a basic shape, they will need to be entered as a combination of a cuboid and holes. We will create our basic unit 1, which contains part of the cruciform element, the water, and the SS316 cylinder. Because we are putting unit 1 into an array, the outside region of unit 1 must be a cuboid so the flat surfaces can be touching. We will then create unit 2, which is one arm of the cruciform. This will be placed as a hole in unit 1 to form the cruciform (see Fig. 103).



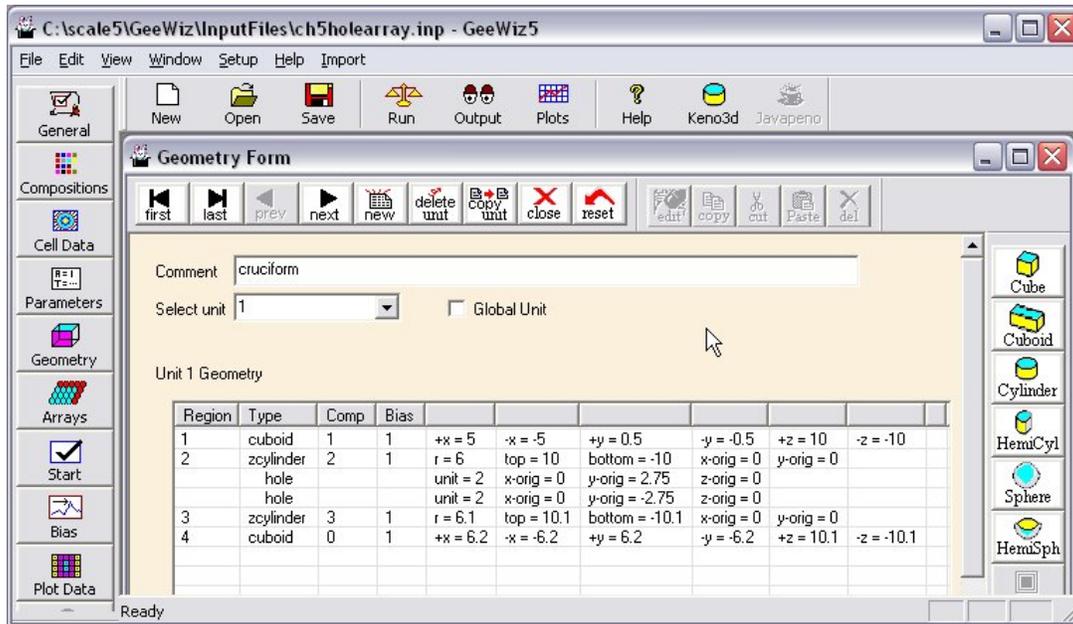
**Fig. 103. Creating cruciform with holes placed next to cuboid.**

We will start with unit 1. Select `cuboid` (this is the horizontal part of the cruciform). For **Mixture** select `1 uc` from the pulldown menu. Enter `5, -5, 0.5, -0.5, 10, -10` for **+X** through **-Z**. This puts the origin in the center of the cruciform and the center of the tank. For the next region, we need to enter the water in which the cruciform will be placed. Select `cylinder` and accept the default **+z** direction. For **Mixture** select `2 h2o` from the pulldown menu. Then enter `6` for the **Radius**, `10` for **Top**, and `-10` for **Bottom**. Now we are ready to place the holes in the water.

Next we must define unit 2 so we can insert it as a hole in unit 1. Click **New** to create unit 2. Now define unit 2 as a `cuboid` with **Mixture** `1 uc`. The **+X** and **-X** should be `0.5`

and  $-0.5$ ; the  $+Y$  and  $-Y$  should be  $2.25$  and  $-2.25$ ; and the  $+Z$  and  $-Z$  should be  $10$  and  $-10$ .

Click **Prev** to return to the previous unit 1 to enter the hole data. Select **Hole** from the right-hand toolbar. For this problem, the hole is unit 2, so set the **Unit** to 2. For the first hole, we will locate its origin above the  $X$ -axis at  $(0, 2.75, 0)$ , so enter 0 for  $X$ , 2.75 for  $Y$ , and 0.0 for  $Z$ . Go to the next geometry line and enter data for the second hole, which will also be **Unit** 2 with an origin below the  $X$ -axis at  $(0, -2.75, 0)$ . The third region in unit 1 is the SS316 cylinder that contains the water and the cruciform element. Enter the data for it. Then the last (fourth) region in unit 1 is the cuboid outside of the steel cylinder, which allows us to use this unit in an array. Because the array pitch in the  $X$ - and  $Y$ -directions is 12.4 cm, the  $+X$ ,  $-X$ ,  $+Y$ , and  $-Y$  entries will be  $+6.2 = (12.4/2)$ . After entering the appropriate data for this cylinder, the geometry form for unit 1 should look like Fig. 104.



**Fig. 104. Geometry input for unit 1.**

Before defining unit 3, which is the global unit, we need to define the array that will be inserted in unit 3. Note that the five individual containers are also in a cruciform shape with one unit in the  $+Y$  position, three units along the  $X$ -axis, and one unit in the  $-Y$  position. Because arrays must be rectangular, we will need to use holes to get a cruciform-shaped array. First we will define an array consisting of the three units along the  $X$ -axis. Then we will place the array in unit 3 along with two holes of unit 1.

Open the **Array** form by selecting the **Arrays** item from the left-hand menu. Then select **Create** from the upper toolbar; this will bring up the array properties form. For this example, the array is not the global array, so we will leave that box unchecked. We want 3 units in the X direction and 1 each in the Y- and Z-directions. Use unit 1 to initialize new array locations. The completed form should look like Fig. 105.

The screenshot shows a dialog box titled "Array Properties". At the top left, there is a checkbox labeled "Global Array" which is unchecked, followed by the text "(Make this the global array)". Below this is a text input field labeled "Number =" containing the value "1". Underneath are three rows of directional settings: "NUX = 3 # of units in X direction", "NUY = 1 # of units in Y direction", and "NUZ = 1 # of units in Z direction". Each of these has a corresponding text input field. At the bottom of the dialog, there is a label "Select unit to initialize new array locations" and a dropdown menu currently showing "1". At the bottom right, there are two buttons: "OK" and "CANCEL", each with a small traffic light icon.

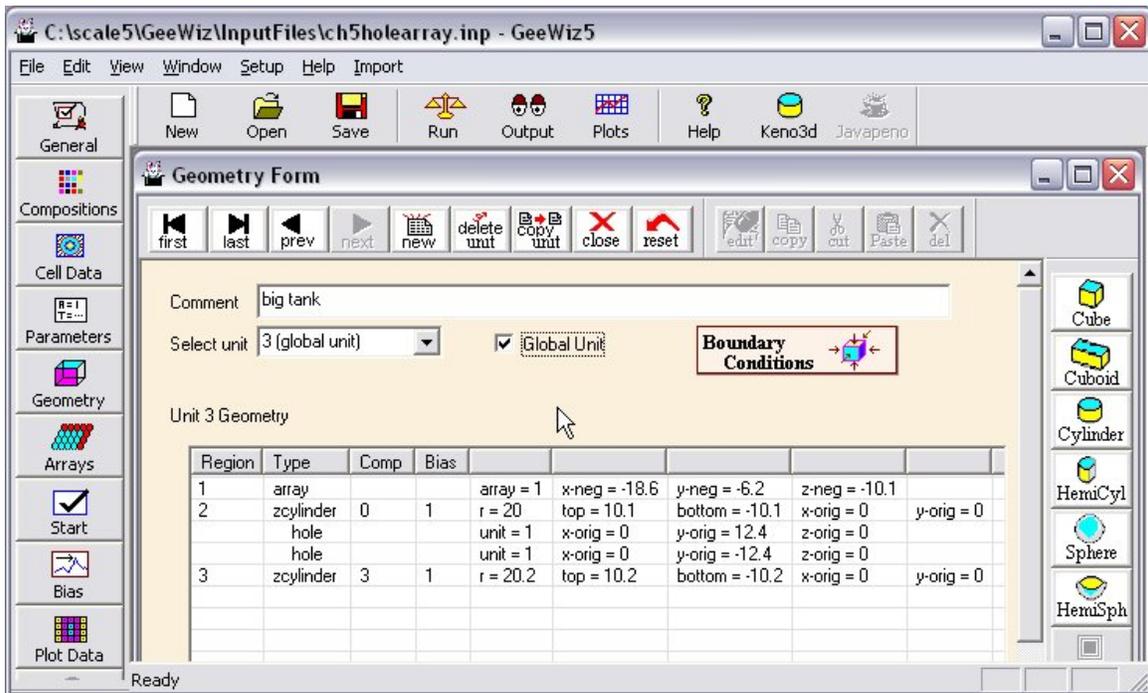
**Fig. 105. Array properties for holes/array example.**

After closing the array properties form the array form should show three squares of the same color in a line. Then **Close** the array form and go back to the geometry summary form. You will need to create a new unit, Unit 3, which will be the global unit. The first entry in the new unit will be the array that was just created. To bring up the array placement form, select **Array** from the right-hand toolbar. The existing array is array 1, and we will need to specify the location of the lower left-hand corner of the array. The lower left-hand corner is located at  $(-18.6, -6.2, -10.1)$ , where **X-neg** is  $(1.5 * \text{the pitch})$ , **Y-neg** is  $(0.5 * \text{the pitch})$ , and **Z-neg** corresponds to the bottom of unit 1. The screen should look like Fig. 106.



**Fig. 106. Array placement data.**

The next region (region 2) is the inside of the large cylinder that holds the array. This cylinder is filled with void, a **Radius** of 20 cm, **Top** of 10.1, and **Bottom** of -10.1. Now that we have a region in which to place the holes, we can complete the cruciform array. We will locate unit 1 as a hole above the X-axis and as a hole below the X-axis. The first hole is Unit 1 with an **X Origin** of 0, a **Y Origin** of 12.4, and a **Z Origin** of 0.0. The second hole is Unit 1 with an **X Origin** of 0, a **Y Origin** of -12.4, and a **Z Origin** of 0.0. The last region (region 3) is the large SS316 cylinder containing the array with a **Radius** of 20.2 cm and heights of  $\pm 10.2$  cm. With the addition of a comment and checking the **Global Unit** box, the completed geometry form for unit 3 should look like Fig. 107.



**Fig. 107. Geometry data for unit 3.**

Save the changes in a new input file and execute SCALE. The calculated  $k_{\text{eff}}$  value is  $0.6199 \pm 0.0025$ .

## 5.5 SUMMARY

This section has helped you to:

- Use GeeWiz to describe hemispheres and hemicylinders.
- Define units for partially filled shapes such as tanks or spheres.
- Understand how holes are used to include multiple non-nested shapes in a unit.
- Create arrays containing basic shapes and holes.

## 6. NONSTANDARD MATERIALS

Now that you have an understanding of the geometry and basic standard composition input requirements, this section provides an explanation of a few commands you might find useful for problems involving compounds or other materials not available in the Standard Composition Library.

### 6.1 WHAT YOU WILL BE ABLE TO DO

- Define user-defined (non-standard) material and use GeeWiz to enter data for it.
- Define a mixture by using a combination of user-defined material and a basic standard composition.

### 6.2 USER-DEFINED MATERIALS

In Sect. 3, you learned how to enter information for elements, isotopes, and compounds found in the Standard Composition Library. However, there are some materials, particularly compounds, that are not available in the Standard Composition Library in SCALE. For these materials, you need to use either the **Alloy or Mix (Wt %)** or the **Compound (atom)** types from the **New Composition** form as shown in Fig. 108. This approach works best for materials where the chemical composition or weight fraction is provided. If number densities are available for each of the constituents in a compound, then use the basic standard composition input to enter each constituent with its appropriate atom density. Materials with weight fractions can be done with either approach but are best entered as basic standard compositions if they appear in that library.

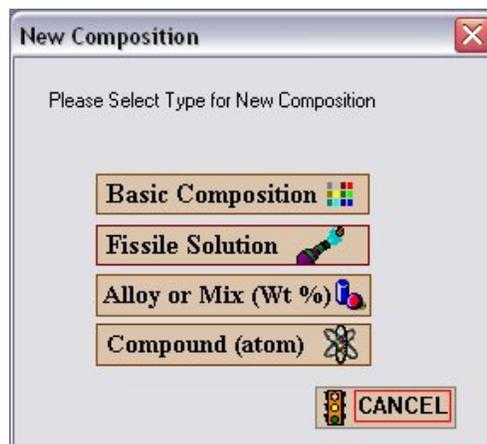
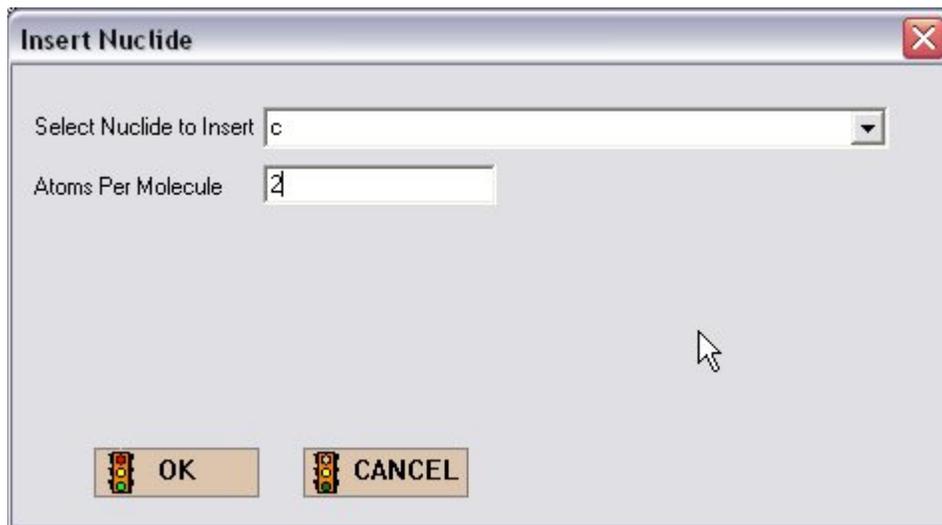


Fig. 108. New compositions type form.

## 6.2.1 Description of User-Defined Material with Chemical Formula

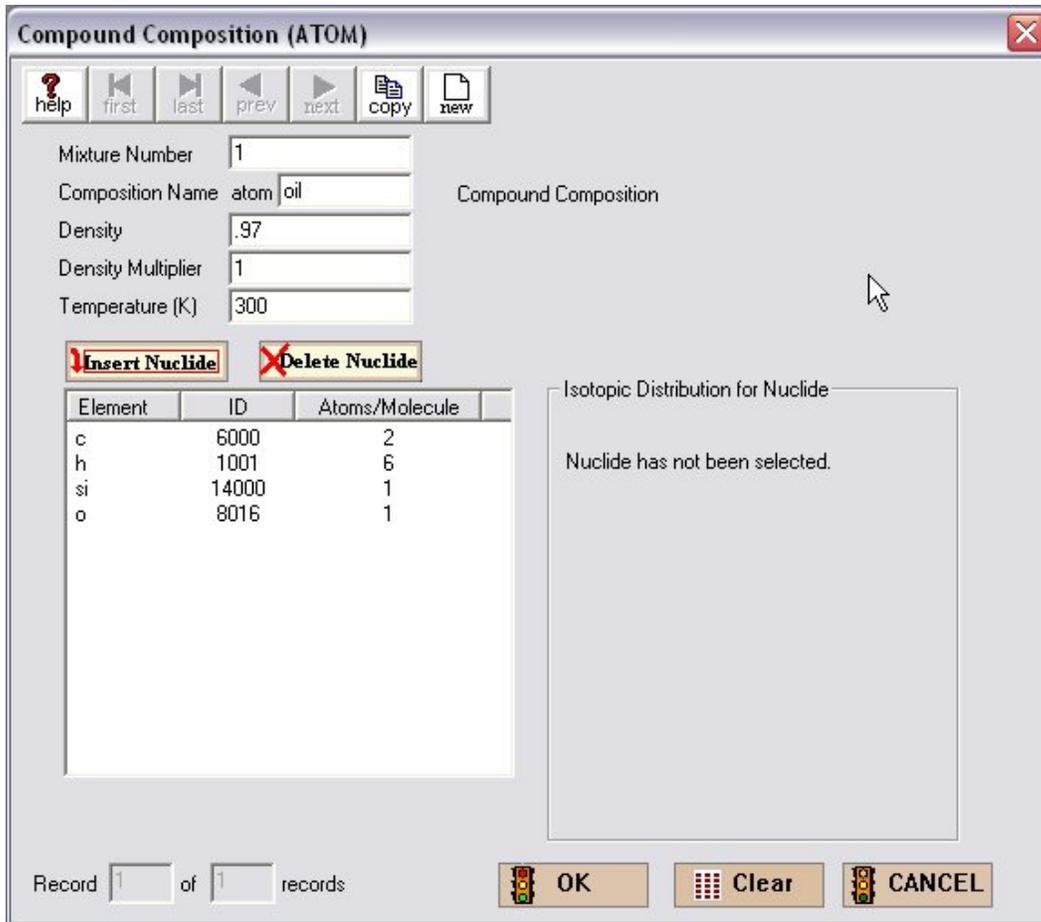
For this example, we will enter the material information for hydraulic fluid,  $C_2H_6SiO$ , with a density of 0.97 g/cc. Click on the **Compound (atom)** type from the **New Composition** form. (**NOTE:** The first four characters of the **Composition name** must be **atom** for a user-designated compound.) For **Composition name** enter **oil**, the “atom” keyword will be added at the beginning to create a material name of **atomoil**. Now enter the **Density** of 0.97 g/cc, and leave the **Density Multiplier** and **Temperature** at the default values. For this material, we know the chemical composition, so we will enter information for each nuclide in terms of atoms per molecule. Select the **Insert Nuclide** box. For each element, select the element name and then enter the atoms per molecule. For example, select **c** for the **Element Name** and enter **2** for **Atoms/Molecule**. The form for carbon should look like Fig. 109.



The image shows a dialog box titled "Insert Nuclide". It has a standard Windows-style title bar with a close button (X) in the top right corner. Inside the dialog, there are two input fields: a dropdown menu labeled "Select Nuclide to Insert" which currently shows "c", and a text box labeled "Atoms Per Molecule" which contains the number "2". At the bottom of the dialog, there are two buttons: "OK" and "CANCEL", each with a small icon of a traffic light to its left. A mouse cursor is visible over the right side of the dialog.

Fig. 109. Insert nuclide form.

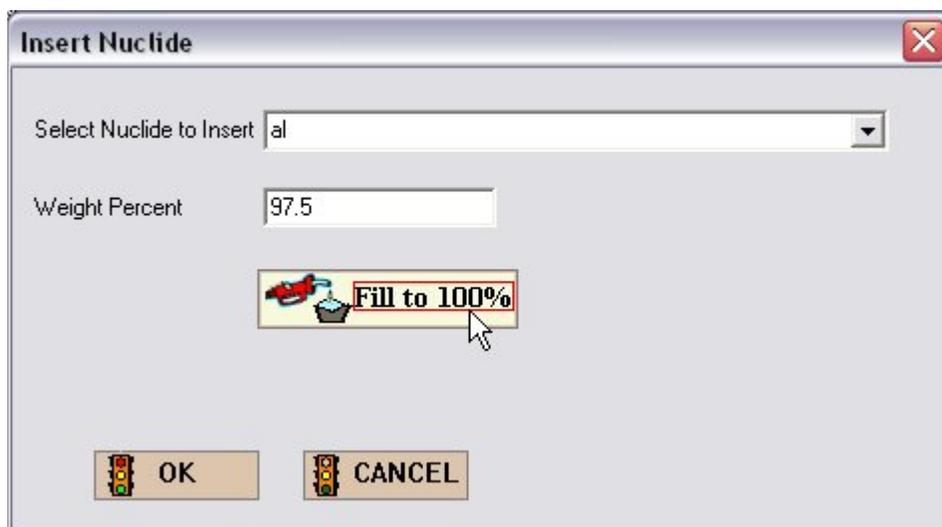
Continue with hydrogen, silicon, and oxygen. The completed form should look like Fig. 110.



**Fig. 110. Compound composition input for hydraulic fluid.**

## 6.2.2 Description of User-Defined Material with Weight Percents and Isotopic Abundance

For this example, we will enter the material information for borated aluminum that is 2.5 wt % boron and has a density of 2.65 g/cc. The boron is 90 wt % B-10 and 10 wt % B-11. For this material, we know the weight percents so we want to enter information in terms of weight percent, which is the **Alloy or Mix (Wt %)** type. For **Composition name** enter `bal` after `wtpt` to create the material `wtptbal`. Now enter the **Density** of 2.65 g/cc and leave the **Density Multiplier** and **Temperature** at the default values. Select the **Insert Nuclide** box. For each nuclide, select the nuclide name and then the weight percent or select **Fill** to 100% if it is the last nuclide. For example, if the information for boron (wt % = 2.5) has already been entered, then select `al` for the **Nuclide** and then move the cursor to the **Weight Percent** box. Then select the **Fill to 100%** option and GeeWiz will put 97.5 in the **Weight Percent** box as shown in Fig. 111.



The image shows a software dialog box titled "Insert Nuclide". It has a standard Windows-style title bar with a close button (X) in the top right corner. Inside the dialog, there is a dropdown menu labeled "Select Nuclide to Insert" with the value "al" selected. Below this is a text input field labeled "Weight Percent" containing the number "97.5". In the center of the dialog is a button with a small icon of a red car and a blue cup, and the text "Fill to 100%". A mouse cursor is pointing at this button. At the bottom of the dialog are two buttons: "OK" and "CANCEL", each with a small traffic light icon to its left.

Fig. 111. Weight percent and fill to 100% option.

After entering the data for both boron and aluminum, we need to enter the isotopics for boron. To bring up the Isotopic Distribution window, click on `boron` in the element list. The default isotopic distribution is that for natural boron, 18.4309% B-10 and 81.5691% B-11. For this material we need to change the composition to 90 wt % B-10 and 10 wt % B-11. Click on **Edit Selection**. This brings up the **Isotopic Distribution** form where you can enter 90.0 for 5010 (B-10) and then Fill to 100% for 5011 (B-11). After doing this, click **OK** on the **Isotopic Distribution** form. The completed form should look like Fig. 112. Click **OK** to save this information.

**Allow or Mixture Composition (WTPT)**

help first last prev next copy new

Mixture Number: 1  
 Composition Name: wtpt bal Weight Percent Mixture or Alloy  
 Density: 2.65  
 Density Multiplier: 1  
 Temperature (K): 300

**Insert Nuclide** **Delete Nuclide**

Element	ID	Weight %
b	5000	2.5
al	13027	97.5

Isotopic Distribution for Nuclide

- 5000
  - 5010 90 wt%
  - 5011 10 wt%

**Edit Selection**

Record 1 of 1 records

OK Clear CANCEL

**Fig. 112. Weight percent form for borated aluminum.**

Note that you cannot mix atom per molecule entries with nuclide weight percents. However, if the isotopics of elements in a compound are given in weight percent, then you can enter the atom per molecule data for the nuclides in the compound and then use the isotopic distribution box to enter the proper isotopic weight percents.

### 6.2.3 Combinations of Basic Standard Compositions and User-Defined Materials to Define a Mixture

For this example, we will enter the material information for a burnable poison, density of 3.7 g/cc, which is a combination of B<sub>4</sub>C and Al<sub>2</sub>O<sub>3</sub>. Note that B<sub>4</sub>C is in the Standard Composition Library, but Al<sub>2</sub>O<sub>3</sub> is not. The material is 1.395 wt % B<sub>4</sub>C with natural boron. We will specify this mixture using a Compound type material for Al<sub>2</sub>O<sub>3</sub> and a basic standard composition for the B<sub>4</sub>C. Select the Compound type material and for **Composition Name** enter alox. Again, the first four characters of the **Composition Name** will be atom. Now for the **Density**, enter the mixture density of 3.7 g/cc. However, the density of the Al<sub>2</sub>O<sub>3</sub> is only a part of the mixture, so we need to enter its weight fraction, (1-0.01395) = 0.98605, as the **Density Multiplier**. We will leave the **Temperature** at its default value.

We know the chemical composition for this material so enter the atoms per molecule information for each nuclide. To start, select al for the **Nuclide** and enter 2 for **Atoms/Molecule**. Continue with oxygen. After both nuclides have been entered, the completed form should look like Fig. 113. After checking the information, select **OK**.

Compound Composition (ATOM)

help first last prev next copy new

Mixture Number 1

Composition Name atom alox Compound Composition

Density 3.7

Density Multiplier .98605

Temperature (K) 300

Insert Nuclide Delete Nuclide

Element	ID	Atoms/Molecule
al	13027	2
o	8016	3

Isotopic Distribution for Nuclide

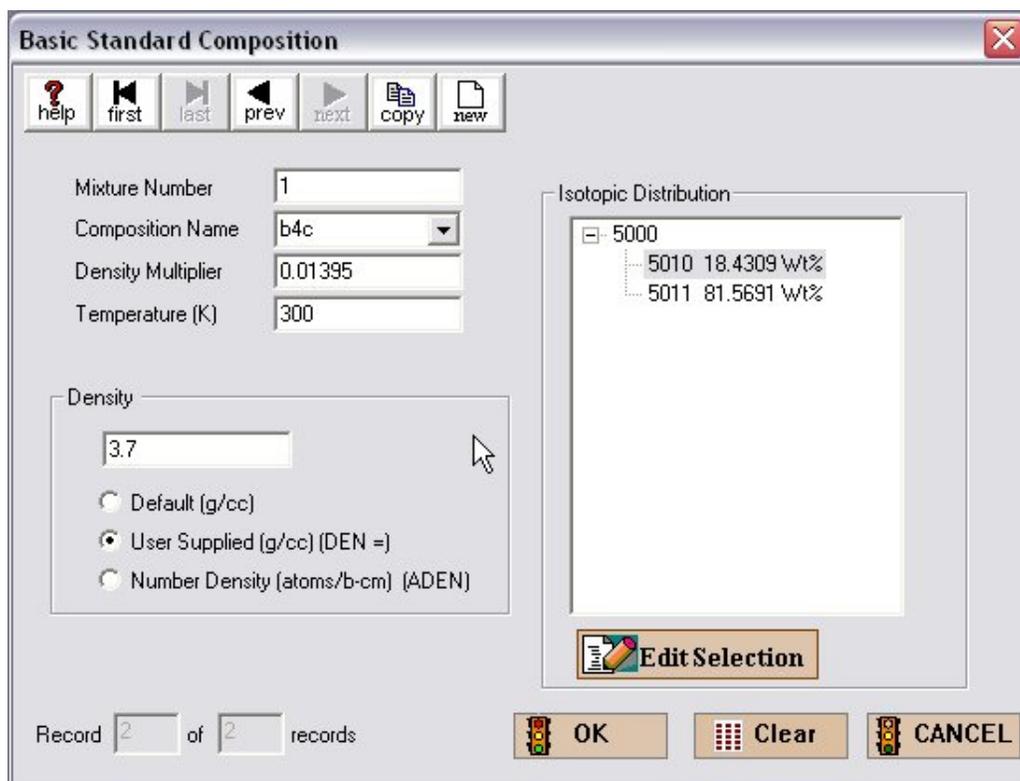
Nuclide has not been selected.

Record 2 of 3 records

OK Clear CANCEL

Fig. 113. Compound composition for Al<sub>2</sub>O<sub>3</sub> in burnable poison mixture.

Now for the  $B_4C$ , click on the **Basic Composition** type. For **Composition Number** change it to be the same as the mixture number (1) for  $Al_2O_3$ , so that the  $B_4C$  will be part of the same mixture as the aluminum oxide. For **Composition Name** select  $b_4c$ , and a **Density Multiplier** of 0.01395 (i.e., the weight fraction of  $B_4C$ ). We will leave the temperature at its default value. Because the boron is natural, we don't need to alter the isotopic distribution. However, it is always a good idea to check the default values so click on the pulldown menu under **Isotopic Compositions**. This brings up 5000, which is the alphanumeric ID for boron ( $Z=5$  and 000 indicating natural isotopes), and the weight percents of the two isotopes in natural boron as shown in Fig. 114. Click **OK** and then enter **User Supplied** under the **Density** box. Then enter the mixture density of 3.7 g/cc. The completed information should look like Fig. 114.



**Fig. 114. Standard composition part of burnable poison mixture.**

This completes the description of the burnable poison mixture using user-defined material and a basic standard composition. Remember that you can have any number of materials with the same composition number as long as you have properly handled the density multipliers to give the correct weight fraction of each material.

## 6.3 SUMMARY

This section has shown you how to use GeeWiz to:

- Define user-defined material based on a known chemical formula.
- Define user-defined material for a mixture with known weight percents of constituents.
- Define a mixture by using a combination of user-defined material and a basic standard composition.

## **7. UNIT CELLS AND BOUNDARY CONDITIONS**

The examples we have used thus far have been limited to relatively large homogeneous systems where the default INFHOMMEDIUM (infinite homogeneous medium) unit cell type was appropriate. In this section, we will look at more heterogeneous systems and learn how to use the other unit cell types appropriately.

### **7.1 WHAT YOU WILL BE ABLE TO DO**

- Understand the difference in cross-section processing for Infinite Homogeneous Medium, Lattice Cell, and Multiregion Analyses.
- Identify the appropriate unit cell type to use for various heterogeneous systems.
- Use GeeWiz to define LATTICECELL and MULTIREGION unit cells.
- Define different boundary conditions for a MULTIREGION unit cell.
- Use the REPLICATE command to model reflectors or materials of a given thickness added to the outside of a shape.
- Use boundary conditions to create reflective boundaries for a KENO V.a global unit.

### **7.2 CALCULATION TYPES FOR PROBLEM-DEPENDENT CROSS SECTIONS**

The Material Information Processor is primarily used to prepare data for creating the problem-dependent cross-section libraries required by the criticality safety sequences. This is particularly important for heterogeneous systems and large regular lattices of slabs, pins, or spheres. The Material Information Processor utilizes a unit cell description to provide information for the resonance self-shielding corrections and the Dancoff corrections that are applied to the cross sections to create a problem-dependent cross-section library. A unit cell is typically a portion of the system containing fuel that can be used to define the neutron spectrum characteristics for part of the problem.

## 7.3 UNIT CELL TYPES

The Material Information Processor offers three types of unit cell calculations: INFHOMMEDIUM, LATTICECELL, and MULTIREGION. Note that you may define multiple unit cells in a single CSAS/KENO V.a input file. Each mixture number may be used in only one unit cell.

### 7.3.1 INFHOMMEDIUM (Infinite Homogeneous Medium)

The INFHOMMEDIUM treatment is best suited for large masses of materials where the size of each material is large compared with the average mean-free path of the material or where the fraction of the material that is a mean-free path from the surface of the material is very small. Every material specified in the problem that is not used in a LATTICECELL or MULTIREGION unit cell is treated as an infinite homogeneous lump. Systems composed of small fuel lumps should not be treated as an infinite homogeneous medium.

### 7.3.2 LATTICECELL

The LATTICECELL treatment is appropriate for large arrays of fuel in slabs, pins/rods, or spherical pellets. The resonances are treated differently, depending on whether the NITAWL processor or the CENTRM processor is specified. When the LATTICECELL treatment is used with NITAWL, the mixtures specified in the cell have resonance self-shielding with Dancoff corrections applied to the cross sections of the nuclides utilized in the cell. When the LATTICECELL treatment is used with CENTRM/PMC, a set of point fluxes are calculated for a set of mesh intervals that make up the unit cell. The cell is assumed to have mirror boundary conditions. The isotopes comprising the mixtures specified in the cell are then collapsed using these point fluxes and point cross sections. Limitations of the LATTICECELL treatment include the following:

1. The cell description is limited to a 1-D cell. Most physical systems consist of 3-D geometry, but in many instances a 1-D representation is adequate, as in the case of a large array of spheres in a regular lattice, a large array of slabs, or a large array of long uniform pins in a regular lattice. A 1-D representation may be inadequate for systems exhibiting a 2-D or 3-D spatial dependence.
2. The LATTICECELL treatment assumes an infinite array of 1-D cells. This assumption is an excellent approximation for large arrays of long fuel pins or large arrays of spherical pellets. The approximation becomes less rigorous for short fuel pins and/or small arrays where multidimensional spatial dependence or leakage can become important.

### 7.3.3 MULTIREGION

The MULTIREGION treatment is appropriate for geometric regions where the geometry effects may be important, but the infinite homogeneous treatment or lattice cell treatment is not general enough. The MULTIREGION unit cell allows more flexibility in the placement of the fuel but requires all regions of the cell to have the same geometric shape (i.e., slab, cylinder, sphere, buckled slab, or buckled cylinder). Lattice arrangements can be approximated by specifying a white boundary condition on the outer boundary. Limitations of the MULTIREGION cell treatment are listed below.

1. A MULTIREGION cell is limited to a 1-D approximation of the system being represented. This constraint is appropriate for a sphere, an infinitely long cylinder, a slab, or an infinite array of slabs.
2. The shape of the outer boundary of the MULTIREGION cell is the same as the shape of the inner regions. Cells with curved outer surfaces cannot be stacked to represent arrays. However, arrays can be represented by making a curved outer region of equal volume to the cuboidal outer region and specifying a white outer boundary condition.
3. The boundary conditions available in a MULTIREGION problem include vacuum (eliminated at the boundary), reflected (reflected about the normal to the surface at the point of impact), periodic (a particle exiting the surface effectively enters an identical cell having the same orientation and continues traveling in the same direction), and white (isotropic return about the point of impact). Reflected and periodic boundary conditions on a slab can represent a real physical situation but are not valid on a curved outer surface.
4. A MULTIREGION cell represents a single cell if the outer boundary has a vacuum boundary condition applied to it. If NITAWL is specified, the cross-section treatment then uses an interlump (i.e., lump-to-lump) Dancoff factor of zero in the geometric correction calculations. If CENTRM is specified, a point flux spectrum is calculated over a set of intervals that make up the unit cell with the incoming flux on the boundary set to zero. This flux spectrum is then used to collapse a set of point cross sections.
5. If the outer boundary of a MULTIREGION cell has a boundary condition other than vacuum, the unit cell approximates an array. If NITAWL is specified, the interlump Dancoff correction is approximated by homogenizing the adjacent zones and computing the transmission through the homogenized material. This value is correct for a slab having a reflected or periodic boundary condition but is inexact for a curved surface. If CENTRM is specified, a point flux spectrum is calculated over a set of intervals that make up the unit cell with the incoming flux to the outgoing flux on the boundary. This flux spectrum is then used to collapse a set of point cross sections. For a slab having a periodic or reflected boundary condition, the incoming and outgoing fluxes are exact, but for a curved surface, the incoming flux is approximated by an isotropic return flux.

6. For NITAWL cases, the intralump (i.e., within the lump) Dancoff factor is determined using homogenized interior zones.

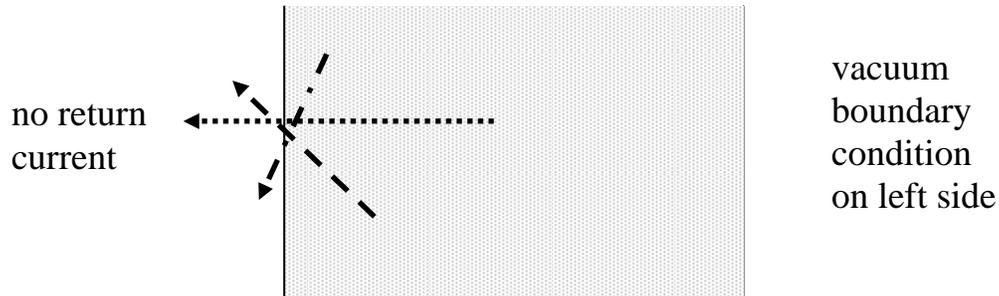
**NOTE:** If you want to apply boundary conditions to your unit cell model, then you must use the MULTIREGION cell treatment.

### 7.3.3.1 Boundary Conditions

For the MULTIREGION unit cell, there are four possible boundary conditions. The default for the left or inner boundary is *Reflected* (required for a cylinder or sphere); the default for the right or outer boundary is *Vacuum*.

#### Vacuum Boundary Condition

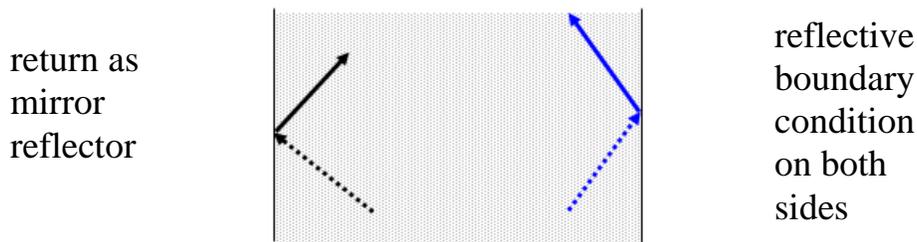
A vacuum boundary condition means that no neutrons will re-enter the boundary. Thus, any neutron exiting the system through a vacuum boundary is permanently lost to the system. This condition is shown in Fig. 115. (NOTE: In the following figures, a dashed arrow indicates neutrons leaving the system. A solid arrow represents those returning to the system. The length of the arrow is proportional to the number of neutrons, so longer arrows represent more neutrons than shorter arrows.)



**Fig. 115. Vacuum boundary conditions.**

## Reflective Boundary Condition

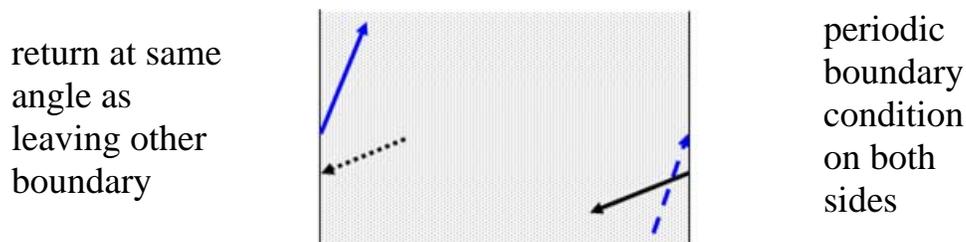
For the reflective boundary condition, the incoming angular flux is set equal to the outgoing angular flux in the direction corresponding to mirror or specular reflection. The reflective boundary should not be used on curved surfaces, that is, the outer boundary of a cylinder or sphere. It is the default (and required) for the left or inner boundary of a cylindrical or spherical system. As shown in Fig. 116, a given quantity of neutrons leaving a boundary (dotted line) in a particular direction will be returned (solid line of same color) to the system with the same quantity but at a mirrored angle to the initial leakage direction.



**Fig. 116. Reflective boundary condition.**

## Periodic Boundary Condition

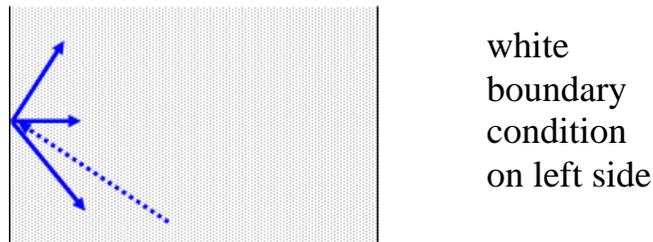
For the periodic boundary condition, the incoming angular flux on a boundary is set equal to the outgoing angular flux on the opposite boundary. Fig. 117 shows the leakage leaving each boundary (dotted lines) being returned at the same quantity and angle on the opposite boundary (solid line of same color). When the periodic boundary condition is used, it must be applied to both opposing boundaries. It should not be used on curved surfaces, that is, either boundary of a cylinder or a sphere.



**Fig. 117. Periodic boundary condition.**

## White Boundary Condition

For the white boundary condition, the incoming angular fluxes are each set equal to a single value chosen such that the net flow across the boundary is zero. The white boundary provides isotropic return (solid lines) at a boundary (see Fig. 118) and is suitable for all geometries. Although the white boundary condition is in a sense nonphysical on a curved surface, it is the best possible approximation of a reflective or repeating boundary condition, such as a lattice cell.



**Fig. 118. White boundary condition.**

## 7.4 UNIT CELL SPECIFICATIONS

Unit cell data are not required for IHFHOMMEDIUM. With the LATTICECELL and MULTIREGION treatments, you must specify the unit cell dimensions and materials to be used in the resonance self-shielding process. The unit cell is always 1-D: infinitely long cylinders, infinite slabs, or spheres. Finite cylinders or slabs can be approximated with geometric buckling in MULTIREGION cells. The configuration of the unit cell depends on the treatment and the type of lattice (if the LATTICECELL treatment is used).

### 7.4.1 LATTICECELL Unit Cell Data

For the LATTICECELL treatment, both “regular” and “annular” cells are allowed. These cells are rigorously constrained as to the placement of fuel, gap, clad, and moderators. Materials not used in the cell are treated as infinite homogeneous media. The “regular” cells allow spherical, cylindrical, or symmetric slab fuel regions that are constrained to a central fuel region surrounded by an optional gap, an optional clad, and an external moderator material. The “annular” cells for spherical, cylindrical, or asymmetric slab configurations are constrained to a central (second) moderator material surrounded by a fuel region having an optional gap and optional clad on both sides of the fuel with an external (first) moderator material.

The unit cell data in a LATTICECELL problem are used (1) to provide the dimensions and shape of the lump and the moderator material for resonance cross-section processing, (2) to provide lattice corrections for the cross-section processing, and (3) to provide information used in creating cell-weighted cross sections when XSDRNPM is executed. CELLMIX= must be specified in the unit cell data if cell-weighted cross sections are used in the problem.

### **7.4.2 MULTIREGION Unit Cell Data**

For the MULTIREGION treatment, the unit cell is more flexible than that of the LATTICECELL treatment. In fact, the MULTIREGION treatment allows complete freedom in the placement of materials but is constrained by shape (i.e., only concentric regions of the same shape are allowed). MULTIREGION does not account for lattice effects, so it is best used for problems where lattice effects are not important.

### **7.4.3 Cell-Weighted Cross Sections**

Cell-weighted cross sections are created by XSDRNPM when CELLMIX= is specified in the unit cell data. The unit cell description is then used by XSDRNPM to calculate the eigenvalue of the cell. For LATTICECELL problems, a white boundary condition is assumed. For MULTIREGION problems, the boundary conditions specified in the unit cell are used. The resultant fluxes are used to weight the cross sections of the materials in the cell and create homogenized cell-weighted cross sections that have the characteristics of the heterogeneous cell configuration. Whenever XSDRNPM is executed for cross-section processing, only the cell-weighted mixture number can be used in the KENO V.a geometry data. The original mixtures used in the unit cell description cannot be used. Refer to the SCALE Manual [Sect. M7.5.12] for more information on cell-weighting.

## **7.5 PROBLEM DESCRIPTIONS**

Two example problems will be used to demonstrate how to enter unit cell data for LATTICECELL and MULTIREGION unit cell types using GeeWiz. The first problem is a 9×9 fuel assembly array of UO<sub>2</sub> fuel rods with Zircaloy-2 cladding. The second problem involves two parallel, fully reflected SS304 slab tanks containing U(93)O<sub>2</sub>F<sub>2</sub> solution.

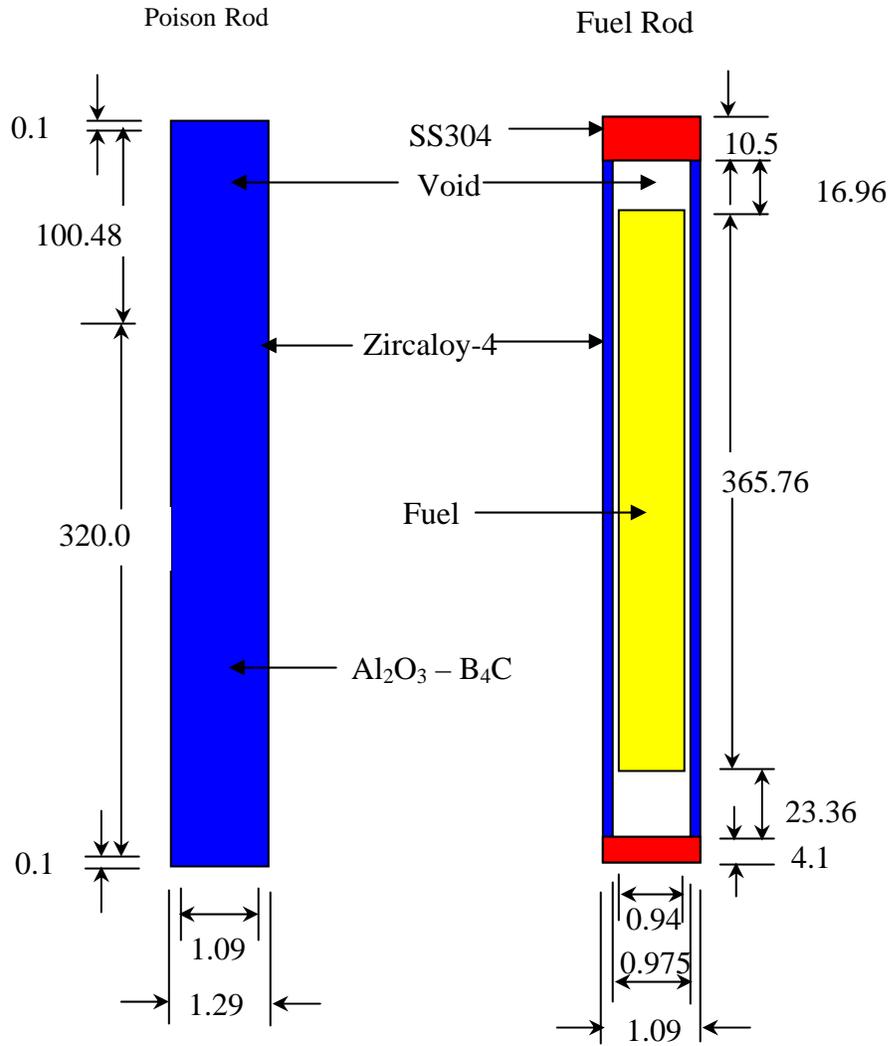
### **7.5.1 Lattice Cell Example: 9 × 9 Fuel Assembly**

This problem is a single fuel assembly at 3.44 wt % enrichment stored in a pool of water at a temperature of 300 K. There is 15.24 cm of water above and below the assembly shroud and 7.62 cm of water on each side of the assembly shroud. The inside dimensions of the shroud are 14.96 cm in the X- and Y-dimensions and 420.68 cm in the Z-dimension. The space between fuel rods is full-density water. The shroud is 304 stainless steel, 0.16 cm thick on all faces. The array of fuel rods and poison rods comprising the assembly is centered within the shroud.

The fuel rods are 0.94 cm in diameter and contain  $\text{UO}_2$  at 92.5% of theoretical density. The active fuel length is 365.76 cm. Each fuel rod is contained within Zircaloy-2 cladding with an inner radius of 0.4875 cm and an outer radius of 0.545 cm. The cladding extends 16.96 cm above the top of the active fuel and 23.36 cm below the bottom of the active fuel. The ends are capped with solid SS304 plugs having the same OD as the cladding. The top plug is 10.5 cm thick and the bottom plug is 4.1 cm thick. The axial configurations of the poison rods and the fuel rods are shown in Fig. 119.

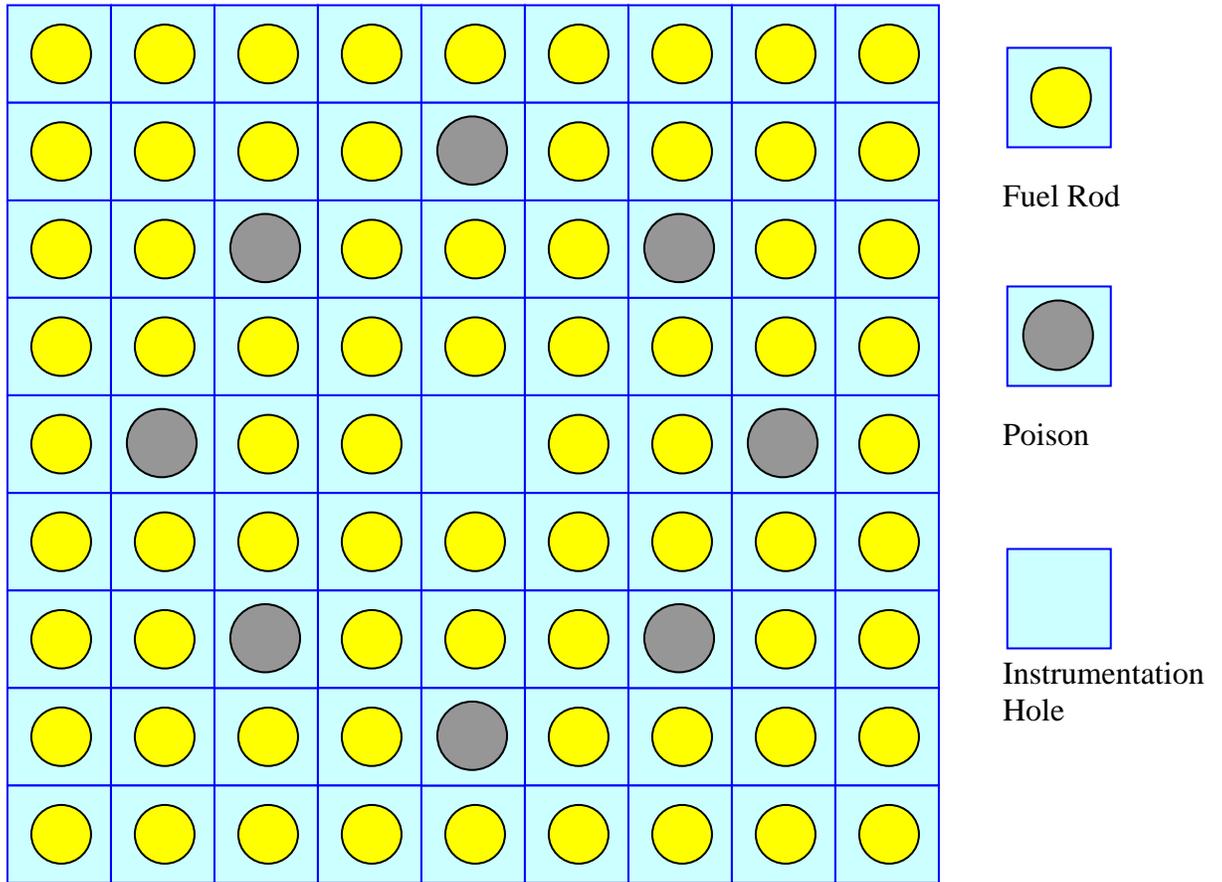
The fuel assembly has a water-filled central instrumentation hole with eight burnable poison rods in various lattice positions, as shown in Fig. 120. The burnable poison rods are composed of  $\text{Al}_2\text{O}_3\text{-B}_4\text{C}$ , having a density of 3.7 g/cc and are 1.260 wt %  $\text{B}_4\text{C}$ . The boron in the  $\text{B}_4\text{C}$  is natural boron. The burnable poison rod has a diameter of 1.09 cm and an active poison length of 320.0 cm. A 100.48 cm void space extends above the active poison rod. The poison rod and void space have a tight fitting 0.1-cm-thick Zircaloy-2 cladding. The rod pitch within the assembly is 1.64 cm.

### Axial Rod Layout



NOT TO SCALE  
(All dimensions in cm)

**Fig. 119. Axial layout of assembly rods.**



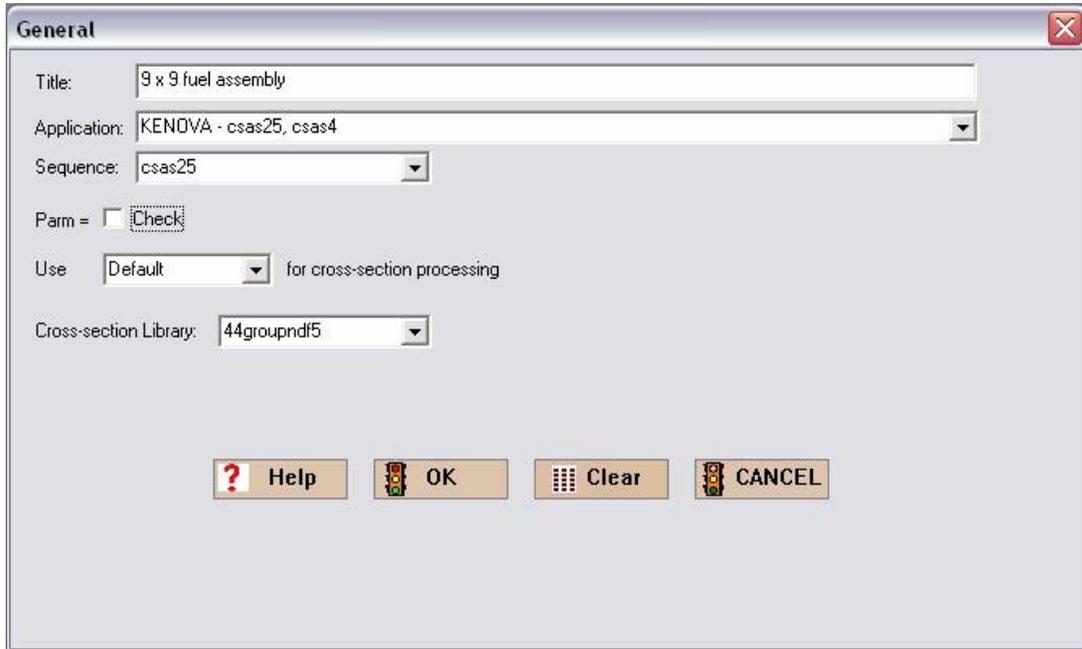
**Fig. 120. Plan view of rod positions in  $9 \times 9$  assembly.**

### 7.5.1.1 General and Material Data

The initial data entry for this example is the same as previous problems. Start the GeeWiz user interface and then select the **New** button from the top toolbar. Select the **General** button on the left-hand side and enter the problem **Title**, **Application**, the **SCALE Sequence**, select `Default` for cross-section processing and the 44-group library as the **Cross-section Library**. Unit Cell information is entered later in GeeWiz. The **General Information** window should look like that in Fig. 121.

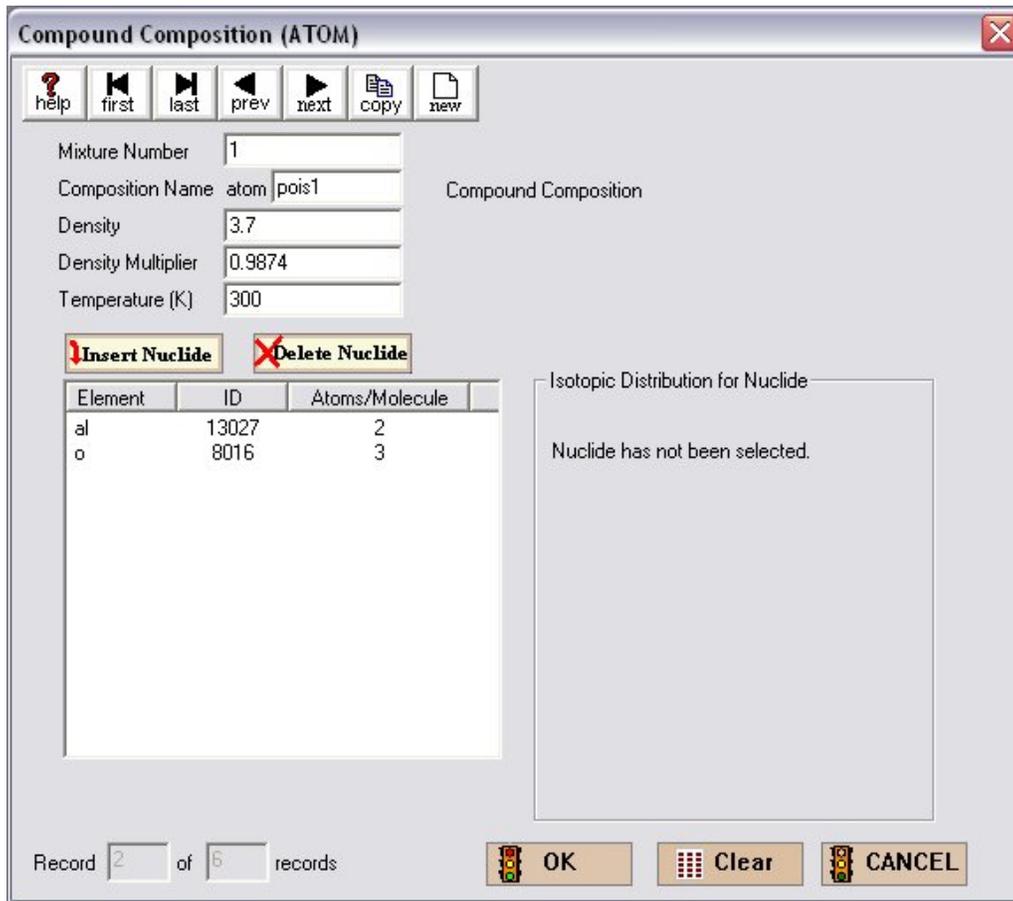
Now we need to enter the **Materials** information. For four of the materials, Basic Standard Compositions can be used: `h2o` (Composition No. 2), `uo2` (Composition No. 3), `zirc2` (Composition No. 4), and `ss304` (Composition No. 5). You should be able to enter the information for these from the problem statement. The default theoretical densities are used for all. All materials have a **Density Multiplier** of 1.0 except `uo2`, which has a **Density**

**Multiplier** of 0.925. Also remember that the  $u_{O2}$  is 3.44 wt %  $^{235}\text{U}$ , so the isotopics need to be entered for this material.



**Fig. 121. General information for lattice problem.**

For the burnable poison, we will enter the data as shown in the example in Sect. 6.2.3. The burnable poison has a density of 3.7 g/cc and is a combination of  $\text{B}_4\text{C}$  and  $\text{Al}_2\text{O}_3$ . The material is 1.260 wt %  $\text{B}_4\text{C}$  with natural boron. As before, we will specify this mixture using a compound material for  $\text{Al}_2\text{O}_3$  and a basic composition for the  $\text{B}_4\text{C}$ . From the composition summary screen, select **Create** and then select **Compound** (atom). For **Mixture Number** enter 1 as we will call this mixture or composition 1. For **Composition Name** enter `pois1`. Now for the **Density**, enter the mixture density of 3.7 g/cc with a **Density Multiplier** of  $(1-0.0126) = 0.9874$ . Then select **Insert Nuclide** to enter the information for `a1` (2 atoms per molecule) and for `o` (3 atoms per molecule). When completed, the input form should look like Fig. 122. Click **OK**.



**Fig. 122. Data for  $\text{Al}_2\text{O}_3$  portion of burnable poison mixture.**

For the  $\text{B}_4\text{C}$ , click the **Create** button, then select **Basic Composition** as the type. Change the **Mixture Number** to 1 so that it will be part of the arbitrary poison mixture. For **Composition Name** select  $\text{b}_4\text{c}$ , and a **Density Multiplier** of 0.0126. Because the boron is natural, we don't need to alter the **Isotopic Distribution**. Select **User Supplied (g/cc)** and enter the mixture **Density** of 3.7 g/cc. The completed information should look like Fig. 123. Click **OK**.

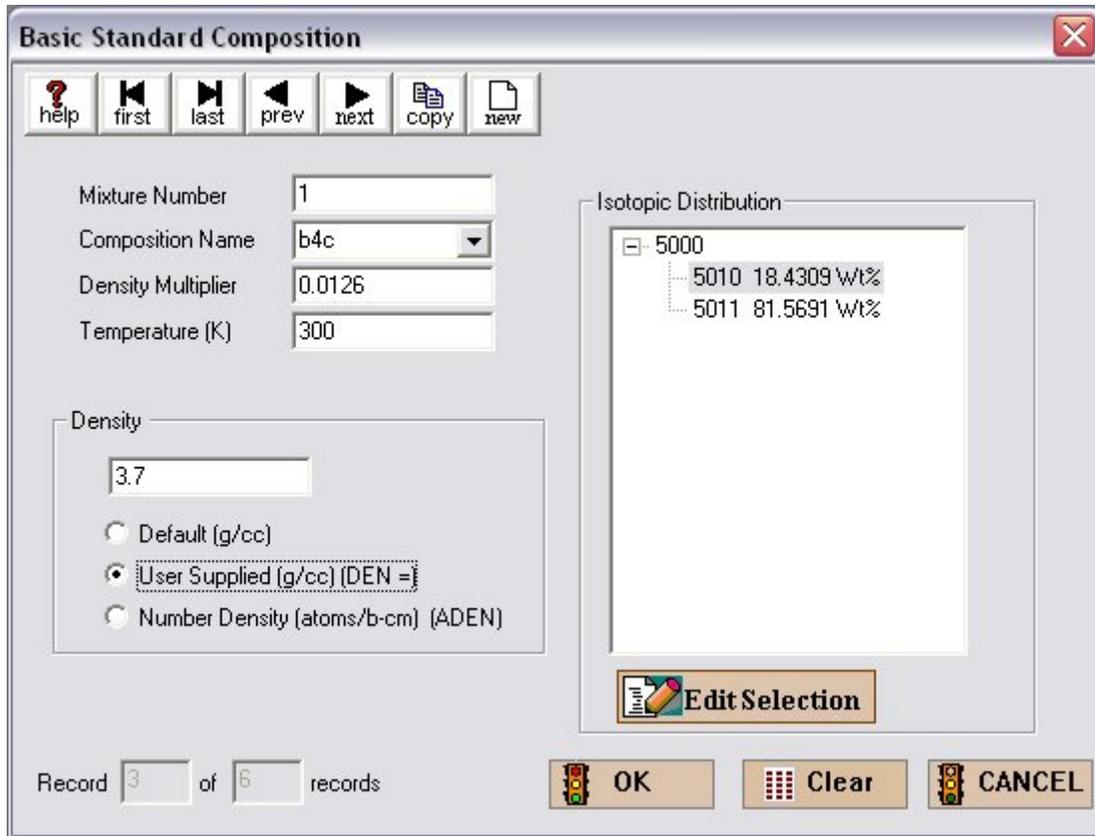


Fig. 123. B<sub>4</sub>C portion of burnable poison mixture.

### 7.5.1.2 Unit Cell Data

Now that we have entered the material information, we are ready to enter the unit cell information for the cross-section treatment. Selecting the **Cell Data** button on the left-hand toolbar will open the **Unit Cell Data** window, where you enter the unit cell data. By default, the **Lattice Cell** tab is active. To create a new lattice cell, click on **New Cell** to bring up the **Lattice Cell Data** form shown in Fig. 124. The first entry is **Type of Lattice**. The menu has a number of choices; those starting with the letter A are for annular lattices. In this problem, we have a regular square pitch lattice, so select **SquarePitch** from the menu. Now we need to give the dimensions of the unit cell and the materials for the fuel, clad, and moderator. First, enter 0.82 (=1.64/2) for the **Half Pitch (cm)** and 0.47 (=0.94/2) for the **Fuel Radius (cm)**. Select the 3 uo2 material from the menu for **Fuel Mixture**. The moderator is water, so select the 2 h2o material from the menu for **Moderator Mixture**. The fuel rods have both a gap and a clad so we need to check the **Clad/Gap Exists** box. Checking this box activates data entry for the **Clad** and the **Gap**.

**Lattice Cell Data**

Unit Cell Description

Type of Lattice: SquarePitch

Half Pitch (cm): 0.82

Fuel Radius (cm): 0.47

Fuel Mixture: 3 uo2

Moderator Mixture: 2 h2o

CELLMIX =

\*\* CELLMIX value should not be an existing mixture number.

Clad/Gap Exists

Clad Radius (cm): 0.545

Clad Mixture: 4 zirc2

Gap Radius (cm): 0.4875

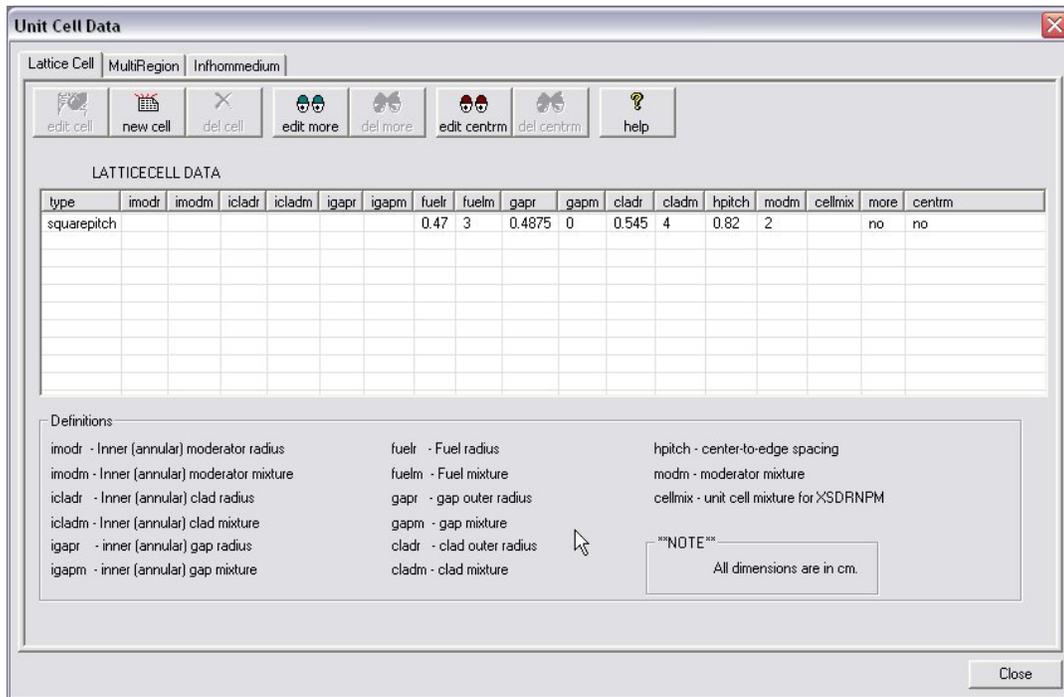
Gap Mixture: 0 void

? Help    OK    CANCEL

**Fig. 124. Lattice cell data.**

For the clad, enter 0.545 ( $=1.09/2$ ) for the **Clad Radius (cm)** and select material 4 zirc2 for the **Clad Mixture**. For the gap, enter 0.4875 ( $=0.975/2$ ) for the **Gap Radius (cm)** and select material 0 void for the **Gap Mixture Number**. Note that the **Gap Radius** is the inner radius of the clad. The completed Lattice Cell form should look like Fig. 124.

Now click **OK** and you will see the information summarized on the **Unit Cell Data** screen shown in Fig. 125. This completes the Unit Cell Data, so save the information by clicking on **Close**.



**Fig. 125. Unit cell data.**

### 7.5.1.3 REPLICATE Command

Before entering the **KENO Geometry** data for this problem, we will introduce another geometry command that you will find useful when describing reflectors and other external shapes. **REPLICATE** is used to generate additional geometry regions having the shape of the previous region. **REPLICATE** can be thought of as adding layers of different materials or reflectors. The **REPLICATE** button is only active when the region to be replicated is highlighted. When selected, it replicates the shape just above it but extends its dimensions by a specified thickness. The required information for the **REPLICATE** command includes the material in the new outer region, the delta dimensions (i.e., thicknesses) beyond the previous region, and the number of replicated regions using these thicknesses. For example, if the previous region is a cuboid, then the delta dimensions are the thickness in the X-max, X-min, Y-max, Y-min, Z-max, and Z-min directions. If the previous region is a cylinder, then the delta dimensions are the additional thickness in the radius and the top and bottom thicknesses.

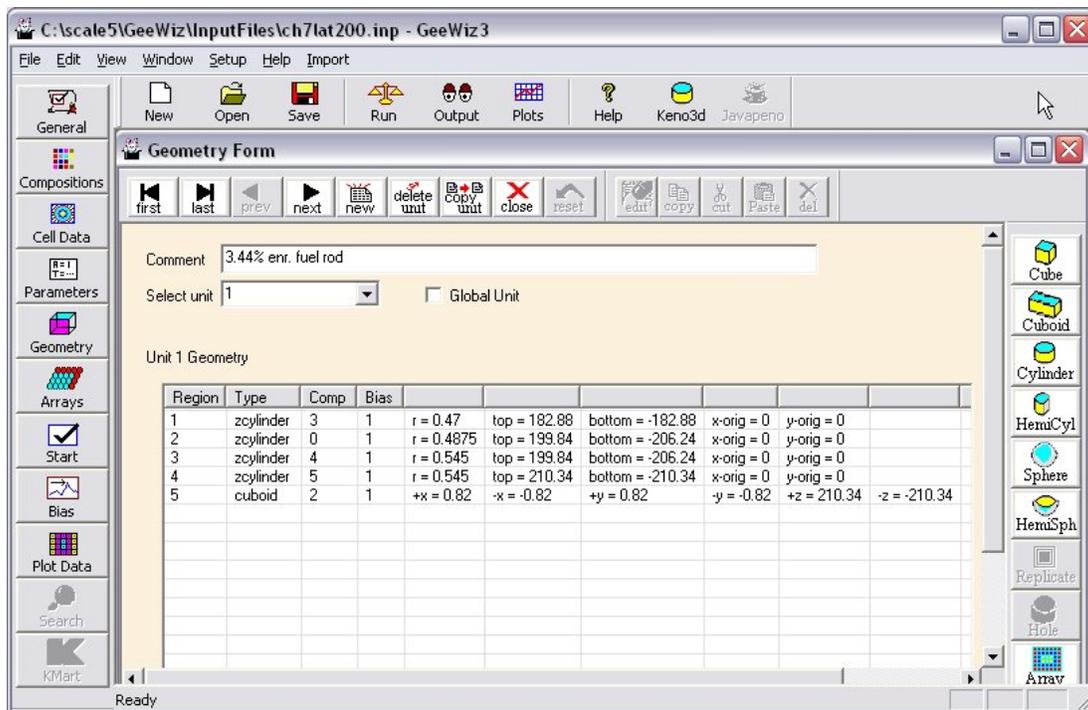
A **REPLICATE** command can follow a **REPLICATE** command, indicating that the second region reproduces the first but is outside it with the given delta dimensions. This capability could be used to model different reflector materials with different thicknesses on different faces, or it could be used when creating a fuel rod with gap and clad. The rod would be a cylinder with a given radius and height. The gap would then replicate the cylinder shape with a

gap radial thickness and delta height above the rod. Then the clad would replicate the gap cylinder with a clad radial thickness and a delta thickness above the top of the gap and below the fuel rod bottom. Note that the deltas can be 0.0 if the surfaces are coincident. An example of the REPLICATE command is given in the next section.

### 7.5.1.4 KENO V.a Data

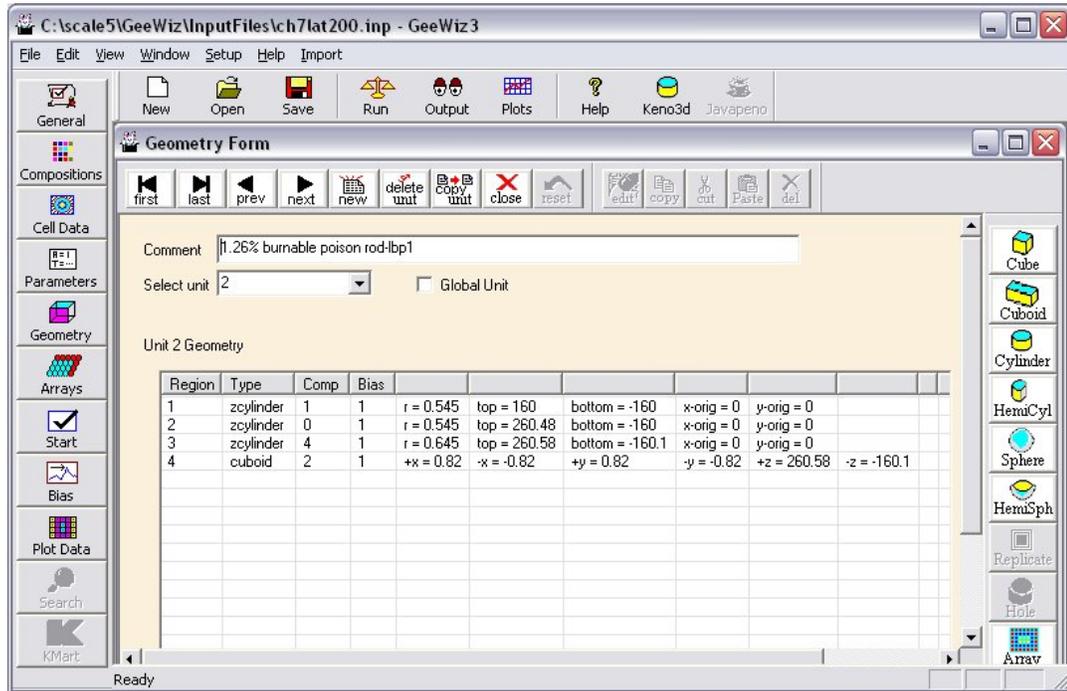
For the KENO input form, select the **Geometry** button. In this problem, we will define four units as follows. Unit 1 will be a fuel rod cell; Unit 2 will be a burnable poison rod cell, Unit 3 will be the instrumentation tube cell, and Unit 4 will be the global unit containing the array of rods and the surrounding shroud and water.

We will start with unit 1. The first shape is the fuel cylinder, which is then enclosed by the gap cylinder, and then the clad cylinder. Enter the data for these three shapes using the dimensions from Fig. 119. The fuel rod has end caps made from SS304; they require a fourth cylinder enclosing the previous three cylinders. The radial dimension of this cylinder is the same as that of the clad cylinder, and the additional height is to account for the cap thickness at the top and bottom of the rod. Remember that any unit used in an array must have flat surfaces where it touches other array elements; so we need a fifth shape, a cuboid that encloses the fuel rod and contains the moderator (water). The X- and Y-dimensions are  $\pm 0.5 * \text{pitch}$  while the Z-dimensions are the same as those for the SS304 end caps. When the data have been entered, the Geometry form should look like Fig. 126.



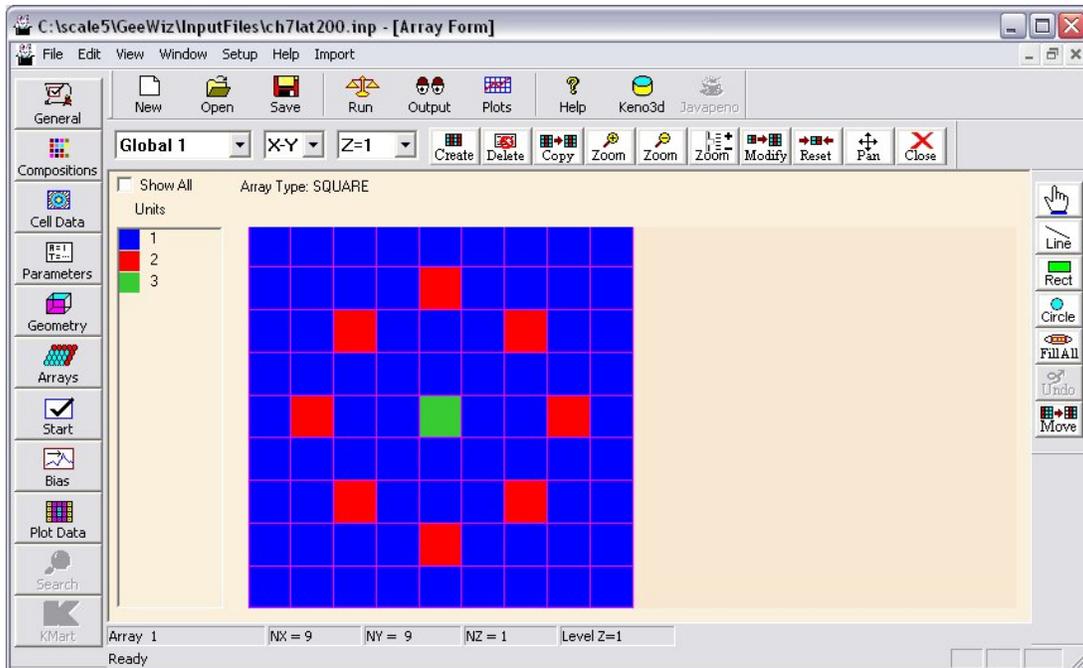
**Fig. 126. Geometry information for a fuel rod.**

Unit 2 is the burnable poison rod. This unit is handled like unit 1 but with three cylindrical shapes instead of four. (The end caps are made of the same material as the cladding.) Enter the data using the dimensions from Fig. 119. Now enclose the cylinders in a cuboid containing the moderator. The X- and Y-dimensions are again  $\pm 0.5 * \text{pitch}$  while the Z-dimensions are the same as those for the `zirc2` cylinder. When the data have been entered, the Geometry form should look like Fig. 127.



**Fig. 127. Geometry information for burnable poison rod.**

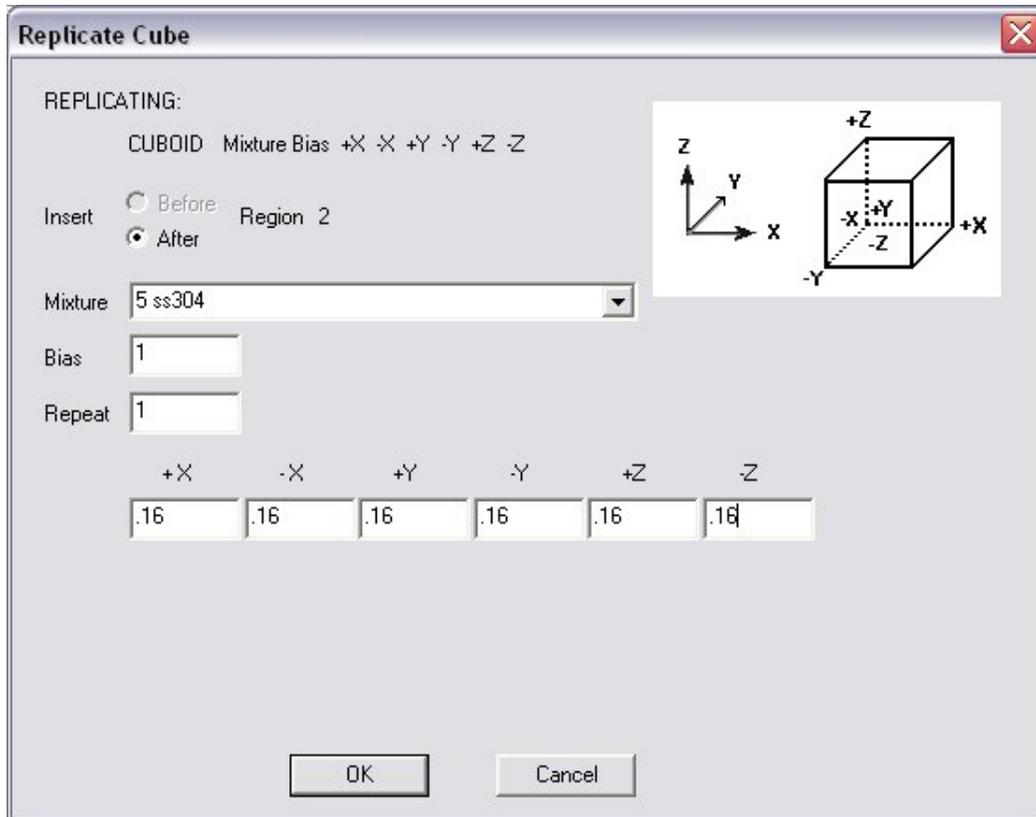
For unit 3, the geometry is quite simple. We have a cuboid containing water with the same dimensions as the cuboid from unit 2. Before defining unit 4, which is the global unit, we need to define the array. In this case, the array is nine units in the X-, nine units in the Y-, and one unit in the Z-directions. Open the **Arrays** window and set up a new array with **NUX** = 9, **NUY** = 9, and **NUZ** = 1. Select Unit 1 as the unit to initialize new locations. Then, using Fig. 120, place the poison rods (unit 2) and the instrumentation tube (unit 3) into their appropriate positions. Provide a comment for the array and then save the information. The screen should look like Fig. 128.



**Fig. 128. Array layout for  $9 \times 9$  fuel assembly problem.**

Now we will enter the data for the global unit, unit 4. The first region in unit 4 will be the array. Parameters for an array as a region in a unit include the Array Number, and the X, Y, and Z coordinates of the lower left-hand corner. For this problem, the **Array No.** is 1, and the lower left-hand corner is located at  $(-7.38, -7.38, -210.34)$ . The **X-neg** is  $-7.38$  ( $9 * \text{the half-pitch}$ ), the **Y-neg** is  $-7.38$  ( $9 * \text{the half-pitch}$ ), and the **Z-neg** is  $-210.34$  (half of the fuel assembly height). These values place the origin at the center of the fuel assembly.

The next region is the cuboid containing the water inside the stainless steel shroud. The shroud is 14.96 cm in width (inside dimension), so the X- and Y-dimensions will be  $\pm 7.48$  while the Z-dimensions are  $\pm 210.34$  (half of the fuel assembly height). The SS304 shroud is a cuboid whose thickness is 0.16 cm greater than the cuboid just entered. For this we will use the REPLICATE command. To do this, select the shape to be replicated; in this case the cuboid of region 2. Then from the right-hand toolbar, select **Replicate** to bring up the **Replicate Cube** form. Notice that the form indicates that you are replicating a cuboid and that the new cuboid will be inserted after region 2. Select 5 ss304 as the **Mixture**; leave the **Bias** as 1 and **Repeat** (number of regions) as 1. Now we need to enter the **delta thicknesses** in the +X, -X, +Y, -Y, +Z, and -Z-directions. These are all 0.16; note that the delta values must always be positive, including the -X, -Y, and -Z deltas. The information should match that in Fig. 129.



**Fig. 129. Replicate screen for stainless steel shroud.**

Note that the **Bias** field contains the Bias ID for that region. Biasing can be used in the outer reflector in KENO V.a to reduce the CPU time needed for tracking neutrons in the reflector. The default Bias ID is 1 (i.e., no biasing) and should be used in all internal regions. Because KENO V.a runs very fast on modern computers, biasing is seldom used and will not be used in this primer.

The last entry handles the water outside the shroud. This is a cuboid shape so we will use REPLICATE to add thickness to the outside of the shroud cuboid (region 3). To do this, select the shape to be replicated; in this case the cuboid of region 3. Then from the right-hand toolbar, select **Replicate** to bring up the **Replicate Cube** form. Notice that the form indicates that you are replicating a cuboid and that the new cuboid will be inserted after region 3. Select 2 h<sub>2</sub>O as the **Mixture**, and leave the **Bias** as 1 and **Repeat** (number of regions) as 1. We have different thicknesses, so we enter the delta thicknesses of 7.62 in the +X, -X, +Y, and -Y directions and 15.24 in the +Z, and -Z directions. After entering this information, click **OK** and return to the Geometry Form for the unit. Unit 4 is the global unit, so we need to check the **Global Unit** box and provide a Comment for this unit. The completed geometry form should look like Fig. 130.

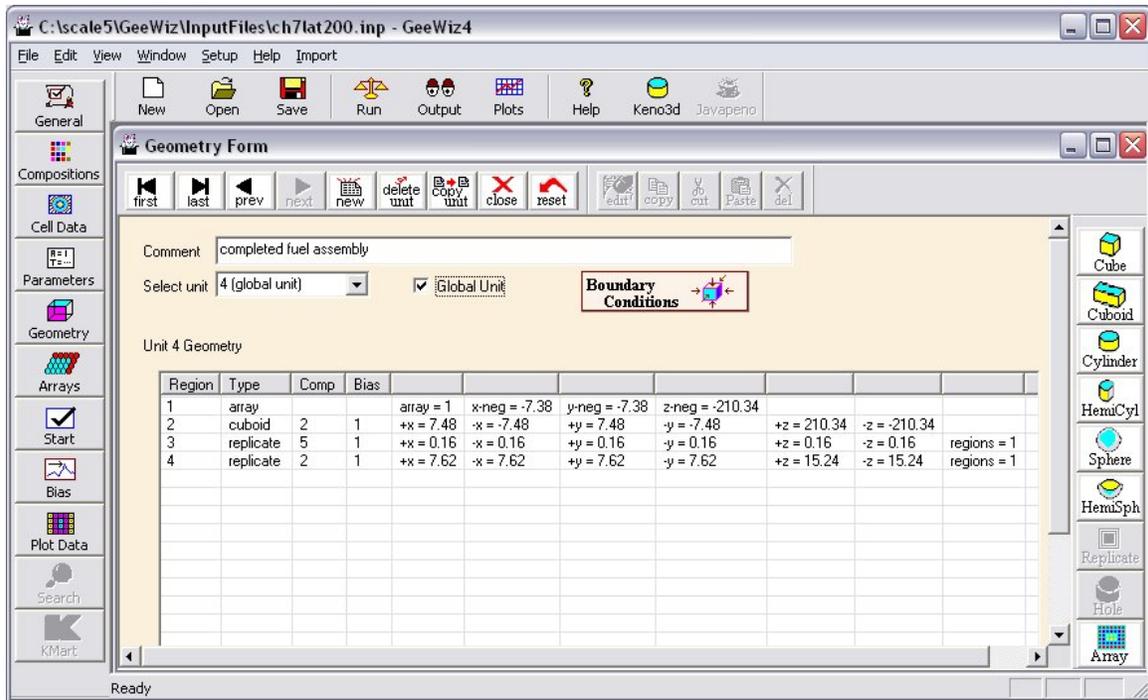


Fig. 130. Global unit for  $9 \times 9$  fuel assembly.

Because this geometry model is more complex than previous examples, we want to run 1003 generations, skipping the first 3 generations. To change the run parameters, select **Parameters** from the left-hand side menu. This brings up the screen shown in Fig. 131. We will change the number of generations (**GEN=**) from 203 to 1003. Then click **OK**.

**Parameter Data** ✖

Key Parameters | Numeric Parameters | Logical Parameters | I/O Unit Numbers

GEN =  # of generations

NPG =  # per generation

NSK =  Generations skipped

RES =  Generations between restart

RND =  Random Number (12 hex digits)

TME =  Execution time (in minutes)

WRS =  Write restart unit number

FAR (Fiss./abs. by region)

GAS (Group average summary)

FDN (Fission densities)

FLX (Print Fluxes)

PLT (create 2-D plots)

RUN (Execute KENO)

MFP (Compute Region Mean Free Paths)

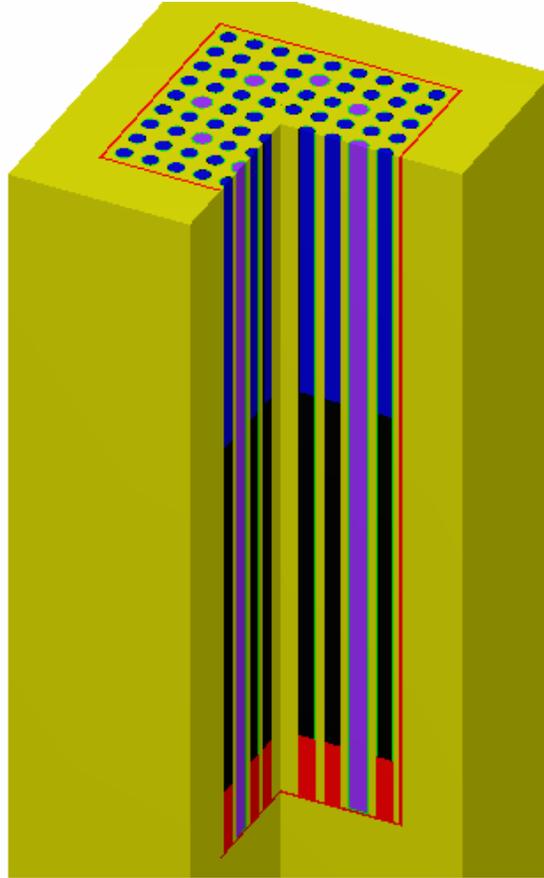
CFX (Compute Flux Densities)

**\*\*Warning! Reset Defaults cannot be cancelled or undone**

Reset

**Fig. 131. Parameters data.**

A cutaway view from KENO3D of the bottom portion of the completed assembly is shown in Fig. 132. This view was obtained by using the **Remove section** button in KENO3D twice. First the top half was removed, then the front right quarter.



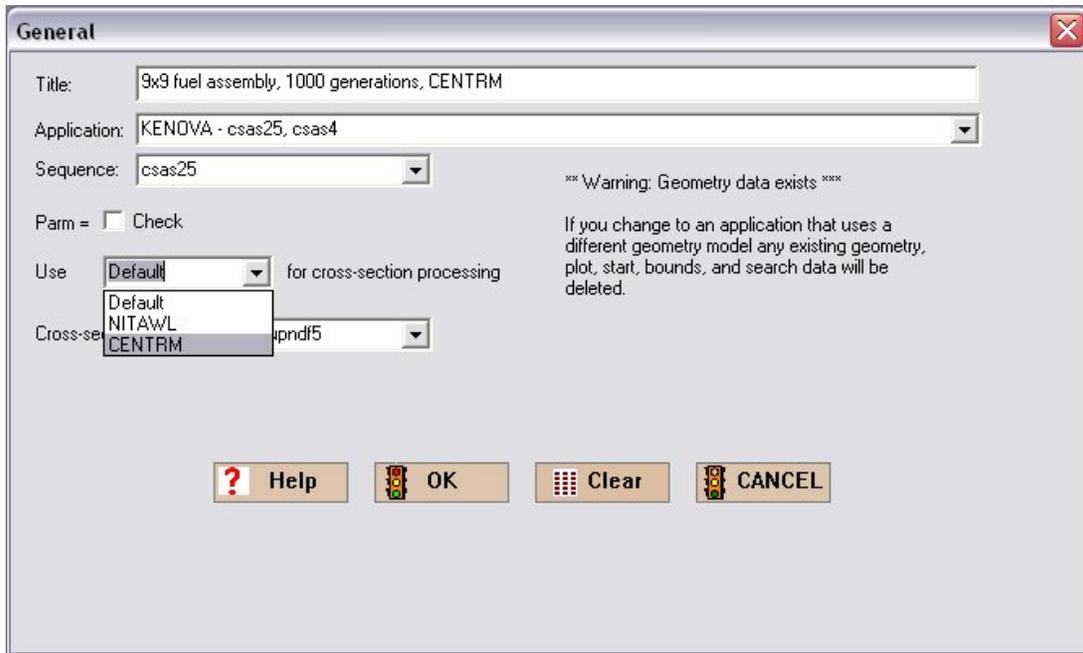
**Fig. 132. 3-D view of bottom part of  $9 \times 9$  array.**

Save the changes in a new input file and execute CSAS. For this problem, 1003 generations were run to stabilize the  $k_{\text{eff}}$ . The calculated  $k_{\text{eff}}$  with 1000 generations is  $0.61514 \pm 0.00072$  while for 200 generations, it is  $0.6118 \pm 0.0018$ .

#### **7.5.1.5 Using CENTRM to Process Cross Sections**

For the above example we used NITAWL, which is the default in SCALE 5, to process the resonances and cross sections. If we want to use CENTRM to process the lattice cell data in SCALE 5, we need to first select the General window and change the cross-section processing option to **CENTRM**, as shown in Fig. 133. You might also want to change the title to indicate CENTRM processing. Click **OK** and then **Save As...** to create a different input file. If you are using SCALE 5.1, no action is required because the default option is CENTRM.

The calculated  $k_{\text{eff}}$  with 1000 generations is  $0.61191 \pm 0.00077$ . If you get a significantly different answer (about 0.50) for  $k_{\text{eff}}$ , this probably indicates that CENTRM cross-section data have not yet been installed on the computer. So you need to install CENTRM cross-section data and rerun the analysis. If the continuous energy CENTRM data have not been installed, CENTRM uses multigroup data instead and prints warning messages that the continuous energy data for each nuclide could not be found. However, the multigroup data have not been resonance self-shielded, and the resulting calculated  $k_{\text{eff}}$  will be significantly lower than it should be.



**Fig. 133. Selecting CENTRM for cross-section processing.**

## 7.5.2 Multiregion Example: Two Parallel Slab Tanks

This problem consists of two parallel slab tanks constructed of 0.5-cm-thick SS304. The material in the tanks is  $U(93)O_2F_2$  with a fuel density of 0.459 g/cc and a solution density of 1.566 g/cc. Each slab tank has internal dimensions of 5 cm thick by 300 cm long by 150 cm high. Each tank is reflected by 5 cm of water on each side in the X-direction (i.e., 10 cm of water between the tanks). There is no reflector material above the tanks or on the ends of the tanks. See Fig. 134.

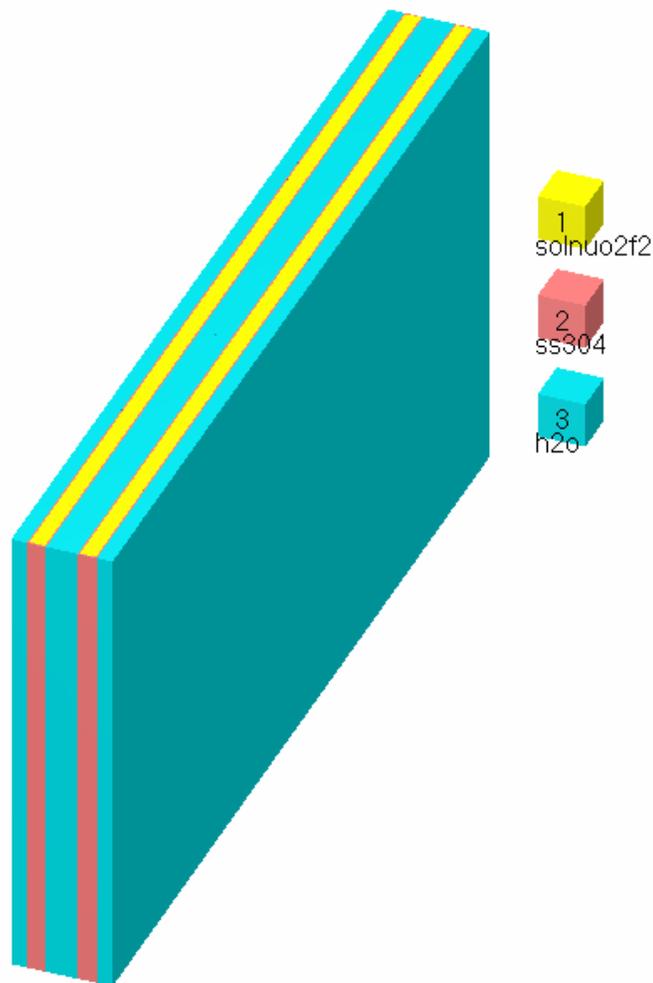
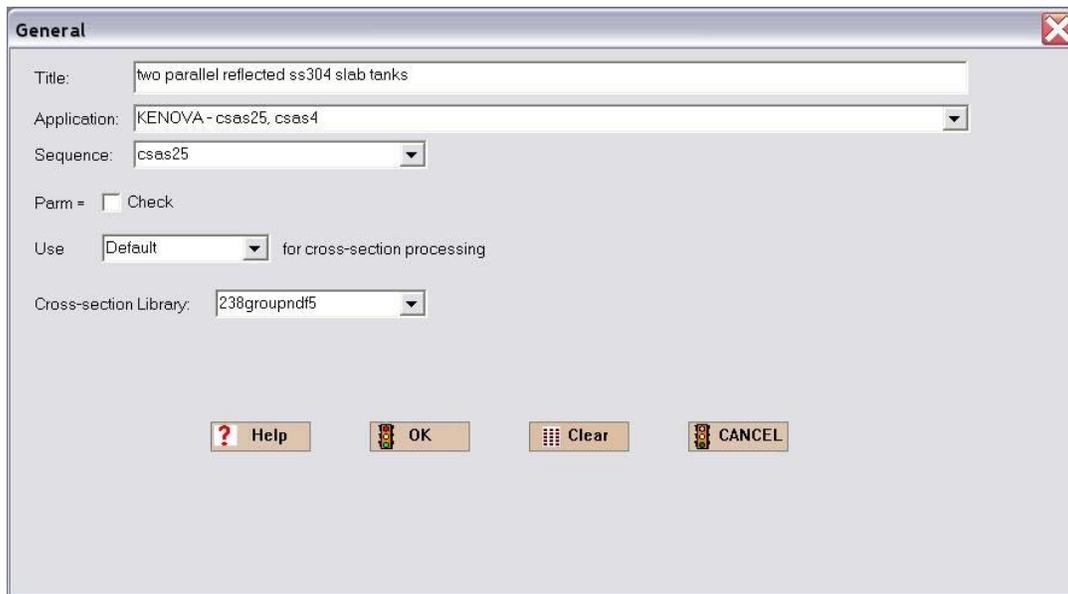


Fig. 134. Two parallel slab tanks.

### 7.5.2.1 General and Material Data

The initial data entry for this example is the same as previous problems. Start GeeWiz and select the **General** button. Enter the problem **Title**, the **Application** and **SCALE Sequence**, and the **Cross-section Library**. We will again use the `Default` for cross-section processing. The **General** information form should look like that in Fig. 135.



**Fig. 135. General information for multiregion problem.**

Now we need to enter the **Materials** information. For the three materials, Fissile Solution (Solution in SCALE 5.1) is used for  $uO_2F_2$  (Composition No. 1); Basic Composition is used for  $ss304$  (Composition No. 2) and  $h_2O$  (Composition No. 3). You should be able to enter the information for these from the problem statement. Remember that the  $UO_2F_2$  is 93 wt %  $^{235}U$ , so the isotopics need to be entered for this material. The solution has a **fuel density** of 459 g/l and a **specific gravity (solution density in SCALE 5.1)** of 1.566. The **acid molarity** is 0. The default theoretical densities are used for the other two materials. If you are using CENTRM for cross-section processing (default in SCALE 5.1), you will need to create two  $ss304$  and two  $h_2O$  mixtures because a unique mixture number is required for each region in the unit cell.



For the **Zone** information, you need to enter the mixture and position starting from the left or innermost and moving toward the right or outermost material. Remember that you are entering the information for a 1-D unit cell. Because the two tanks are symmetric, we will start with the centerline through the water between the two tanks and will work out to the external water reflector. For **Zone 1**, select 3 h2o as the **Mixture No.**, then enter 5.0 for the **Outside Cumulative Radius or Thickness (cm)**. For **Zone 2**, select 2 ss304 as the **Mixture No.**, and enter 5.5 (i.e., = 5.0 cm water + 0.5 cm SS304) for the **Cumulative Thickness (cm)**. For **Zone 3**, select 1 solnuo2f2 as the **Mixture No.**, then enter 10.5 for the **Outside Cumulative Radius or Thickness (cm)**. For **Zone 4**, select 2 ss304 as the **Mixture No.**, and enter 11.0 for the **Cumulative Thickness (cm)**. Finally for **Zone 5**, select 3 h2o as the **Mixture No.**, and then enter 16.0 (i.e., = 11.0 + 5.0) for the **Cumulative Thickness (cm)**. The completed **Multiregion Cell Data** form should look like Fig. 137. Note that if CENTRM is being used, each zone must contain a unique mixture number.

Multiregion Cell Data

Geometry Type: Slab

Left (Inner) Boundary Condition: Reflected

Right (Outer) Boundary Condition: Vacuum

Origin: 0

CELLMIX =

\* CELLMIX value should not be an existing mixture number.

\*\*\* Distance should increase with each zone.

Zone	Mixture	Distance from center-line (cm) ***
1	3	5
2	2	5.5
3	1	10.5
4	2	11
5	3	16

? Help    OK    CANCEL

**Fig. 137. Multiregion unit cell description.**

### 7.5.2.3 KENO V.a Data

For the KENO input form, select the **Geometry** button. In this problem, we will define one unit. Unit 1 will be a slab tank with fuel, stainless steel container, and water reflector. Because the two tanks are arranged symmetrically, we will use a mirror boundary condition to model the entire system.

The first region is the cuboid of fuel ( $5 \times 300 \times 150$  cm), which is then enclosed by the SS304 tank (0.5 cm thick) on five sides (not including the top), and by the 5-cm water reflector in the X-direction. Enter the data for these two shapes using the REPLICATE command as described earlier. We will use the center of the slab tank as the origin for the dimensions. For the SS304 tank, we add 0.5 cm on all sides but +Z where we enter 0. Remember, when using the REPLICATE command, all values must be non-negative, because they represent thicknesses. Also, remember to enter the **Repeat** for both the SS304 tank and the water reflector as 1. For the water reflector, the REPLICATE command is again used, but only the +X, and -X values are non-zero. Click **Global Unit**, and the **Boundary Conditions** button appears on the Geometry form. The Geometry form for the completed unit should look like Fig. 138.

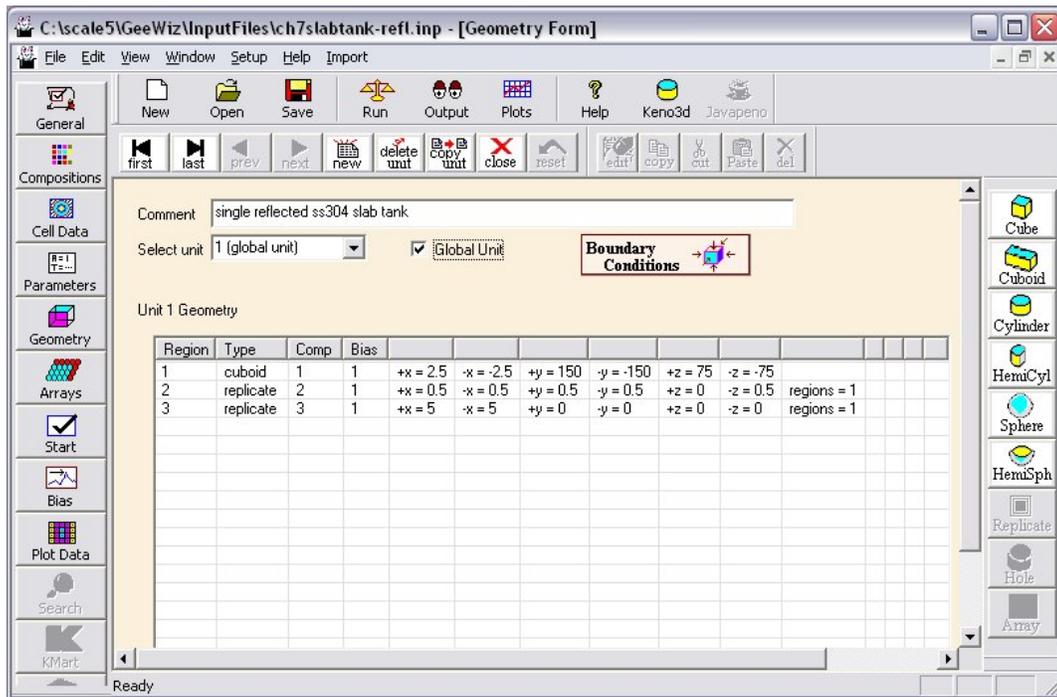
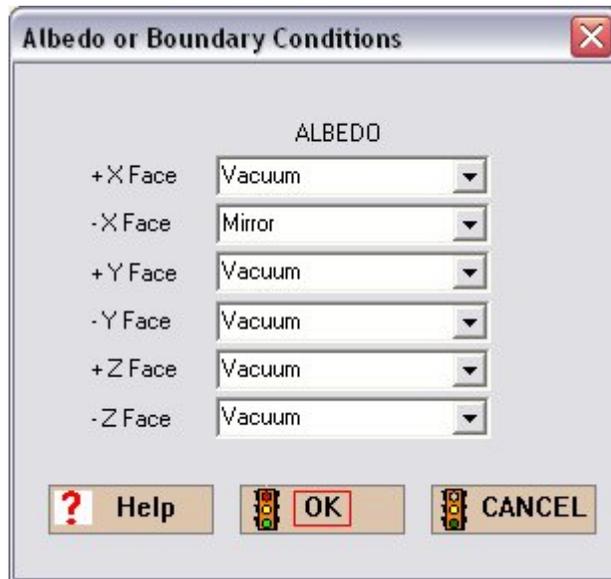


Fig. 138. Geometry information for slab tank.

Click on the **Boundary Conditions** button to open the **Boundary Conditions** form for the global unit. The default boundary conditions are vacuum. Change the boundary condition for the **-X** face to mirror. This setup will simulate an array of two tanks side-by-side. The form should look like that in Fig. 139.

Close all forms, save the changes in a new input file, and execute CSAS. The calculated  $k_{\text{eff}}$  value is  $0.9540 \pm 0.0022$ .



**Fig. 139. Boundary conditions form.**

## 7.6 SUMMARY

This section helped you to:

- Understand the difference in cross-section processing for Infinite Homogeneous Medium, Lattice Cell, and Multiregion Analyses.
- Identify the appropriate unit cell type to use for various heterogeneous systems.
- Use GeeWiz to define LATTICECELL and MULTIREGION unit cells.
- Define different boundary conditions for a MULTIREGION unit cell.
- Use the REPLICATE command to model reflectors or materials of a given thickness added to the outside of a shape.
- Use boundary conditions to create reflective boundaries for the KENO V.a global unit.

## 8. PLOTTING AND VISUALIZATION

A strongly recommended practice for all KENO users is to visually check their geometry models prior to performing calculations. This section discusses the use of the two-dimensional (2-D) and three-dimensional (3-D) plotting and visualization tools available with KENO V.a and GeeWiz.

### 8.1 WHAT YOU WILL BE ABLE TO DO

- Generate 2-D color plots of KENO V.a geometry models.
- Interactively view 3-D wireframe and rendered images of KENO V.a geometry models using KENO3D.
- Plot calculated results overlain on the 3-D geometry model using KMART and KENO3D.

### 8.2 CREATING AND VIEWING 2-D COLOR PLOTS

CSAS and KENO V.a have the built-in capability to produce plots of 2-D KENO V.a geometry slices. These plots can be generated without performing a calculation by using the PARM=CHECK option in the CSAS/KENO V.a general input. This option provides the user with the capability to check their geometry model prior to performing calculations.

To demonstrate the 2-D plotting capability, use GeeWiz to open the  $9 \times 9$  fuel assembly model that was generated in the previous section. Click on the **Plot Data** button on the left-hand toolbar to open the form in Fig. 140.

**Screen Plotting Data**

help first last prev next new copy delete

Title: \_\_\_\_\_

Do not generate this plot

Plot Type:  Mixture  Unit Number

Plot Orientation:  XY  XZ  YZ

Upper Left Corner	X	Y	Z
	-7.48	7.48	0
Lower Right Corner	7.48	-7.48	0

Scaling Parameters (Specify only one)

Number of Pixels Across (NAX): 0

Number of Pixels Down (NDN): 0

Colors:  GeeWiz Colors  User Specified Colors  SCALE Defaults

Legend:

- 1 atompis1 b4c
- 2 h2o
- 3 uo2
- 4 zirc2
- 5 ss304

Plot 1 of 1 plots

OK CANCEL

**Fig. 140. Screen plotting data form.**

Note that you can choose from **X–Y**, **X–Z**, and **Y–Z** plots, and you can plot by **Mixture** or **Unit Number**. Mixture plots are typically performed, because they show the geometry using a unique color for each material in the model. The coordinates of the **Upper Left Corner** and the **Lower Right Corner** of the plot must be specified by the user. The direction that does not vary in the plot (e.g., **Z** in an **X–Y** plot) must have the same coordinate values for both corners. In SCALE 5.1, GeeWiz will automatically calculate the coordinate values for the corners based on the coordinates of the global unit. It will choose the minimum and maximum values of the two directions that vary and the midpoint of the third direction that does not vary.

In this case, by default GeeWiz has set the coordinates for an **X–Y** plot through the center of the model (**Z=0**). If you are using SCALE 5, you will need to manually enter the coordinates for the **Upper Left Corner** (**X=-7.48**, **Y=7.48**, **Z=0**) and the **Lower Right Corner** (**X=7.48**, **Y=-7.48**, **Z=0**). You will also need to enter a **Title** for the plot and one of the **Scaling Parameters** (**NAX** or **NDN**). You must define the size in pixels of the color PNG file

in one dimension. KENO V.a automatically calculates the size of the other dimension for a plot that is proportionally scaled. Enter a value of 800 pixels for **NAX**. This value is typically a good size for most cases. The resolution of the plot is proportional to the number of pixels, so increasing the value of **NAX** or **NDN** will improve the resolution of the plot.

Note that you can select the color for each mixture in the plot. For a new plot, GeeWiz displays its default color palette. You can change any color by clicking on the **User Specified Colors** button and then clicking on the color you want to change. A color palette is then displayed. The GeeWiz default color for mixture 1 in SCALE 5 is gray, which is the same color used by KENO V.a to plot void (mixture 0) regions. If you are using SCALE 5, you should change the color of mixture 1 to another color. The completed form should look like Fig. 141. Click **OK** to close the form.

**Screen Plotting Data**

help first last prev next new copy delete

Title: x-y plot of fuel assembly

Do not generate this plot

Plot Type:  Mixture  Unit Number

Plot Orientation:  XY  XZ  YZ

	X	Y	Z
Upper Left Corner	-7.48	7.48	0
Lower Right Corner	7.48	-7.48	0

Scaling Parameters (Specify only one)

Number of Pixels Across (NAX): 800

Number of Pixels Down (NDN): 0

Colors:  GeeWiz Colors  User Specified Colors  SCALE Defaults

- 1 atmpois1 b4c
- 2 h2o
- 3 uo2
- 4 zirc2
- 5 ss304

Plot 1 of 1 plots

OK CANCEL

**Fig. 141. Screen plot form for X-Y plot.**

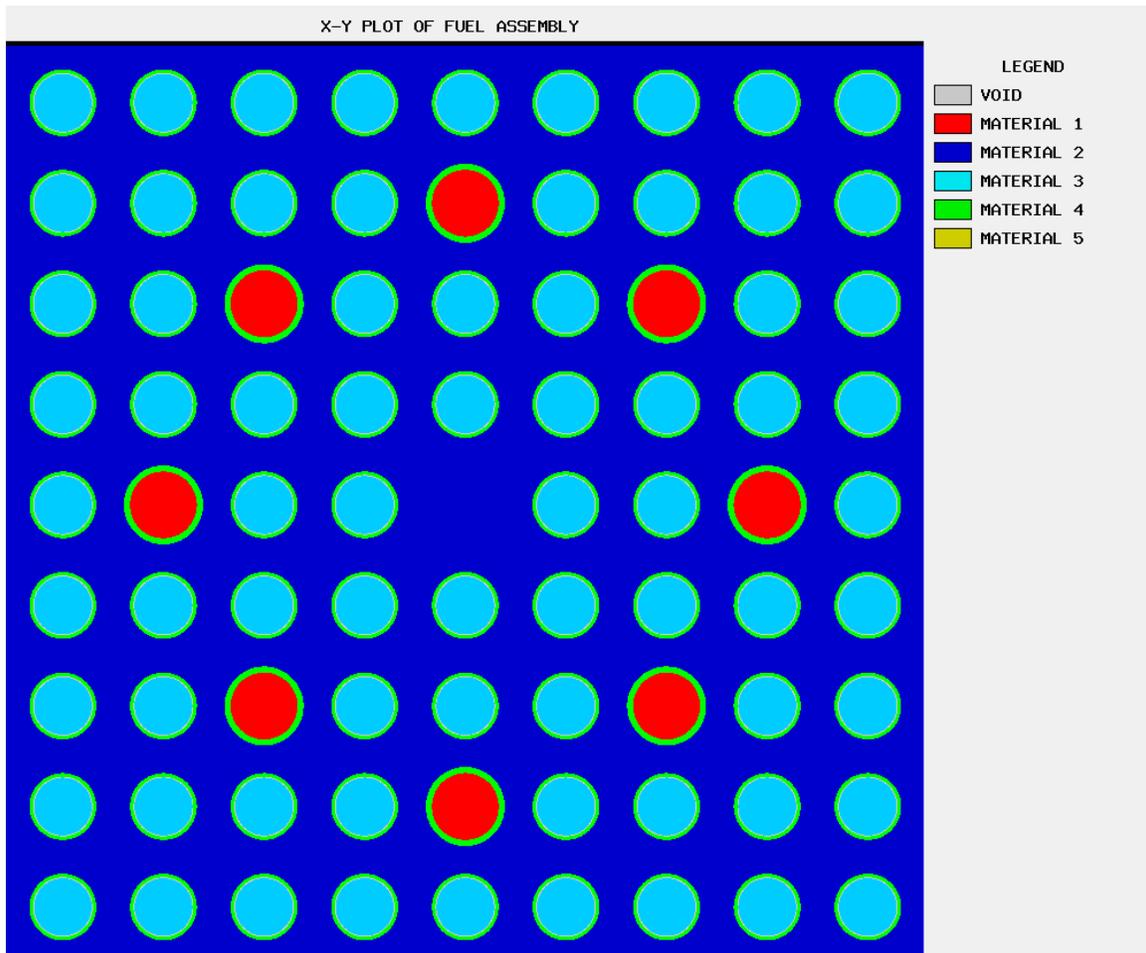
Click on the **General** button on the left-hand toolbar to open the general information form. Click on the **Parm=Check** box so that CSAS will perform only input checking and plotting without calling KENO V.a. Click **OK** to close the form. Then click on the **Run** button. When the job has finished, close the DOS window and click on the **Plots** button on the main toolbar. If a program for viewing plots has not been specified previously, the form in Fig. 142 will be displayed.



**Fig. 142. Graphics file viewer setup form for 2-D plots.**

Click on the **Browse** button to open an Explorer window to find the graphics viewing program that you want to use. The PNG files can be viewed by many different graphics viewers, such as IrfanView (<http://www.irfanview.com>), and web browsers, such as Internet Explorer.

Once the viewing program has been identified, the plot will be displayed. It should look like Fig. 143.



**Fig. 143. X-Y plot of  $9 \times 9$  fuel assembly.**

### 8.3 INTERACTIVE 3-D VISUALIZATION WITH KENO3D

KENO3D enables KENO V.a and KENO-VI users to interactively display their 3-D geometry models. The interactive options include:

- Shaded or wireframe images
- Standard views, such as top view, side view, front view, and isometric (3-D) view
- Rotating the model
- Zooming in on selected locations
- Selecting parts of the model to display
- Editing colors and displaying legends
- Displaying properties of any unit in the model

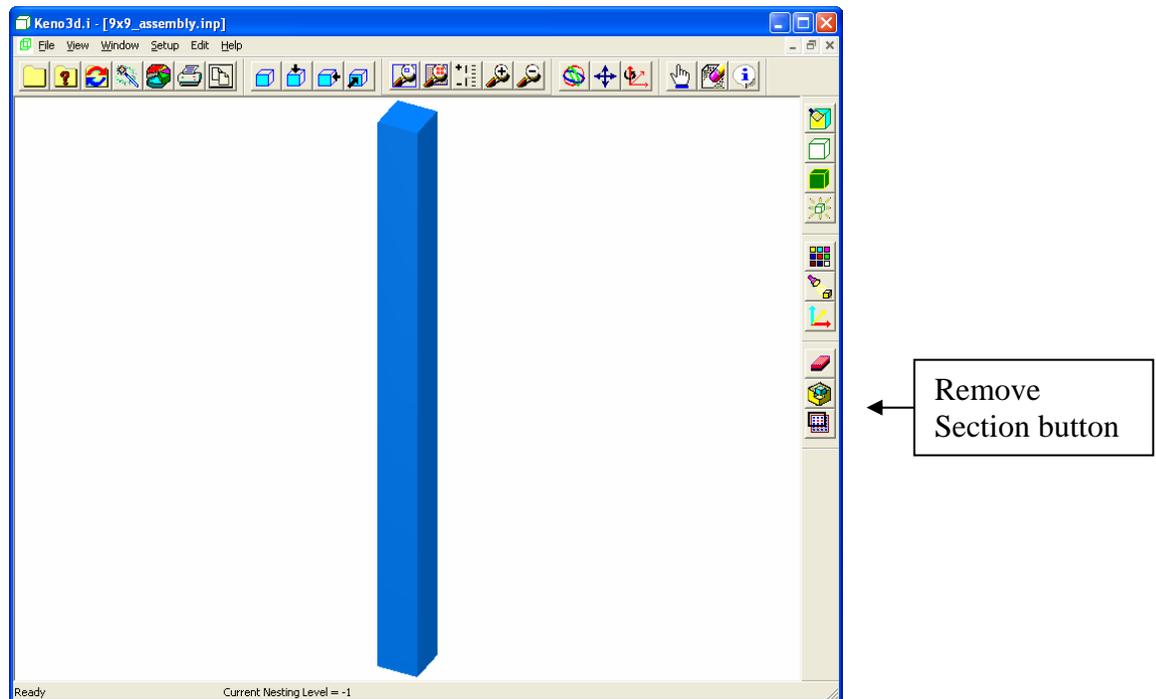
- Creating cut-away views
- Removing units from the model
- Copying images to clipboard or saving images to common graphics formats.

KENO3D reads CSAS/KENO V.a or CSAS6/KENO-VI input files and can be opened directly from GeeWiz. It attempts to verify that the KENO geometry input is “legal,” i.e., it conforms to the code input guidelines. KENO3D prints a warning message for illegal geometry input and, if possible, displays the illegal KENO geometry to facilitate debugging of the input.

KENO3D has a fully integrated help system to aid users in learning how to use it. Only a brief demonstration of how to use KENO3D will be presented here. Users are strongly encouraged to follow the tutorials in the KENO3D help files to quickly learn how to use the many powerful options.

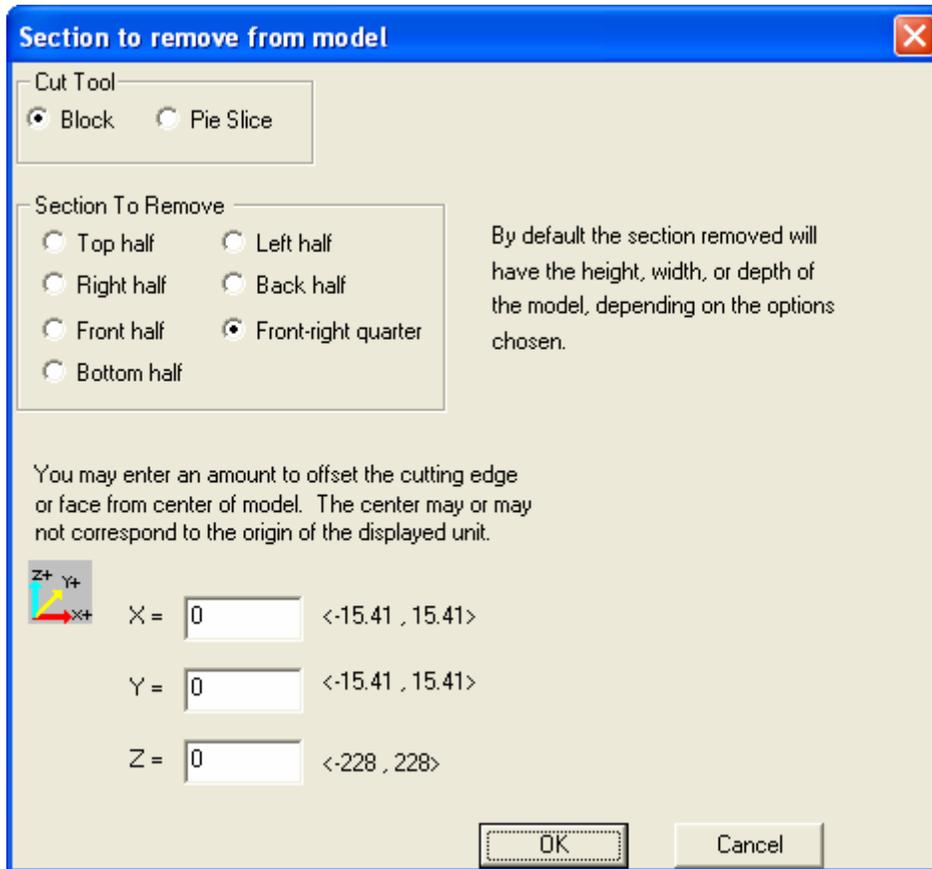
KENO3D has several unique options that provide users with increased flexibility in visualizing portions of a model in greater detail or for visualizing parts of larger models that may be too big to provide a useful image when viewed in their entirety.

To display the  $9 \times 9$  fuel assembly in KENO3D, click on the KENO3D button on the main toolbar in GeeWiz. KENO3D opens the file and displays the geometry as shown in Fig. 144.

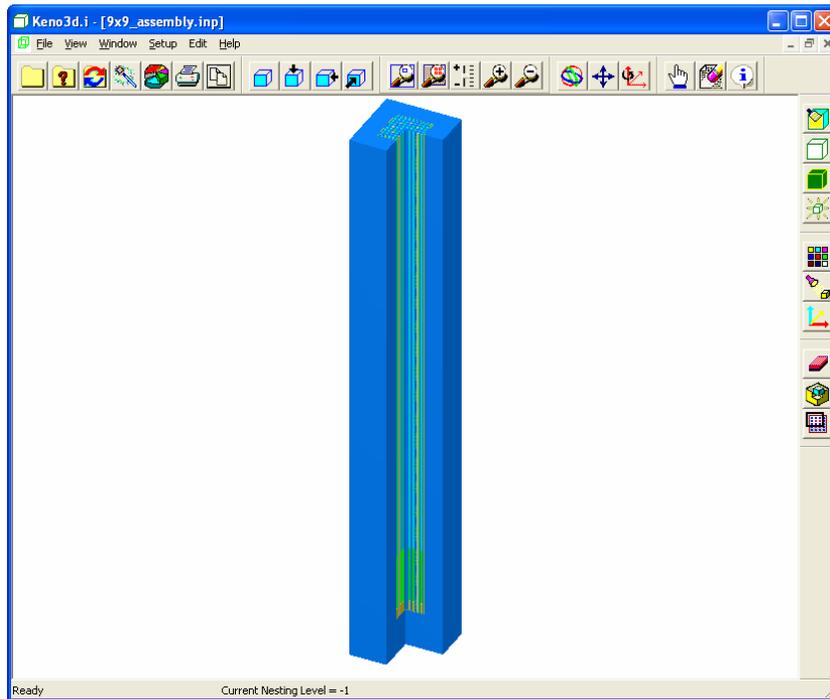


**Fig. 144. Initial isometric view of  $9 \times 9$  fuel assembly.**

This isometric view shows the water reflector that surrounds the outer stainless steel shroud. Next click on the **Remove Section** button (see arrow in Fig. 144). This opens the **Remove Section** dialog form shown in Fig. 145. Click on the **Top half** radio button under **Section to Remove** and click **OK**. This action removes the top half of the model. Click the **Remove Section** button again and click **OK** to remove the **Front-right quarter**. Click on the blue magnifying glass button (**Zoom all**) on the top toolbar. The image should now look similar to Fig. 146.



**Fig. 145. Remove section dialog form.**

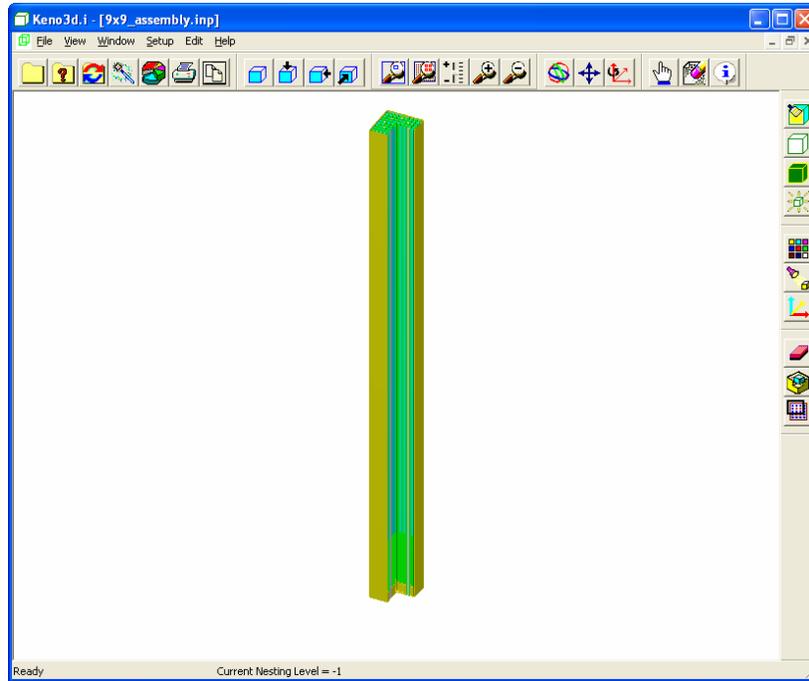


**Fig. 146. Cutaway view of bottom half of assembly.**

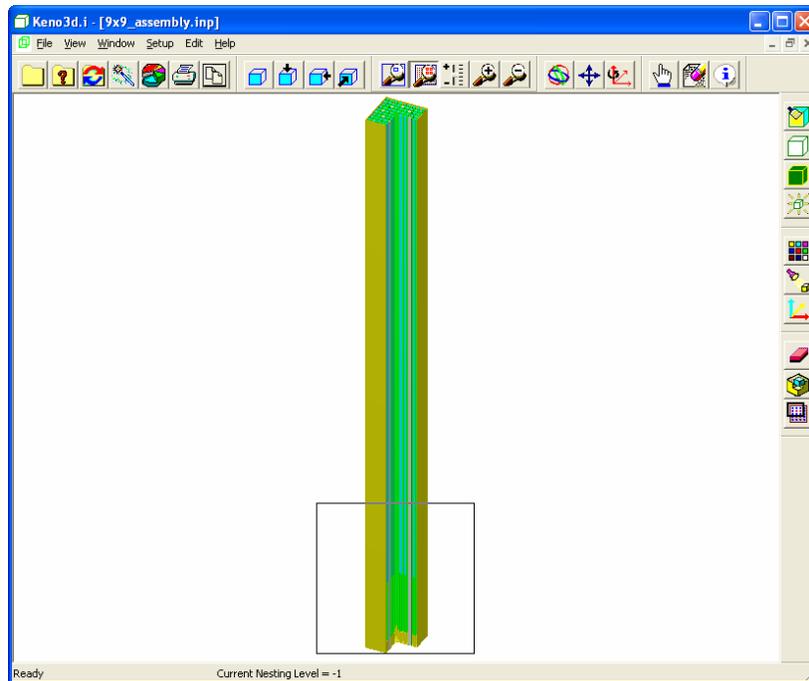
Next, hide the water so that the stainless steel shroud and the fuel assembly are more easily visible. Click on the **eraser** button on the top toolbar and select 0 void and 2 h2o under **Select mixture(s) to hide** and click **OK**. The image now looks like Fig. 147.

We want to zoom in on the bottom part of the fuel assembly so we can see the details more clearly. To do this, click on the **Zoom Window** button (red magnifying glass on the top toolbar). Then hold down the left mouse button and drag to make a window around the bottom portion of the assembly (Fig. 148). Once the window is satisfactory, release the left mouse button and then click to zoom in on that part of the model.

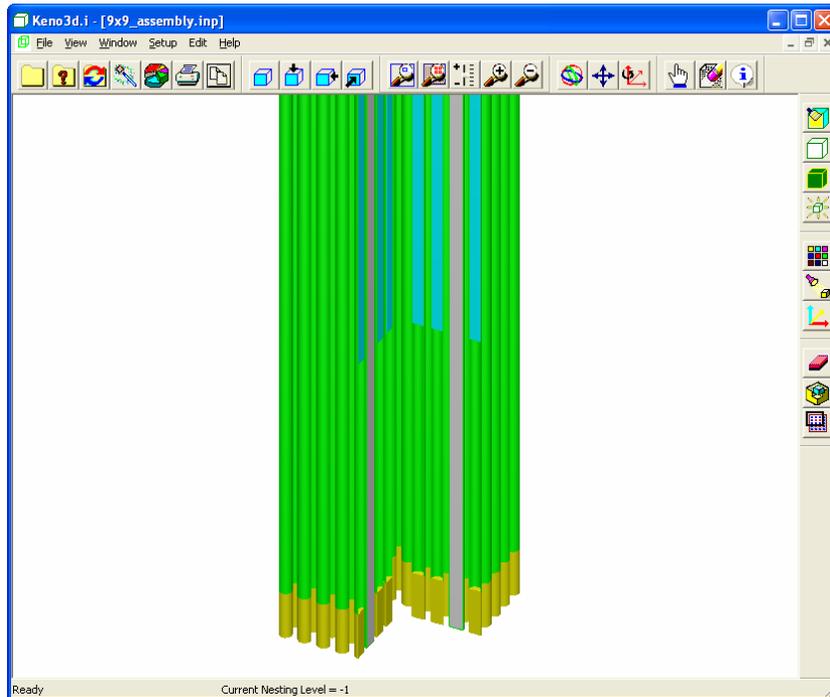
Now we will hide the stainless steel shroud. Click on the **Display Properties** button (pointing finger on top toolbar). Then click on the shroud. It will be highlighted in red with an information window about it. Click on the **Hide Selected Body** button. The view now looks like Fig. 149. Click **Close** to close the Display Properties dialog box.



**Fig. 147. Cutaway view with water hidden.**

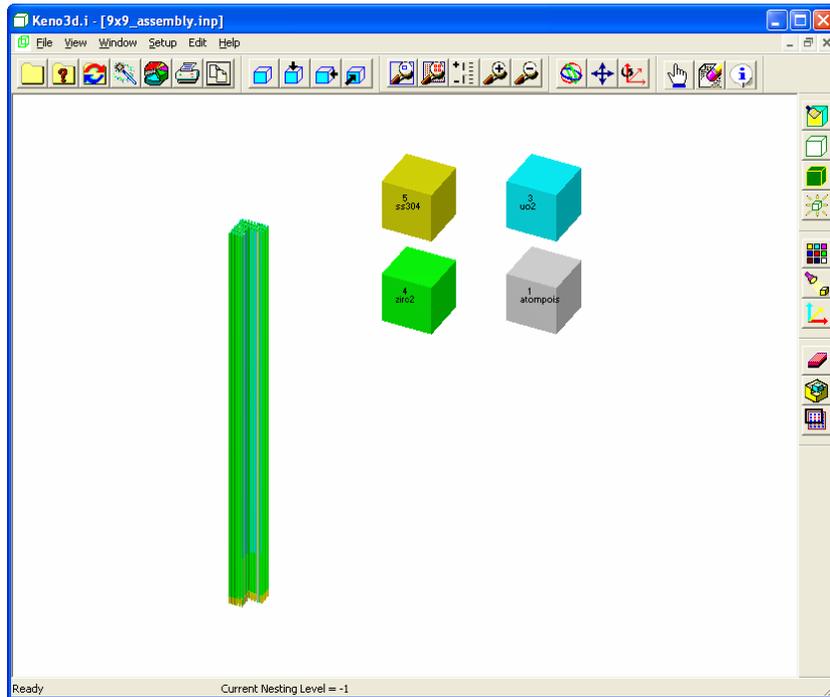


**Fig. 148. Zoom window on bottom portion of fuel assembly in shroud.**



**Fig. 149. Zoomed view of fuel assembly bottom with shroud hidden.**

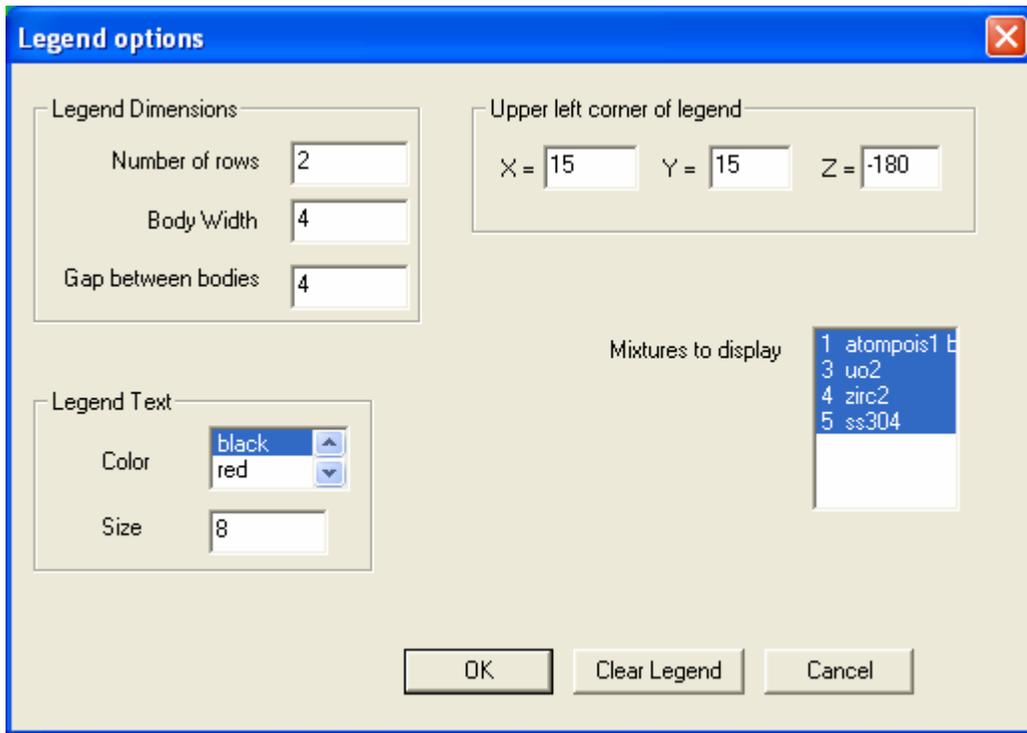
Now we can clearly see the structure of the fuel and burnable poison rods. It would be helpful to have a legend that labels the different components in the view. Click on the **Display Legend** button on the right toolbar and click **OK** on the **Legend options** form to display the legend with the default settings. The view in Fig. 150 now appears.



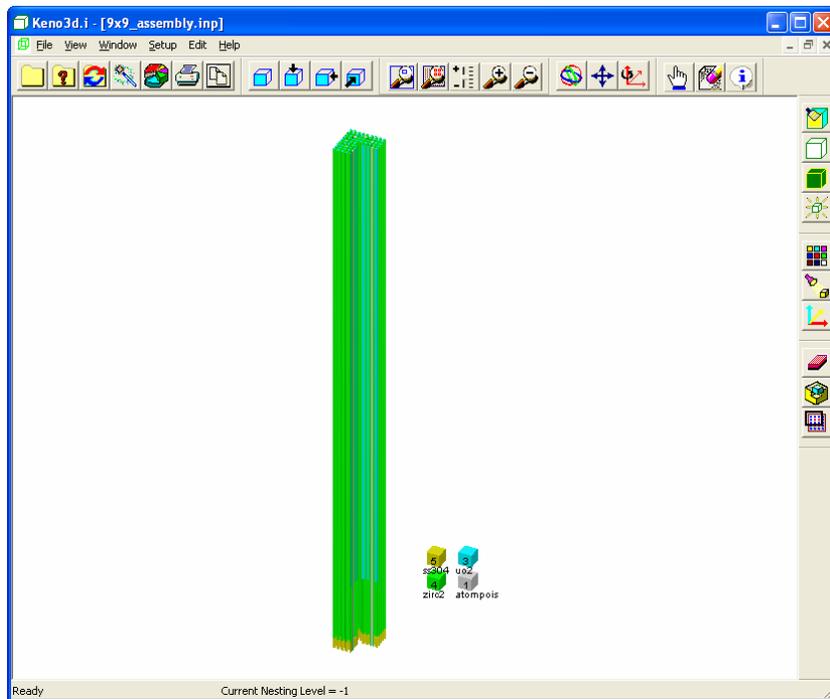
**Fig. 150. View with default legend.**

Adding the legend has removed the focus on the zoom window and has returned the view of the bottom half of the fuel assembly. In addition, the legend is too large and not positioned near the bottom of the fuel assembly. We can correct this by changing the display legend options. Click on the **Display legend** button again. Change the **Body Width** and **Gap between bodies** to 4. Set the **Upper left corner of legend** to **X= 20, Y= 20, and Z= -180**. Set the **Size of the Legend Text** to 8. (See Fig. 151.) Click **OK** and the screen looks like Fig. 152.

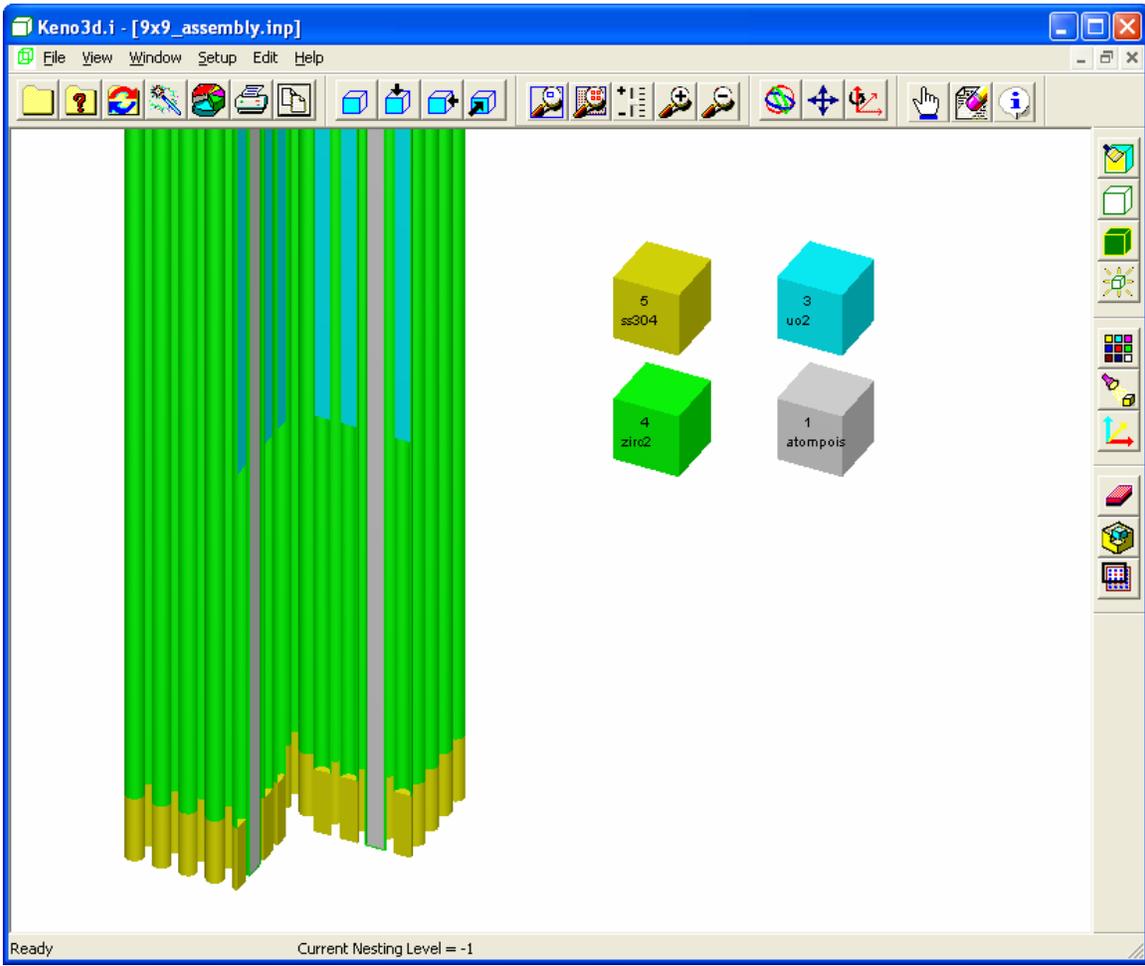
Finally, to obtain the zoomed image of the fuel assembly bottom with the modified legend, click on the **Zoom window** button and draw the zoom window around the bottom of the fuel assembly and the legend. Click and the final image in Fig. 153 appears.



**Fig. 151. Modified legend options.**



**Fig. 152. Image with modified legend.**



**Fig. 153. Final image with legend.**

## 8.4 PLOTTING CALCULATED RESULTS WITH KMART AND KENO3D

KMART (KENO Module for Activity-Reaction Rate Tabulation) is a tool that post-processes information from a KENO V.a run to provide reaction rates by nuclide and the collapsing and printing of fluxes. [Details on KMART are provided in Sect. M17.3 of the SCALE Manual.] KENO3D has the capability to plot the calculated results produced by KENO V.a/KMART overlaid on the 3-D geometry model.

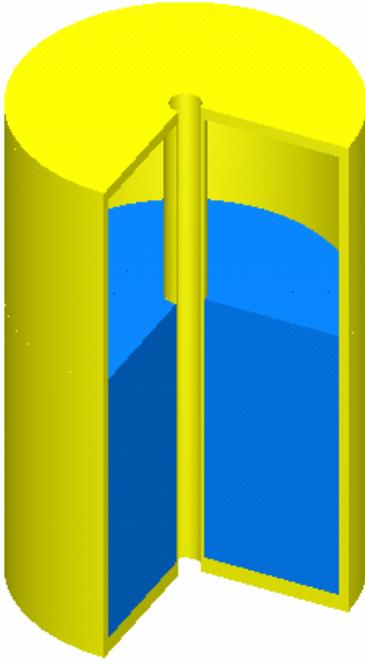
There are a few items of which the KENO V.a user must be aware when utilizing KMART. First, KMART uses a restart file for its evaluations. Thus the user must make sure that a restart unit number (**WRS=**) is identified, and the generations between restart (**RES=**) must be greater than zero in the KENO parameter input. Secondly, if detailed reaction rates or fluxes are desired, then the user must modify the geometry input to create finer regions to provide more detail for the plot. KENO V.a collects calculated data on a unit and region basis. The level of detail in the results is directly dependent upon the level of detail in the individual geometry regions. As an example, if it is desired to model the SHEBA solution reactor, a simple KENO V.a. file might look like the one in Fig. 154. A view of the model in KENO3D is shown in Fig. 155.

```

'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
sheba 2
238groupndf5
read comp
  solnuo2f2      1 978 0.25 DEN=2.1092 1 293 92234 0.027 92235 4.998 92236 0.049
92238 94.926 end
  ss304s      2 den=7.8419 1 293 end
end comp
read parameter
  npg=2000
  res=100
  flx=yes
  fdn=yes
  wrs=35
  mkp=yes
  fmp=yes
  mku=yes
  fmu=yes
end parameter
read geometry
unit 1
com='section 0 - 5.0 of solution in the tank'
  zcylinder 0 1 2.54 44.8 0
  zcylinder 2 1 3.175 44.8 0
  zcylinder 1 1 24.4475 44.8 0
  zcylinder 2 1 25.4 44.8 0
  cuboid 0 1 25.4 -25.4 25.4 -25.4 44.8 0
unit 10
com='bottom of tank'
  zcylinder 0 1 2.54 2.8575 0
  zcylinder 2 1 25.4 2.8575 0
  cuboid 0 1 25.4 -25.4 25.4 -25.4 2.8575 0
unit 11
com='void section of tank'
  zcylinder 0 1 2.54 76.5175 44.8
  zcylinder 2 1 3.175 76.5175 44.8
  zcylinder 0 1 24.4475 76.5175 44.8
  zcylinder 2 1 25.4 76.5175 44.8
  cuboid 0 1 25.4 -25.4 25.4 -25.4 76.5175 44.8
unit 12
com='top of tank'
  zcylinder 0 1 2.54 1.905 0
  zcylinder 2 1 25.4 1.905 0
  cuboid 0 1 25.4 -25.4 25.4 -25.4 1.905 0
end geometry
read array
ara=1 nux=1 nuy=1 nuz=4 gbl=1
fill 10 1 11 12
end fill
end array
end data
end

```

**Fig. 154. Simple SHEBA-II input file.**

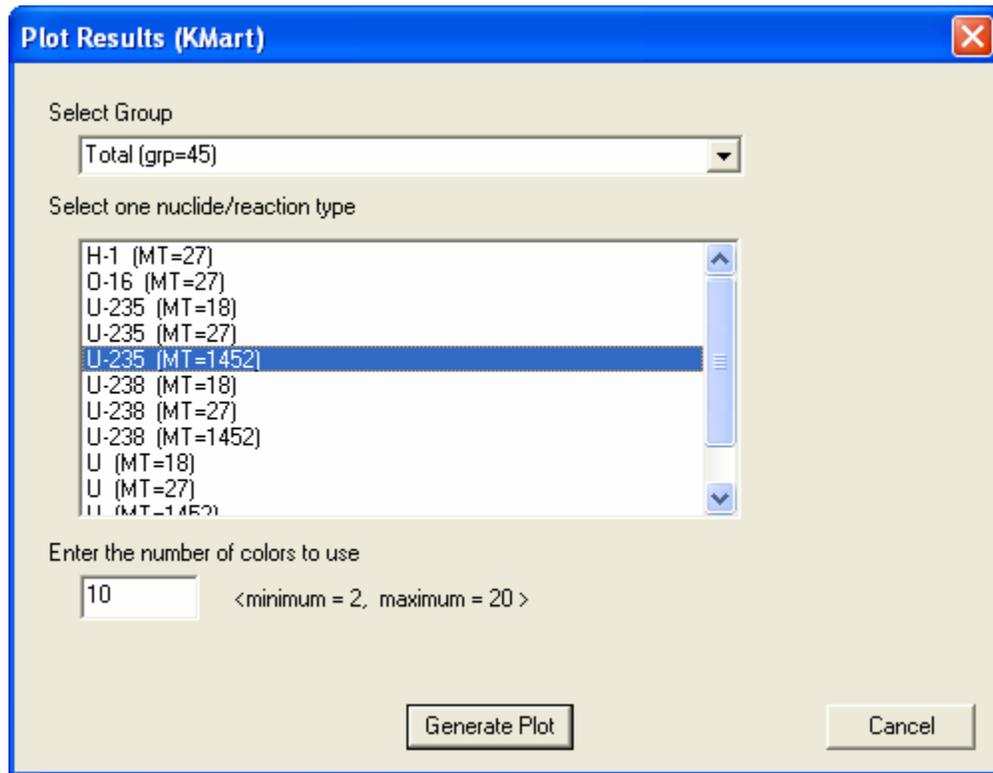


**Fig. 155. Simple model of SHEBA-II.**

However, if you want to look at reaction rates, fluxes, or neutron production rates, then you need to divide the solution into finer segments. So for this example, you might want to create sections that are 5 cm in height and 3 cm in radius. The input file with the associated KMART input can be found in the Keno3d\Examples folder in SCALE. Open the input file sheba.inp in GeeWiz. Click on the **KMart** button to view the **KMART parameters** input data (Fig. 156). The **Activity by group** and **Reaction rates per unit volume** flags are checked. The compositions specified include  $^1\text{H}$  (1001),  $^{16}\text{O}$  (8016),  $^{235}\text{U}$  (92235),  $^{238}\text{U}$  (92238), and U. The reaction types include absorption (27), fission (18), and neutron production ( $\text{nu} * \text{fission} = 1452$ ). Click on the **Insert** button to view the **KMart Activity** form (Fig. 157). On this form you can select any nuclide in the model and the associated reaction type that you want. The definition for each reaction type is shown in the list. [These reaction type numbers are also documented in Sect. F3.B of the SCALE Manual.] Click **Cancel** to remove the forms from the screen.



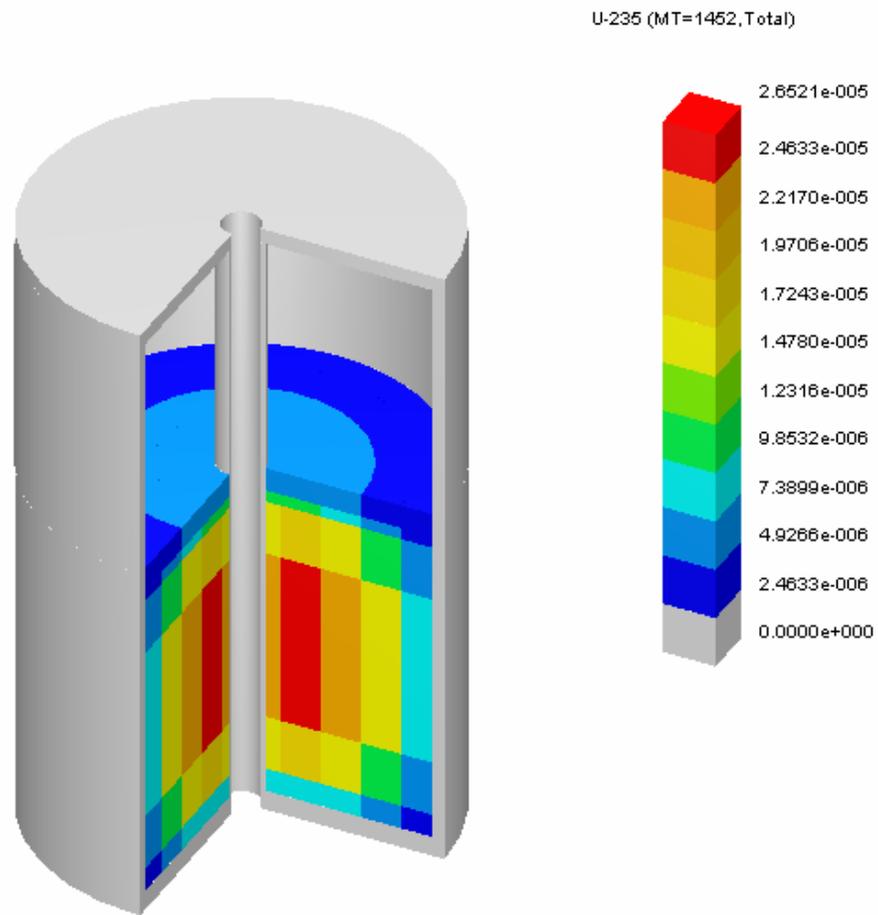
We will use KENO3D to plot the neutron production. Click on the **KENO3D** button in GeeWiz to display the model. Click on the **Remove Section** button and click **OK** to remove the front right quarter. The view should look like Fig. 155. The output and KMART files are included in the KENO3D\Examples folder, so we can plot the KMART data. Click **View** and then **Plot KMart data** to open the **Plot Results (KMART)** form (Fig. 158).



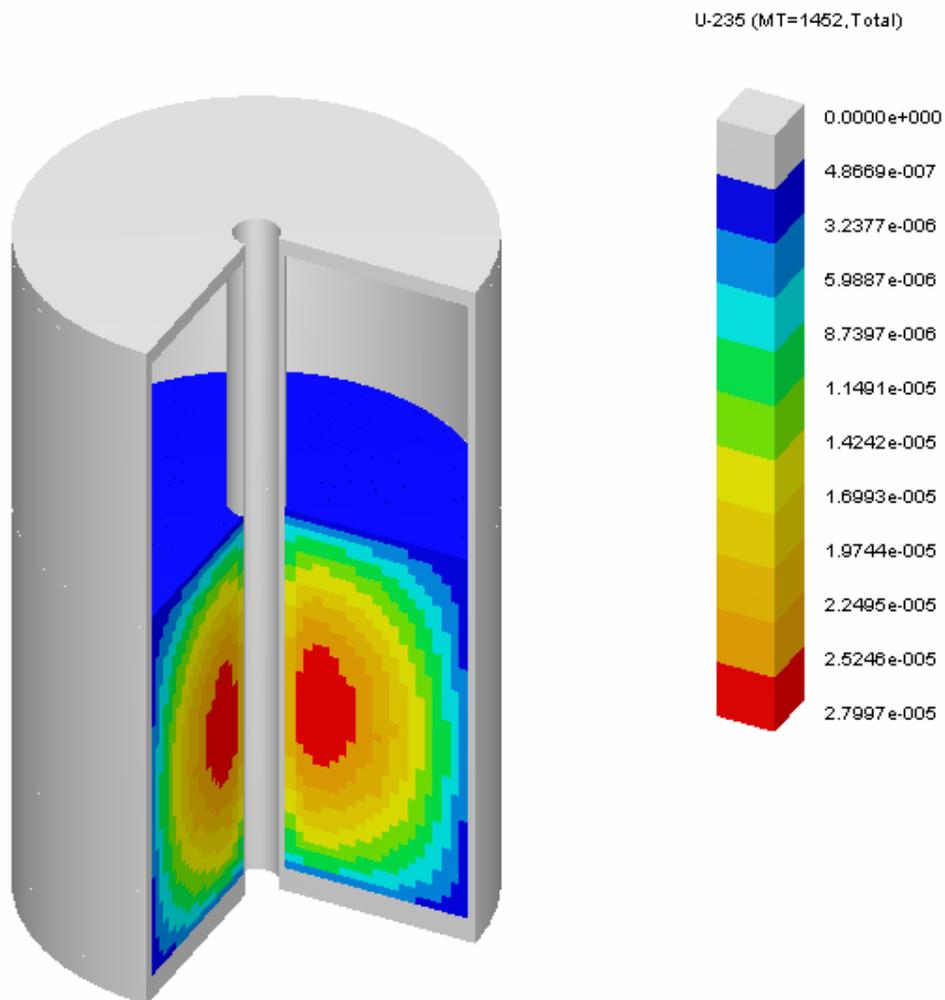
**Fig. 158. Plot results (KMART) form.**

Under **Select Group**, click on **Total (grp=45)** to select the total reaction rate over all energy groups. Click on **U-235 (MT=1452)** to select the  $^{235}\text{U}$  neutron production. Click on **Generate Plot**. Then click on the **Display Legend** button. The neutron production plot (Fig. 159) appears on the screen.

Note that the KENO3D view of the model appears the same as the simple model in Fig. 155, but dividing it into smaller segments allows KMART to produce neutron production plots like Fig. 159. Dividing the model into even smaller segments can result in a much higher resolution plot, as shown in Fig. 160.



**Fig. 159. SHEBA-II  $^{235}\text{U}$  neutron production.**



**Fig. 160. Higher resolution plot of SHEBA-II neutron production.**

## 8.5 SUMMARY

This section has helped you to:

- Generate 2-D color plots of KENO V.a geometry models.
- Interactively view 3-D wireframe and rendered images of KENO V.a geometry models using KENO3D.
- Plot calculated results overlain on the 3-D geometry model using KMART and KENO3D.



## 9. CONCLUSION

Congratulations! If you have completed all previous sections, you now should be able to:

- Describe the structure of SCALE/KENO V.a input files, such as the sequence, the materials, and the KENO information.
- Use the GeeWiz user interface to create and run SCALE/KENO V.a input files to model criticality problems and view results.
- Find and interpret  $k_{\text{eff}}$  information from your output and perform simple checks for reasonableness on your output.

Additional information and help can be obtained at the SCALE website [www.ornl.gov/sci/scale](http://www.ornl.gov/sci/scale). There you can find:

- Current and past issues of the SCALE Newsletter,
- SCALE training course information, and
- SCALE Notebook with answers to many user questions.

The 3-D illustrations in this primer were generated with the KENO3D interactive visualization tool. For more information about KENO3D, including how to order, visit the KENO3D website at [www.ornl.gov/sci/scale/keno3d](http://www.ornl.gov/sci/scale/keno3d).

User assistance is also available by e-mail at [scalehelp@ornl.gov](mailto:scalehelp@ornl.gov).



## 10. REFERENCES

1. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations*, ORNL/TM-2005/39, Version 5, Vols. I–III, April 2005. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-725.
2. S. M. Bowman, W. C. Jordan, J. F. Mincey, C. V. Parks, and L. M. Petrie, *Experience with the SCALE Criticality Safety Cross-Section Libraries*, NUREG/CR-6686 (ORNL/TM-1999/322), U.S. Nuclear Regulatory Commission, Oak Ridge National Laboratory, October 2000.
3. H. C. Paxton and N. L. Pruvost, *Critical Dimensions of Systems Containing U-235, Pu-239, and U-233*, 1986 Revision, LA-10860-MS, July 1987, Los Alamos National Laboratory.
4. NEA Nuclear Science Committee, *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, DVD, NEA/NSC/DOC(95)03, September 2005 Edition, Nuclear Energy Agency, OECD.



**APPENDIX A**  
**CROSS-SECTION LIBRARIES**



# APPENDIX A

## CROSS-SECTION LIBRARIES<sup>a</sup>

### A.1. INTRODUCTION

This section describes the cross-section libraries currently available in the SCALE system. There are six cross-section libraries distributed with SCALE 5 that were designed primarily for criticality analysis. Three of these libraries contain ENDF/B-IV data and are not being distributed in SCALE 5.1: the 218-group ENDF/B-IV library, the 27-group ENDF/B-IV library (27GROUPNDF4), and the 27-group depletion library (27BURNUPLIB).

The 238-group library (238GROUPNDF5) is the most complete library in SCALE 5. This library contains data for all ENDF/B-V nuclides and has 148 fast and 90 thermal groups. Most resonance nuclides in the 238-group library have resonance data in the resolved resonance region and Bondarenko factors in the unresolved resonance region. The 44-group library (44GROUPNDF5) is a broad-group version of 238GROUPNDF5 designed for analysis of light-water-reactor (LWR) fresh and spent fuel systems and has been extensively validated against LWR critical experiments. The 238- and 44-group libraries are the preferred criticality safety analysis libraries in SCALE 5. The Hansen-Roach 16-group library (HANSEN-ROACH) is based on the original Hansen and Roach data. Important nuclides not available in the library were added by collapsing the 218-group ENDF/B-IV library to the 16-group structure. Although the library was originally developed for fast systems, a modification to the  $\sigma_p$  data for <sup>238</sup>U has allowed it to be successfully used as a general-purpose library. The Hansen-Roach library is not recommended, but it is included in SCALE for historical reasons.

A new ENDF/B-VI library is being added in SCALE 5.1. The V6-238 library is a 238-group ENDF/B-VI library with the same energy group structure as the 238GROUPNDF5 library. Extensive validation of this library has been performed with critical experiments from the following categories: high-enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), plutonium (Pu), mixed oxide (MOX), and <sup>233</sup>U.

### A.2. DESCRIPTION OF THE SCALE CROSS-SECTION LIBRARIES

The neutron energy group structure of each of the SCALE neutron libraries is given in the SCALE Manual [Vol. 3, Sect. M4, Tables M4.2.1 and M4.2.2].

---

<sup>a</sup> The information in this appendix is taken from Sect. M4.3 of the SCALE Manual.

### A.2.1. THE 238-GROUP ENDF/B-V LIBRARY (238GROUPNDF5)

The 238-group ENDF/B-V library is a general-purpose criticality analysis library and the most complete library available in SCALE. This library is also known as the LAW (Library to Analyze Radioactive Waste) Library. The library contains data for all nuclides (more than 300) available in ENDF/B-V processed by the AMPX-77 systems.<sup>A.1</sup> It also contains data for ENDF/B-VI evaluations of <sup>14</sup>N, <sup>15</sup>N, <sup>16</sup>O, <sup>154</sup>Eu, and <sup>155</sup>Eu, as discussed in the SCALE manual [Sect. M4.2.5]. A special nuclide set, identified by nuclide ID number 900, contains dose factors based on the ANSI/ANS 6.1.1-1977 standard (dose factor ID 9029) and on the more recent ANSI/ANS 6.1.1-1991 standard (dose factor ID 9031). The library has 148 fast groups and 90 thermal groups (below 3 eV). [The group structure is listed in Table M4.2.2.]

Most resonance nuclides in the 238 group and 44 group have resonance data (to be processed by NITAWL-II) in the resolved resonance range and Bondarenko factors (to be processed by BONAMI) for the unresolved range. Both libraries contain resolved resonance data for *s*-wave, *p*-wave, and *d*-wave resonances ( $\ell = 0$ ,  $\ell = 1$ , and  $\ell = 2$ , respectively) as shown in the SCALE manual [Table M4.2.6]. These data can have a significant effect on results for undermoderated, intermediate-energy problems. Resonance structures in several light-to-intermediate mass “nonresonance” ENDF nuclides (i.e., <sup>7</sup>Li, <sup>19</sup>F, <sup>27</sup>Al, <sup>28</sup>Si) are accounted for using Bondarenko shielding factors. These structures can also be important in intermediate energy problems. [Nuclides with thermal scattering data are listed in Table M4.2.7.]

All nuclides in the 238-group LAW Library use the same weighting spectrum, consisting of

1. Maxwellian spectrum (peak at 300 K) from  $10^{-5}$  to 0.125 eV,
2. a 1/E spectrum from 0.125 eV to 67.4 keV,
3. a fission spectrum (effective temperature at 1.273 MeV) from 67.4 keV to 10 MeV, and
4. a 1/E spectrum from 10 to 20 MeV.

A plot of this spectrum is shown in the SCALE manual [Fig. M4.2.1].

All nuclides use a  $P_5$  Legendre expansion to fit the elastic and discrete level inelastic scattering processes in the fast range, thereby making the library suitable for both reactor and shielding applications. A  $P_3$  fit was used for thermal scattering. All other scattering processes use  $P_0$  fits. A special material is included in the library with an identifier of 99, which contains 238-group weighting spectra for collapsing the 238-group library using the MALOCS module to produce an application-specific collapsed library.

Several spectra are included:

1. spectrum based on a fuel cell from a  $17 \times 17$  Westinghouse LWR assembly and identified by 9001,
2. spectrum designed for use with the Molten Salt Reactor Experiment (MSRE) fuel storage tanks at ORNL and identified by 9002,
3. average spectrum in a 27-cm carbon steel shield for use in cask shielding studies and identified by 9003,
- 4,5. average spectra in an 18.6-cm lead/13-cm resin shield for use in shielding cask studies (the flux in the lead region is identified by 9004 and that in the resin region by 9005),
6. average spectrum in a 50-cm concrete shield for cask shielding studies and identified by 9006, and
7. spectrum in an infinite medium of hydrogen and  $^{235}\text{U}$  with  $H/X = 300$ .

In cases 3 through 6, the spent fuel source was a  $15 \times 15$  Westinghouse LWR assembly with initial enrichment of 3.0 wt % and burned to 30 GWd/MTU and cooled for 5 years.

Data testing has been performed for 33 benchmarks, including 28 Cross Section Evaluation Working Group (CSEWG) benchmarks. Results obtained for these benchmarks are very close to those obtained by other data testers using different ENDF/B-V-based cross-section libraries. There is considerable improvement in the trend of  $k_{\text{eff}}$  vs leakage obtained with the use of the ENDF/B-VI oxygen evaluation. The LAW-238 library appears to be acceptable for general use in criticality and reactor physics applications. The library has had minimal testing for shielding applications and should be evaluated by the user for applicability.

### **A.2.2. THE 44-GROUP ENDF/B-V LIBRARY (44GROUPNDF5)**

The 44-group ENDF/B-V library has been developed for use in the analysis of fresh and spent fuel and radioactive waste systems. Collapsed from the fine-group 238GROUPNDF5 cross-section library, this broad-group library contains all nuclides (more than 300) from the ENDF/B-V data files. Broad-group boundaries were chosen as a subset of the parent 238GROUPNDF5 boundaries, emphasizing the key spectral aspects of a typical LWR fuel package. Specifically, the broad-group structure was designed to accommodate the following features: two windows in the oxygen cross-section spectrum; a window in the cross section of iron; the Maxwellian peak in the thermal range; and the 0.3-eV resonance in  $^{239}\text{Pu}$  (which, due to its low energy, cannot be properly modeled via the SCALE Nordheim Integral Treatment module NITAWL-II). The resulting boundaries represent 22 fast and 22 thermal energy groups; the full group structure is compared to that of the 238-group library in the SCALE Manual

[Table M.4.2.2]. The fine-group 238GROUPNDF5 cross sections were collapsed into this broad-group structure using a fuel cell spectrum calculated based on a  $17 \times 17$  Westinghouse pressurized-water reactor (PWR) assembly.

Because of the significantly improved and conservative behavior of the ENDF/B-VI  $^{16}\text{O}$  evaluation under conditions where higher-order scattering terms are important (e.g., high leakage geometries), this cross section has been included in the 238-group and 44-group libraries as the default for  $^{16}\text{O}$ . The ENDF/B-V evaluation is available within the library as cross-section number 801601 and may be copied into an AMPX working library using AJAX for subsequent use in calculations. Similarly, ENDF/B-VI evaluations of  $^{14}\text{N}$  and  $^{15}\text{N}$  are included in the library; however, ENDF/B-V versions remain the default for these isotopes. The ENDF/B-VI nitrogen data were processed using the same methods used for  $^{16}\text{O}$ , and, like oxygen, were tested to see if significant differences between ENDF/B-V and ENDF/B-VI could be identified. No significant differences have been identified; however, because they had already been processed into AMPX master library format and were readily available, ENDF/B-VI  $^{14}\text{N}$  and  $^{15}\text{N}$  cross sections are included in the library as cross sections 701401 and 701501, respectively. Finally, ENDF/B-VI evaluations of  $^{154}\text{Eu}$  and  $^{155}\text{Eu}$  are also included in the library as default cross sections 63154 and 63155, respectively. The more recent ENDF/B-VI evaluations include resonance parameters not included in previous evaluations and yield energy-dependent cross sections significantly different from those obtained using ENDF/B-V cross sections. Comparisons of depletion/decay calculations to experimental isotopic measurements have indicated that the ENDF/B-VI europium evaluations are more accurate than those available in ENDF/B-V. However, as with  $^{16}\text{O}$ , ENDF/B-V cross sections are available within the library, as isotopes 631541 and 631551. The 44GROUPNDF5 library was tested against its parent library using a set of 33 benchmark problems in order to demonstrate that the collapsed set was an acceptable representation of 238GROUPNDF5, except for intermediate energy systems. Validation of the library within the SCALE system was based on a comparison of calculated values of  $k_{\text{eff}}$  with that of 93 experiments, 92 critical and 1 subcritical. The experiments primarily consisted of various configurations of LWR-type fuel representative of transportation and storage conditions. Additional experiments were included to allow comparison with results obtained in earlier validation of the 27GROUPNDF4 library.

Results show that the broad 44-group structure is an acceptable representation of its parent 238-group library for thermal as well as hard fast spectrum systems. Accurate broad-group analyses of intermediate spectrum systems will require either a more detailed group structure in this energy range or a more appropriate collapsing spectrum. Further, validation calculations indicate that the 44-group library is an accurate tool in the prediction of criticality for arrays of LWR-type fuel assemblies, as would be encountered in fresh or spent fuel transportation or storage environments. Validation results for LWR-type  $\text{UO}_2$  fuel show virtually no bias. A positive bias of 0.5 to 1% has been observed for very thermal MOX systems. The bias is caused by inadequate representation of plutonium cross sections, possibly in the ENDF/B-V data. These validation results are consistently better than those seen for the same cases using the 27GROUPNDF4 library and make the 44GROUPNDF5 library the recommended library for thermal and many hard fast spectrum systems. For intermediate energy systems, the parent 238GROUPNDF5 library is recommended.

### A.2.3. THE HANSEN-ROACH LIBRARY (HANSEN-ROACH)

The Hansen-Roach 16-group library is based on the original Los Alamos report by Hansen and Roach.<sup>A.2</sup> Important nuclides not available in the original library were added by collapsing the 218-group ENDF/B-IV library to the 16-group structure. [Table M4.A.6 in Appendix M4.A of the SCALE Manual gives a complete list of the nuclides available in this library and the source of the data.] Resonance nuclides in the original Hansen-Roach library had cross sections tabulated at several  $\sigma_p$  values. To make these cross sections compatible with the SCALE system, an infinite dilution library was defined for each resonance nuclide and Bondarenko data were generated for the remaining values of  $\sigma_p$ . The implementation of the Hansen-Roach library in SCALE departs significantly from historical use of the Hansen-Roach library. In the past the shielded cross-section set used in a Hansen-Roach calculation was determined by calculating a  $\sigma_p$  value using a single value of the potential scatter cross section for each nuclide.

As implemented in SCALE,  $\sigma_p$  is calculated on a group-wise basis using the total cross section. Cross-section shielding is then done on a group-wise basis. The original Hansen-Roach library did not carry total cross sections, *per se*, but had a total cross section that included a transport correction. In order to implement the Hansen-Roach library in SCALE, an infinite dilute 16-group total cross section was generated from the SCALE 27-group library and was added to the Hansen-Roach library as MT-201. The Bondarenko iteration in BONAMI automatically uses MT-201 when it is present in a library. The addition of the 16-group total cross sections allowed the original SCALE control modules to perform automatic problem-dependent cross-section processing using BONAMI.

The Hansen-Roach library was developed primarily for fast systems. There are 12 fast groups and four thermal groups (groups below 3 eV). However, thermal upscatter is not included in the original Hansen-Roach data. The cross sections are generally  $P_0$  cross sections that are transport corrected to account for leakage. The exceptions are hydrogen and deuterium, which are  $P_1$  transport-corrected cross sections. All of the nuclides added to the original library were generated to  $P_3$ . One significant modification was made to  $^{238}\text{U}$  in the original library such that the library more accurately calculated low-enriched uranium systems. This was the Knight modification to the  $\sigma_p$  data for  $^{238}\text{U}$  such that the 2% enriched green block experiments were accurately calculated. While the library was originally developed for fast systems, the Knight modification has allowed it to be successfully used as a general-purpose library. The areas of applicability have been periodically documented at the Oak Ridge facilities in validations against critical experiments. The library continues to be widely used because it is well known. Areas of validation include HEU-metal, compounds and solutions, moderated LEU systems, and plutonium-metal and solution systems. The Hansen-Roach cross-section set is known to have a 1.5 to 2% negative bias for some highly enriched uranyl nitrate systems and to have a 1 to 1.5% positive bias for highly thermal  $^{239}\text{Pu}$  systems. Other areas of bias tend to be geometry and composition dependent (the reader is referred to the various validation reports for specific areas

of applicability). [In the SCALE Manual, Tables M4.2.8 and M4.2.9 show Hansen-Roach nuclides that have resonance and thermal scattering data, respectively.]

### **A.3. EXPERIENCE WITH THE SCALE CRITICALITY SAFETY CROSS-SECTION LIBRARIES**

The following information is excerpted from Ref. A.3.

This report provides detailed information on the SCALE criticality safety cross-section libraries. Areas covered include the origins of the libraries, the data on which they are based, how they were generated, past experience and validations, and performance comparisons with measured critical experiments and numerical benchmarks.

The performances of the SCALE criticality safety cross-section libraries on various types of fissile systems are examined in detail. Most of the performance areas are demonstrated by examining the performance of the libraries versus critical experiments to show general trends and weaknesses. In areas where directly applicable critical experiments do not exist, performance is examined based on the general knowledge of the strengths and weaknesses of the cross sections. In this case, the acceptability of applying a particular SCALE library to the specific fissile system of interest relies upon experience in the use of that library and comparisons with the results of other libraries on the same systems.

This report should aid in establishing when a SCALE cross-section library would be expected to perform acceptably and where there are known or suspected deficiencies that would cause the calculations to be less reliable. To determine the acceptability of a library for a particular application, the calculational bias of the library should be established by directly applicable critical experiments.

This report provides detailed information on the SCALE criticality-safety cross-section libraries. Areas covered include the origins of the libraries, the data on which they are based, how they were generated, past experience and validations, and performance comparisons with measured critical experiments and numerical benchmarks. Performance results of each library for seven different application areas are summarized in Table A.1.

The remainder of this section contains a brief summary of each library.

**Table A.1. Summary of SCALE library performance for various applications<sup>a</sup>**

Problem type	Cross-section library		
	SCALE 16-group Hansen-Roach	44-group ENDF/B-V	238-group ENDF/B-V
Fast HEU	Very good 0.995 ± 1%	Very good 1.00 ± 1%	Very good 0.995 ± 1%
Thermal HEU	Very poor 2% high to 4% low	Poor 1.00 ± 3%	Poor 1.00 ± 2%
LWR lattices	Fair ± 1.5% bias vs energy	Very good 1.00 ± 1%	Very good 0.995 ± 1%
Homogeneous LEU	Poor ± 2% bias vs energy	Fair 1.01 ± 1.5%	Fair 1.005 ± 1.5%
<sup>239</sup> Pu	Very poor up to 5% high bias vs energy	Fair 1.01 ± 1.5%	Fair 1.005 ± 1.5%
MOX lattices	Very poor 3% high to 1% low	Excellent 1.003 ± 0.6%	Very good 1.00 ± 1% small bias vs energy
<sup>233</sup> U	Poor Thermal: 0.99 ± 2% Fast: 1.0 ± 1%	Good Thermal: 1.00 ± 1.5% Fast: 0.997 ± 0.5%	Good Thermal: 0.995 ± 1.5% Fast: 0.999 ± 0.4%

<sup>a</sup> This table is based on Table 8.1 of Ref. A.3.

### A.3.1. SCALE 16-GROUP HANSEN-ROACH LIBRARY

1. How the library was generated or collapsed:

The library was generated from available data of 1960 vintage. It was originally intended for fast calculations (six fast groups), and later extended to 16 groups, covering the full energy range. Most of the data is  $P_0$  transport-corrected data, but hydrogen and deuterium are  $P_1$  data with a  $P_2$  transport correction. The  $^{238}\text{U}$  data in the resonance range were adjusted to give good results for the Physical Constant Test Reactor (PCTR) experiments.<sup>A.4-A.6</sup>

2. Known biases/weaknesses in original data for this library:

The age and sparseness of the base data (pre-ENDF) are the major weaknesses. Temperature effects and thermal upscatter are not treated.

3. Application areas where the library performs well:

The library performs well for small, high-enriched  $^{235}\text{U}$  metal systems at room temperature and fairly well for many LEU thermal systems.

4. Application areas where the library performs poorly:

Optimally moderated uranyl nitrate solutions underpredict by as much as 2.5 to 3% in  $k_{\text{eff}}$ . Other thermal HEU systems may vary from 2% high to 4% low. Plutonium systems may be high by 2 to 4%. Thermal  $^{233}\text{U}$  systems can underpredict  $k_{\text{eff}}$  by 2 to 3%.

### A.3.2. SCALE 238-GROUP ENDF/B-V LIBRARY

1. How the library was generated or collapsed:

The library was generated from ENDF/B-V data, using a  $\chi(E)$ -1/E-Maxwellian spectrum. The integrating function makes it more difficult to collapse a general-purpose broad-group library that is valid over a large range of problems. It contains all nuclides (over 300) in ENDF/B-V plus data for ENDF/B-VI evaluations of  $^{14}\text{N}$ ,  $^{15}\text{N}$ ,  $^{16}\text{O}$ ,  $^{154}\text{Eu}$ , and  $^{155}\text{Eu}$ .

2. Known biases/weaknesses in original data for this library:

The  $^{235}\text{U}$  fission data and the  $^{238}\text{U}$  capture data are slightly too high. There may be a problem with the thermal plutonium cross sections.

3. Application areas where the library performs well:

Generally, this library has done very well for high-enriched fast systems and low-enriched thermal homogeneous and lattice systems. Results for MOX lattices and  $^{233}\text{U}$  systems are good, too. This library is recommended as the best library in SCALE for general-purpose criticality safety analyses.

4. Application areas where the library performs poorly:

This library has problems with intermediate-energy problems that involve nuclides with cross-section structure without resonance parameters. Although any intermediate-energy problems are suspect because of the scarcity of critical experiments, this library performs better than any other library in SCALE.

### A.3.3. SCALE 44-GROUP ENDF/B-V LIBRARY

1. How the library was generated or collapsed:

The library was collapsed from the 238-group library, using an LWR flux spectrum. Consequently, the library does well predicting LWR lattices but not as well for other types of systems.

2. Known biases/weaknesses in original data for this library:

Same as the 238-group library. Because of the 1/E weighting in the 238-group library, this library is not a good general-purpose library.

3. Application areas where the library performs well:

LWR and MOX lattices are the library's strong points, and it is the recommended SCALE library for these applications. It calculates highly enriched metal systems well. It also predicts  $^{233}\text{U}$  systems reasonably well. For other types of systems, the more the spectrum differs from a LWR spectrum, the more likely it is that the calculated  $k_{\text{eff}}$  will show a bias.

4. Application areas where the library performs poorly:

The 44-group library has all the shortcomings of the 238-group library as well as not being able to calculate homogeneous thermal, epithermal, and intermediate-energy systems as accurately as the 238-group library.

## A.4. REFERENCES

- A.1. N. M. Greene, J. W. Arwood, R. Q. Wright, and C. V. Parks, *The LAW Library – A Multigroup Cross-Section Library for Use in Radioactive Waste Analysis Calculations*, ORNL/TM-12370, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, August 1994.
- A.2. G. E. Hansen and W. H. Roach, *Six and Sixteen Group Cross-Sections for Fast and Intermediate Critical Assemblies*, LA-2543-MS, Los Alamos Scientific Laboratory, November 1961.
- A.3. S. M. Bowman, W. C. Jordan, J. F. Mincey, C. V. Parks, and L. M. Petrie, *Experience With the SCALE Criticality Safety Cross-Section Libraries*, NUREG/CR-6686 (ORNL/TM-1999/322), U.S. Nuclear Regulatory Commission, Oak Ridge National Laboratory, October 2000.
- A.4. H. E. Handler, *Progress Report on Experiments to Determine Infinite Multiplication Factors of Enriched  $UO_3-H_2O$  Mixtures*, HW-51168, Hanford Atomic Products Operation, July 1, 1957.
- A.5. H. E. Handler and R. E. Trumble, Jr., *Infinite Multiplication Constants of Enriched  $UO_3-H_2O$  Mixtures*, Preliminary Report by Hanford Atomic Products Operation, October 16, 1957.
- A.6. V. I. Neeley and H. E. Handler, *Measurement of Multiplication Constant for Slightly Enriched Homogeneous  $UO_3$ -Water Mixtures and Minimum Enrichment for Criticality*, HW-70310, Hanford Atomic Products Operation, August 21, 1961.

**APPENDIX B**

**INPUT FILES FOR EXAMPLE PROBLEMS**



## APPENDIX B

### INPUT FILES FOR EXAMPLE PROBLEMS

#### SECTION 2 – SCALE/KENO V.a *QUICKSTART*

##### 2.3.1. Jezebel (jezebel.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
jezebel problem, bare plutonium sphere with nickel shell
238groupndf5
read comp
  pu-239      1 0 0.037047 293 end
  pu-240      1 0 0.001751 293 end
  pu-241      1 0 0.000117 293 end
  gallium     1 0 0.001375 293 end
  nickel      2 0 0.091322 293 end
end comp
read celldata
  multiregion spherical right_bdy=vacuum left_bdy=reflected origin=0 end 1
  6.38493 2 6.39763 end zone
end celldata
read geometry
global unit 1
com='jezebel core with nickel plating'
  sphere 1 1 6.38493
  sphere 2 1 6.39763
end geometry
end data
end
```

## SECTION 3 – MATERIAL INFORMATION INPUT

### 3.5.1. Bare <sup>235</sup>U Metal Cylinder (bare\_u235\_cyl.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
example problem 1
238groupndf5
read comp
  u-235      1 den=18.742 1 300 end
end comp
read geometry
global unit 1
com='bare cylinder'
  zcylinder 1 1 7.82  7.82  -7.82
end geometry
end data
end
```

### 3.5.2. Bare U(93.7) Metal Cylinder (bare\_u\_cyl.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
ch. 3 example problem 2
238groupndf5
read comp
  u      1 den=18.742 1 300 92235 93.71 92238 6.29 end
end comp
read geometry
global unit 1
com='bare cylinder'
  zcylinder 1 1 7.82  7.82  -7.82
end geometry
end data
end
```

### 3.5.3. Bare U(93.7)O<sub>2</sub> Cylinder (bare\_uo2\_cyl.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
ch. 3 example problem 3
238groupndf5
read comp
  uo2          1 0.95 300 92235 93.71 92238 6.29 end
end comp
read geometry
global unit 1
com='bare cylinder'
  zcylinder 1 1 12.8 12.8 -12.8
end geometry
end data
end
```

### 3.5.4. Bare U(30.3)O<sub>2</sub>F<sub>2</sub> Solution Cylinder (bare\_uo2f2\_cyl.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
ch. 3 example problem 4
238groupndf5
read comp
  u-235        1 0 0.0005637 300 end
  u-238        1 0 0.0012802 300 end
  f            1 0 0.0036844 300 end
  o            1 0 0.0335605 300 end
  h            1 0 0.0597522 300 end
end comp
read geometry
global unit 1
com='uo2f2 (30.3) cylinder'
  zcylinder 1 1 15.225 15.225 -15.225
end geometry
end data
end
```

## SECTION 4 – GEOMETRY INPUT

### 4.2.2. Z-Cylinder (z-cyl.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
single material, z-axis cylinder
238groupndf5
read comp
  u-235      1 den=18.742 1 300 end
end comp
read geometry
global unit 1
com='single z axis cylinder'
  zcylinder 1 1 7.82 7.82 -7.82
end geometry
end data
end
```

### 4.2.3. Z-Cylinder Offset 2 cm from Origin (z-cyl\_2cm\_offset.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
single material, z-axis cylinder
238groupndf5
read comp
  u-235      1 den=18.742 1 300 end
end comp
read geometry
global unit 1
com='single z axis cylinder with origin 2cm above bottom'
  zcylinder 1 1 7.82 13.64 -2
end geometry
end data
end
```

#### 4.2.4. X-Cylinder (x-cyl.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
single material, x-axis cylinder
238groupndf5
read comp
  u-235      1 den=18.742 1 300 end
end comp
read geometry
global unit 1
com='single x axis cylinder with origin at bottom'
  xcylinder 1 1 7.82 15.64 0
end geometry
end data
end
```

#### 4.5.1. Reflected Pu Metal Cylinder (pu\_cyl\_reflected.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
reflected pu(5) cylinder h/d=7.16
238groupndf5
read comp
  pu          1 den=15.44 1 300 94239 95 94240 5 end
  c-graphite  2 den=1.6  1 300 end
end comp
read geometry
global unit 1
com='reflected cylinder'
  zcylinder 1 1 2.86 40.96 0
  zcylinder 2 1 20.64 58.74 -17.78
end geometry
end data
end
```

#### 4.5.2. <sup>235</sup>U Sphere with Graphite and Water Reflectors (u235\_sphere\_graphite\_h2o\_refl.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
u-235 sphere with graphite and water reflectors
238groupndf5
read comp
  u-235      1 den=18.74 1 300 end
  c-graphite 2 den=1.65 1 300 end
  h2o        3 1 300 end
end comp
read geometry
global unit 1
com='nested shapes, sphere inside cylinder inside cube'
  sphere 1 1 7
  zcylinder 2 1 10 10 -10
  cube 3 1 12 -10
end geometry
end data
end
```

#### 4.6.1. $2 \times 2 \times 2$ Array of U(93.2) Metal Cylinders (2c8\_array.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
2c8 array
238groupndf5
read comp
  u          1 den=18.76 1 300 92234 1 92235 93.2 92236 0.2 92238 5.6 end
end comp
read geometry
unit 1
com='unit cell'
  zcylinder 1 1 5.748 10.765 0
  cuboid 0 1 6.87 -6.87 6.87 -6.87 11.8875 -1.1225
end geometry
read array
ara=1 nux=2 nuy=2 nuz=2 gbl=1
fill 8*1
end fill
end array
end data
end
```

## 4.6.2. Stack of Six Disks and Flat Plate (stack\_disks\_plate.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
array of disks and plates
238groupndf5
read comp
  c-graphite  1 den=1.65 1 300 end
  u           2 den=18.74 1 300 92234 1 92235 93.2 92236 0.2 92238 5.6 end
  al          3 1 300 end
end comp
read geometry
unit 1
com='disk 1'
  zcylinder 1 1 10  1.25  -1.25
  cuboid 0 1  15  -15  15  -15  1.25  -1.25
unit 2
com='disk 2'
  zcylinder 2 1 10  2  -2
  cuboid 0 1  15  -15  15  -15  2  -2
unit 3
com='square plate'
  cuboid 3 1  15  -15  15  -15  1.5  -1.5
end geometry
read array
ara=1 nux=1 nuy=1 nuz=7  gbl=1
com='stacked array'
fill 1 2 1 2 1 2 3
end fill
end array
end data
end
```

## SECTION 5 – ADVANCED GEOMETRY INPUT

### 5.2.2. Flat-Bottomed Spherical Tank—SCALE 5 (flat\_bottom\_sphere.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
flat bottom sphere
238groupndf5
read comp
  solnpu(no3)4      1 39 0.4 DEN=1.103 1 300 94239 95.4 94240 4.6 end
  ss316             2 1 300 end
end comp
read geometry
global unit 1
com='flat bottom sphere'
  hemisphe+z 0 1 19.5 chord -13.8
  hemisphe+z 1 1 19.5 chord 16
  hemisphe+z 2 1 19.622 chord 16.122
end geometry
end data
end
```

### Flat-Bottomed Spherical Tank—SCALE 5.1 (flat\_bottom\_sphere\_5.1.inp)

```
'Input generated by GeeWiz 5.02 Compiled on 04-29-2005
=csas25
flat bottom sphere
238groupndf5
read composition
  solution  mix=1  rho[pu(no3)4]=39 94239 95.4
                                94240 4.6
                                molar[hno3]=0.4
                                density=1.103 temperature=300 vol_frac=1
  end solution
  ss316      2 1 300  end
end composition
read geometry
global unit 1
com='flat bottom sphere'
  hemisphe+z 0 1 19.5 chord -13.8
  hemisphe+z 1 1 19.5 chord 16
  hemisphe+z 2 1 19.622 chord 16.122
end geometry
end data
end
```

### 5.3.1. Simple Hole (simple\_hole.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
ch 5 holes example
238groupndf5
read comp
  u-235      1 den=18.7 1 300 end
  ss316     2 1 300 end
  c-graphite 3 1 300 end
end comp
read geometry
unit 1
com='u-235 cylinder'
  zcylinder 1 1 6.85 10 -10
global unit 2
com='steel cylinder'
  cuboid 3 1 -2 -14 14 2 10 -10
  zcylinder 0 1 20 10 -10
  hole 1 6 -6 0
  zcylinder 2 1 20.2 10.2 -10.2
end geometry
end data
end
```

### 5.4.1. Five Cylinders with Cruciforms (5\_cyls\_cruciforms.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
holes and arrays
238groupndf5
read comp
  uc          1 1 300 92235 93.2 92238 6.8 end
  h2o         2 1 300 end
  ss316       3 1 300 end
end comp
read geometry
unit 1
com='cruciform'
  cuboid 1 1 5 -5 0.5 -0.5 10 -10
  zcylinder 2 1 6 10 -10
  hole 2 0 2.75 0
  hole 2 0 -2.75 0
  zcylinder 3 1 6.1 10.1 -10.1
  cuboid 0 1 6.2 -6.2 6.2 -6.2 10.1 -10.1
unit 2
com='tops'
  cuboid 1 1 0.5 -0.5 2.25 -2.25 10 -10
global unit 3
com='big tank'
  array 1 -18.6 -6.2 -10.1
  zcylinder 0 1 20 10.1 -10.1
  hole 1 0 12.4 0
  hole 1 0 -12.4 0
  zcylinder 3 1 20.2 10.2 -10.2
end geometry
read array
ara=1 nux=3 nuy=1 nuz=1
com='central array'
fill 3*1
end fill
end array
end data
end
```

## **SECTION 6 – ARBITRARY MATERIALS**

No Example Problems.

## SECTION 7 – UNIT CELLS AND CROSS-SECTION PROCESSING

### 7.5.1. 9 × 9 Fuel Assembly (9x9\_assembly.inp)

```
'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25 parm=centrm
9x9 fuel assembly, 1000 generations, CENTRM
44groupndf5
read comp
  uo2          3 0.925 300 92235 3.44 92238 96.56 end
  atompois1    1 3.7 2 13027 2 8016 3 0.9874 300 end
  b4c          1 den=3.7 0.0126 300 end
  h2o          2 1 300 end
  zirc2        4 1 300 end
  ss304        5 1 300 end
end comp
read celldata
  latticecell squarepitch fuelr=0.47 3 gapr=0.4875 0 cladr=0.545 4
  hpitch=0.82 2 end
end celldata
read parameter
  gen=1003
  fdn=yes
end parameter
read geometry
unit 1
com='3.44% enr. fuel rod'
  zcylinder 3 1 0.47 182.88 -182.88
  zcylinder 0 1 0.4875 199.84 -206.24
  zcylinder 4 1 0.545 199.84 -206.24
  zcylinder 5 1 0.545 210.34 -210.34
  cuboid 2 1 0.82 -0.82 0.82 -0.82 210.34 -210.34
unit 2
com='1.26% burnable poison rod-lbp1'
  zcylinder 1 1 0.545 160 -160
  zcylinder 0 1 0.545 260.48 -160
  zcylinder 4 1 0.645 260.58 -160.1
  cuboid 2 1 0.82 -0.82 0.82 -0.82 260.58 -160.1
unit 3
com='central water unit for assembly'
  cuboid 2 1 0.82 -0.82 0.82 -0.82 260.58 -160.1
global unit 4
com='3.44% enr. fuel assembly'
  array 1 -7.38 -7.38 -210.34
  cuboid 2 1 7.48 -7.48 7.48 -7.48 210.34 -210.34
  replicate 5 1 0.16 0.16 0.16 0.16 0.16 0.16 1
  replicate 2 1 7.62 7.62 7.62 7.62 15.24 15.24 1
end geometry
read array
```

```

ara=1 nux=9 nuy=9 nuz=1
fill 13*1 2 6*1 2 3*1 2 12*1 2 2*1 3 2*1 2 12*1 2 3*1 2 6*1 2 13*1
end fill
end array
end data
end

```

## 7.5.2. Two Parallel Slab Tanks (slab\_tanks.inp)

```

'Input generated by GeeWiz 5.01a Compiled on March-03-2005
=csas25
two parallel reflected ss304 slab tanks
238groupndf5
read comp
  solnuo2f2      1 459 0 DEN=1.566 1 300 92235 93 92238 7 end
  ss304          2 1 300 end
  h2o            3 1 300 end
end comp
read celldata
  multiregion slab right_bdy=vacuum left_bdy=reflected origin=0 end 3 5 2
5.5 1 10.5 2 11 3 16 end zone
end celldata
read geometry
global unit 1
com='single reflected ss304 slab tank'
  cuboid 1 1 2.5 -2.5 150 -150 75 -75
  replicate 2 1 0.5 0.5 0.5 0.5 0 0.5 1
  replicate 3 1 5 5 0 0 0 0 1
end geometry
read bnds
  +xb=vacuum
  -xb=mirror
  +yb=vacuum
  -yb=vacuum
  +zb=vacuum
  -zb=vacuum
end bnds
end data
end

```

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