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

**R. D. Busch  
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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 CSPAN for Input**

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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 4.4a, which includes the Criticality Safety Processor for Analysis (CSPAN) input processor for Windows personal computers (PCs). A second edition of the primer, which uses the new KENO Visual Editor, is currently under development at ORNL and is planned for publication in late 2003. Each example in this first edition of the primer uses CSPAN 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 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 which are covered in detail in the example problems in that section. Upon completion of the primer, a new user should be comfortable using CSPAN 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

With the closure of many experimental facilities, the nuclear criticality safety analyst is increasingly required to rely on computer calculations to identify safe limits for the handling and storage of fissile materials. However, in many cases, the analyst has little experience with the specific codes available at their facility. This primer will help you, the analyst, understand and use the SCALE/KENO V.a Monte Carlo code for nuclear criticality safety analyses. It assumes that you have a college education in a technical field. There is no assumption of familiarity with Monte Carlo codes in general or with 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 4.4a,<sup>1</sup> which includes the Criticality Safety Processor for Analysis (CSPAN) input processor. Each of the examples will use CSPAN to provide the framework for data input. Although the focus is on using CSPAN to enter the information, the input files are provided and are suitable for use with previous versions of SCALE (SCALE 4.3, 4.4). 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 CSPAN, the input, or the SCALE/KENO V.a options in detail; but rather it introduces the CSPAN input processor 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 which are then covered in detail in the example problems in that section. It is expected that upon completion of the primer, you will be comfortable using CSPAN 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 80 to 90% of the 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) plots and 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 analyst using SCALE/KENO V.a. Complete descriptions are provided in the SCALE/KENO V.a manual.<sup>1</sup> 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 while the documentation 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. The 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 Roman font. Information that you type into an input file (or provide to the CSPAN Input Processor) 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 CSPAN will be highlighted in **bold font**. Because the primer often references the SCALE/KENO V.a 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 out of 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 reading through the primer and practicing the examples will save many hours of possible confusion and embarrassment later. After studying the primer, you will find it a valuable tool to help expedite accurate criticality analyses with SCALE/KENO V.a.

## 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 provided the technical capabilities of the individual modules with which they were familiar. With this proposal, the concept of the Standardized Computer Analyses for Licensing Evaluation (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 4.4a. 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-II, 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 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 module is the primary criticality safety control module for the calculation of the neutron multiplication factor ( $k_{eff}$ ) 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 three-dimensional (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. 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. Thus, in the SCALE sequences, BONAMI is always used in conjunction with NITAWL-II, so that even if no resonance processing is performed, BONAMI converts the master library into an AMPX working library.

NITAWL-II 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.

An additional function of NITAWL is its conversion of cross-section libraries from the master library format to a problem-dependent working library format.

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 the preparation of cell-averaged cross sections for subsequent system analysis and for 1-D criticality safety analysis.

KENO V.a is a multigroup Monte Carlo code employed to determine  $k_{eff}$  for 3-D 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 KENO3D 3-D visualization tool.

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 analytic sequence designated by =CSAS25 follows the execution path BONAMI, NITAWL-II, and KENO V.a. The sequence =CSAS4 follows the same execution path but repeats the three modules for each pass as part of a search for the geometry dimension or material concentration that provides the minimum, maximum, or specified  $k_{eff}$  value. The above sequences are modified to include cell-weighting with XSDRNPM if =CSAS2X or =CSAS4X is designated. As the geometry package for KENO-VI is different than 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 non-orthogonal geometry).

Other sequences are available to obtain  $k_{eff}$  via a 1-D XSDRNPM model or to simply prepare problem-dependent cross-section processing for subsequent use in analyses with individual codes. A Windows graphical user interface (GUI) named CSPAN is available for preparing CSAS input.

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> Other frequently used libraries include the 27-group ENDF/B-IV and the 16-group Hansen-Roach neutron libraries.

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 foreign 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 CSPAN input processor to create a SCALE/KENO V.a input file.
- Set up and run a simple criticality problem on SCALE/KENO V.a.
- Find and interpret  $k_{eff}$  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 CSPAN input processor.

### 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 CSPAN to enter SCALE/KENO V.a input data right away, so we walk through this sample 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 CSPAN 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 it easier to set up the geometry before identifying the materials.

### 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  $^{239}\text{Pu}$  =  $3.7047\text{E}-2$  atoms/b-cm

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

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

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

Spherical nickel coating: thickness = 0.0127 cm

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

### 2.3.2. CSPAN Input – General Information

Now you are ready to begin entering the example problem. First start the CSPAN input processor. You should see a screen that looks like Fig. 1.

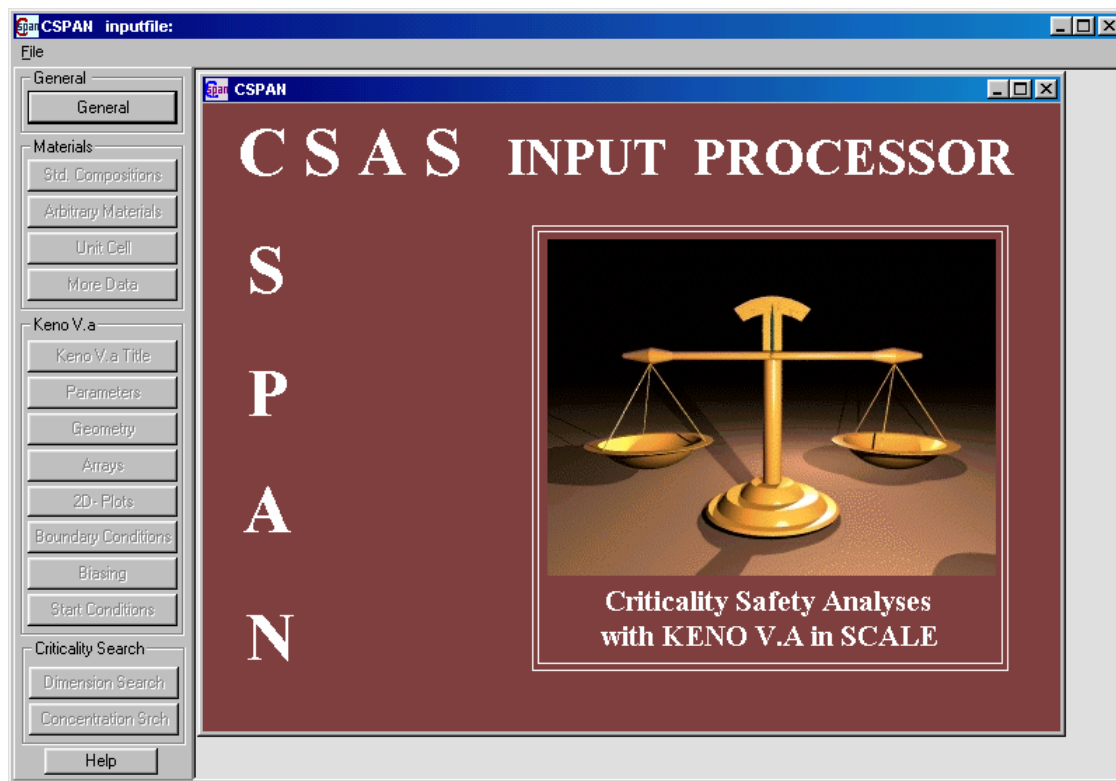
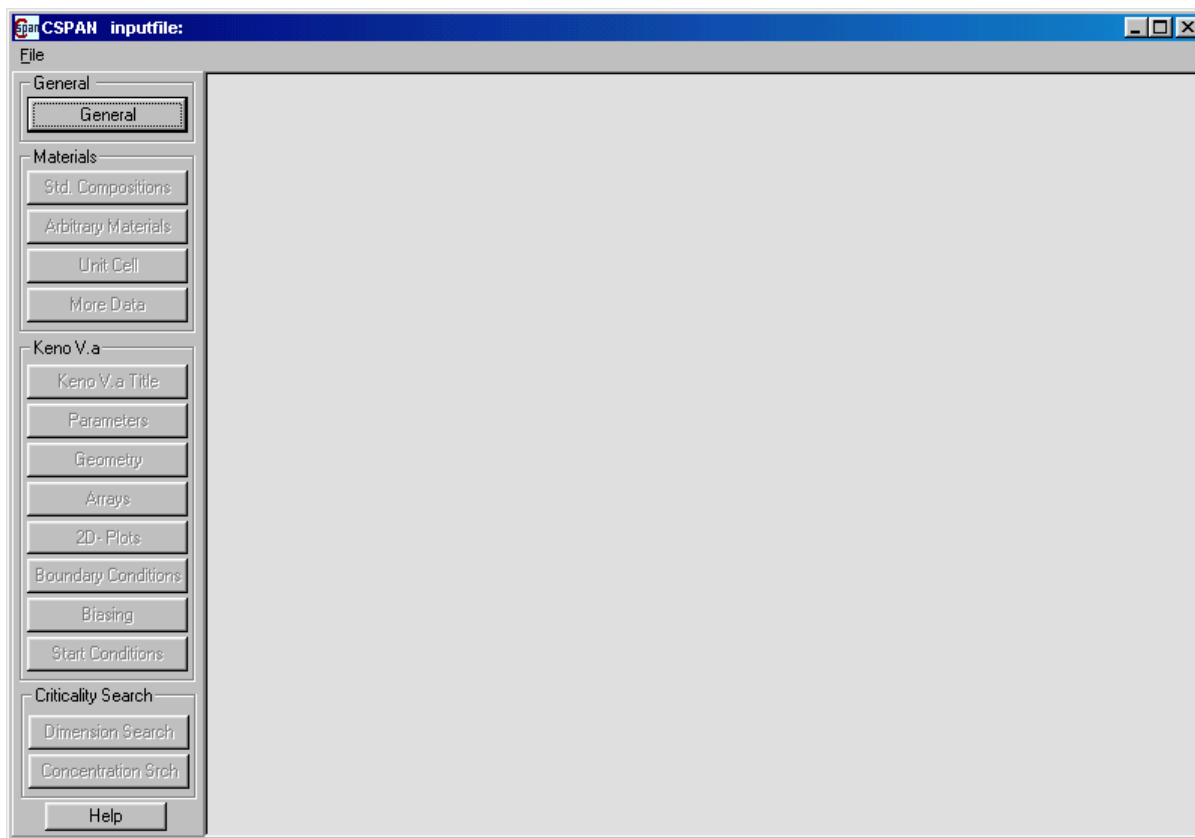


Fig. 1. CSPAN start screen.

The first step is to select **File** and then select **New Problem**. This should bring up a screen as shown in Fig. 2.



**Fig. 2. First screen for new problem input.**

Clicking on the **General** button on the left hand side menu will bring up a window as shown in Fig. 3. In this window, you enter the **Title**, the **SCALE Sequence**, the **Cross-section Library**, and the **Unit Cell Type** information. Other parameter information can be entered if desired. The version of SCALE should already be selected, based on the version installed on your PC. CSPAN must know the version of SCALE to determine the location of the SCALE Standard Composition and cross-section libraries on the user's PC. CSPAN reads these libraries to generate the list of available standard compositions for the selected cross-section library. Some users may have more than one version installed on their PC. Other users may run SCALE on a workstation and just use CSPAN to create input files. If SCALE is not installed on the user's PC, the SCALE Standard Composition and cross-section libraries must be installed under the CSPAN directory. CSPAN searches each hard drive on the user's PC for installations of SCALE 4.4 or 4.4a in the default directories. It will only allow a user to check a version that is installed. CSPAN writes and reads a CSPAN.INI file that contains the SCALE version last selected by the user. Unless the user decides to execute a different version, the option will not

have to be changed again. CSPAN reads the Standard Composition Library and the selected cross-section library. CSPAN will not execute unless these files are available.

Enter the **Title** as follows:

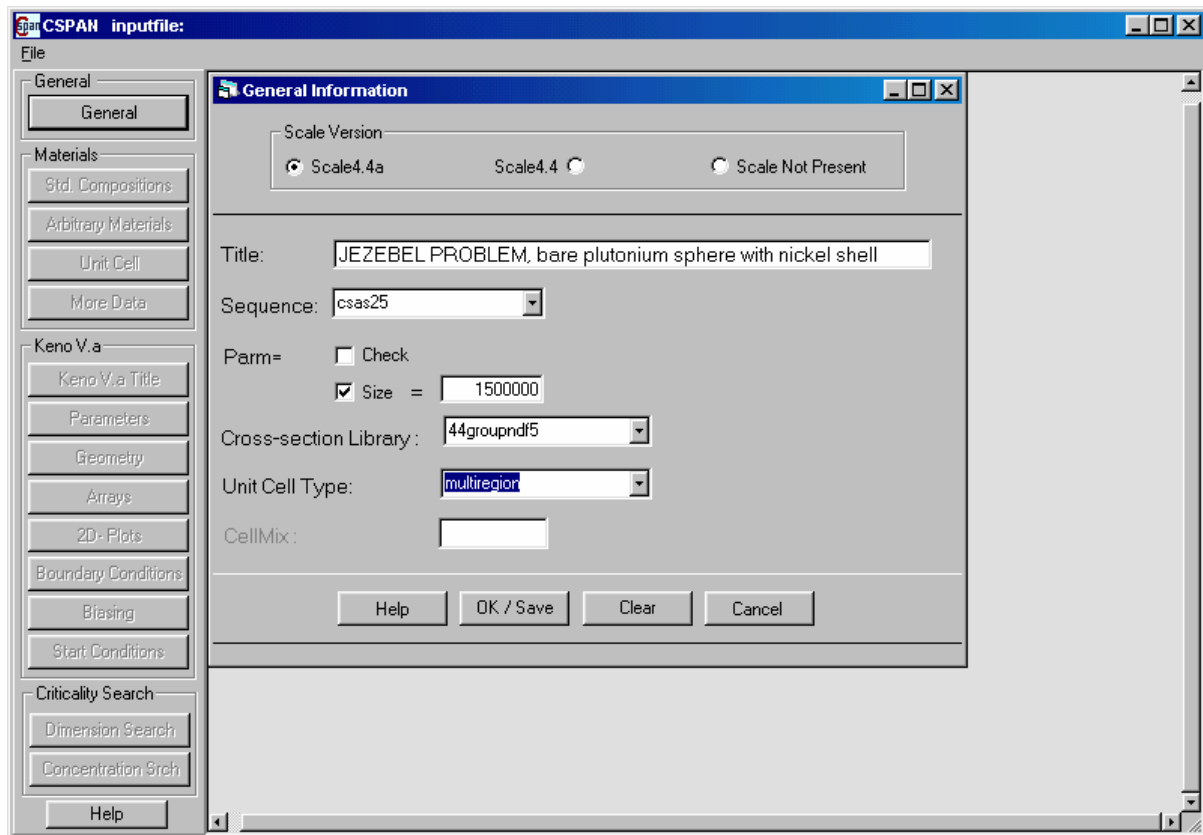
JEZEBEL PROBLEM, bare plutonium sphere with nickel shell

Again note that information to be entered into CSPAN will appear in the Courier font. Select csas25 as the sequence. Under the **Parm=** line, click on the **Size** box and enter 500000 after the = sign.

The image shows a screenshot of the CSPAN software interface. The main window is titled "CSPAN inputfile:". On the left is a vertical menu with categories: "General" (containing a "General" button), "Materials" (containing "Std. Compositions", "Arbitrary Materials", "Unit Cell", and "More Data" buttons), "Keno V.a" (containing "Keno V.a Title", "Parameters", "Geometry", "Arrays", "2D Plots", "Boundary Conditions", "Biasing", and "Start Conditions" buttons), and "Criticality Search" (containing "Dimension Search" and "Concentration Search" buttons). At the bottom of the menu is a "Help" button. The main area of the window displays the "General Information" form. This form includes a "Scale Version" section with three radio buttons: "Scale4.4a" (selected), "Scale4.4", and "Scale Not Present". Below this is a "Title:" label followed by a text input field. The "Sequence:" label is followed by a dropdown menu showing "select a value". The "Parm=" label is followed by two checkboxes: "Check" and "Size". The "Size" checkbox is selected, and it is followed by an equals sign and a text input field. Below this is a "Cross-section Library:" label followed by a dropdown menu showing "select a value". The "Unit Cell Type:" label is followed by a dropdown menu showing "select a value". The "CellMix:" label is followed by a text input field. At the bottom of the form are four buttons: "Help", "OK / Save", "Clear", and "Cancel".

**Fig. 3. General information form.**

For **Cross-section Library**, select 44groupndf5, and for **Unit Cell Type**, select multiregion. The **General Information** screen should look like that in Fig. 4.



**Fig. 4. General information for example problem.**

Now select **OK/Save** to save this information in a temporary file. Later you will save all of the input information under a file name. As soon as OK/Save is selected, the four buttons under **Materials** on the left are activated.

### 2.3.3. Materials

The next section of CSPAN 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 **Std. Compositions** from the menu on the left hand side of CSPAN. This button opens the form for specifying the materials in the model.

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. As the first four materials are mixed together, they will be part of composition number 1. You will enter four materials for composition 1. The entry for the first material, pu-239, should look like that in Fig. 5. The composition number should already be set to 1 and then you select pu-239 from the list of materials in the library. 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  $3.7047\text{e-}2$ . After entering the data, select **OK/Save** to save this information and go to the next material.

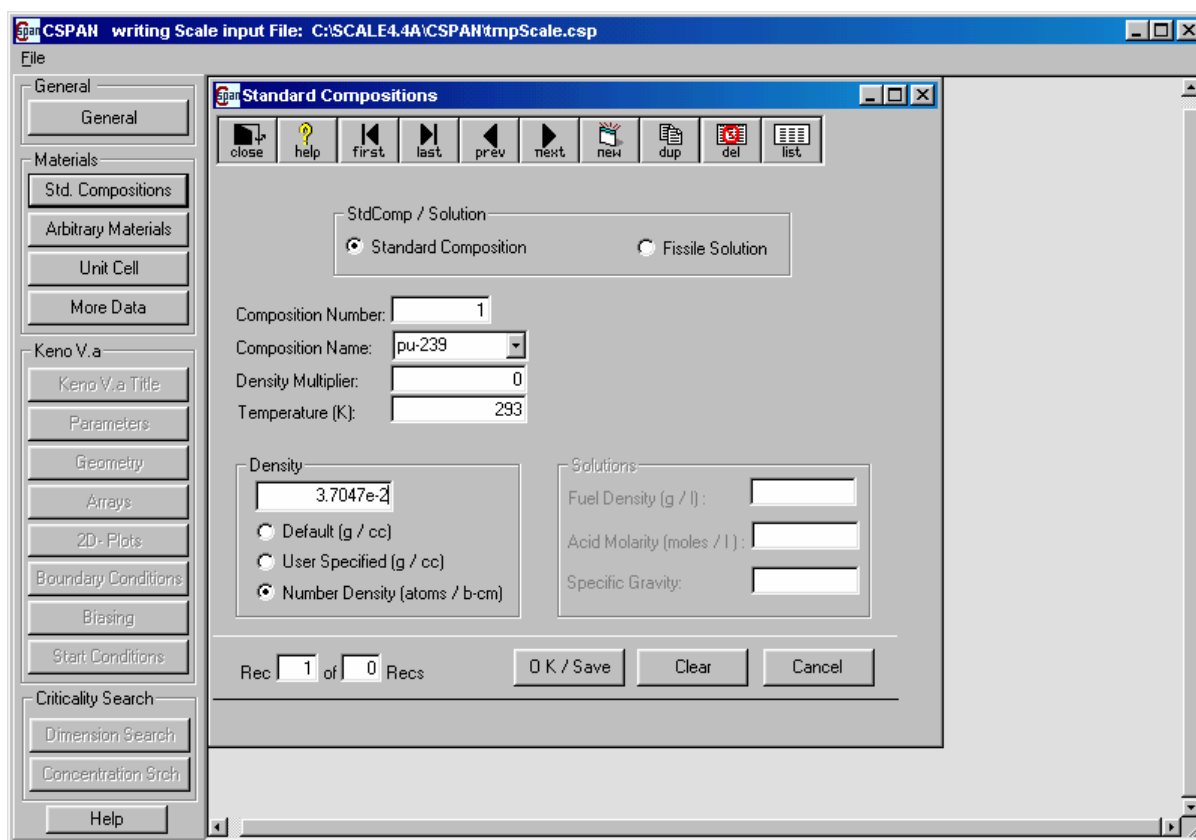


Fig. 5. Data for  $^{239}\text{Pu}$  in composition 1.

The entries for the next two materials should look like those shown in Fig. 6 and Fig. 7. Note that CSPAN automatically updates the composition number when you go to a new screen, so you will need to reset it back to 1 for the pu240, pu-241, and gallium entries.



CSPAN writing Scale input File: C:\SCALE4.4A\CSPAN\mpScale.csp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

Geometry

Arrays

2D-Plots

Boundary Conditions

Biasing

Start Conditions

Criticality Search

Dimension Search

Concentration Search

Help

Standard Compositions

close help first last prev next new dup del list

StdComp / Solution

☒ Standard Composition ☐ Fissile Solution

Composition Number: 1

Composition Name: pu-240

Density Multiplier: 0

Temperature (K): 293

Density

1.751e-3

☐ Default (g / cc)

☐ User Specified (g / cc)

☒ Number Density (atoms / b-cm)

Solutions

Fuel Density (g / l):

Acid Molarity (moles / l):

Specific Gravity:

Rec 2 of 1 Recs

O K / Save Clear Cancel

Fig. 6. Data for  $^{240}\text{Pu}$  in composition 1.

CSPAN writing Scale input File: C:\SCALE4.4A\CSPAN\mpScale.csp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

Geometry

Arrays

2D-Plots

Boundary Conditions

Biasing

Start Conditions

Criticality Search

Dimension Search

Concentration Search

Help

Standard Compositions

close help first last prev next new dup del list

StdComp / Solution

☒ Standard Composition ☐ Fissile Solution

Composition Number: 1

Composition Name: pu-241

Density Multiplier: 0

Temperature (K): 293

Density

1.17e-4

☐ Default (g / cc)

☐ User Specified (g / cc)

☒ Number Density (atoms / b-cm)

Solutions

Fuel Density (g / l):

Acid Molarity (moles / l):

Specific Gravity:

Rec 3 of 2 Recs

O K / Save Clear Cancel

Fig. 7. Data for  $^{241}\text{Pu}$  in composition 1.

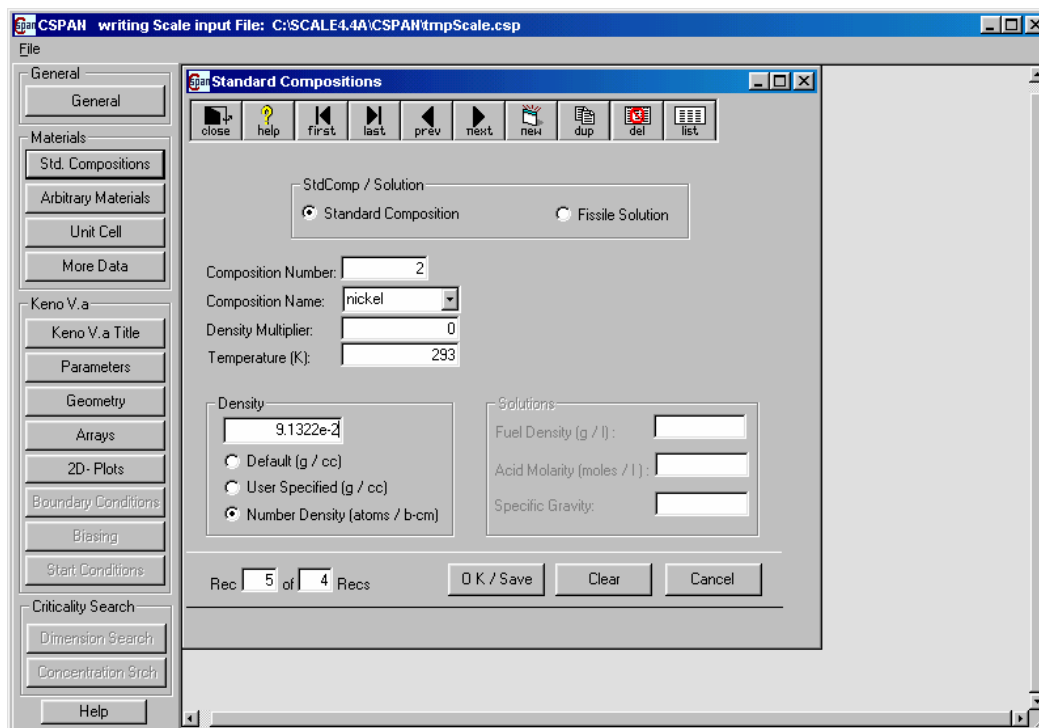
The last composition 1 material is gallium with its data entered as shown in Fig. 8. Note that before saving this screen, the notation in the lower left hand corner indicates that it is **Rec 4 of 3 Recs**. This means that the previous 3 records have been saved, but this one has not yet been saved. After entering the data for gallium, select **OK/Save** to complete the information for composition 1.

The screenshot shows the 'Standard Compositions' dialog box within the CSPAN application. The title bar reads 'CSPAN writing Scale input File: C:\SCALE4.4A\CSPAN\tmpScale.csp'. The left sidebar contains a 'File' menu and several categories of options: 'General' (with a 'General' button), 'Materials' (with 'Std. Compositions', 'Arbitrary Materials', 'Unit Cell', and 'More Data' buttons), 'Keno V.a' (with 'Keno V.a Title', 'Parameters', 'Geometry', 'Arrays', '2D- Plots', 'Boundary Conditions', 'Biasing', and 'Start Conditions' buttons), and 'Criticality Search' (with 'Dimension Search' and 'Concentration Search' buttons). A 'Help' button is at the bottom of the sidebar.

The main area of the dialog box is titled 'Standard Compositions' and includes a toolbar with icons for close, help, first, last, prev, next, new, dup, del, and list. Below the toolbar, there are radio buttons for 'StdComp / Solution' with 'Standard Composition' selected and 'Fissile Solution' unselected. The 'Composition Number' is set to 1, and the 'Composition Name' is 'gallium'. The 'Density Multiplier' is 0, and the 'Temperature (K)' is 293. The 'Density' section shows a value of 1.375e-3 with three radio buttons: 'Default (g / cc)' (unselected), 'User Specified (g / cc)' (unselected), and 'Number Density (atoms / b-cm)' (selected). The 'Solutions' section has three empty input fields for 'Fuel Density (g / l)', 'Acid Molarity (moles / l)', and 'Specific Gravity'. At the bottom, it shows 'Rec 4 of 3 Recs' and buttons for 'OK / Save', 'Clear', and 'Cancel'.

**Fig. 8. Data for gallium in composition 1.**

The next information is for the second composition, which has only one material, nickel, in this example problem. The information for nickel is entered in the same manner as was done for the first four materials. Remember to make sure that the **Composition Number** is 2 and that you have selected **Number Density** to allow you to enter  $9.1322\text{e-}2$ . The completed screen for nickel should look like that shown in Fig. 9.



**Fig. 9. Data for nickel in composition 2.**

This completes the data for the standard compositions; however, unit cell information is still required. To enter this information, select **Unit Cell** from the left-hand side CSPAN menu.

The MULTIREGION unit cell data should be entered as shown in Fig.10. The **Geometry Type** should be Spherical, the **Inner Boundary** reflected, and the **Outer Boundary** vacuum. Then the **Zone Dimensions** should be entered with the first mixture having a **Radius** of 6.38493 cm and the second mixture having a **Radius** of 6.39763 cm. Once the screen looks like Fig. 10, select **OK/Save** to retain this information.

CSPAN writing Scale input File: C:\SCALE4.4A\CSPAN\tmpScale.csp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

Geometry

Arrays

2D-Plots

Boundary Conditions

Biasing

Start Conditions

Criticality Search

Dimension Search

Concentration Strch

Help

Multiregion Unit Cell Specifications

### MULTIREGION UNIT CELL

Type of Geometry: Spherical

Left (inner) Boundary Condition: Reflected

Right (outer) Boundary Condition: Vacuum

Dy:

Dz:

Origin: 0

Zone	Mixture No.	Outside Cumulative Radius or Thickness (cm)	Zone	Mixture No.	Outside Cumulative Radius or Thickness (cm)
1	1 pu-239,pu-	6.38493	6	select a valu	
2	2 nickel	6.39763	7	select a valu	
3	select a valu		8	select a valu	
4	select a valu		9	select a valu	
5	select a valu		10	select a valu	

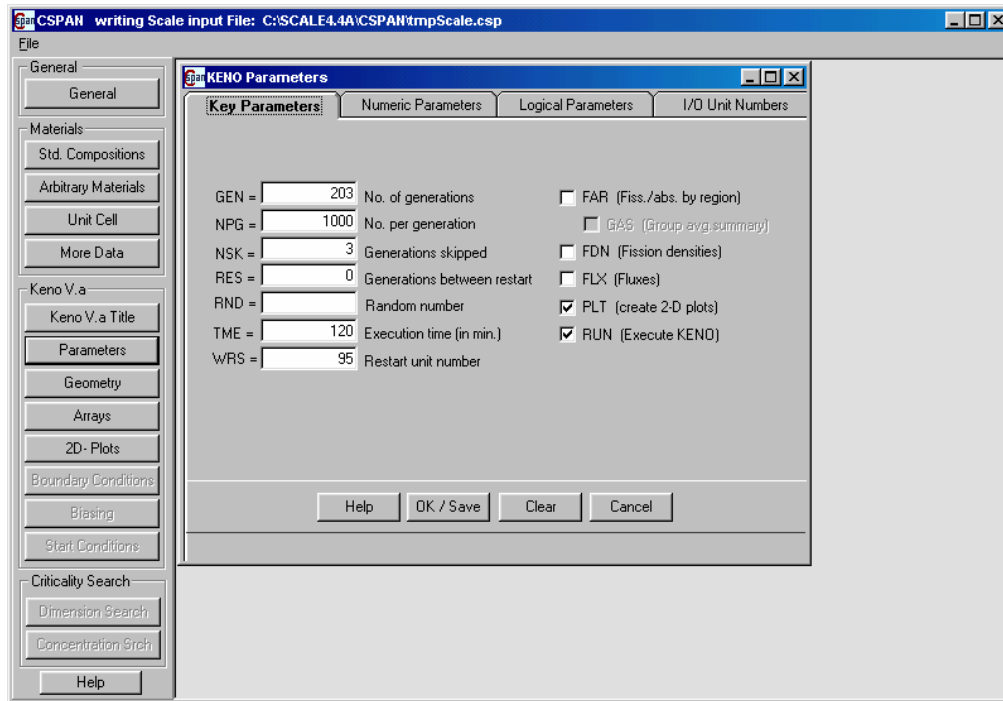
page 1 of 0

Help Prev Page Next Page OK / Save Clear Cancel

Fig. 10. Multiregion unit cell data.

#### 2.3.4. KENO V.a

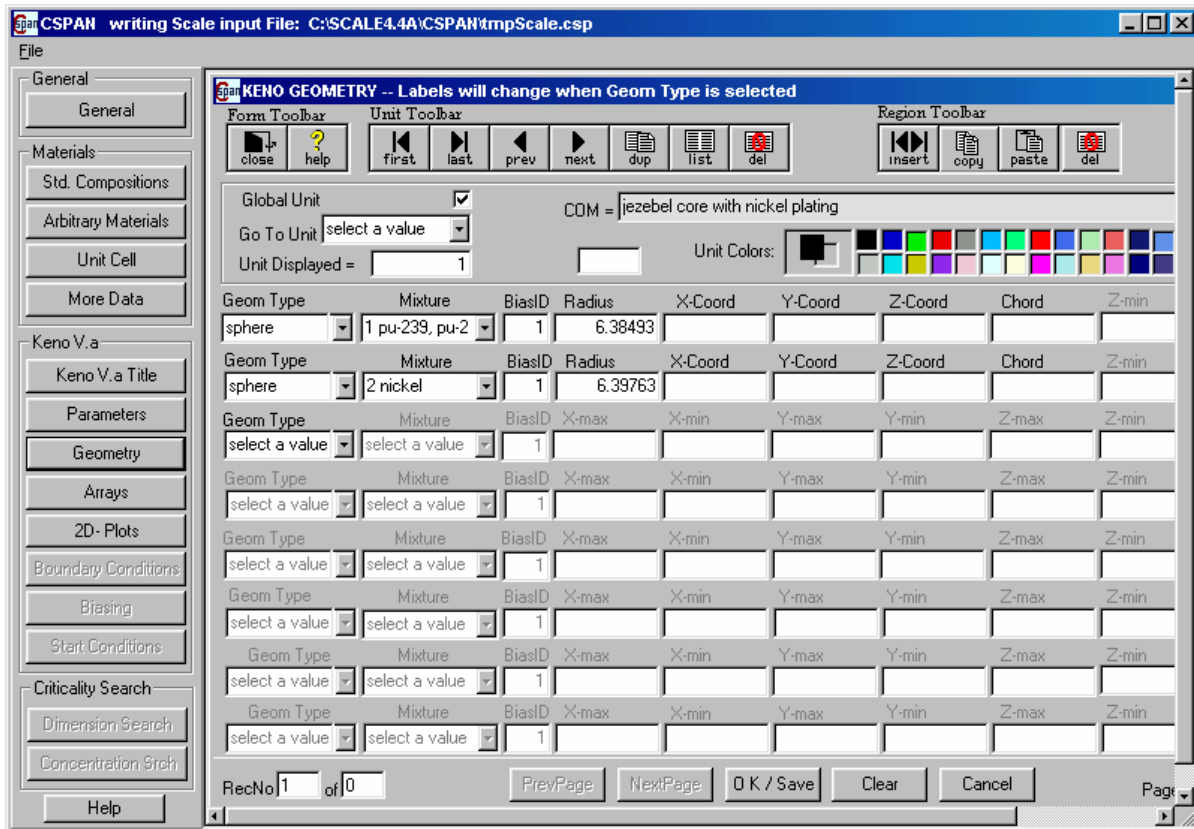
The next section of CSPAN input provides information required to run a KENO V.a analysis of the problem. The first entry is the title, which will appear in the KENO run. If you want a different title for KENO than you used for the problem as a whole, you enter it here by selecting **KENO V.a Title** from the menu on the left hand side of CSPAN. This brings up the **Title** entry form. The next screen is for the KENO **Parameters** and should look like Fig. 11. We will use the default values.



**Fig. 11. KENO parameters window.**

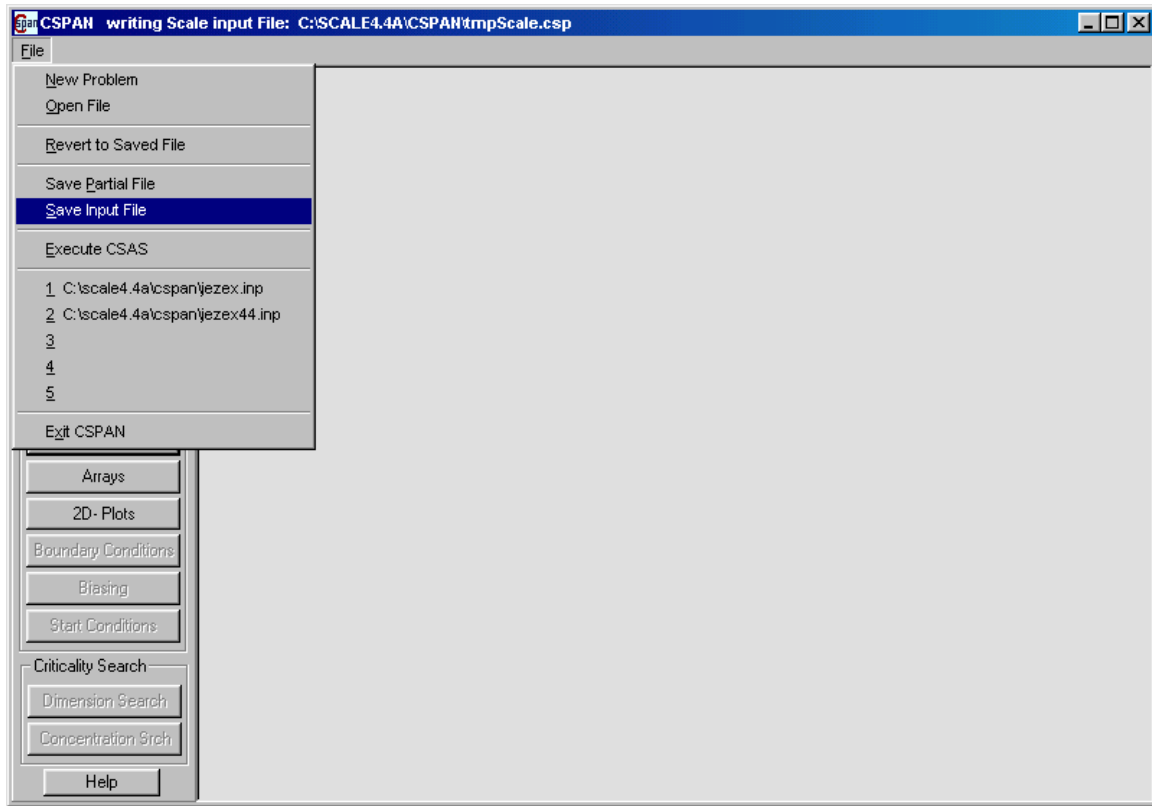
Select **OK/Save** to retain these values. Now select **Geometry** from the CSPAN menu on the left-hand side. This opens the **KENO Geometry** window.

You first need to check the box beside **Global Unit** by clicking on the box. The global unit in KENO is the outermost unit that defines the entire system to be analyzed. Then enter a comment next to **COM=**. The comment for this problem should read, *jezebel core with nickel plating*. Then enter the **Geom Type**, **Mixture**, and **Radius** for the two regions as shown in Fig. 12. Note the radii entered are the same radii entered in the unit cell data.



**Fig. 12. KENO geometry window.**

Now select **OK/Save** to retain this data. 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 CSPAN screen. This will bring up the pulldown menu as shown in Fig. 13. From the pulldown menu, select **Save Input File** and then enter the file name, such as jezebel.



**Fig. 13. Pulldown menu for saving input file.**

## **2.4. RUNNING SCALE/KENO V.a**

To run SCALE/KENO V.a, use the same pulldown menu as used to save the input file. From the pulldown menu, select **Execute CSAS**. 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. 14.

```

C:\WINDOWS\system32\cmd.exe

generation      generation      elapsed time      average
generation      k-effective      minutes      k-effective
191      1.01315E+00      1.45833E-01      9.97124E-01
192      9.87929E-01      1.46667E-01      9.97075E-01
193      9.96235E-01      1.47333E-01      9.97071E-01
194      9.65482E-01      1.48000E-01      9.96906E-01
195      1.03552E+00      1.48667E-01      9.97106E-01
196      9.73993E-01      1.49500E-01      9.96987E-01
197      1.04380E+00      1.50333E-01      9.97227E-01
198      9.83291E-01      1.50833E-01      9.97156E-01
199      1.02881E+00      1.51500E-01      9.97317E-01
200      9.86798E-01      1.52333E-01      9.97264E-01

jezebel problem, bare plutonium sphere with nickel shell as multiregion

generation      generation      elapsed time      average
generation      k-effective      minutes      k-effective
201      1.02110E+00      1.52833E-01      9.97384E-01
202      1.00224E+00      1.53667E-01      9.97408E-01
203      1.01887E+00      1.54500E-01      9.97515E-01

SCALE-4.4a job jezebel is finished.
Output is stored in jezebel.out.

```

Fig. 14. DOS Window showing completed run.

Note that it indicates **SCALE-4.4a job jezebel is finished.** where the job name is the name of the input file. 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 a **.out** extension. The elapsed time in the DOS window may not match that shown in Fig. 14 as each computer has different clock speeds.

## 2.5. SCALE OUTPUT

First, let's assume that the run was successful. The output for this problem consists of the following sections:

- echo of input,
- CSAS25 information and brief review of input values,
- BONAMI data from cross-section processing,
- NITAWL data from resonance treatment, and
- KENO V.a information.

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**. 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, nu-bar, 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. 15. Following the neutron parameters table is a table providing the calculated  $k_{eff}$  of the problem versus number of initial generations skipped. For the example problem, the calculated  $k_{eff}$  after skipping 3 initial generations is  $0.99739 \pm 0.00189$  as shown in Fig. 15. Also note that the smallest standard deviation for the example problem occurs after skipping 6 initial generations. This  $k_{eff}$  is used in the plot of generations skipped, which will be discussed in Sect. 3.

jezexmp44.out - WordPad

File Edit View Insert Format Help

199	1.02881E+00	7.47833E-01	9.97317E-01	1.88355E-03	0.00000E+00
200	9.86798E-01	7.48667E-01	9.97264E-01	1.87476E-03	0.00000E+00
201	1.02110E+00	7.66167E-01	9.97384E-01	1.86916E-03	0.00000E+00
202	1.00224E+00	7.67000E-01	9.97408E-01	1.85995E-03	0.00000E+00
203	1.01887E+00	7.68000E-01	9.97515E-01	1.85375E-03	0.00000E+00

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

jezebel problem, bare plutonium sphere with nick

lifetime = 3.87220E-09 + or - 1.02472E-11                      generation time = 3.07283E-09 + or - 1

nu bar = 3.13506E+00 + or - 6.85491E-04                      average fission group = 7.76907E+00 + or - 7

energy(ev) of the average lethargy causing fission = 1.19197E+06 + or - 3

no. of initial generations skipped	average k-effective	deviation	67 per cent confidence interval	95 per cent confidence interval	99 confid
3	0.99739	+ or - 0.00189	0.99550 to 0.99927	0.99361 to 1.00116	0.9917
4	0.99731	+ or - 0.00187	0.99544 to 0.99917	0.99357 to 1.00104	0.9917
5	0.99714	+ or - 0.00189	0.99525 to 0.99904	0.99335 to 1.00093	0.9914
6	0.99679	+ or - 0.00184	0.99495 to 0.99864	0.99310 to 1.00048	0.9912
7	0.99677	+ or - 0.00187	0.99490 to 0.99864	0.99302 to 1.00052	0.9911
8	0.99694	+ or - 0.00205	0.99490 to 0.99899	0.99285 to 1.00104	0.9908

For Help, press F1

**Fig. 15. KENO output for example problem.**

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 below in Fig. 16.

```

module csas25    will be called
  JEZEBEL PROBLEM, bare plutonium sphere with nickel shell
  44groupndf5 multiregion
  pu-239          1 0   3.7047E-2      293.0    end
  pu-240          1 0   1.751E-3       293.0    end
  pu-241          1 0   1.17E-4        293.0    end
  gallium         1 0   1.375E-3       293.0    end
  nickel          2 0   9.1322E-2      293.0    end
    end comp
  Spherical      end
  1 6.38493
  2 6.39763
    end zone

  JEZEBEL PROBLEM, bare plutonium sphere with nickel shell as multiregion
  read geom
  '
  global unit 1
  com='jezebel core with nickel plating'
  sphere      1   1 6.38493
  sphere      2   1 6.39763
    end geom
  end data

```

**Fig. 16. Example problem output echo of input file.**

## 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 CSPAN input processor to create a SCALE/KENO V.a input file.
- Set up and run a simple criticality problem on SCALE/KENO V.a.
- Find and interpret  $k_{eff}$  information from your output and perform simple checks for reasonableness on 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 CSPAN Input Processor. From this you gained confidence in using the code and some experience with CSPAN. 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 five main cross-section libraries available for criticality safety analyses.
- Use the CSPAN input processor 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 provide automated, problem-dependent, cross-section processing followed by calculation of the  $k_{eff}$  for the system being modeled. These control sequences activate the cross-section processing codes BONAMI and NITAWL-II to provide resonance-corrected cross sections. CSAS sequences ending with “X” utilize XSDRNPM to provide cell-weighted cross sections for a homogenized unit cell and/or the  $k_{eff}$  for a 1-D system model. ICE is used by CSASI and CSASIX to provide a Monte Carlo-formatted mixed (i.e., macroscopic) cross-section library. KENO V.a uses the processed cross sections and calculates the  $k_{eff}$  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. A search capability is achieved in the CSAS4 and CSAS4X sequences by repeatedly activating the control module MODIFY to alter the dimensions or the nuclide concentrations and the functional modules BONAMI, NITAWL, and KENO V.a to perform resonance processing and calculate the  $k_{eff}$  for the new dimensions or concentrations. Table 1 lists the control sequences and the modules they invoke.

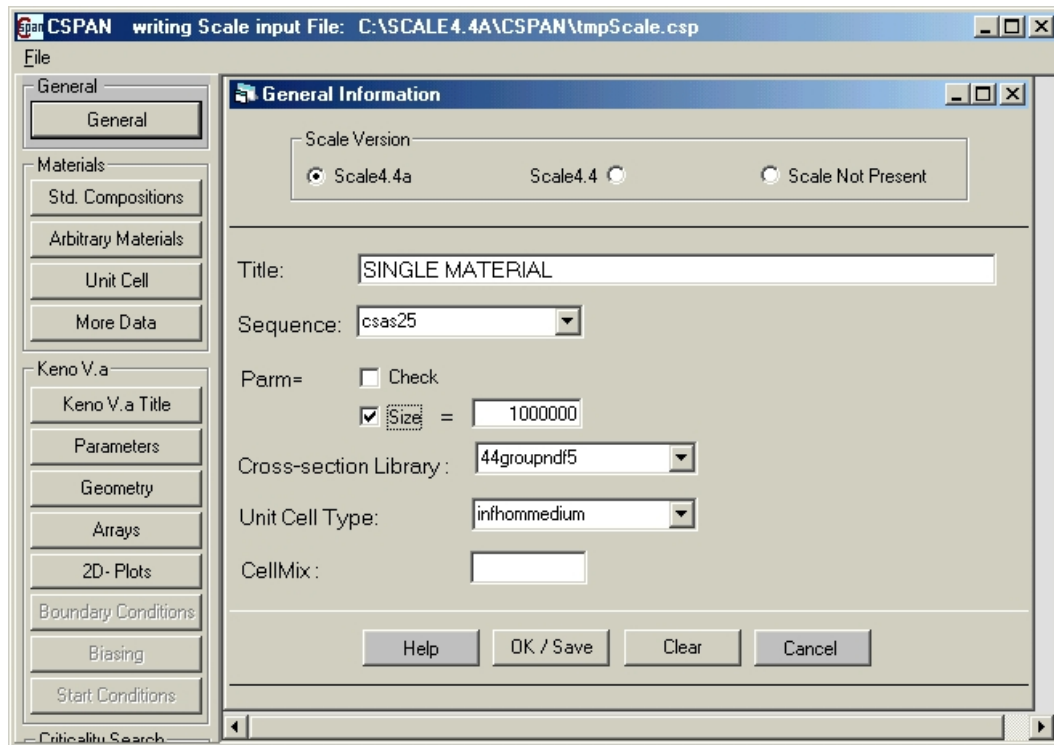
**Table 1. CSAS sequences for criticality safety**

Control module	Search function	Functional modules executed by the control module				
CSASI	No search	BONAMI	NITAWL-II		ICE	
CSASIX	No search	BONAMI	NITAWL-II	XSDRNPM	ICE	
CSASN	No search	BONAMI	NITAWL-II			
CSAS1X	No search	BONAMI	NITAWL-II	XSDRNPM		
CSAS25	No search	BONAMI	NITAWL-II		KENO V.a	
CSAS2X	No search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	
CSAS4	Search	BONAMI	NITAWL-II		KENO V.a	MODIFY <sup>a</sup>
CSAS4X	Search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	MODIFY <sup>a</sup>

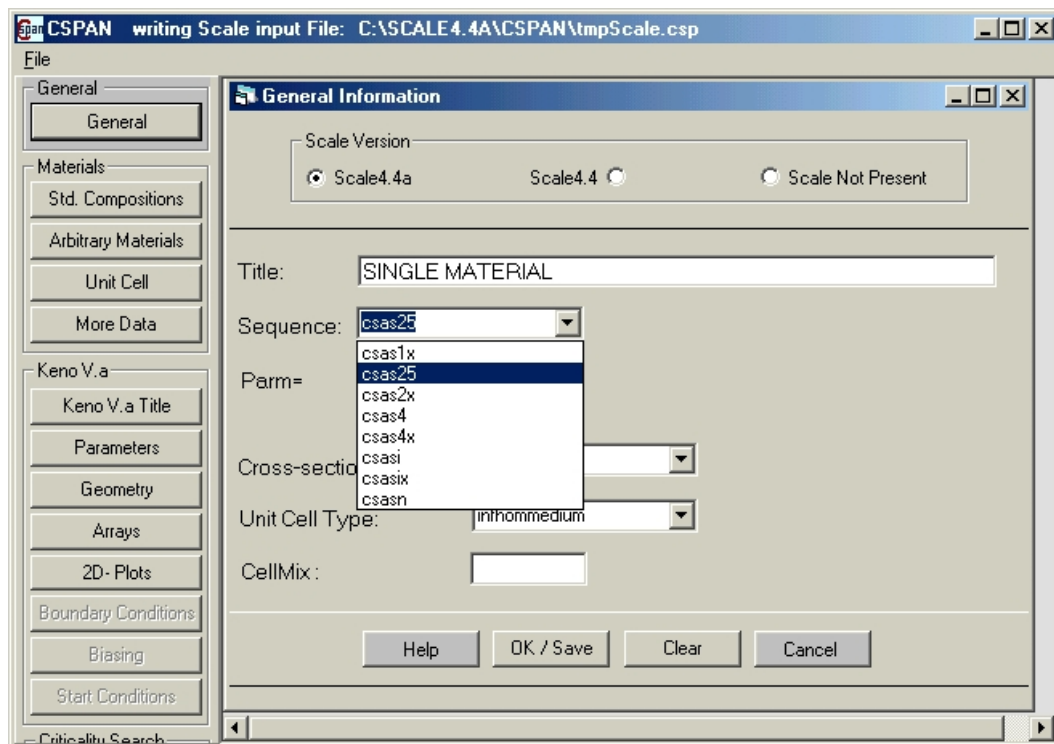
<sup>a</sup> MODIFY is a control module.

For most criticality applications, CSAS25 and CSAS2X will be the sequences used. The CSAS25 sequence is used most often for KENO V.a criticality calculations. For those unusual cases where homogenization of the fuel, clad, and moderator in the KENO model is needed, the CSAS2X sequence should be used to generate cell-weighted cross sections.

The selection of a sequence is done through the **General Information** window (Fig. 17) of CSPAN. Click on the **General** button to open this window. Information in this window includes the version of SCALE you are using as determined by CSPAN, a **Title** for the problem and the **Sequence** that you want to execute. The available sequences are listed on a pulldown menu as shown in Fig. 18. Select the sequence you want by clicking on it.



**Fig. 17. General information window in CSPAN.**

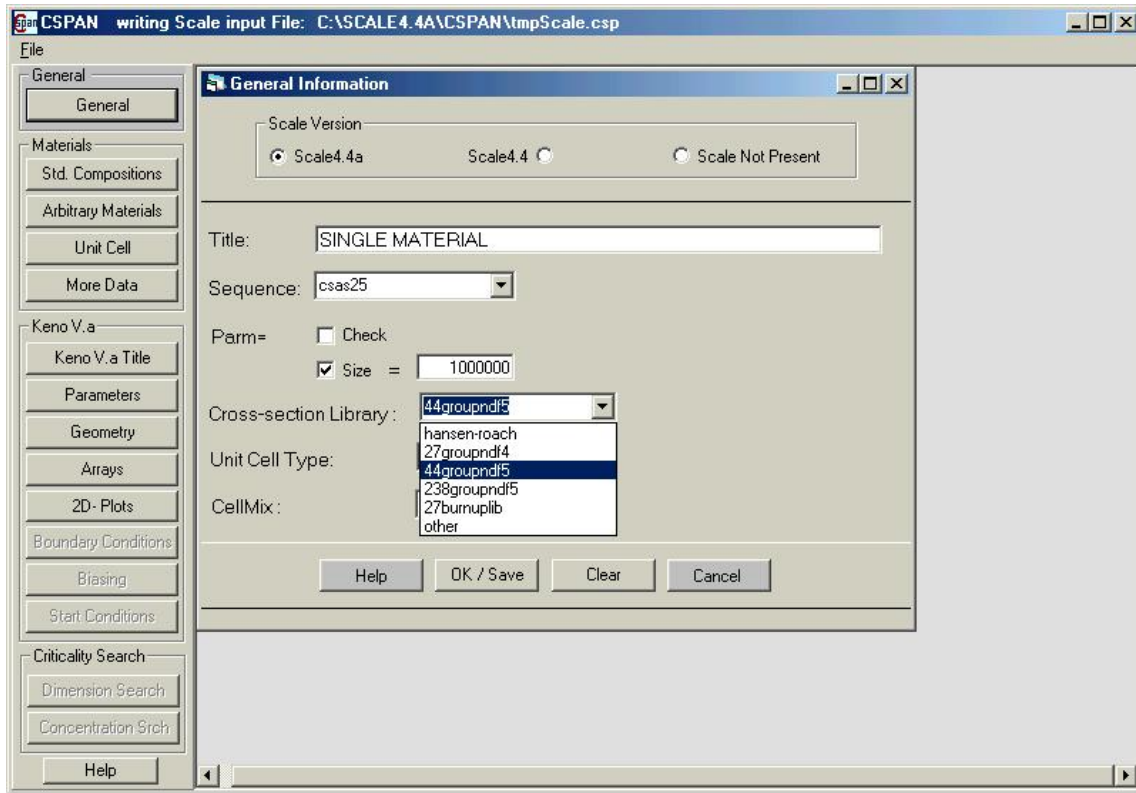


**Fig. 18. Criticality safety sequence pulldown menu.**

### 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 nine cross-section libraries distributed with SCALE, five of which are typically used 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 27-group library (27GROUPNDF4) is the broad-group library collapsed from the 218-group, ENDF/B-IV library and has 14 fast and 13 thermal groups. This library has been extensively validated against critical experiments. The 27-group burnup library (27BURNULIB) contains the data from 27GROUPNDF4 plus pre-release ENDF/B-V fission product data. The 238-group library (238GROUPNDF5) is the most complete library in SCALE. 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. The 44-group library is recommended for LWR systems, and the 238-group library is recommended for all other types of systems. It must be noted that the 238-group library requires more computer resources and time for the cross-section preparation. For the 238GROUPNDF5 and 218GROUPNDF5 libraries, it is suggested that the size parameter in the General Information window (see Fig. 19) be set to at least 500,000 or larger. See Appendix A for a more detailed discussion of the cross-section libraries.

A library is selected in CSPAN from the pulldown menu for **Cross-section Library** (See Fig. 19). Table 2 lists the standard SCALE cross-section libraries, along with the alphanumeric name and the main source of data for each library.



**Fig. 19. Cross-section library pulldown menu.**

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

Alphanumeric name	Primary data source
HANSEN-ROACH	Hansen-Roach 16-group library
27GROUPNDF4	ENDF/B-IV 218-group library
27BURNUPLIB	ENDF/B-IV 27-group library and pre-release ENDF/B-V
44GROUPNDF5	ENDF/B-V 44-group library
238GROUPNDF5	ENDF/B-V 238-group library

The criticality sequences access BONAMI first to process nuclides with Bondarenko data. The master library output from BONAMI is input to NITAWL-II, where resonance data are processed via the Nordheim integral treatment and an AMPX working-format library is produced.

### 3.4. MATERIAL INPUT

Information on materials in a system is entered into CSPAN, which puts that information in the format required by the **M**aterial **I**nformation **P**rocessor (MIP). The MIP utilizes this data along with standardized procedures to provide data to create problem-dependent cross-section libraries. Input data to CSPAN identifies the materials from the Standard Compositions 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 cell-weighting calculation. These input data include (1) the Standard Composition data (a standardized alphanumeric name, mixture number, and other data to define materials, including volume fraction or percent theoretical density, temperature, and isotopic distribution), that are used in the standardized number density calculations, 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 three fissile solutions ( $\text{UO}_2\text{F}_2$ ,  $\text{UO}_2(\text{NO}_3)_2$ , and  $\text{Pu}(\text{NO}_3)_4$ ) available for which the user can specify the heavy metal, acid, and water components.

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 293 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 CSPAN. These problems examine uranium in a bare (unreflected) finite cylinder with four different material compositions: pure  $^{235}\text{U}$  metal, U(93.7) metal,  $\text{U}(93.7)\text{O}_2$ , and  $\text{U}(30.3)\text{O}_2\text{F}_2$  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 $^{235}\text{U}$ Metal Cylinder

The metal cylinders in the bare metal cylinder problems have an effective radius of 7.82 cm with a critical height of 15.64 cm ( $H/D=1$ ). A cylinder containing pure  $^{235}\text{U}$  is modeled first to demonstrate using CSPAN to enter a single isotope (see Fig. 20). 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.

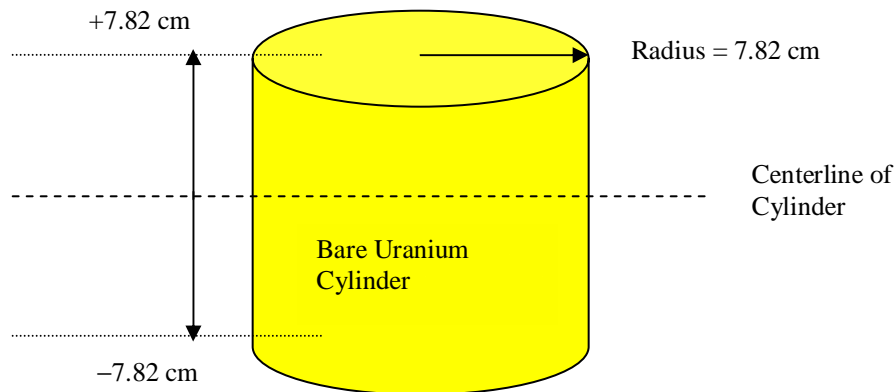
*Core Material ( $\rho_{\text{mix}} = 18.742 \text{ g/cc-mixture}$ )*

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

Configuration 1. *Bare Uranium Cylinder*

Radius = 7.82 cm

Height =  $\pm 7.82 \text{ cm}$

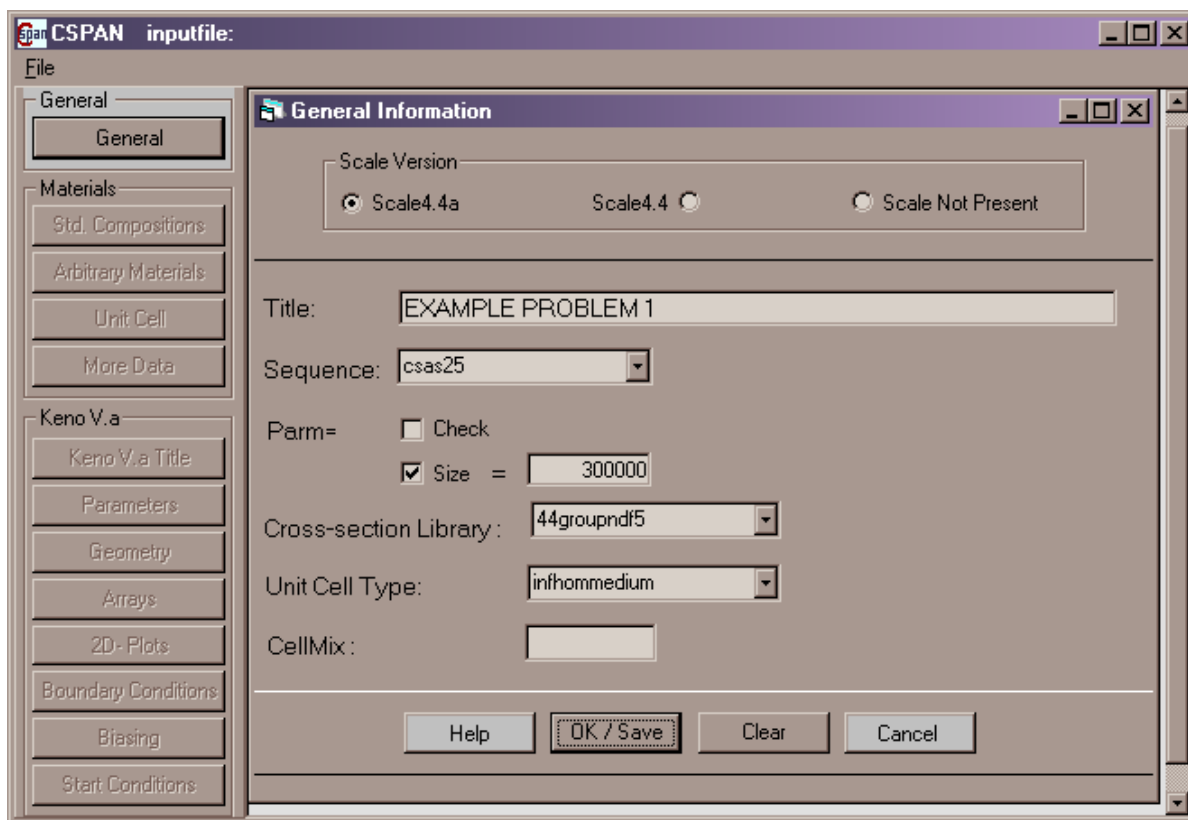


**Fig. 20. Configuration 1 geometry.**

The initial data entry for this example is the same as that described in the *Quickstart* section. Start the CSPAN input processor 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. The version of SCALE should already be selected as SCALE 4.4a. Now enter the title as follows:

#### EXAMPLE PROBLEM 1

Again note that information to be entered into CSPAN will appear in the Courier font. Now select `csas25` as the sequence. Under the **Parm=** line, check the **Size** box and enter 300000 after the = sign. For **Cross-section Library**, select `44groupndf5`, and for **Unit Cell Type**, select `inhommedium`. The general information screen should look like that in Fig. 21.



**Fig. 21. Example 1 general information window.**

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 CSPAN's Materials windows. There are four basic material input screens: **Std. Compositions**, **Arbitrary Materials**, **Unit Cell** and **More Data**. Most problems will use the **Std. Compositions** screen as shown in Fig. 22. For this example problem, we will select **Compositions**. The **Composition 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)**: (293). Now we need to enter the density by selecting **User Specified (g/cc)** and then entering the value 18.742 in the data entry box. The completed screen should look like Fig. 22.

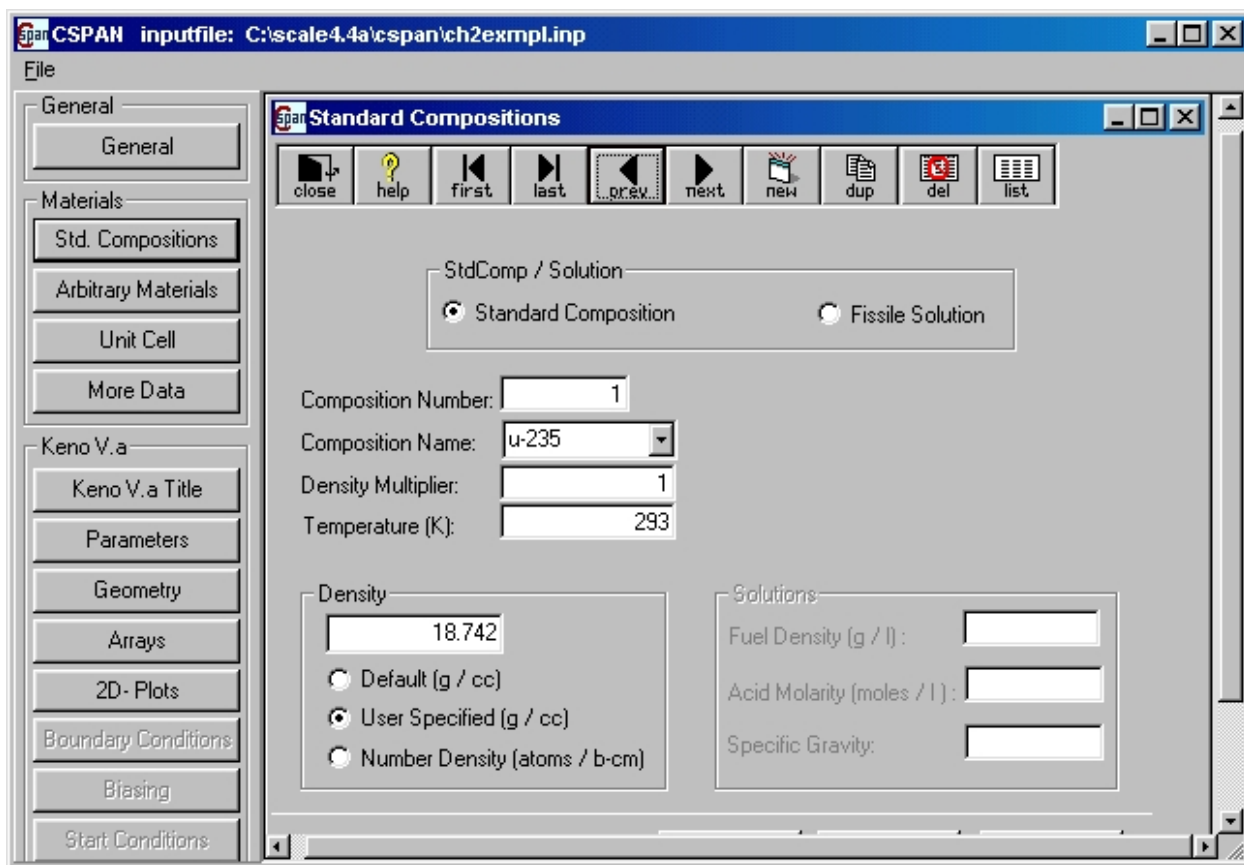


Fig. 22. Example 1 standard compositions window.

For this example,  $^{235}\text{U}$  is the only material (the **Arbitrary Materials** screen is not required) so select **OK/Save** and then **close** the **Std. Composition** window. Because the **Unit Cell Type** selected in the **General** window was infinite homogeneous medium, the **Unit Cell** data are not required.

The **More Data** window may also be skipped, because it is used for additional details on cross-section processing or when running XSDRNPM. The materials input data required for this example is now complete.

### 3.5.1.2. KENO V.a input

With this simple geometry, only a few entries are needed to complete the KENO input data.

The only KENO V.a input required for this problem is the geometry. Click on the **Geometry** button. Select the **Global Unit** box, and enter a comment in the **COM=** box. Then under **Geom Type** select cylinder and then for **Orientation of cylinder** select cylinder again. For **Mixture** select 1 u-235 from the pulldown menu. Then enter 7.82 for the **Radius**, 7.82 for the **H-Max**, and -7.82 for the **H-Min**. This completes the **Geometry** window information and it should look like Fig. 23.

**Fig. 23. Example 1 KENO geometry window.**

After checking that the input data match, select **OK/Save**. This completes the information required for the first example. Select **File**, then **Save Input File**. After saving, select **Execute CSAS** from the **File** menu. CSPAN opens a DOS window that shows the progress of the calculation. The beginning of the job should look like Fig. 24. The screen will show the input and output file names and then indicate which programs are being executed. When KENO V.a (a.k.a. o0o009) is started, the title is displayed and then the calculated  $k_{eff}$  from each generation are shown.

```

C:\scale4.4a\cspan>C:
C:\scale4.4a\cspan>cd C:\scale4.4a\cspan
C:\scale4.4a\cspan>c:\SCALE4.4a\cmds\scale44 ch2exmpl
*****
*   Now executing SCALE4.4a installed on drive c:
*   Input file = ch2exmpl.inp  Output file=ch2exmpl.out
*****

Now executing csas
Now executing o0o008
Now executing o0o002
Now executing o0o009
bare cylinder with u-235

      generation      generation      elapsed time      average
generation      k-effective      minutes      k-effective
      1          9.27886E-01      1.28333E-02      1.00000E+00
      2          1.01533E+00      1.56667E-02      1.00000E+00

```

Fig. 24. SCALE output in DOS window at job initiation.

When the run is completed, the DOS window should look like that in Fig. 25. If the job does not run successfully, try checking the error message with those given in Appendix B to determine how to fix the problem.

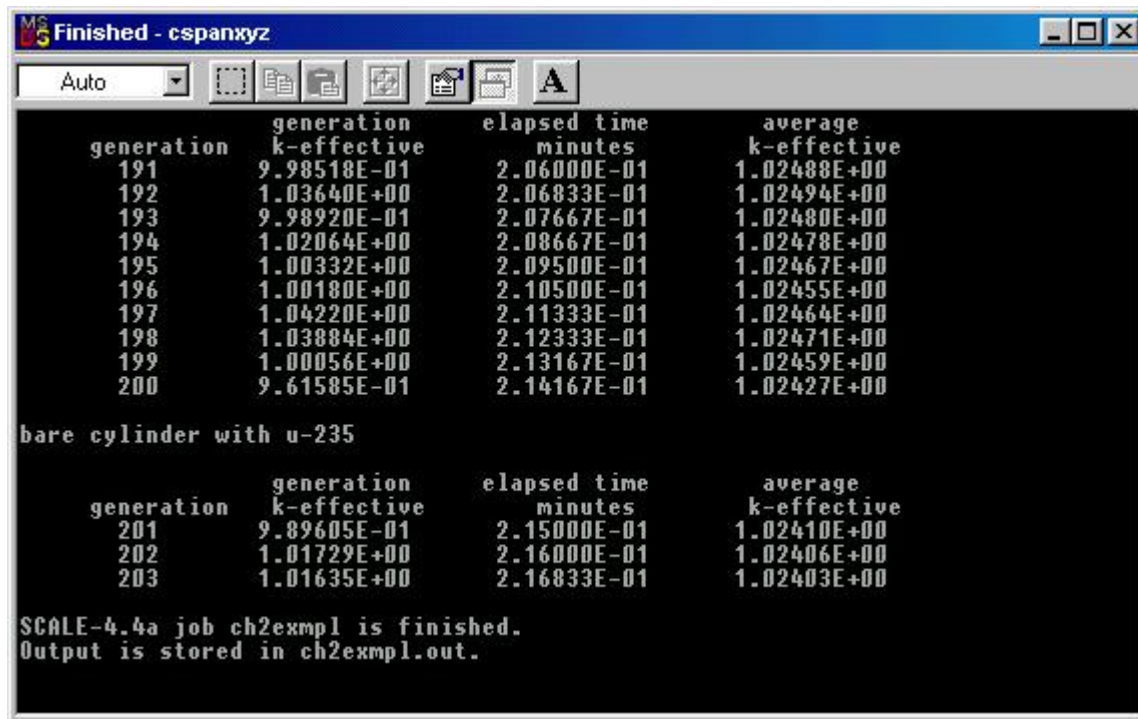


Fig. 25. SCALE output in DOS window at job completion.

### 3.5.1.3. Basic output

There are many pages in the output file. Each module has a section of output, starting with CSAS, then BONAMI, NITAWL-II, and finally 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  $k_{eff}$  values by generation along with elapsed time and average  $k_{eff}$ . 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 on the spectrum of the system modeled. 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 5.65 nanoseconds and the relatively high energy, 0.92 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 EALF is relatively insensitive to group structure and can thus be used to compare results from different libraries.

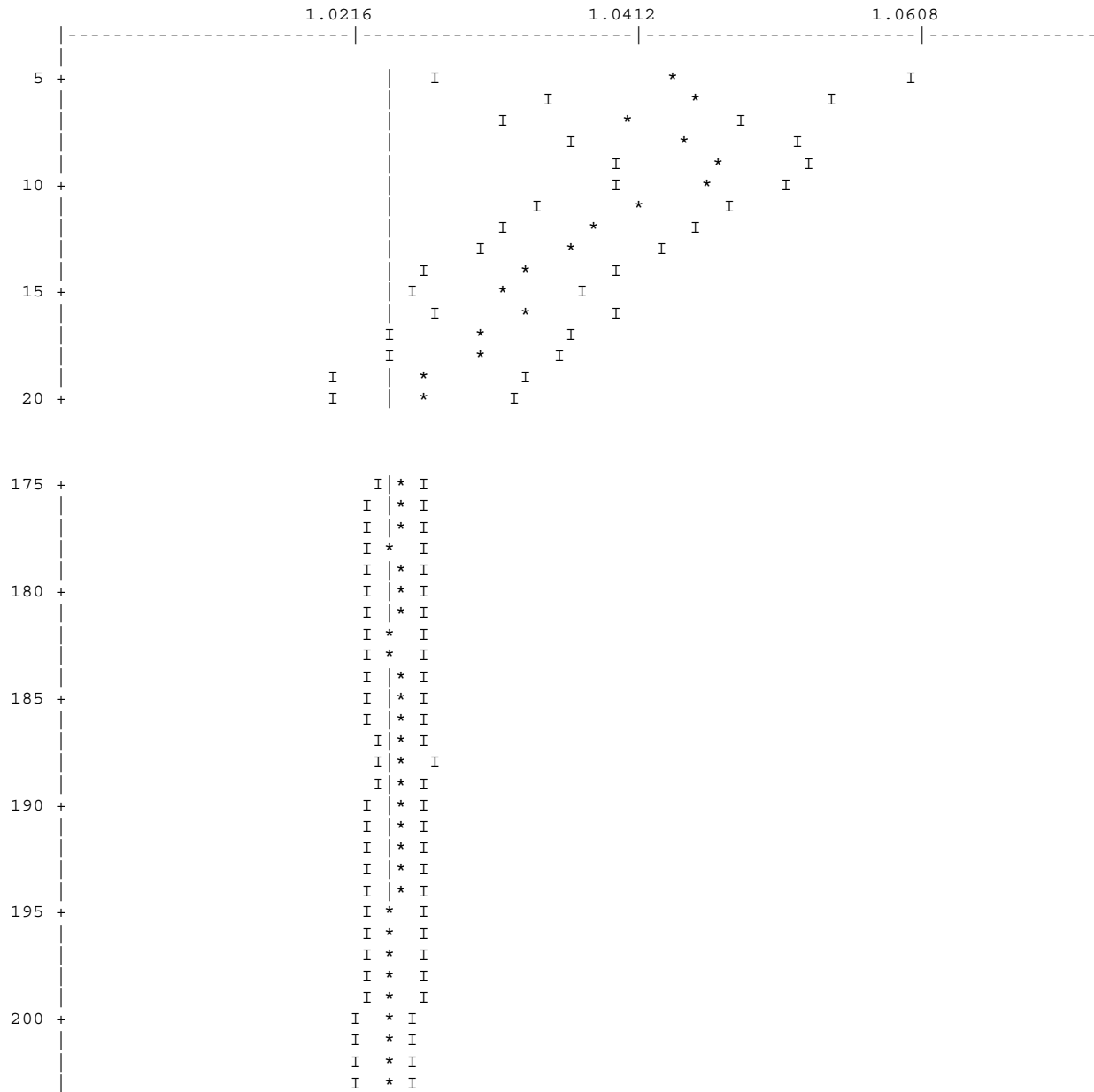
The final  $k_{eff}$  edit prints the average  $k_{eff}$  and its associated deviation and the limits of  $k_{eff}$  for the 67, 95, and 99% confidence intervals ( $\pm 1\sigma$ ,  $\pm 2\sigma$  and  $\pm 3\sigma$ ). The number of histories used in calculating the average  $k_{eff}$  is also printed. These results are based on skipping increasing numbers of the initial generations. Fig. 26 shows an abbreviated version of the table without the 95 and 99% confidence intervals. The user should carefully examine the final  $k_{eff}$  edit to determine if the average  $k_{eff}$  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  $k_{eff}$  becomes stable.

no. of initial generations skipped	average k-effective	deviation	67 per cent confidence interval	number of histories
3	1.02407	+ or - 0.00194	1.02213 to 1.02600	200000
4	1.02388	+ or - 0.00190	1.02198 to 1.02578	199000
5	1.02386	+ or - 0.00172	1.02214 to 1.02558	198000
6	1.02374	+ or - 0.00190	1.02184 to 1.02565	197000
7	1.02373	+ or - 0.00191	1.02182 to 1.02564	196000

**Fig. 26. Example of the final k-effective edit.**

Following the final  $k_{eff}$  edit are two plots of average  $k_{eff}$ : (1) versus the number of generations run and (2) versus the number of generations skipped. The limits of one standard deviation ( $\sigma$ ) are plotted on either side of each average  $k_{eff}$ . In the first plot (Fig. 27), KENO omits the calculated  $k_{eff}$  of the first NSK generations (number of generations skipped) in the calculation of the average  $k_{eff}$ . The dotted line represents the value of the average  $k_{eff}$  corresponding to the smallest deviation when the average  $k_{eff}$  and its deviation are computed for each generation over the range from NSK +1 through the total number of generations (NGEN). Fig. 27 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  $k_{eff}$  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 indicated by the stability of the average  $k_{eff}$  and by the minimum variance in  $k_{eff}$  near the end of the problem.

plot of average k-effective by generation run.  
the line represents  $k\text{-eff} = 1.0248 \pm 0.0019$  which occurs for 198 generations run.



**Fig. 27. Plot of average k-effective by generation run.**



The second output plot graphically depicts the average  $k_{eff}$  by generation skipped from the final  $k_{eff}$  edit in Fig. 26 for all generations from NSK+1 to NGEN. The dotted line represents the value of the average  $k_{eff}$  corresponding to the smallest deviation in the plot. An easy way to conceptualize the data in this plot is to think of each average  $k_{eff}$  as the average when the data for all previous generations is 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  $k_{eff}$  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. 28. (**NOTE:** No leakage is associated with faces having 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 close to 1. For this example, 43.5% of the neutrons were absorbed while 56.6% leaked from the system. The number of fissions printed for the system total, in this case **1.02407**, should be and is the same as the first  $k_{eff}$  printed in the final  $k_{eff}$  edit. The total elapsed time, **0.14967 minutes**, and final random number, **24A5341A654D**, are printed at the end of this edit.

group	fission fraction	fissions	percent deviation	absorptions	percent deviation	leakage	percent deviation
1	0.0072	7.41526E-03	4.1647	1.97080E-03	4.1647	2.41737E-03	4.4811
2	0.0159	1.63314E-02	2.1401	4.79939E-03	2.1401	6.48347E-03	2.2936
3	0.0293	2.99764E-02	1.3519	9.69229E-03	1.3519	1.81249E-02	1.5210
4	0.1041	1.06590E-01	0.6385	3.80169E-02	0.6385	6.38463E-02	0.7640
5	0.0634	6.48956E-02	0.8379	2.45028E-02	0.8379	3.68816E-02	0.9856
6	0.0185	1.89377E-02	1.6531	7.29196E-03	1.6531	1.02639E-02	1.9360
7	0.0926	9.48213E-02	0.7918	3.73444E-02	0.7918	5.28146E-02	0.8183
8	0.1076	1.10204E-01	0.6323	4.48522E-02	0.6323	6.46361E-02	0.7746
9	0.1537	1.57441E-01	0.5447	6.70177E-02	0.5447	9.40372E-02	0.6144
10	0.2138	2.18901E-01	0.4761	9.92882E-02	0.4761	1.34137E-01	0.4542
11	0.1585	1.62306E-01	0.5538	8.04732E-02	0.5538	7.32025E-02	0.5648
12	0.0309	3.16932E-02	1.3545	1.72089E-02	1.3545	8.89726E-03	1.9290
13	0.0021	2.12914E-03	5.4681	1.22250E-03	5.4681	5.24633E-04	6.3423
14	0.0022	2.25795E-03	5.7365	1.29339E-03	5.7365	3.00736E-04	8.9611
15	0.0002	1.59183E-04	20.2626	9.22796E-05	20.2626	9.83681E-06	56.5089
16	0.0000	6.28053E-06	100.0000	3.68840E-06	100.0000	0.00000E+00	0.0000
groups 17 through 43 removed as they have all zero entries							
44	0.0000	0.00000E+00	0.0000	0.00000E+00	0.0000	0.00000E+00	0.0000
system total =	1.02407E+00		0.1605	4.35071E-01	0.1617	5.66577E-01	0.1223
elapsed time	0.14967 minutes						
random number=	24A5341A654D						

**Fig. 28. Fraction of interactions by group.**

The last section of the output contains the frequency distributions that indicate the number of generations whose  $k_{eff}$  is within a specified interval. The intervals are determined by the code based on the upper and lower limits of the calculated  $k_{eff}$  for all generations. One asterisk is printed for each generation  $k_{eff}$ . The distributions should be reasonably symmetrical and bell-shaped for a good statistical analysis of  $k_{eff}$  (Fig. 29).

For this example, the  $k_{eff}$  with the minimum standard deviation was calculated as  $1.02386 \pm 0.00172$  for five generations skipped which is greater than critical as expected due to the buckling conversion from a sphere to a square cylinder.

```

                                frequency for generations    4 to  203

0.9543 to 0.9669      *
0.9669 to 0.9796      **
0.9796 to 0.9922      *****
0.9922 to 1.0049      *****
1.0049 to 1.0175      *****
1.0175 to 1.0302      *****
1.0302 to 1.0428      *****
1.0428 to 1.0555      *****
1.0555 to 1.0681      *****
1.0681 to 1.0808      *****
1.0808 to 1.0934
1.0934 to 1.1061
1.1061 to 1.1187
1.1187 to 1.1314      *

                                frequency for generations    54 to  203

0.9543 to 0.9669      *
0.9669 to 0.9796      *
0.9796 to 0.9922      *****
0.9922 to 1.0049      *****
1.0049 to 1.0175      *****
1.0175 to 1.0302      *****
1.0302 to 1.0428      *****
1.0428 to 1.0555      *****
1.0555 to 1.0681      *****
1.0681 to 1.0808      *****
1.0808 to 1.0934
1.0934 to 1.1061
1.1061 to 1.1187
1.1187 to 1.1314      *

                                frequency for generations   104 to  203

0.9543 to 0.9669      *
0.9669 to 0.9796      *
0.9796 to 0.9922      *****
0.9922 to 1.0049      *****
1.0049 to 1.0175      *****
1.0175 to 1.0302      *****
1.0302 to 1.0428      *****
1.0428 to 1.0555      *****
1.0555 to 1.0681      *****
1.0681 to 1.0808      **
1.0808 to 1.0934
1.0934 to 1.1061
1.1061 to 1.1187
1.1187 to 1.1314      *

                                frequency for generations   154 to  203

0.9543 to 0.9669      *
0.9669 to 0.9796
0.9796 to 0.9922      ****
0.9922 to 1.0049      *****
1.0049 to 1.0175      *****
1.0175 to 1.0302      *****
1.0302 to 1.0428      *****
1.0428 to 1.0555      **
1.0555 to 1.0681      **
1.0681 to 1.0808      *
1.0808 to 1.0934
1.0934 to 1.1061
1.1061 to 1.1187
1.1187 to 1.1314

```

**Fig. 29. Calculated k-effective by generation frequency plot.**

### 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 a critical height of 15.64 cm ( $H/D=1$ ). The geometry is unchanged from that shown in Fig. 20. 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 18.7 g/cc.

*Core Material ( $\rho_{\text{mix}} = 18.7$  g/cc-mixture)*

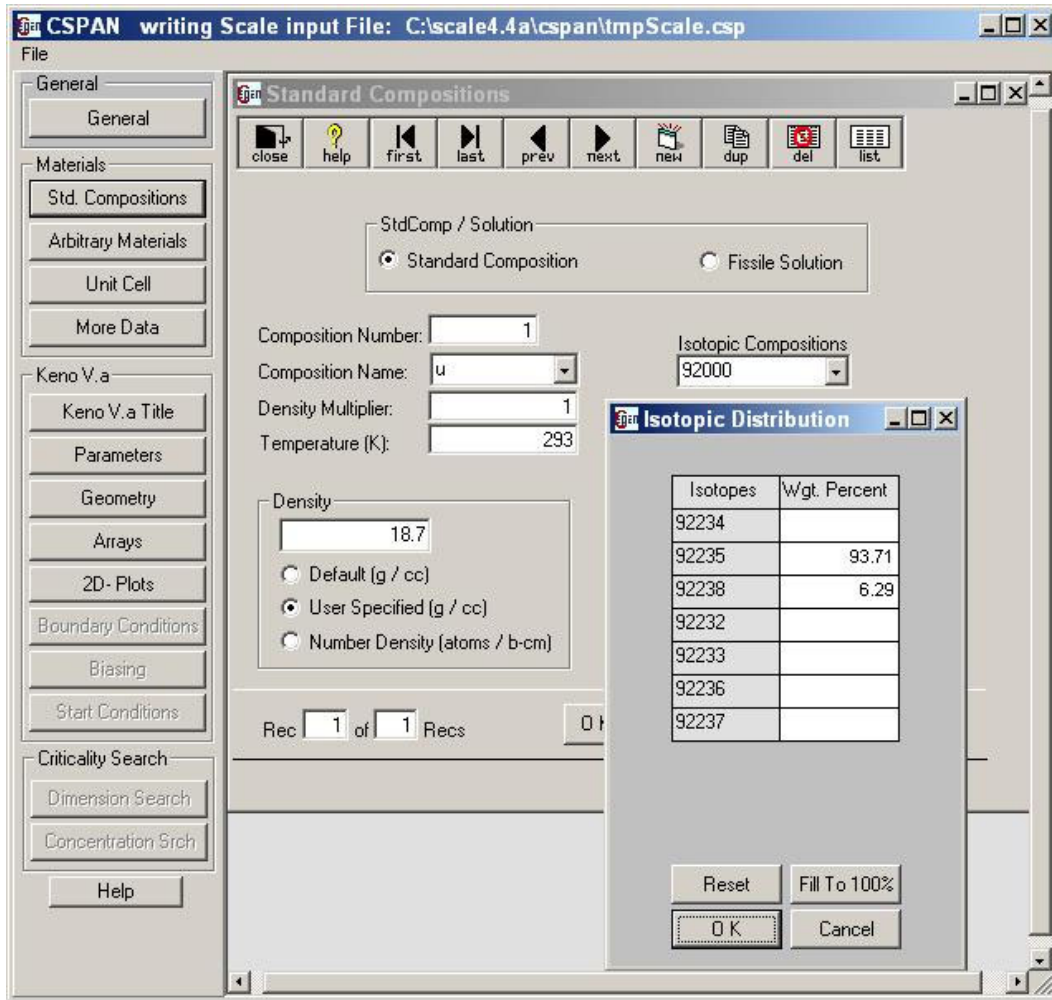
U metal (93.71 wt %  $^{235}\text{U}$  and 6.29 wt %  $^{238}\text{U}$ )

The data entry is the same as for the first problem. The only change will be 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 **Std. Compositions**. The **Composition Number:** starts with 1. Under **Composition Name:** scroll down the menu and select **u**. This brings up a window to the right-labeled **Isotopic Compositions**. It then asks you to select a **Value**. For **Uranium**, the only option is 92000. Clicking on this opens another window with the seven isotopes of uranium listed. We need to enter the isotopic composition 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. 30).



**Fig. 30. Isotopic distribution window.**

After selecting **OK**, the composition box disappears and you can enter the density multiplier of 1.0, and then the density by selecting **User Specified (g/cc)** and then entering the value 18.7 in the data entry box. The information should look like Fig. 30.

For this example, u is the only material (again, the **Arbitrary Materials** screen is not required) so select **OK/Save** and then **Close**.

### 3.5.2.2. KENO V.a input

This completes the information required for the second example. Select **File**, then **Save Input File**. For the filename, you need to use a different name than before; something like U93\_cylinder. After saving, select **Execute CSAS** from the **File** menu. A DOS window will open and show the progress of the calculation. For this example,  $k_{eff}$  was calculated as  $0.99380 \pm 0.00178$ , for three generations skipped which is quite 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 critical radius is 12.8 cm with a 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 wt % <sup>235</sup>U and 6.29 wt % <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 title and unit cell information as for the previous two examples.

#### 3.5.3.1. Material input

For this problem, we will again select **Standard Composition**. The **Composition Number:** starts with 1. Under **Composition Name:** scroll down the menu and select uo2. This again brings up a window to the right labeled **Isotopic Compositions** so that you can specify the uranium composition. For uranium, the only option is 92000. Selecting this option opens a window with the seven isotopes of uranium listed. 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 change that to 0.95\*10.96 or 10.412 g/cc. The data for this problem should look like Fig. 31, although the isotopic screen will not be visible after you have entered the density multiplier.

For this example, uo2 is the only material so select **OK/Save** and then **close** the **Std. Composition** screen. This completes the materials input data required for this example.

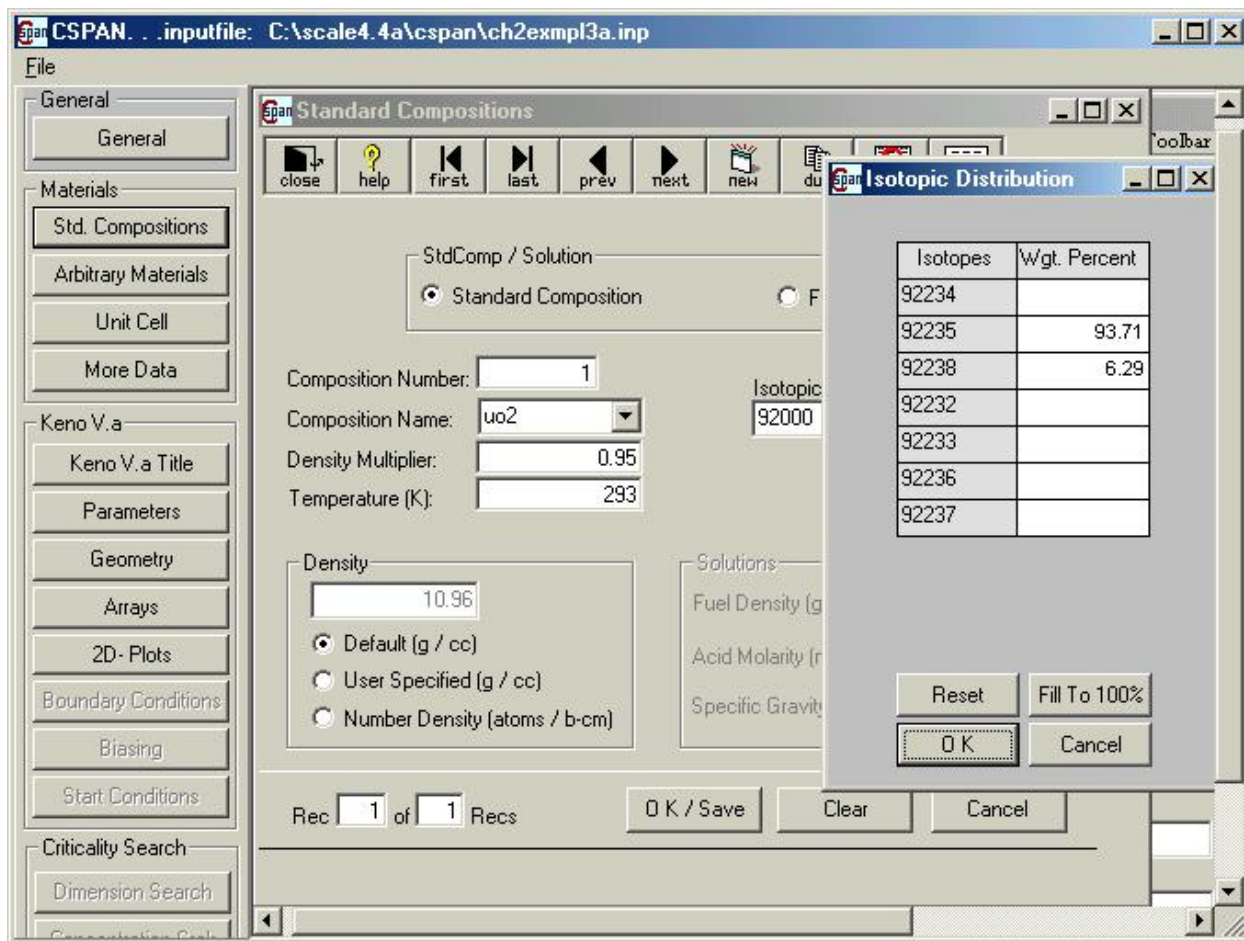


Fig. 31. Standard composition input for U(93.71)O<sub>2</sub>.

### 3.5.3.2. KENO V.a input

Open the **Geometry** window. Select the **Global Unit** box, and enter a comment in the **COM=** box. Then under **Geom Type** select cylinder and then for **Orientation of cylinder** select cylinder again. For **Mixture** select 1 u from the pulldown menu. Then enter 12.8 for the **Radius**, 12.8 for **H-Max**, and -12.8 for **H-Min**. This completes the **Geometry** screen information. This completes the information required for the third example. Select **File**, then **Save Input File**. After saving, select **Execute CSAS** from the **File** menu. A DOS window opens and displays the progress of the calculation. For this example,  $k_{eff}$  was calculated as  $0.99227 \pm 0.00178$  for nine generations skipped which is quite 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 is 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. CSPAN has a special entry screen for fissile solutions, but you need the fuel atom density (in this case, <sup>235</sup>U + <sup>238</sup>U), 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 calculate atom densities for H, O, F, <sup>235</sup>U, and <sup>238</sup>U for entry in CSPAN. The calculated atom densities are:

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

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

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

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

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

$$N_U = 1.8439 \times 10^{-3} \text{ atoms-U(30.3) / b-cm}$$

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, we will again select **Standard Composition**. As the materials are mixed together and we are entering atom densities, they will all be part of composition number 1. You will enter four materials (U, H, O, and F) for composition 1. The first will be uranium. The **Composition Number:** starts with 1. Under **Composition Name:** scroll down the menu and select u. This again brings up a box to the right labeled **Isotopic Compositions** so that you can specify the uranium composition. Select 92000 and a window opens with the seven isotopes of uranium listed. We need to enter the isotopic composition of the uranium (in weight percent) for the problem, which is 30.3 for <sup>235</sup>U and 69.7 for <sup>238</sup>U. (For the <sup>238</sup>U, you can also select the entry in the box and then click below where it says **Fill to 100%**. CSPAN will automatically determine the remaining percentage and enter it in the selected isotope box. Then select **OK**; leave the density multiplier at 1.0. In the density boxes below, select **Number Density (atoms/b-cm)**. Enter the uranium atom density of  $1.8439 \times 10^{-3}$  as 1.8439e-3. (You can also enter the density as 0.0018439.). The screen should look like Fig. 32.



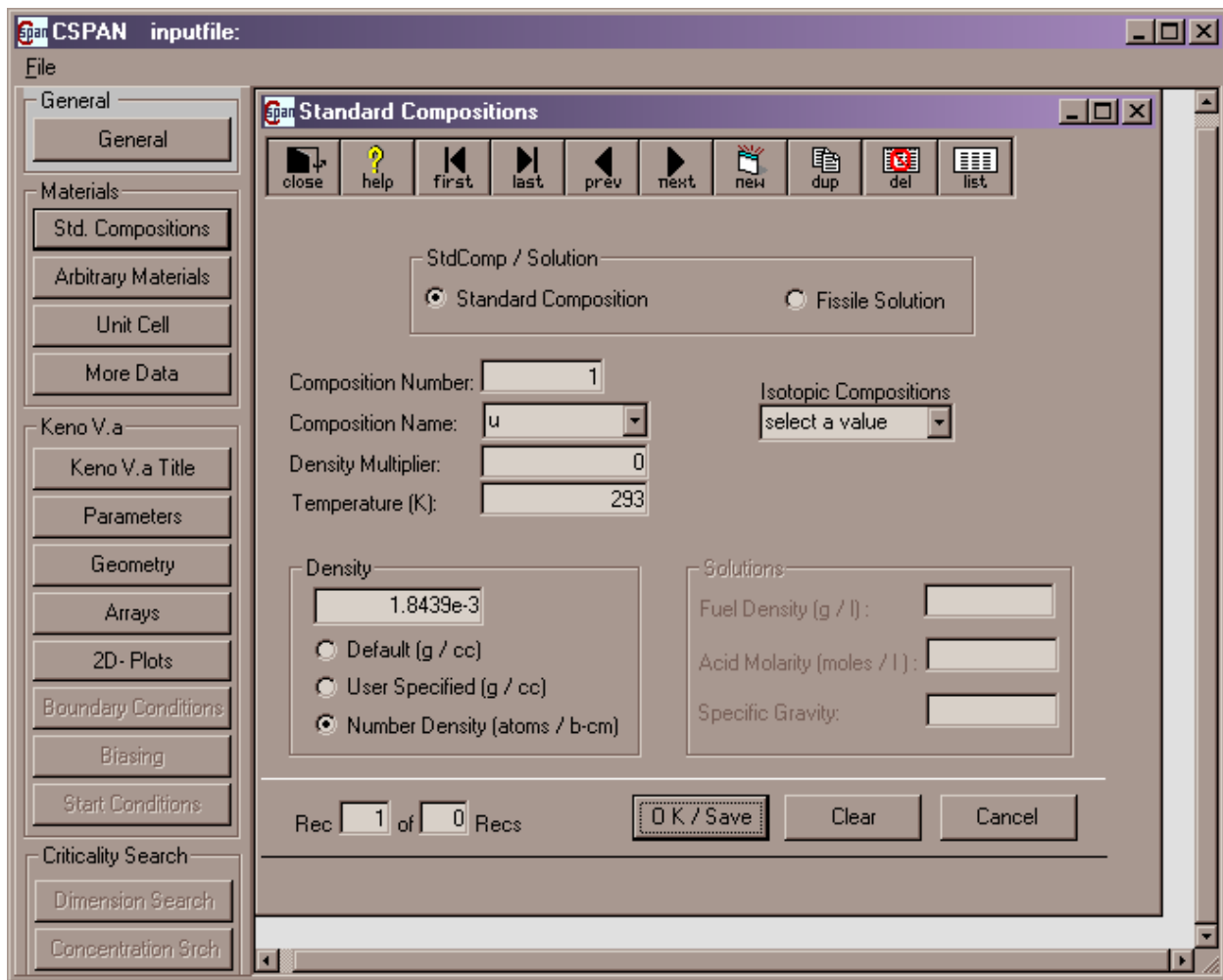


Fig. 32. Standard composition input for U in  $U(30.3)O_2F_2$ .

Note that CSPAN automatically updates the composition number when you go to a new screen, so you will need to reset it back to 1 for the **h**, **o**, and **f** entries. For each of these materials, enter the atom density as given above. Then select **OK/Save**. This completes the materials input data required for this example.

#### 3.5.4.2. KENO V.a input

Open the **Geometry** screen. Select the **Global Unit** window, and enter a comment in the **COM=** field. Then under **Geom Type** select **cylinder** and then for **Orientation of cylinder** select **cylinder** again. For **Mixture** select 1 u, fluorine, h from the pulldown menu. Then enter 15.225 for the **Radius**, 15.225 for **H-Max**, and -15.225 for **H-Min**. This completes the **Geometry** information. This completes the information required for the third example. Select **File**, then **Save Input File**. After saving, select **Execute CSAS** from the **File** menu. A DOS window opens and shows the progress of the analysis. For this example,  $k_{eff}$  was calculated as  $0.99457 \pm 0.00264$  for six generations skipped 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 CSPAN input processor 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 third section you ran a number of simple geometries with various material compositions. You used the CSPAN input processor 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 CSPAN 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

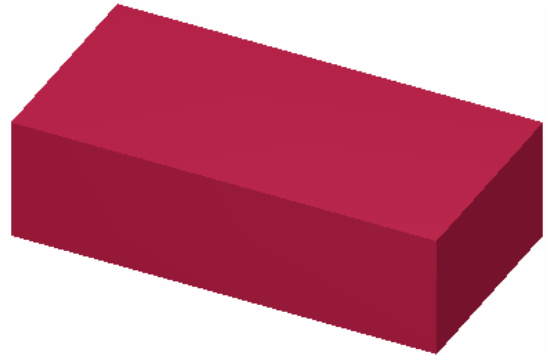
SCALE / KENO V.a uses a set of basic shapes to build the geometry models. You have used CSPAN to enter data on cylinders in Sect. 3. This shape and the other basic shapes are described in Table 3 and depicted in Fig. 33.

**Table 3. Basic shapes**

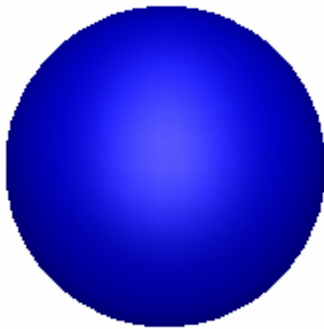
<b>Keyword</b>	<b>Description</b>
<b>CUBE</b>	Box with equal X, Y, and Z dimensions
<b>CUBOID</b>	Box or rectangular parallelepiped; X, Y, and Z dimensions are not necessarily equal
<b>SPHERE</b>	Sphere
<b>CYLINDER</b>	Cylinder that has its length along the X, Y, or Z axis
<b>HEMISPHERE</b>	Partial sphere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



Cube



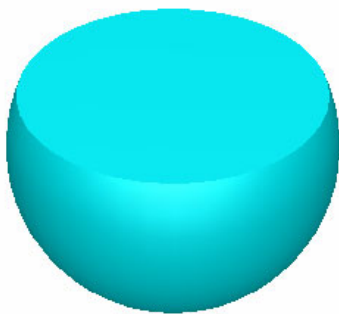
Cuboid



Sphere



Cylinder



Hemisphere



Hemicylinder

**Fig. 33. KENO V.a basic geometry shapes.**

Although there are six shapes listed, CSPAN considers the last two to be subsets of the basic shapes. Thus, the geometry options in CSPAN show cylinder, cuboid, cube, and sphere as the basic shapes.

After selecting sphere, you are given the option to make it a hemisphere; similarly with cylinders and hemicylinders. A description of the options for each basic shape can be found in the KENO V.a manual [Sect. F11.4.9].

Each shape has a set of quantitative information needed to describe its size and location. This information is entered in the **KENO Geometry** window as shown in Fig. 34.

Geom Type	Mixture	BiasID	Radius	H-Max	H-Min	X-coord	Y-coord	Chord	Chord
cylinder	1 u	1	4	10	-2				
Geom Type	Mixture	BiasID	X-Max	X-Min	Y-Max	Y-min	Z-Max	Z-Min	Chord
cuboid	1 u	1	5	0	5	0	6	-6	
Geom Type	Mixture	BiasID	X-Max	X-Min	Y-max	Y-min	Z-max	Z-min	Chord
cube	1 u	1	6	-6					
Geom Type	Mixture	BiasID	Radius	X-Coord	Y-Coord	Z-Coord	Chord	Z-min	Chord
sphere	1 u	1	10						
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							

**Fig. 34. KENO geometry input window.**

As shown in Fig. 34, the description of a cylinder requires the Radius and maximum height (**H-Max**) and minimum height (**H-Min**) data as a minimum. For a cuboid, the **X-Max** and **X-Min**, **Y-Max** and **Y-Min**, and **Z-Max** and **Z-Min** data are necessary to specify the shape. Because a cube is a cuboid with equal sides, only **X-Max** and **X-Min** 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 CSPAN, 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 along the Z-axis is identical to the first example problem in Sect. 3. A summary of the input information follows and is illustrated in Fig. 35.

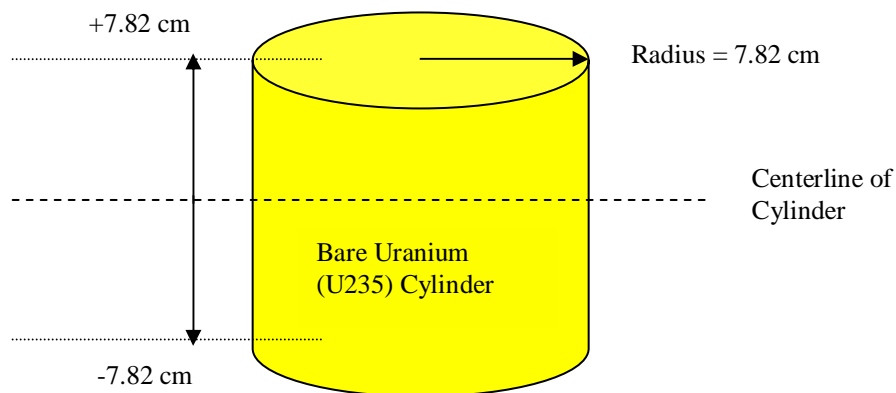
*Core Material ( $\rho_{mix} = 18.742$  g/cc-mixture)*

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

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

Radius = 7.82 cm

Height =  $\pm 7.82$  cm



**Fig. 35. Configuration 1 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.

#### 4.2.2.1. KENO V.a input

With this simple geometry, only a few entries are needed to complete the KENO geometry input data. As we did in Sect. 3, click on the **Geometry** button. Select the **Global Unit** box, and enter a comment in the **COM=** box. Then under **Geom Type** select cylinder and for **Orientation of cylinder** select cylinder again. (**NOTE:** The orientation of the keyword `cylinder` is along the **Z-axis**, and is identical to `zcylinder` so it will provide the

correct geometry for this problem.) For **Mixture** select 1 u-235 from the pulldown menu. Then enter 7.82 for the **Radius**, 7.82 for **H-Max**, and -7.82 for **H-Min**. This completes the **Geometry** screen information and it should look like Fig. 36.

**Fig. 36. KENO geometry input for configuration 1.**

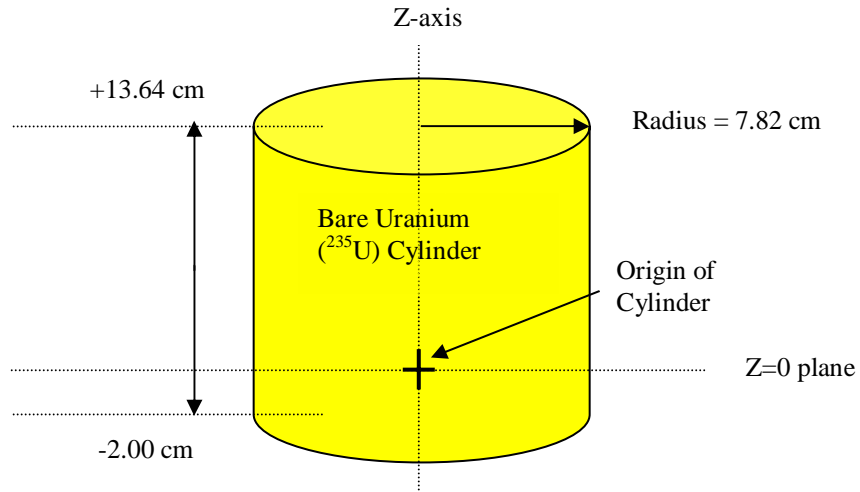
After checking that the input data match, select **OK/Save**. This completes the information required for the first example. Select **File**, then **Save Input File**. After saving, select **Execute CSAS** from the **File** menu. This will bring up a DOS window, which shows the progress of the analysis. When the run is completed, the DOS window will indicate that the job is completed and the name of the output file.

#### 4.2.2.2. Basic output

To make sure the input is correct, check the value of  $k_{eff}$ . As in the first example of the previous section, it should be  $1.02386 \pm 0.00172$  for five generations skipped. Once again, the  $k_{eff}$  is above critical, as we modeled a pure  $^{235}\text{U}$  system compared to 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 **H-Max** and **H-Min**. For example, suppose we want to locate the origin at a point 2 cm above the base of the cylinder, as shown in Fig. 37.



**Fig. 37. Configuration 2 geometry.**

Using the configuration 1 input file, you should only need to change the height parameters on the **Geometry** screen.



#### 4.2.3.1. KENO V.a input

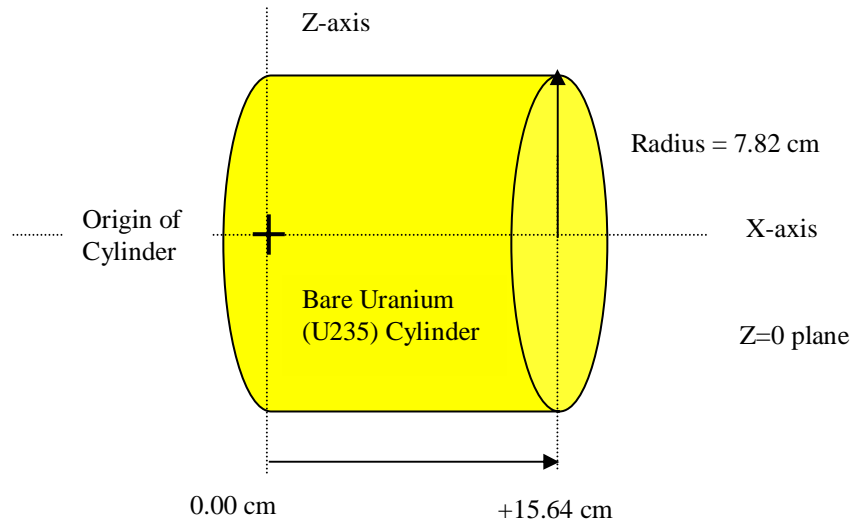
The new **Geometry** screen should look like Fig. 38.

**Fig. 38. KENO geometry input for configuration 2.**

Save the changes in a new input file and execute CSAS. As no changes were made to the physical system, the  $k_{eff}$  value for this run should be within a standard deviation of that from the previous run. The  $k_{eff}$  calculated was  $1.02386 \pm 0.0017$  for five generations skipped which is the same as previously calculated.

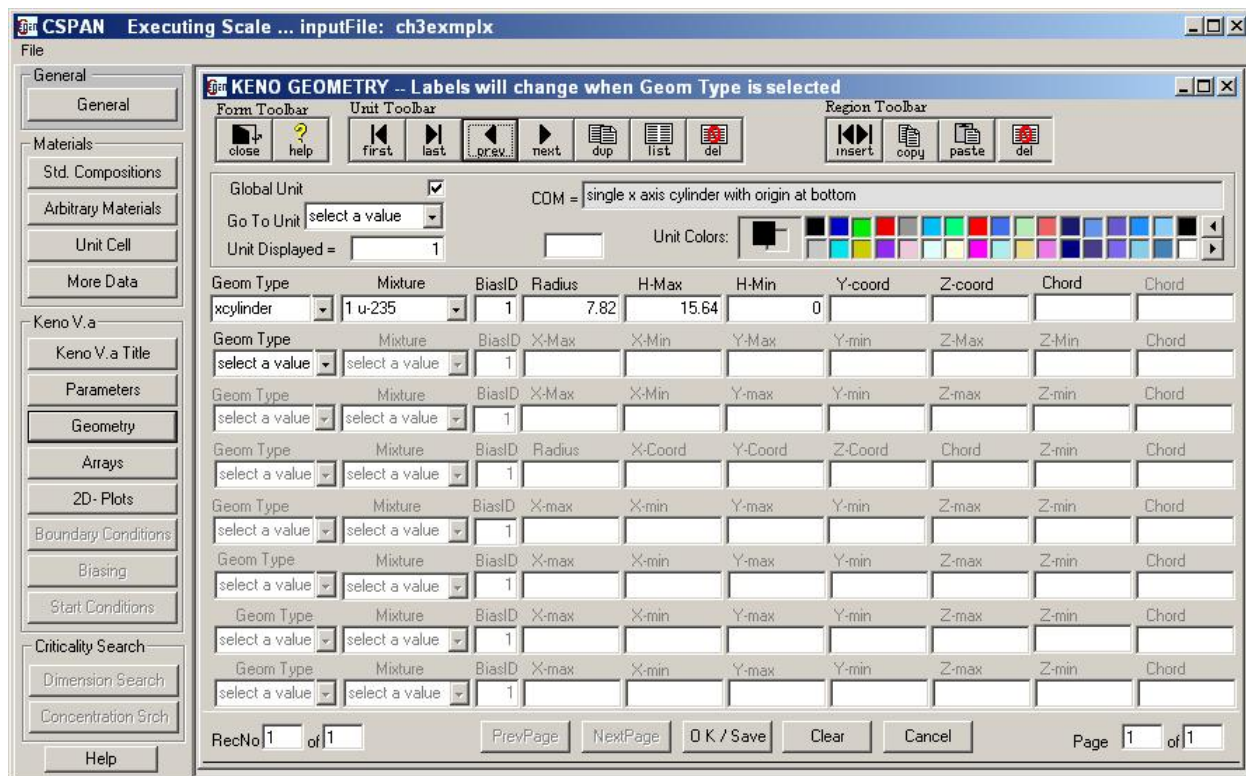
#### 4.2.4. Bare Metal Cylinder Along X-Axis With Origin Located at Cylinder Base

The next problem is for a horizontal cylinder with the origin located at the base as in Fig. 39. We need to change to an `xcylinder` and alter the values of **H-Max** and **H-Min** to locate the origin at the desired point. (**NOTE:** When entering Max and Min values, the Min value can be positive, negative, or zero, but it must be less than the Max value.)



**Fig. 39. Configuration 3 geometry.**

Using the configuration 1 input file, you need to change the **cylinder orientation**, and **height parameters** on the **Geometry** screen. That means for this problem, you need to select **xcylinder**, enter a **radius** of 7.82, a **H-Max** of 15.64, and a **H-Min** of 0.00 as shown in Fig. 40.



**Fig. 40. KENO geometry input for configuration 3 geometry.**

Save the changes in a new input file and execute CSAS. Again, as no changes were made to the physical system, the  $k_{eff}$  value for this run should be within two standard deviations of those from the previous runs. The  $k_{eff}$  calculated was  $1.02165 \pm 0.00162$  for five generations skipped which is within two standard deviations of  $1.02386 \pm 0.0017$  for five generations skipped as previously calculated.

The same approach applies to locating the origin of cubes and cuboids. You enter values of the Max and Min 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 COMMANDMENTS

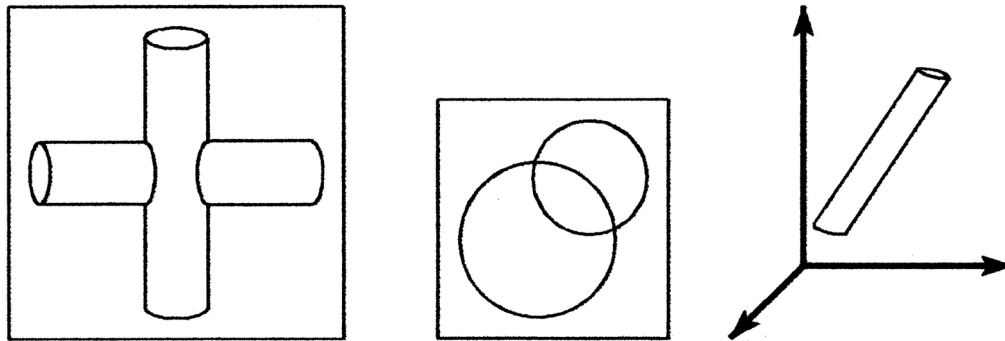
There are seven basic rules or commandments that guide the geometry input to SCALE / KENO V.a.

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. 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. 41 shows some situations that are not allowed.

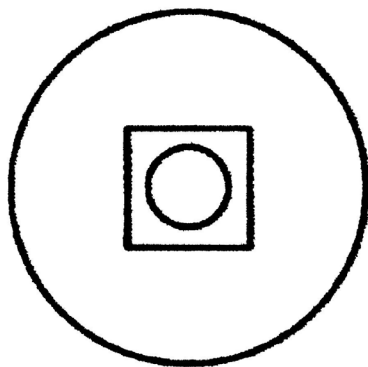
Unless special options (e.g., HOLES — discussed in Sect. 5) are invoked, each geometric region in a UNIT must completely enclose each interior region. However, regions can touch at points of tangency and share faces. See Fig. 42 for examples of allowable situations.



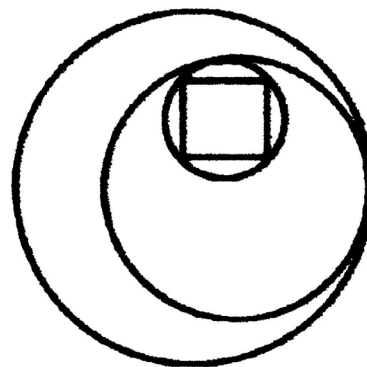
**INTERSECTING REGIONS   INTERSECTING REGIONS   ROTATED REGION**

**Fig. 41. Examples of geometry not allowed in KENO V.a.**

**ORNL-DWG 83-14791**



**REGIONS ENCOMPASSING  
INTERIOR REGIONS**



**REGIONS ENCOMPASSING  
REGIONS AND TOUCHING**

**Fig. 42. Examples of correct KENO V.a units.**

A UNIT can be thought of as an outside 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 shapes 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 understand how to enter KENO geometry information for nested regions in a UNIT via CSPAN, 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 bare 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. 43).

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

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

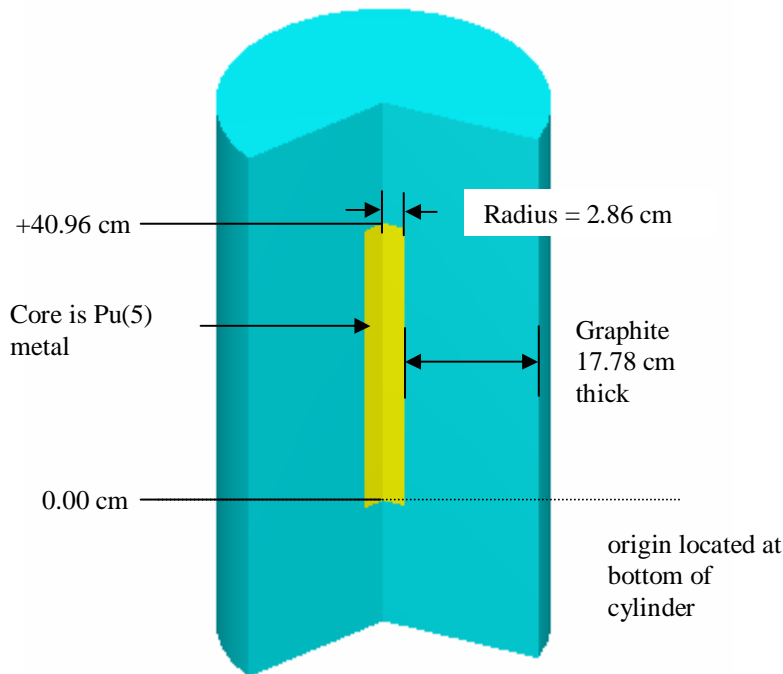
Core Radius = 2.86 cm

Core Height =  $\pm 20.48$  cm

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

Graphite

Reflector Thickness = 17.78 cm



**Fig. 43. 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 Commandments 1 and 2. Open the **Geometry** window. Select the **Global Unit** window, and enter a comment in the **COM=** box. Then under **Geom Type** select cylinder and for **Orientation of cylinder** select cylinder again. For **Mixture** select 1 pu from the pulldown menu. Then enter 2.86 for the **Radius**, 40.96 for **H-Max**, and 0.0 for **H-Min**. 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. To enter the data for the reflector, go to the next **Geom Type** line. (**NOTE:** Each **Geom Type** line is a new region in the UNIT.) Select cylinder and for **Orientation of cylinder** select cylinder again. For **Mixture** select 2 c from the pulldown menu. Then enter 20.64 ( $= 2.86 + 17.78$ ) for the **Radius**, 58.74 ( $= 40.96 + 17.78$ ) for **H-Max**, and -17.78 for **H-Min**. This completes the geometry input (see Fig. 44).

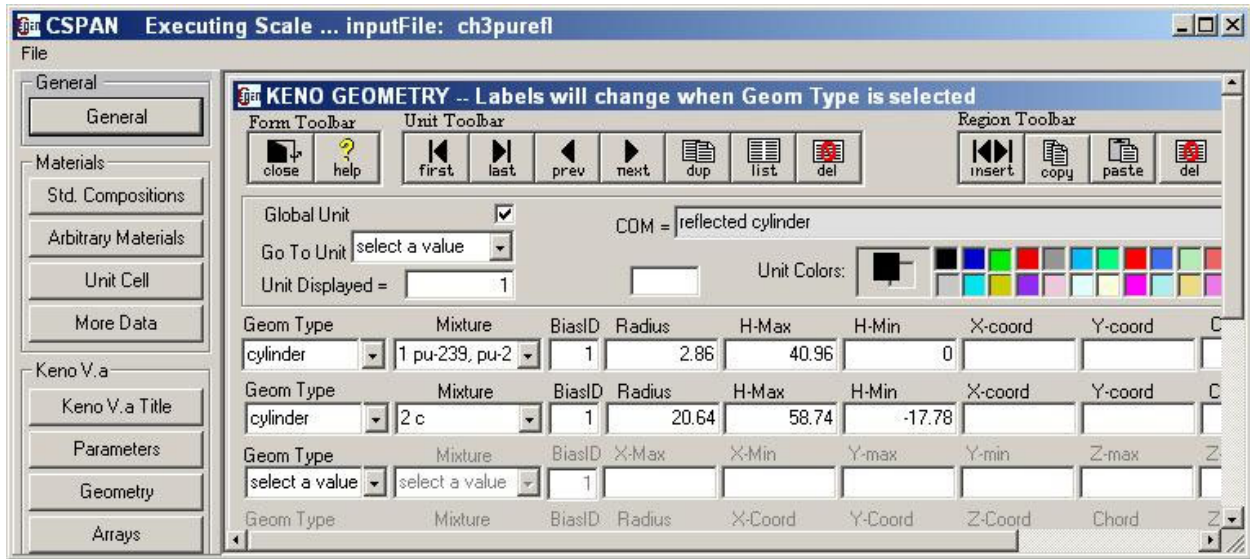


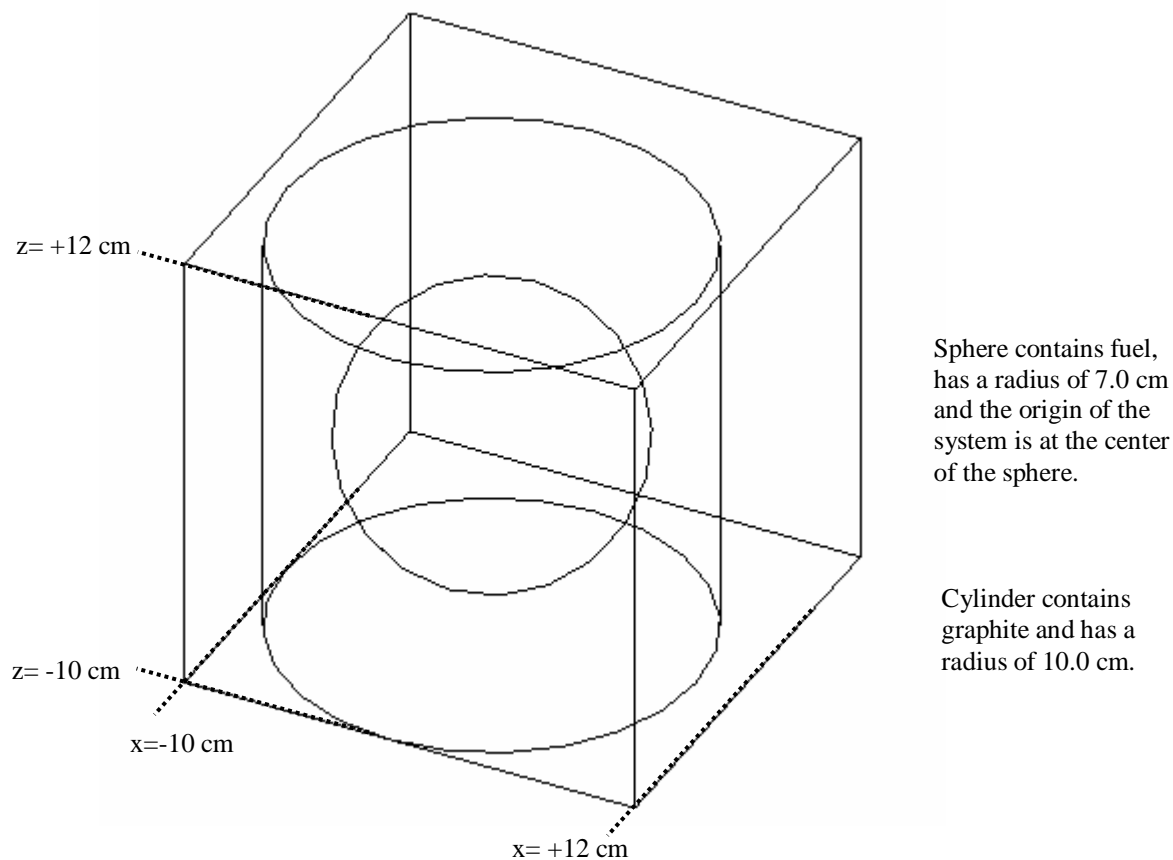
Fig. 44. KENO geometry input for reflected Pu cylinder.

Save the changes in a new input file and execute CSAS. As this is a critical experiment, the  $k_{eff}$  value for this run should be close to 1.0. However, calculated  $k_{eff}$  was  $0.97271 \pm 0.00196$  for seven generations skipped which is not within two standard deviations of 1.0. 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

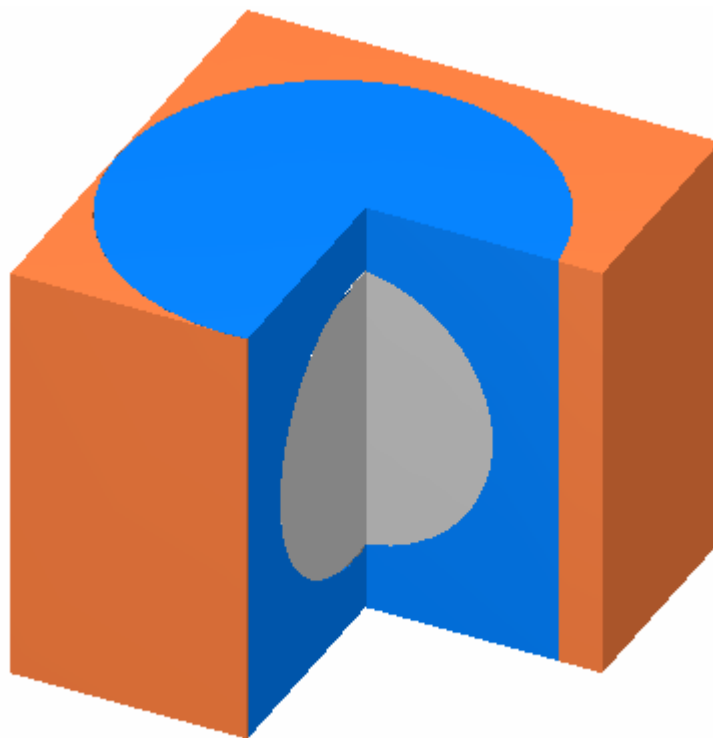
This problem consists of a metal  $^{235}\text{U}$  sphere inside a graphite cylinder inside a cube of water. The center of the sphere and cylinder are offset such that the outside edge of the cylinder touches two of the outside edges of the cube (see Fig. 45). This is consistent with Commandment 3, which indicates regions may share boundaries but 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. 45.  $^{235}\text{U}$  sphere surrounded by graphite and water.**

A cutaway view of the geometry is shown in Fig. 46. 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.

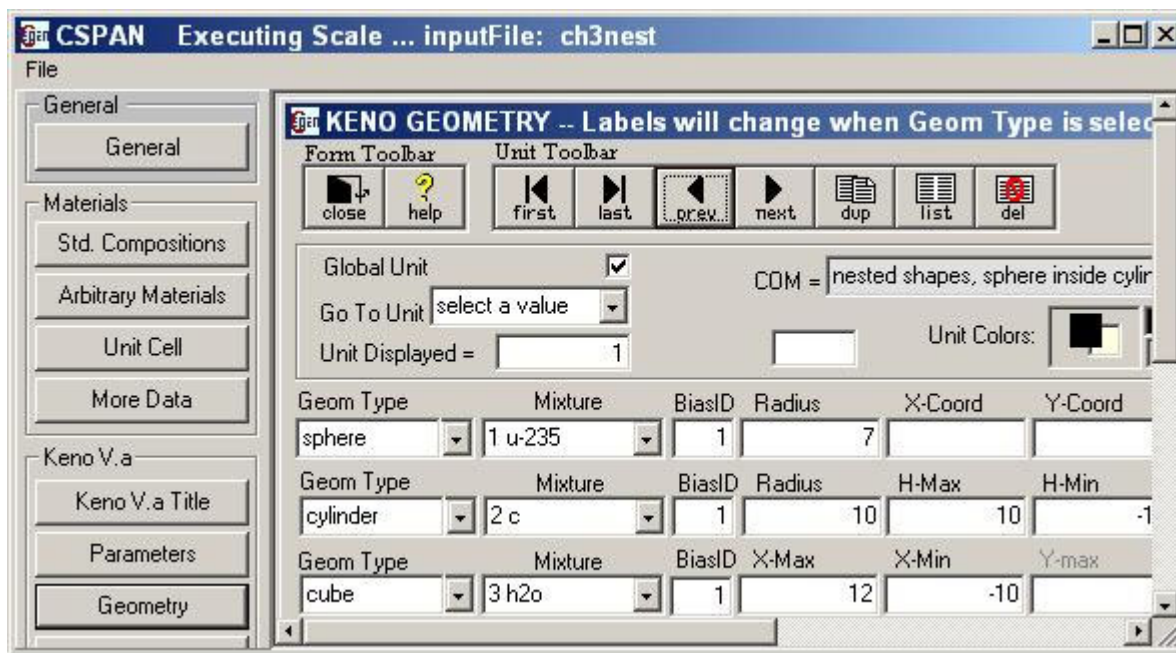


**Fig. 46. Cutaway view of  $^{235}\text{U}$  sphere inside graphite and water.**

Using your knowledge from previous sections, you should be able to open a new file, 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 the previous example. Open the **Geometry** screen. Select the **Global Unit** box, and enter a comment in the **COM=** box. Then under **Geom Type** select sphere and select sphere from the popup list of spherical shapes. 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. To enter the data for the graphite reflector, go to the next **Geom Type** line. Select cylinder and then select cylinder from the popup list of cylindrical shapes. For **Mixture** select 2 c from the pulldown menu. Then enter 10 for the **Radius**, 10 for **H-Max**, and -10 for the **H-Min**. This creates a cylinder centered around the sphere. To enter the data for the outside water reflector, go to the next **Geom Type** line. Select cube 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-Max**, and -10 for the **X-Min** 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 is 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. 47).



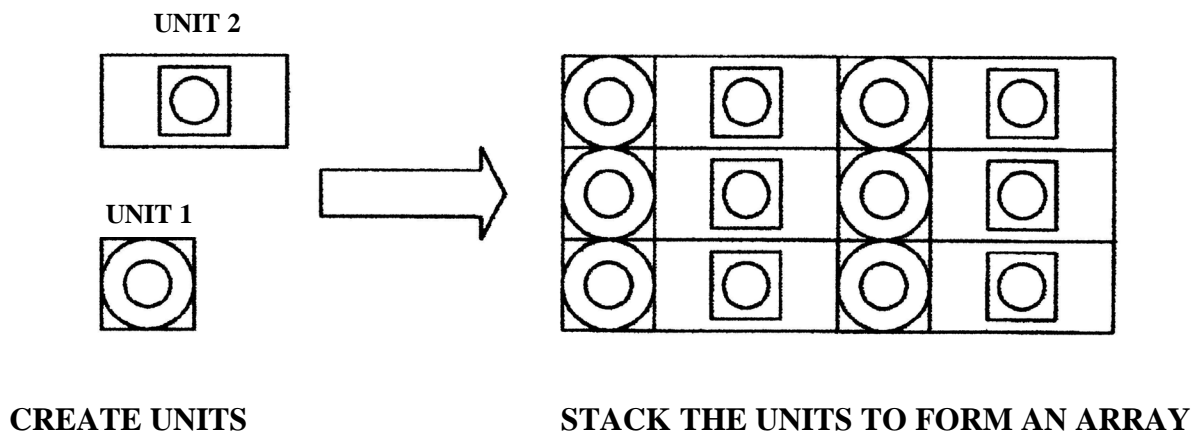
**Fig. 47. KENO geometry input for  $^{235}\text{U}$  sphere in graphite and water.**

Save the changes in a new input file and execute CSAS. The calculated  $k_{eff}$  was  $0.99705 \pm 0.00169$  for six generations skipped.

## 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. 48 for a typical example.



**Fig. 48. 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. 49 for an example of an array composed of units containing HOLES and arrays.

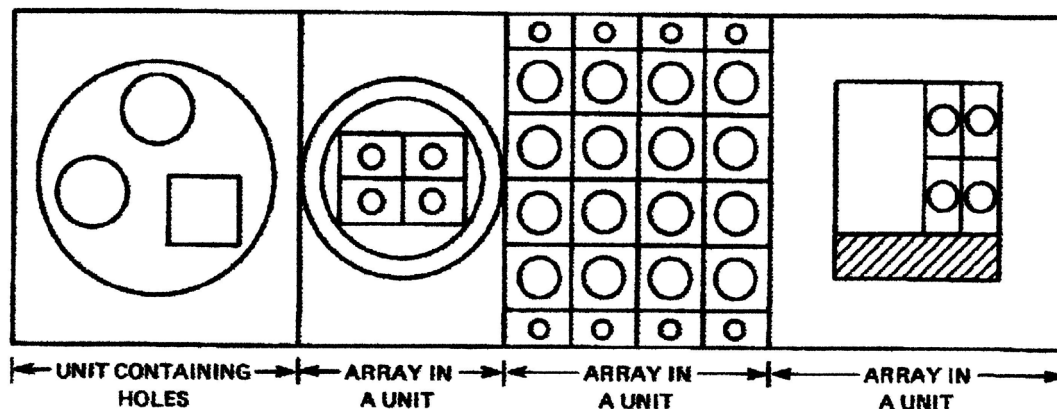


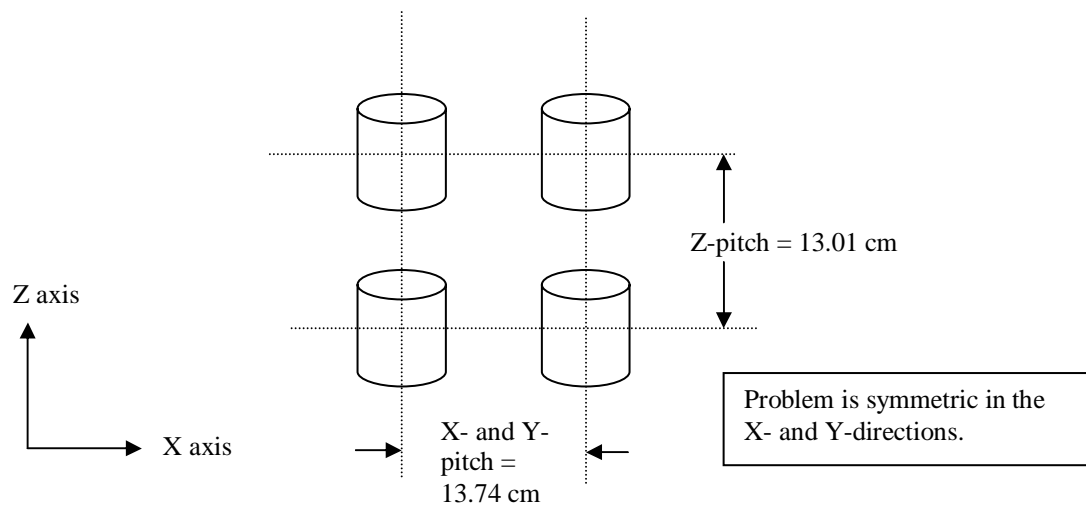
Fig. 49. Example of an array composed of units containing arrays and HOLES.

The focus of this section will be on simple arrays; that is, arrays containing multiple entries of a single UNIT or arrays with multiple UNITs of nominally different sizes.

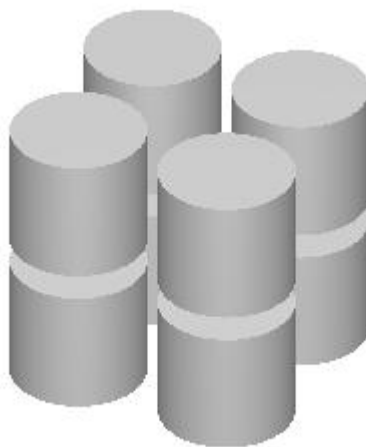
#### 4.6.1. Arrays With Single UNITs

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 13.1125 in the Z-direction. There are no external reflectors or other materials in the array. The geometry is shown in Figs. 50 and 51.

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, these 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. 50. 2x2x2 array geometry.**

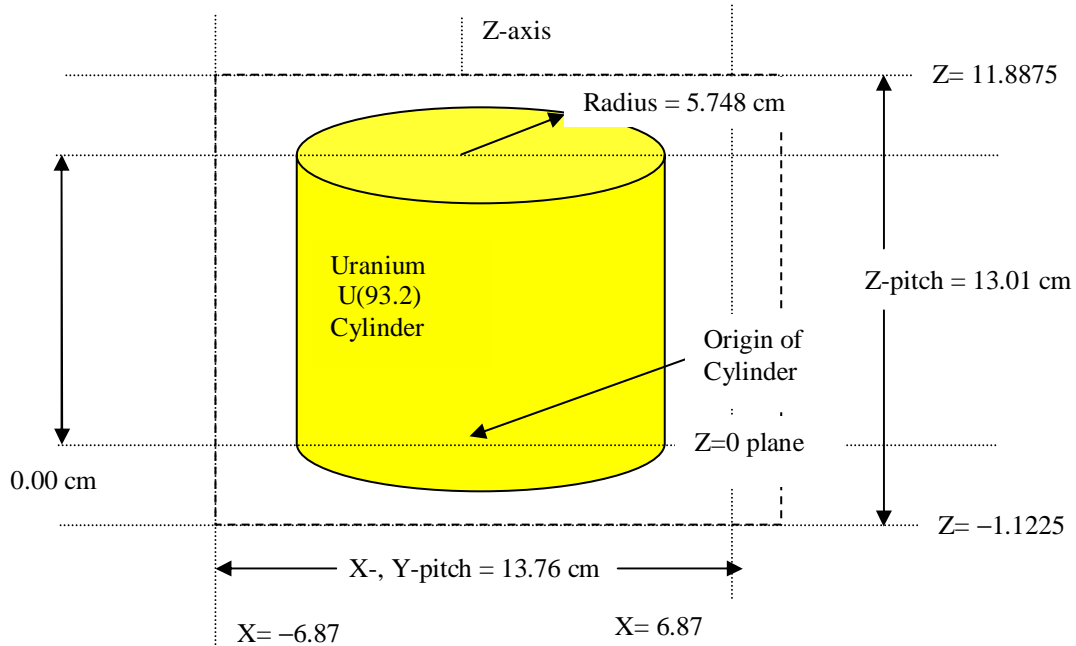


**Fig. 51. 3-D view of array.**

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 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 eight entries of the same UNIT. 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 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 **H-Max** for the cylinder will be 10.765 and the **H-Min** will be 0.0. For the cuboid, the origin is located in the middle in the X- and Y-directions so the **X-Max** and **Y-Max** will be 6.87 while the **X-Min** and **Y-Min** 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  $= 10.765 + 1.1225 = 11.8875$  and the bottom Z-coordinate  $= 0.0 - 1.1225 = -1.1225$ . These parameters are sufficient for describing the single array element as shown in Fig. 52.



**Fig. 52. Single array element (cuboid enclosing a cylinder).**

Describe the geometry by opening the **Geometry** window. As this is not the global unit, we will leave the **Global Unit** box blank, but we do need to enter a comment in the **COM=** box. Then under **Geom Type** select **cylinder** and for type of cylinder select **cylinder** again. For **Mixture** select **1 u** from the pulldown menu, and then enter **5.748** for the **Radius**, **10.765** for **H-Max**, and **0.0** for **H-Min**. 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, go to the next **Geom Type** line. Select **cuboid** and for **Mixture** select **0 void** from the pulldown menu. Then enter **6.87** for **X-Max** and **Y-Max**, **-6.87** for **X-Min** and **Y-Min**, **11.8875** for **Z-Max**, and **-1.1225** for **Z-Min**. This creates a cuboid around the cylinder with the proper spacing. This completes the geometry input (see Fig. 53), but we still need to enter the **Array** data.



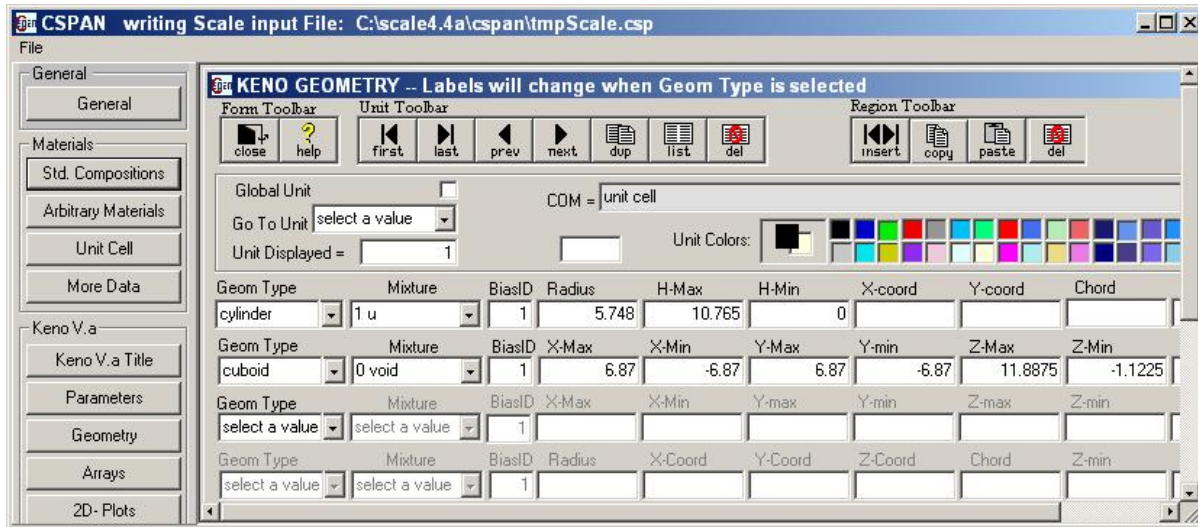


Fig. 53. Single UNIT geometry for array.

Now describe the array by opening the **Arrays** window (Fig. 54).

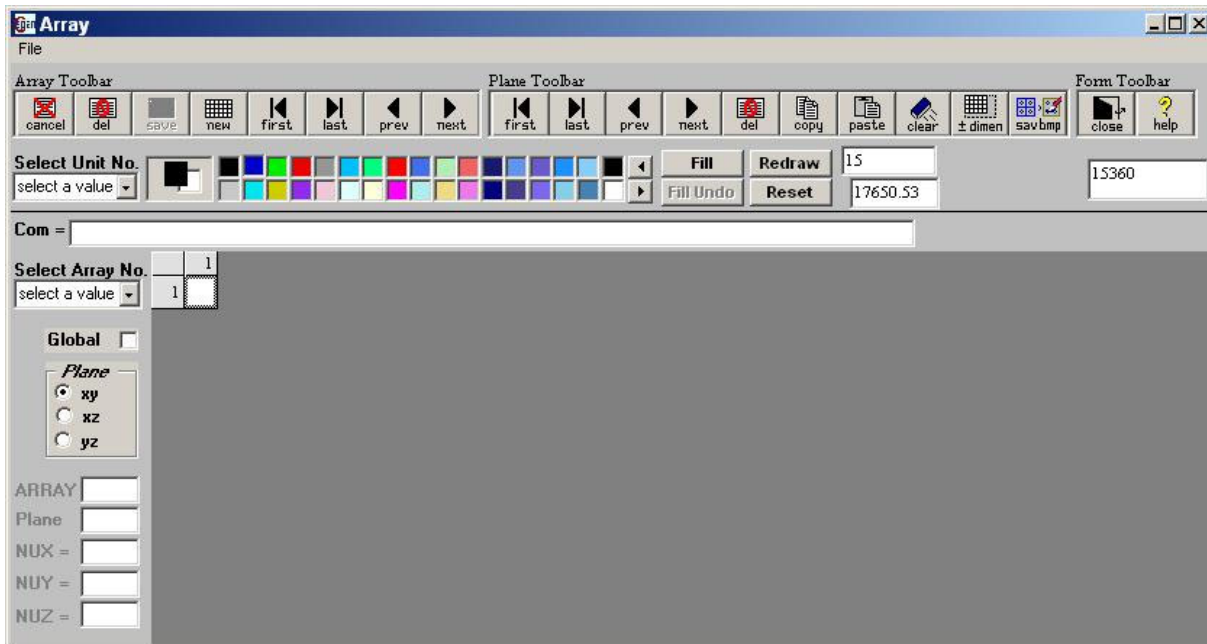
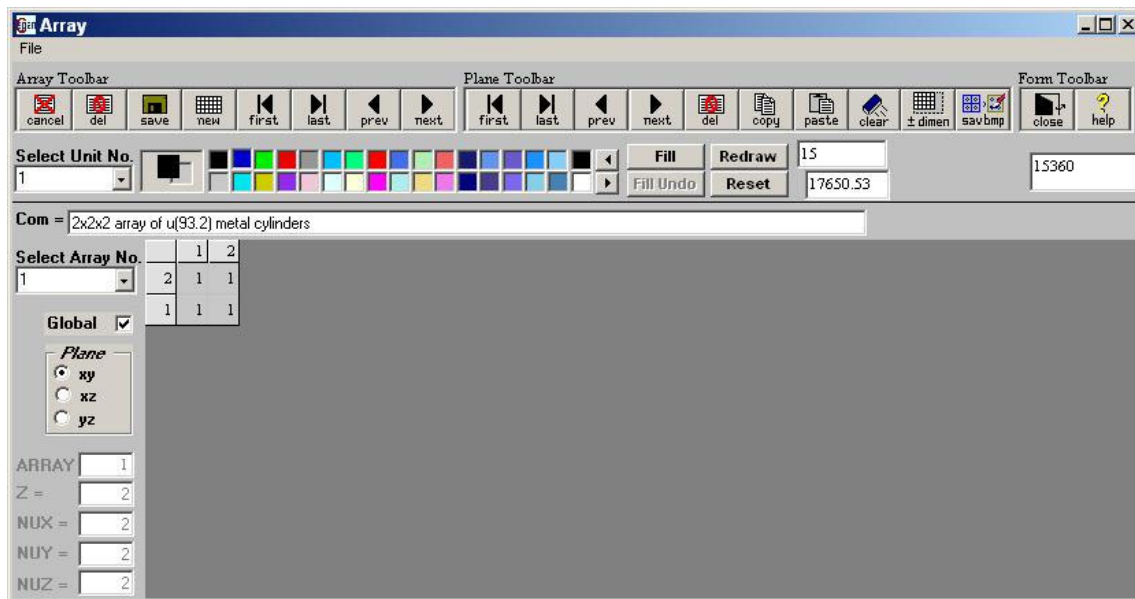


Fig. 54. Array screen from CSPAN.

The **Array** window is set up with three toolbars across the top. The leftmost toolbar (**Array Toolbar**) is for actions relating to arrays (e.g., deleting an entire array or creating a new array). The toolbar in the center (**Plane Toolbar**) is for actions relating to planes, or layers, within an array. The rightmost toolbar (**Form Toolbar**) relates to the **Array** window, or form, and allows you to close the form or get help on a topic. Below the toolbars is the data entry area, with the largest area for entering unit numbers in each plane of an array.

To enter the array data, first click on **New** on the **Array Toolbar**. This will open a window where you will enter the **dimensions** of the array. For this problem, 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. Then click **OK**. This will display a grid of the first plane on the screen in the upper left-hand corner of the blank area. The grid shows a 2×2 arrangement for the XY Plane as indicated to the side. Once you have the 2×2 layout, then you need to tell CSPAN which **UNITs** go in which positions in that layer. For this problem, there is only one **UNIT** so that will need to be filled in the four positions. The fastest way to do this is click on the **Select Unit No.** pulldown menu and then select 1. Then click to select the lower left corner of the grid. Next click on the **Fill** button just below the **Plane Toolbar**. This will fill all positions in the plane with the selected unit number, in this case, 1. As there are two XY planes. We need to fill the second plane in the same manner. Click on the **Next** icon on the **Plane Toolbar**. A new grid should appear and the Z index on the left hand side of the screen should now read 2. Repeat the fill process by selecting the lower left-hand corner of the layer and then click the **Fill** button. Now you need to provide a comment for the array, e.g., 2×2×2 array of U (93.2) metal cylinders, and check the **Global** box. The array is the outermost unit in this model so it is the Global Unit for this problem. The completed screen should look like Fig. 55. After you have checked your input, click on the **Save** icon on the **Array Toolbar**. This will save the array information. To finish, click on the **Close** icon on the **Form Toolbar**.

Save the changes in a new input file and execute CSAS. The calculated  $k_{eff}$  for this critical experiment was  $1.00225 \pm 0.00198$  for four generations skipped.

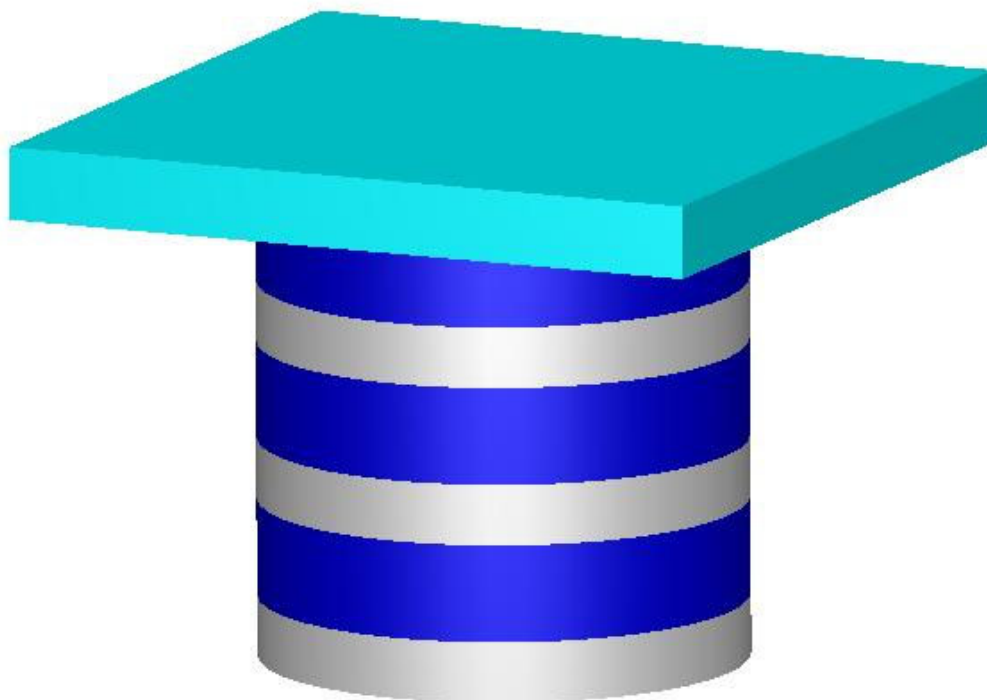


**Fig. 55. Array screen for 2×2×2 array.**

#### 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. 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 18.76 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 bottom disk is graphite followed by uranium, graphite, uranium, graphite, and uranium as the top disk. The top plate is aluminum of nominal density, 30×30-cm-square and 3-cm-thick. There are no external reflectors or other materials in the array. The geometry is shown in Fig. 56.

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. In this case that means 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. 56. Geometry of stack.**

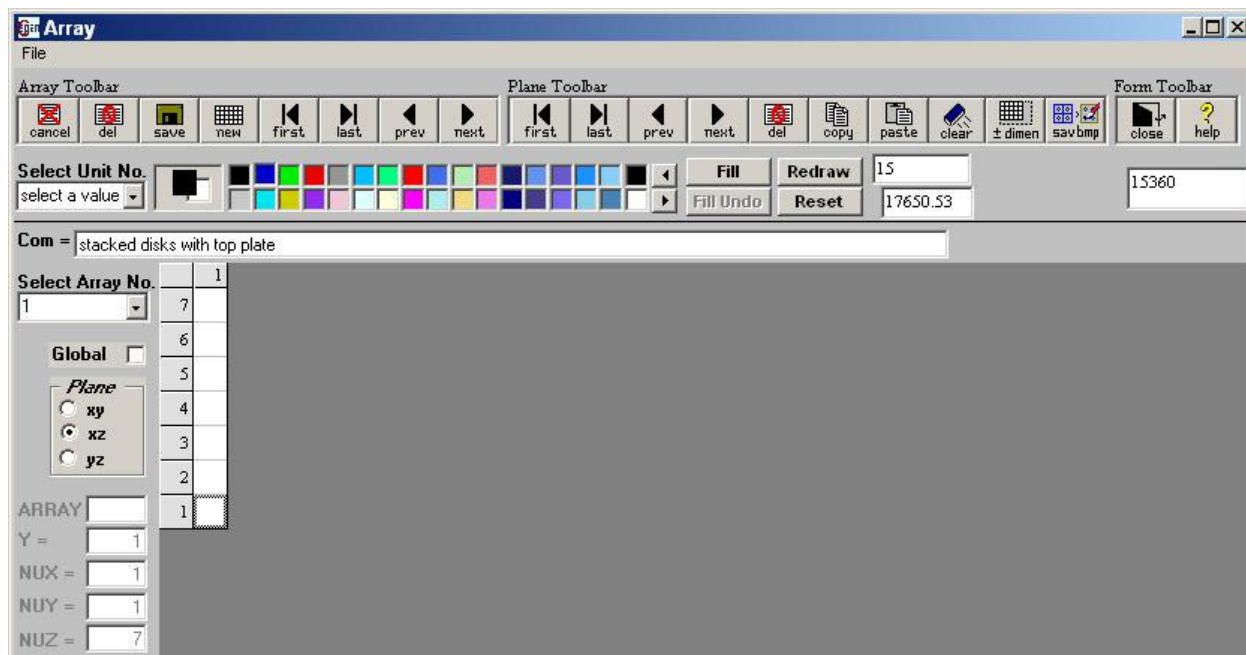
Using your knowledge from previous sections, you should be able to open a new file, enter the title, cross section and material information for the graphite, uranium (including the isotopic composition weight percentages) and aluminum.

Describe the geometry by opening the **Geometry** window. As this is not the global unit, we will leave the **Global Unit** box blank, but we do need to enter a comment in the **COM=** box. Then under **Geom Type** select **cylinder** and for **Configuration** select **cylinder** again. For **Mixture** select **1 c** from the pulldown menu, then enter **10** for the **Radius**, **1.25** for **H-Max**, and **-1.25** for **H-Min**. This puts the origin at the center of the cylinder; this is now the origin for the UNIT and for all other shapes in the UNIT. 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, go to the next **Geom Type** line. Select **cuboid** and for **Mixture** select **0 void** from the pulldown menu. Then enter **15** for **X-Max** and **Y-Max**, **-15** for **X-Min** and **Y-Min**, **1.25** for **Z-Max**, and **-1.25** for **Z-Min**. This creates a cuboid around the cylinder with the proper spacing.

Now describe the uranium cylinder by clicking the **Next** icon on the **Geometry** screen. As this is not the global unit, we will leave the **Global Unit** box blank, but we do need to enter a comment in the **COM=** box. Then under **Geom Type** select **cylinder** and for **Configuration** select **cylinder** again. For **Mixture** select **2 u** from the pulldown menu, then enter **10** for the **Radius**, **2** for the **H-Max**, and **-2** for the **H-Min**. 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, go to the next **Geom Type** line. Select **cuboid** and for **Mixture** select **0 void** from the pulldown menu. Then enter **15** for **X-Max** and **Y-Max**, **-15** for **X-Min** and **Y-Min**, **2** for **Z-Max**, and **-2** for **Z-Min**. This creates a cuboid around the cylinder with the proper spacing.

Now describe the aluminum plate by clicking the **Next** icon on the **Geometry** screen. As this is not the global unit, we will leave the **Global Unit** box blank, but we do need to enter a comment in the **COM=** box. Then under **Geom Type** select **cuboid** and for **Mixture** select **3 al** from the pulldown menu. Then enter **15** for **X-Max** and **Y-Max**, **-15** for **X-Min** and **Y-Min**, **1.5** for **Z-Max**, and **-1.5** for **Z-Min**. This completes the geometry input, but we still need to enter the array data.

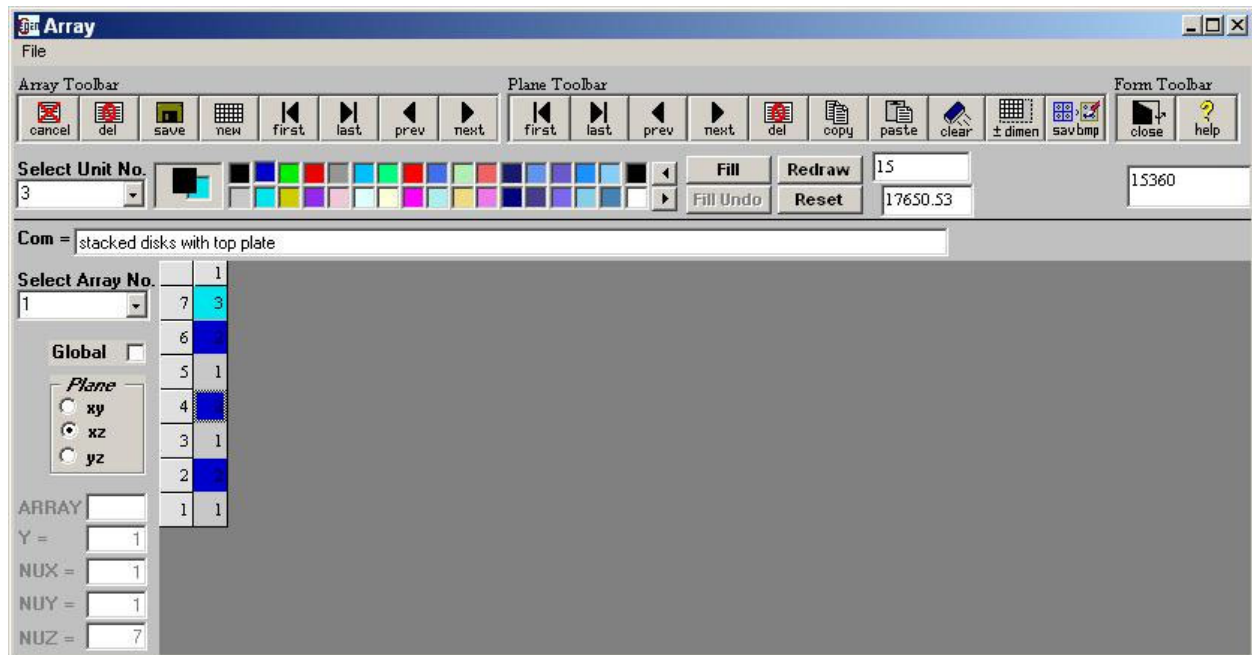
To enter the array data, first click on **New** on the **Array Toolbar**. This will bring up a screen where you will enter the dimensions of the array. For this problem, the array is 1 unit in the X-direction, 1 unit in the Y-direction, and 7 units in the Z-direction, so enter **7** for **NUZ**. Notice that it has already identified the array as number 1. 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 1×1 array as you are looking at the XY plane. Click on XZ plane to display the 1×7 array as shown in Fig. 57.



**Fig. 57. Array screen for stacked disks problem.**

Because we have three different UNITS, we need to tell CSPAN which unit to put in each array position. Click on the **Select Unit No.** pulldown menu and then select 1. Then click to select position 1 in the array. Clicking again will fill that position with the number 1. Repeat the process for positions 3 and 5. Then click on the **Select Unit No.** pulldown menu and select 2. Select position 2 and then click to fill with unit 2; do the same for positions 4 and 6. Finally, select unit 3 and use it to fill position 7. Now you need to provide a comment for the array, e.g., array of stacked disks and square plate, and check the **Global** box. When completed, the array screen should look like Fig. 58. After you have checked your input, then click on the **Save** icon under the **Array Toolbar**. This will save the array information. To finish, click on the **Close** icon under the **Form**.

Save the changes in a new input file and execute CSAS. The calculated  $k_{eff}$  was  $0.94795 \pm 0.00164$  for three generations skipped.



**Fig. 58. Completed array screen for stacked disks problem.**

## 4.7. SUMMARY

This section has helped you to:

- Use CSPAN 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 HOLE.

## **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 CSPAN 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. 59.
<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. 60.



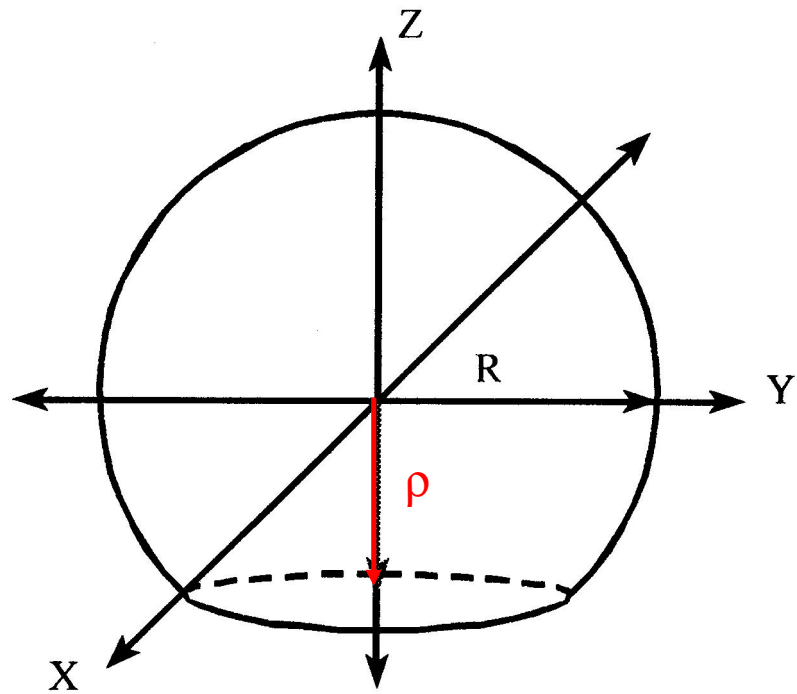


Fig. 59. Parameters for a hemisphere.

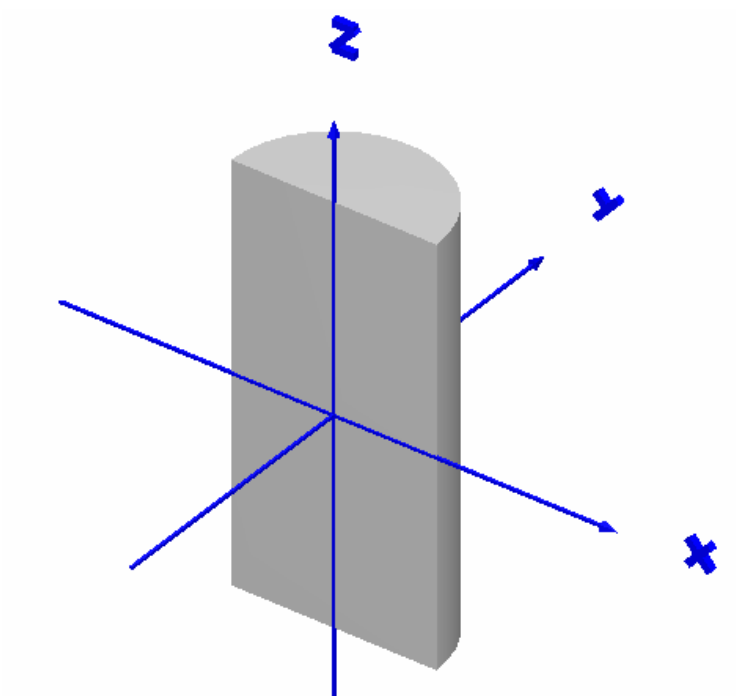
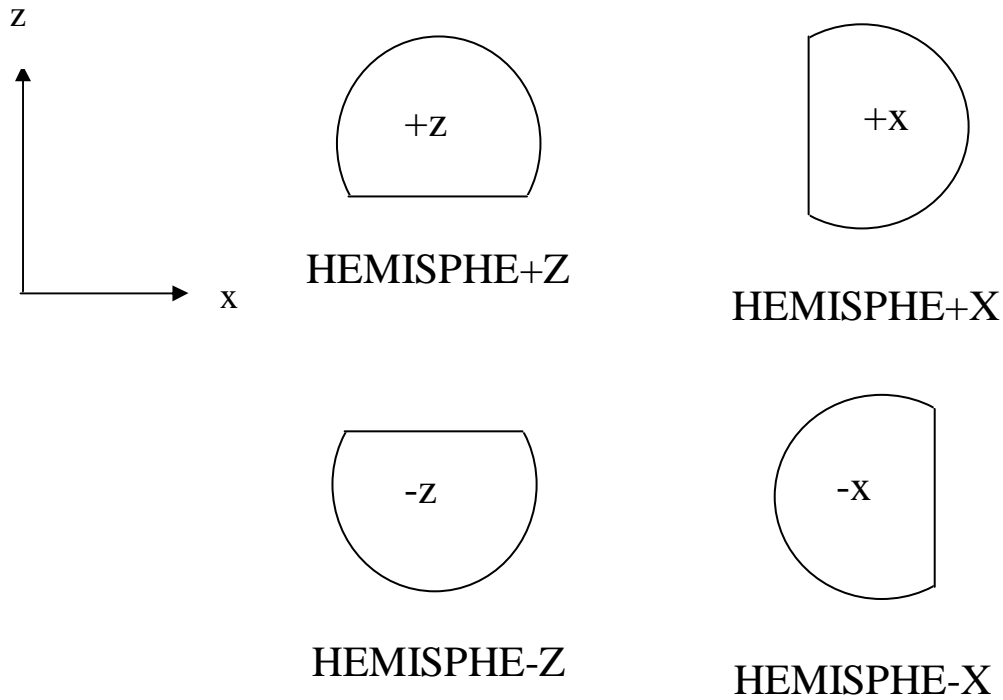


Fig. 60. ZHEMICYCL+Y example.

### 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. 61 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 +, while if it is in the negative direction, the sign is -.



**Fig. 61. Direction of curvature.**

The location of the flat surface is defined by the chord  $\rho$ , 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 +). Another way of looking at hemispheres is: a positive  $\rho$  indicates a volume more than half a sphere and a negative  $\rho$  indicates a volume less than half a sphere ( $\rho = 0$  is exactly half a sphere). See Fig. 62 for examples.

### HEMISPHE-Z or #HEMICYL-Z

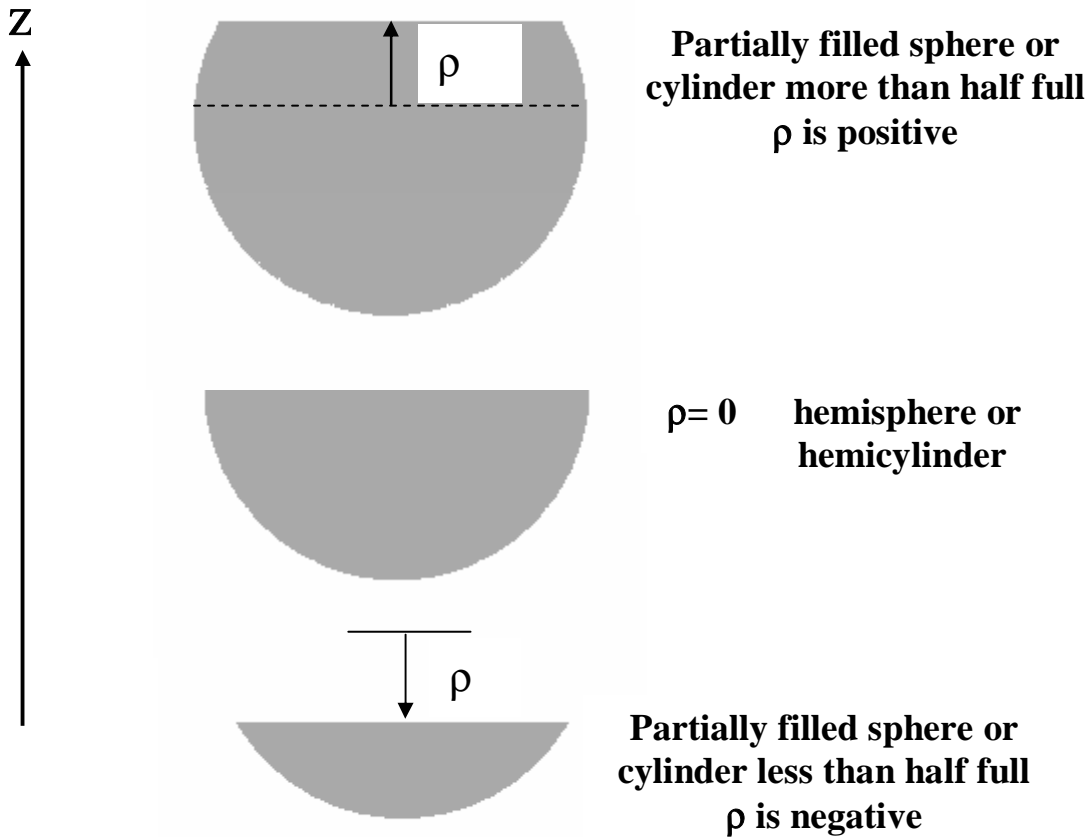
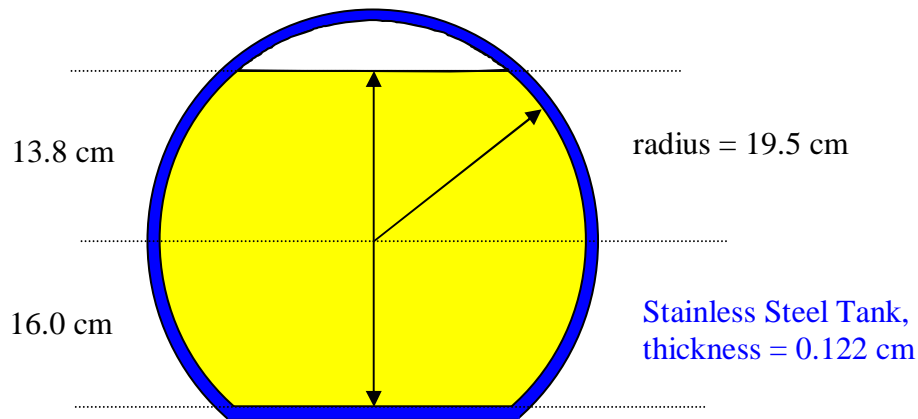


Fig. 62. Use of  $\rho$  to characterize flat surface.

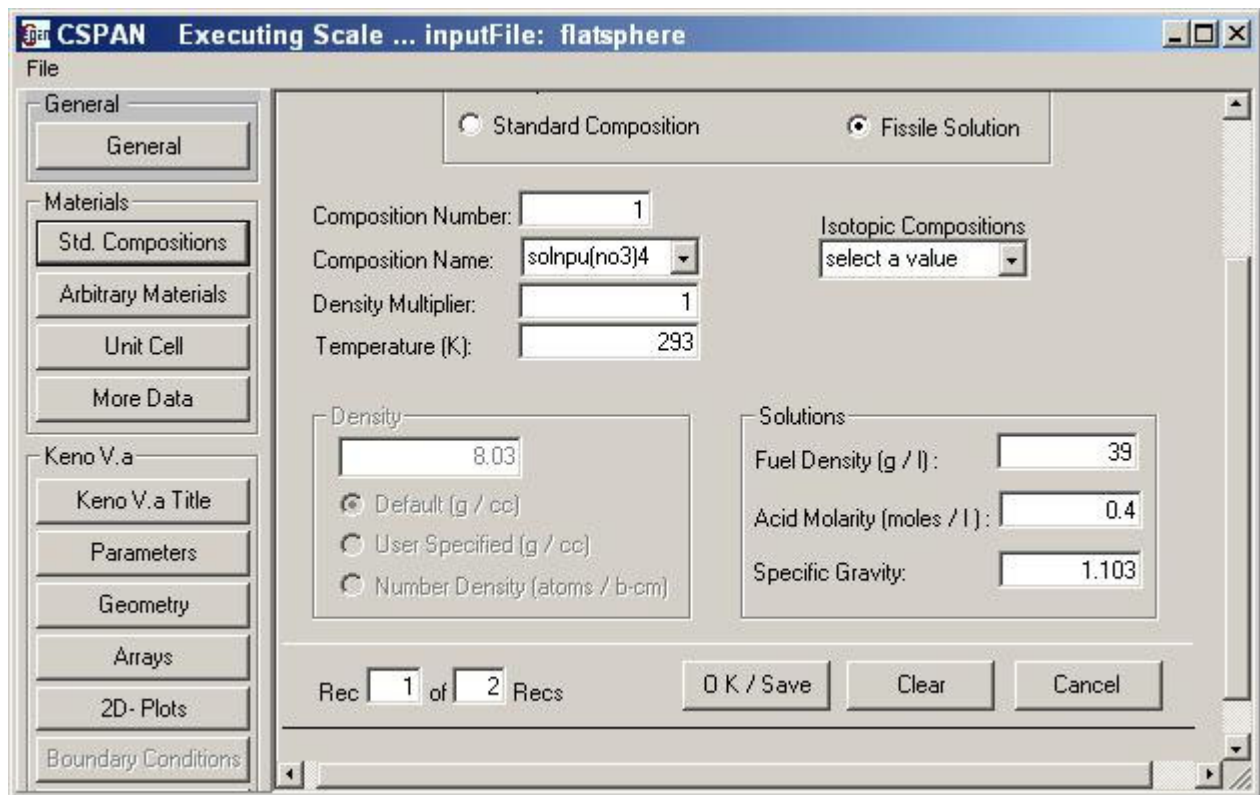
#### 5.2.2. Flat-Bottomed Spherical Tank

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. 63. The solution characteristics are: 39-g Pu / liter, acid molarity of 0.4 moles / liter, and a specific gravity of 1.103.



**Fig. 63. Flat-bottom sphere.**

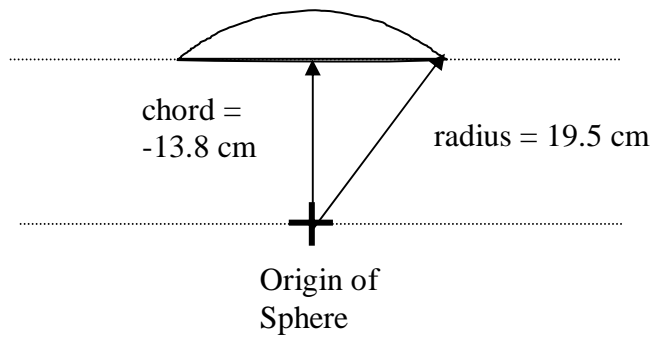
By now, you should be comfortable using CSPAN to enter the **General** information with the title, sequence, unit cell type, and cross-section library. As this is the first example we have done where the fissile material is in solution, we will walk through that process. For this problem, we again open the **Std. Compositions** window. However, instead of selecting **Standard Composition**, this time we will select **Fissile Solution**. Under **Composition Name:** there are only three choices provided on the menu: `solnuo2f2`, `solnuo2(no3)2`, and `solnpu(no3)4`. For this problem, select `solnpu(no3)4`. Under **Isotopic Compositions**, select 94000, 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. CSPAN 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 screen should look like Fig. 64. Click **OK/Save**. Then for Composition 2, select `ss316` (i.e., stainless steel type 316) and accept the default values by clicking on **OK/Save**. This completes the material input for this example.



**Fig. 64. Material input for fissile solution.**

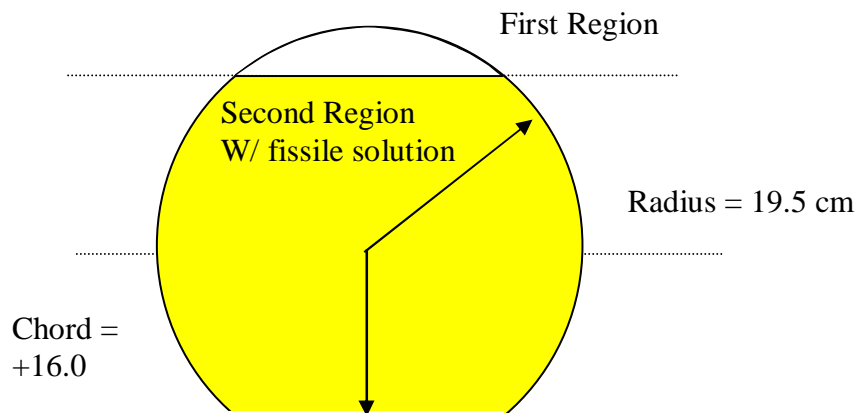
For this geometry, there will be three hemispheres in one UNIT, and that UNIT will be the Global Unit for the problem. Remember that nested shapes must not intersect so the first shape listed in the geometry must be completely contained within the second shape, which must be completely contained in the 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.

Open the **Geometry** window. Select the **Global Unit** box, and enter a comment in the **COM=** box. Then under **Geom Type** select sphere and for the type of spherical shape, select hemisphere+z, which puts 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 the **Chord**. 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. 65.



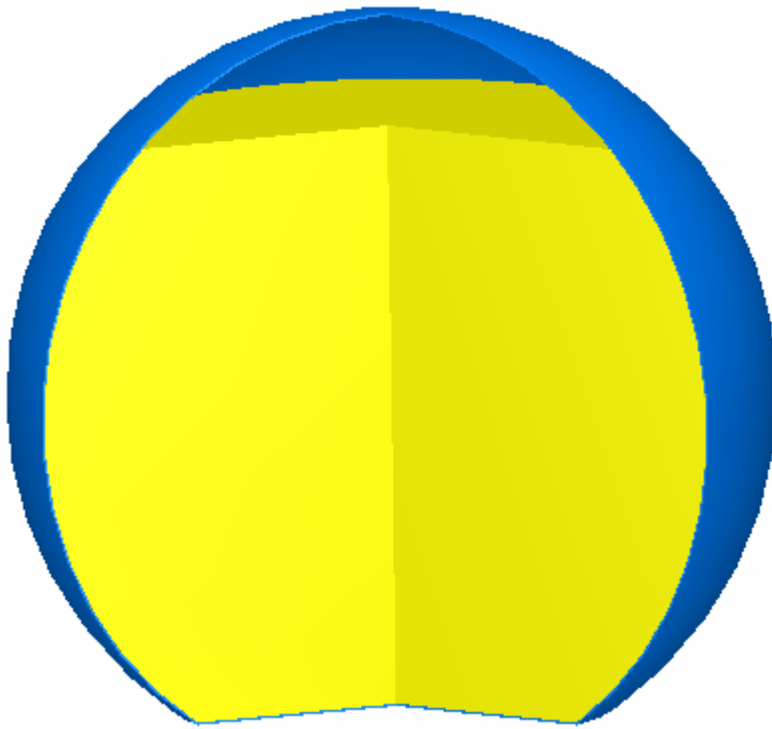
**Fig. 65. Hemisphere containing void.**

Remember as we enter a second shape 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. So, under the next **Geom Type** select `sphere` and for the spherical type, select `hemisphe+z`, which puts the flat surface perpendicular to the Z-axis and the curved part in the positive Z-direction. For **Mixture** select `1 solnpu(no3)4` from the pulldown menu. Then enter 19.5 for the **Radius**, and 16.0 for the **Chord**. 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. 66.

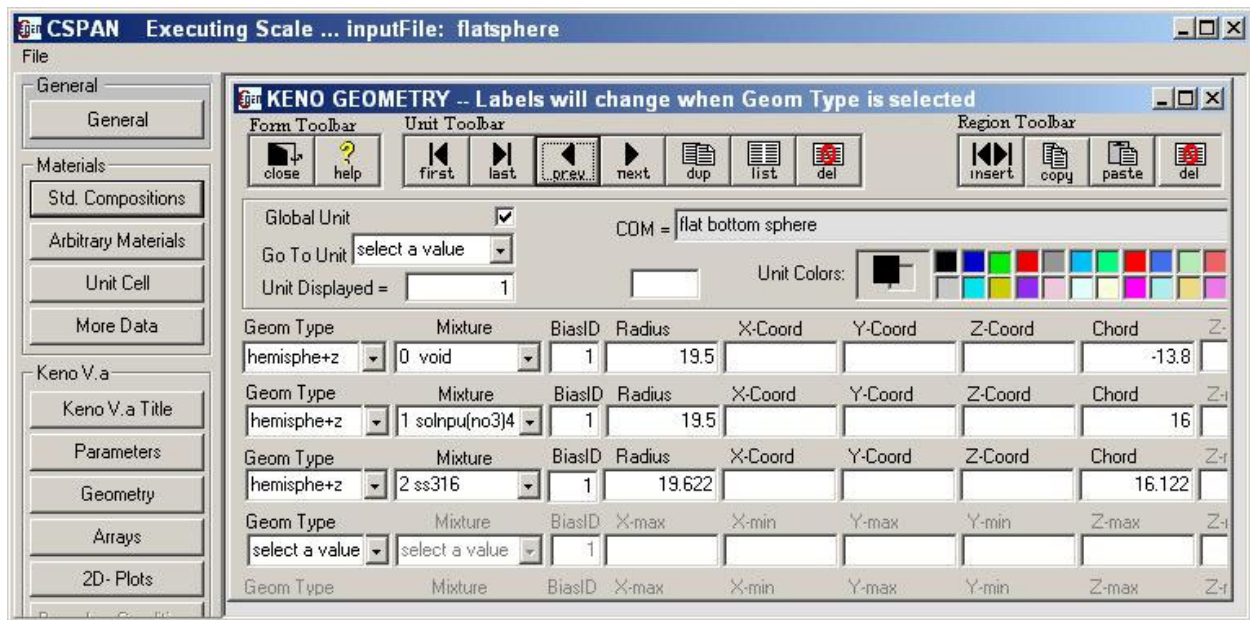


**Fig. 66. First and second regions.**

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. This will fill the thin outer edge of the hemisphere with stainless steel. So, under the next **Geom Type** select sphere and for the spherical type, select hemisphe+z. 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 the **Chord**. 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. 67. The complete geometry input is shown in Fig. 68.



**Fig. 67. 3-D view of nested hemispheres.**



**Fig. 68. Geometry input for flat bottom sphere problem.**

After checking that the input data match, select **OK/Save**. Select **File**, then **Execute CSAS**. The calculated  $k_{eff}$  was  $1.00053 \pm 0.00188$  for four generations skipped.

### 5.3. HOLES

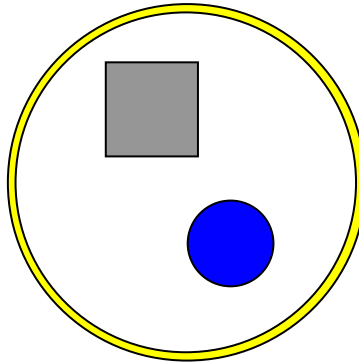
For many problems, the requirement of nested shapes does not interfere with creating an accurate model. However, there will be times when a unit contains more than one shape and these shapes are not nested. For these situations, KENO V.a uses a shape called a HOLE. There are four basic rules for HOLES.

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.



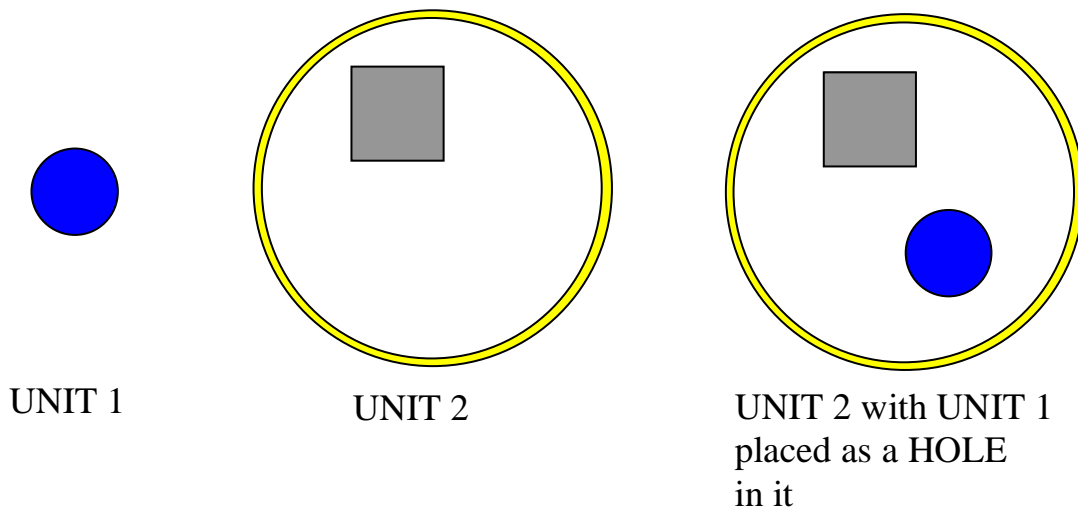
### 5.3.1. Simple HOLE Example

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. 69.



**Fig. 69. HOLE example problem.**

Because the graphite box and the uranium cylinder are not nested, they can not be entered in the normal manner. What we need to do is create 2 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. 70.

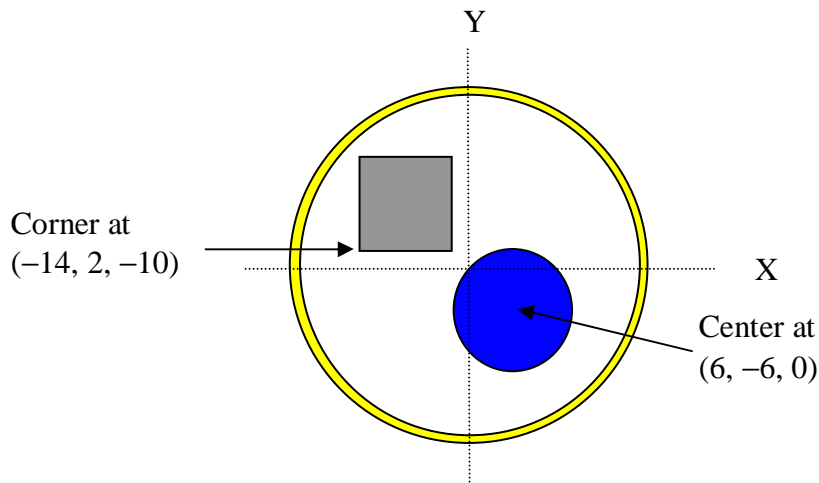


**Fig. 70. Using a HOLE to place one UNIT inside another.**

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 at 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. 70.

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. 71.



**Fig. 71. 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 above. Open the **Geometry** window. For UNIT 1, enter a comment in the **COM=** box. Then under **Geom Type** select **cylinder** and for the

cylinder type select `cylinder` again. For **Mixture** select `u-235` from the pulldown menu. Then enter `6.85` for the **Radius**, `10.0` for **H-Max**, and `-10.0` for **H-Min**. This puts the origin at the center of the cylinder. 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. Save this information and go to the next unit.

UNIT 2 will be the global unit so check that box and enter an appropriate comment. 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-Max**, **X-Min**, **Y-Max**, **Y-Min**, **Z-Max**, and **Z-Min** values. As the coordinates of the lower-left hand corner are  $(-14, 2, 0)$  then **X-Min** will be  $-14$ , **Y-Min** will be  $2$ , and **Z-Min** will be  $-10$ . The maximum values are calculated by adding the appropriate dimension to the minimum values. Thus for **X-Max**, 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. The third region 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 2. 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, under **Geom Type** select `hole`. There is no entry for **Mixture**, but it does indicate that the **Unit** is `1`. If there were other units, then you would change the number to select the appropriate UNIT. The next 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 at  $(6, -6, 0)$  with respect to the SS316 cylinder origin. Enter `6` for the **X-Origin**, `-6` for the **Y-Origin**, and `0.0` for the **Z-Origin**. The last region in UNIT 2 is the outside of the SS316 cylinder. After entering the appropriate data for this cylinder, the geometry form for UNIT 2 should look like Fig. 72.

CSPAN writing Scale input File: C:\SCALE4.4\CSpan\tmpScale.csp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

Geometry

Arrays

2D Plots

Boundary Conditions

Biasing

Start Conditions

Criticality Search

Dimension Search

Concentration Search

Help

KENO GEOMETRY -- Labels will change when Geom Type is selected

Form Toolbar

Unit Toolbar

Region Toolbar

Global Unit ☒ COM = steel cylinder

Go To Unit select a value

Unit Displayed = 2

Unit Colors:

Geom Type	Mixture	Bias/D	X-Max	X-Min	Y-Max	Y-Min	Z-Max	Z-Min
cuboid	3 c	1	-2	-14	14	2	10	-10

Geom Type	Mixture	Bias/D	Radius	H-Max	H-Min	X-coord	Y-coord	Chord
cylinder	0 void	1	20	10	-10			

Geom Type	Mixture	Unit	X-Origin	Y-Origin	Z-Origin	Y-min	Z-max	Z-min
hole	select a value	1	6	-6	0			

Geom Type	Mixture	Bias/D	Radius	H-Max	H-Min	X-coord	Y-coord	Chord
cylinder	2 ss316	1	20.2	10.2	-10.2			

Geom Type	Mixture	Bias/D	X-max	X-min	Y-max	Y-min	Z-max	Z-min
select a value	select a value	1						

Geom Type	Mixture	Bias/D	X-max	X-min	Y-max	Y-min	Z-max	Z-min
select a value	select a value	1						

Geom Type	Mixture	Bias/D	X-max	X-min	Y-max	Y-min	Z-max	Z-min
select a value	select a value	1						

Geom Type	Mixture	Bias/D	X-max	X-min	Y-max	Y-min	Z-max	Z-min
select a value	select a value	1						

RecNo 2 of 2

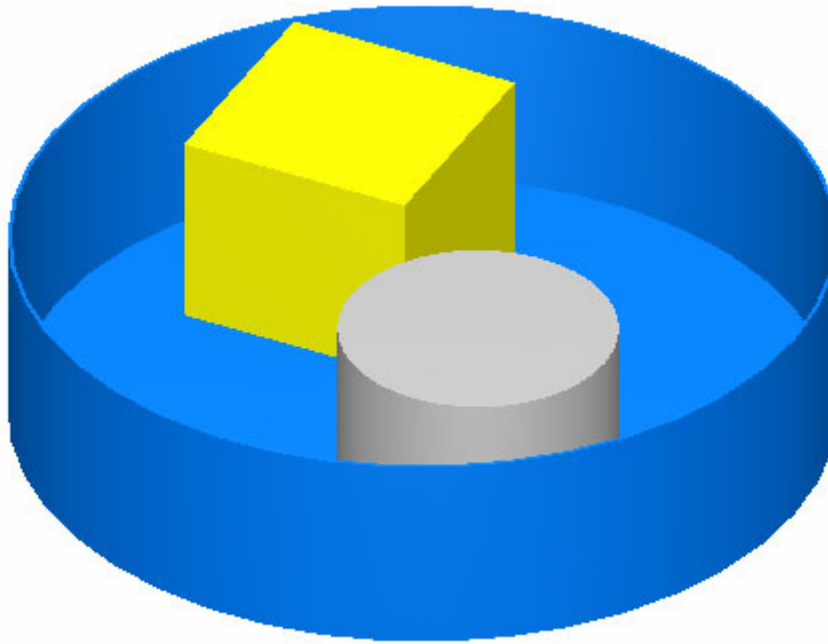
PrevPage NextPage OK / Save Clear Cancel

Page 1

**Fig. 72. UNIT 2 geometry input for HOLE example.**

After checking that the input data match, select **OK/Save**. Save the input file and execute CSAS. The  $k_{eff}$  calculated was  $1.00042 \pm 0.00173$  for seven generations skipped.

The completed geometry for this problem should look like Fig. 73. (The top half of the system has been removed for viewing.)



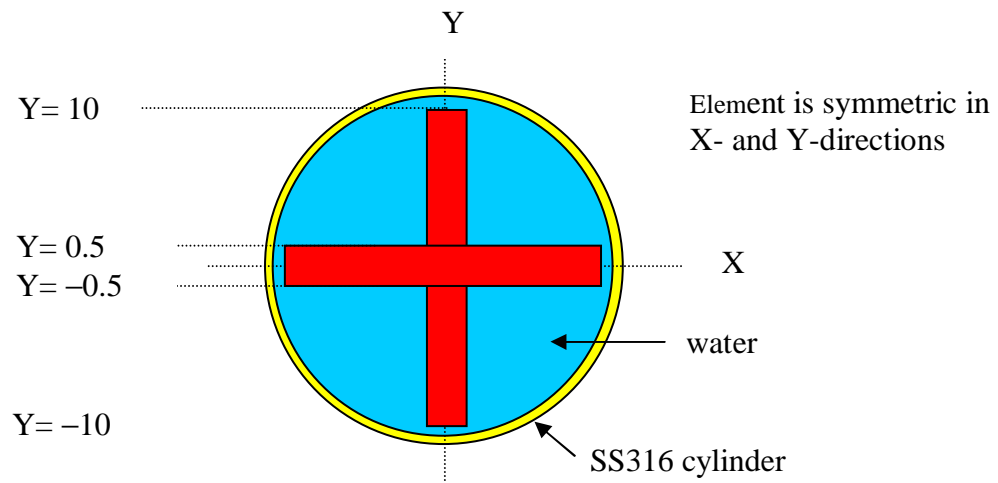
**Fig. 73. 3-D view of geometry for HOLE example problem.**

## **5.4. USING HOLES AND ARRAYS**

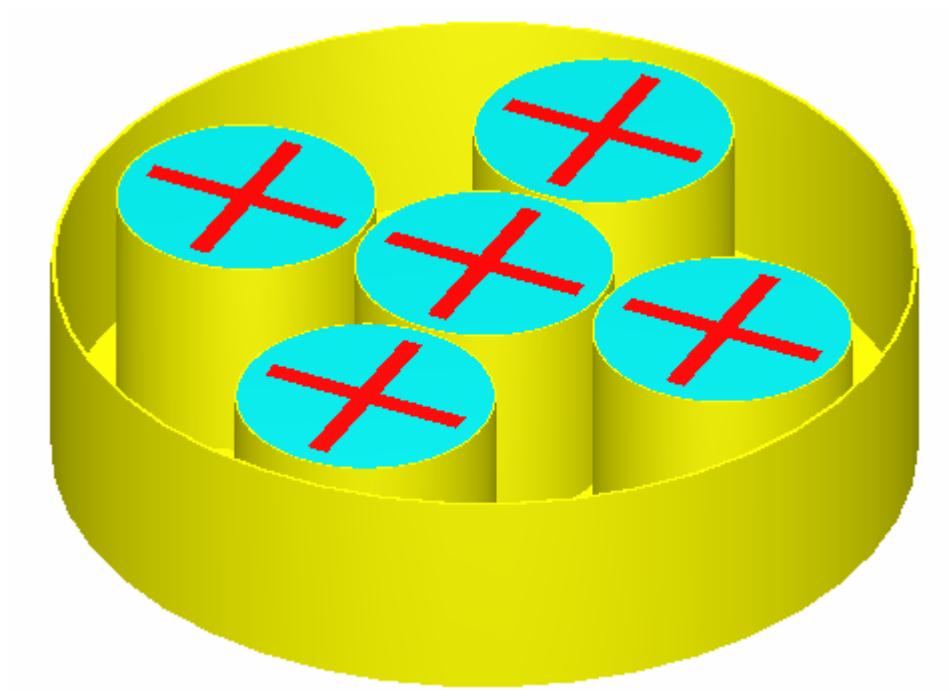
Many problems involve an array of items such as fuel pins. This example problem demonstrates how to enter data for a UNIT containing a HOLE and then use that UNIT in an ARRAY.

### **5.4.1. Shipping Container With 5 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. 74). 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 12.0 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, inside height of 20.2 cm, and radial/axial thicknesses of 0.2 and 0.1 cm. The problem geometry is shown in Fig. 75.

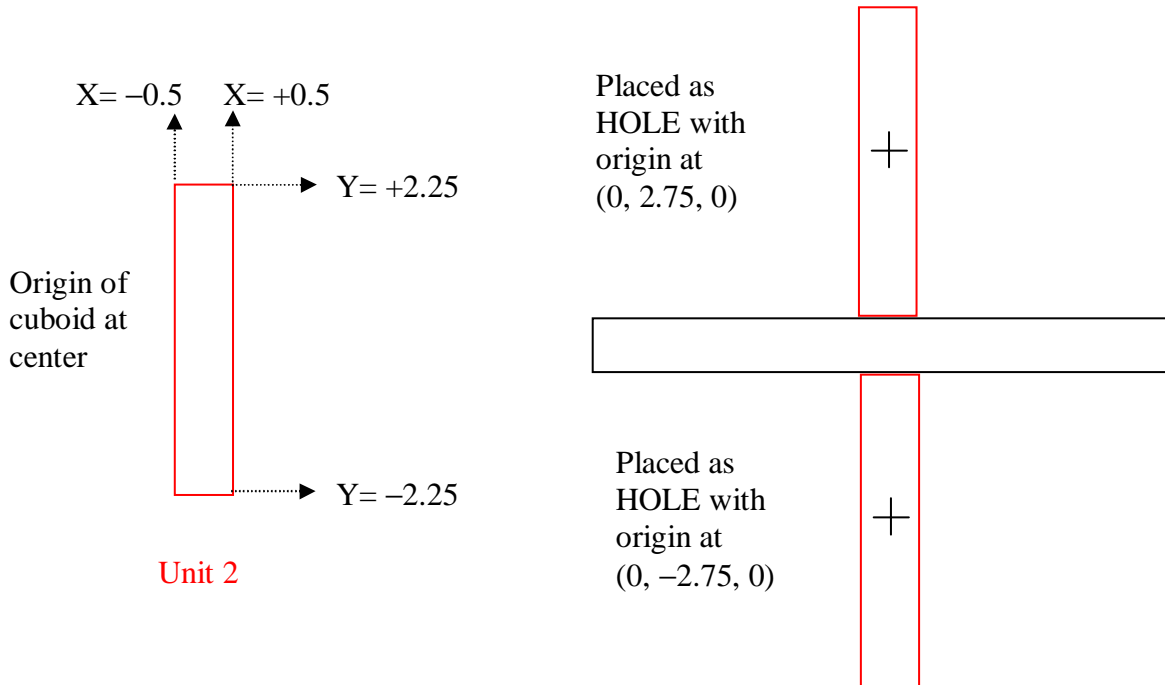


**Fig. 74. SS316 cylinder with U(93.2)C cruciform.**



**Fig. 75. 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 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 touch. 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. 76).



**Fig. 76. Creating cruciform with HOLES placed next to cuboid.**

We will start with UNIT 1. Open the **Geometry** window and enter a comment in the **COM=** box. Then under **Geom Type** 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-Max** through **Z-Min**. 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 for the cylinder type select **cylinder** again. For **Mixture** select 2 **h2o** from the pulldown menu. Then enter 6 for the **Radius**, 10 for **H-Max**, and -10 for **H-Min**. Now we are ready to place the HOLES in the water.

To enter the HOLE data, under **Geom Type** select **hole**. 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 the **X-Origin**, 2.75 for the **Y-Origin**, and 0.0 for the **Z-Origin**. Go to the next geometry line and enter data for the second HOLE whose origin will be below the

X-axis at (0, -2.75, 0). The next region in UNIT 1 is the SS316 cylinder that contains the water and the cruciform element. Enter the data for it. Then the last region in UNIT 1 is the cuboid outside of the steel cylinder, which allows us to put this unit into an array. Because the pitch in the X- and Y-directions is 12.4 cm, the **X-Max**, **X-Min**, **Y-Max**, and **Y-Min** entries will be + or -6.2 = (12.4/2). After entering the appropriate data for this cylinder, the geometry form for UNIT 1 should look like Fig. 77.

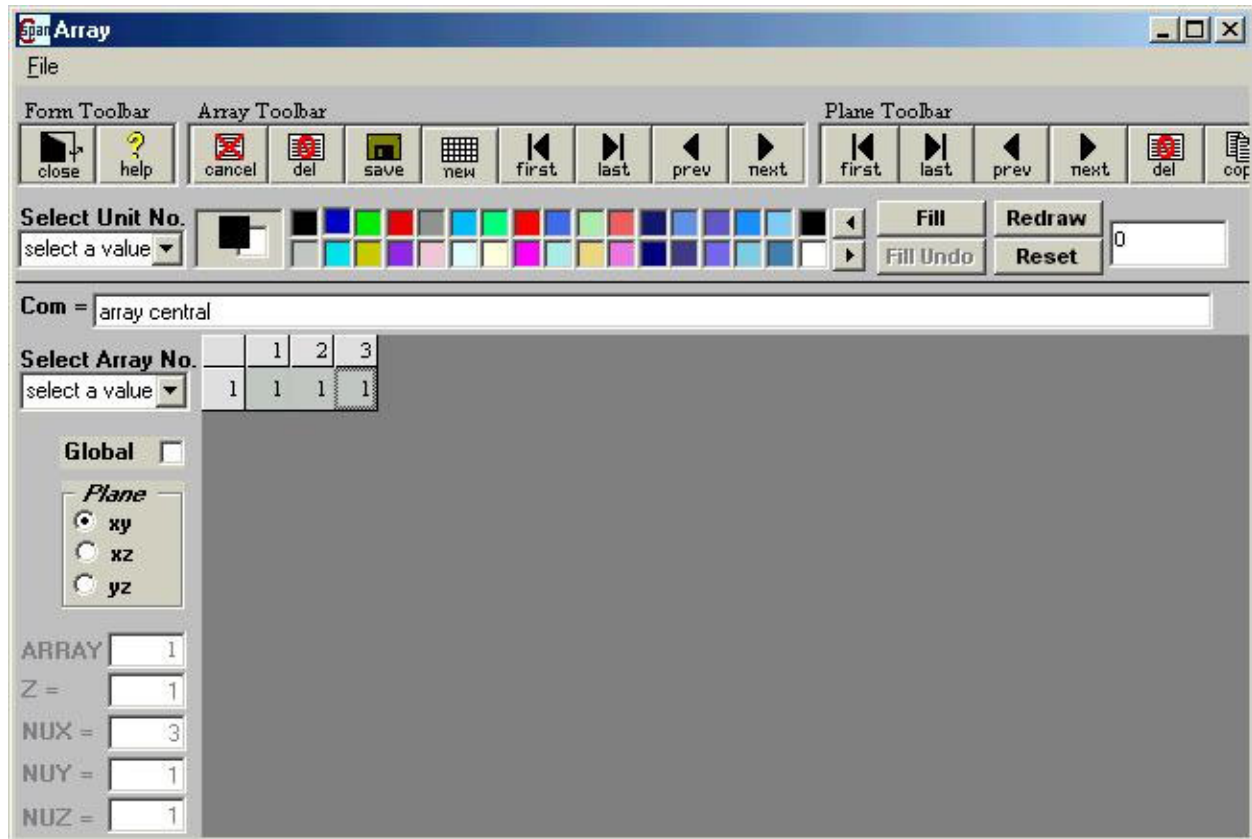
**Fig. 77. Geometry input for UNIT 1.**

Notice that UNIT 2 does not have to be defined before you use it as a HOLE, but it must be defined before the problem is run. Now define UNIT 2 as a cuboid with material 1 uc. The **X Max** and **X-Min** should be 0.5, and -0.5; the **Y-Max** and **Y-Min** should be 2.25 and -2.25; and the **Z-Max** and **Z-Min** should be 10 and -10.

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** window and set up a new array with 3 units in the X-direction and 1 each in the Y- and Z-directions. Fill the array with UNIT 1 in each position. The screen should look like Fig. 78. Provide a comment for the array and then save the information.



**Fig. 78. Array data.**

Now we will enter the data for the global unit, UNIT 3. The first region in UNIT 3 will be the array. Parameters for an array as a region in a UNIT include the **Array Number**, and the **X-Min**, **Y-Min**, and **Z-Min** coordinates of the lower left hand corner. For this problem, the **Array No.** is 1, and the lower left hand corner is located at (-18.6, -6.2, -10.1). The **X-Min** is (1.5 \* the pitch), the **Y-Min** is (0.5 \* the pitch), and the **Z-Min** corresponds to the bottom of UNIT 1.

The next region is the inside of the large cylinder that holds the array. This cylinder has void material in it, a **Radius** of 20 cm, **H-max** of 10.1, and **H-min** 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 has an **X-Origin** of 0, a **Y-Origin** of -12.4, and a **Z-Origin** of 0.0. The last region is the large SS316 cylinder containing the array with a **Radius** of 20.2 cm and heights of  $\pm 10.2$  cm. The completed **Geometry** form for UNIT 3 should look like Fig. 79.

**CSPAN** inputfile: E:\holearray.inp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

**Geometry**

Arrays

2D-Plots

Boundary Conditions

Biassing

**KENO GEOMETRY -- Labels will change when Geom Type is selected**

Form Toolbar: close, help

Unit Toolbar: first, last, prev, next, dup, list, del

Region Toolbar: insert, copy, paste

Global Unit: ☒ COM = big tank

Go To Unit: select a value

Unit Displayed = 3

Unit Colors: [Color palette]

Geom Type	Mixture	BiasID	ArrayNo	X-min	Y-min	Z-min	Chord
array			1	-18.6	-6.2	-10.1	

Geom Type	Mixture	BiasID	Radius	H-Max	H-Min	X-coord	Y-coord
cylinder	0 void	1	20	10.1	-10.1		

Geom Type	Mixture	UnitNo	X-Origin	Y-Origin	Z-Origin	Z-Coord	Chord
hole	select a value	1	0	12.4	0		

Geom Type	Mixture	UnitNo	X-Origin	Y-Origin	Z-Origin	Y-min	Z-max
hole	select a value	1	0	-12.4	0		

Geom Type	Mixture	BiasID	Radius	H-Max	H-Min	X-coord	Y-coord
cylinder	3 ss316	1	20.2	10.2	-10.2		

Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max
select a value							

**Fig. 79. Geometry data for UNIT 3.**

Save the changes in a new input file and execute CSAS. The calculated  $k_{eff}$  was  $0.61975 \pm 0.00191$  for five generations skipped.

## 5.5. SUMMARY

This section has helped you to:

- Use CSPAN 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. ARBITRARY 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 an arbitrary material and use CSPAN to enter data for it.
- Define a mixture by using a combination of an arbitrary material and a basic standard composition.

### 6.2. ARBITRARY 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 the **Arbitrary Materials** input in CSAS. This approach works best for materials where the chemical composition 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.

#### 6.2.1. Description of an Arbitrary 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 **Arbitrary Materials** button. [NOTE: The first four characters of the Composition name must be `arbm` for an arbitrary material.] For **Composition name** choose something like `arbm oil`. 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 want to enter information in terms of atoms per molecule. So select the **Atoms Per Molecule** box. Now for each element, select the element name and then enter the atoms per molecule. To start, select `c` for the **Element Name** and enter 2 for **Atoms/Molecule**. Continue with hydrogen, silicon, and oxygen. The completed form should look like Fig. 80. Click on **OK/Save**.

**CSPAN** writing Scale input File: C:\scale4.4a\cspan\tmpScale.csp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

Geometry

Arrays

2D-Plots

Boundary Conditions

Biased

Start Conditions

Criticality Search

Dimension Search

Concentration Srch

**Arbitrary Materials**

close help first last prev next new dup del list

Composition Number: 1

Composition Name: ARBMoil

Density: 0.97

Density Multiplier: 1

Temperature(K): 293

☐ Weight Percent

☒ Atoms Per Molecule

Elements

Element Name	Atoms/Molecule	Multiple Isotopes
c	2	Isotopic Distribution
h	6	Isotopic Distribution
si	1	Isotopic Distribution
o	1	Isotopic Distribution
select a value		Isotopic Distribution
select a value		Isotopic Distribution

Record 1 of 0 Records Page 1 of 0

Prev Page Next Page OK/Save Clear Cancel

**Fig. 80. Arbitrary materials input.**

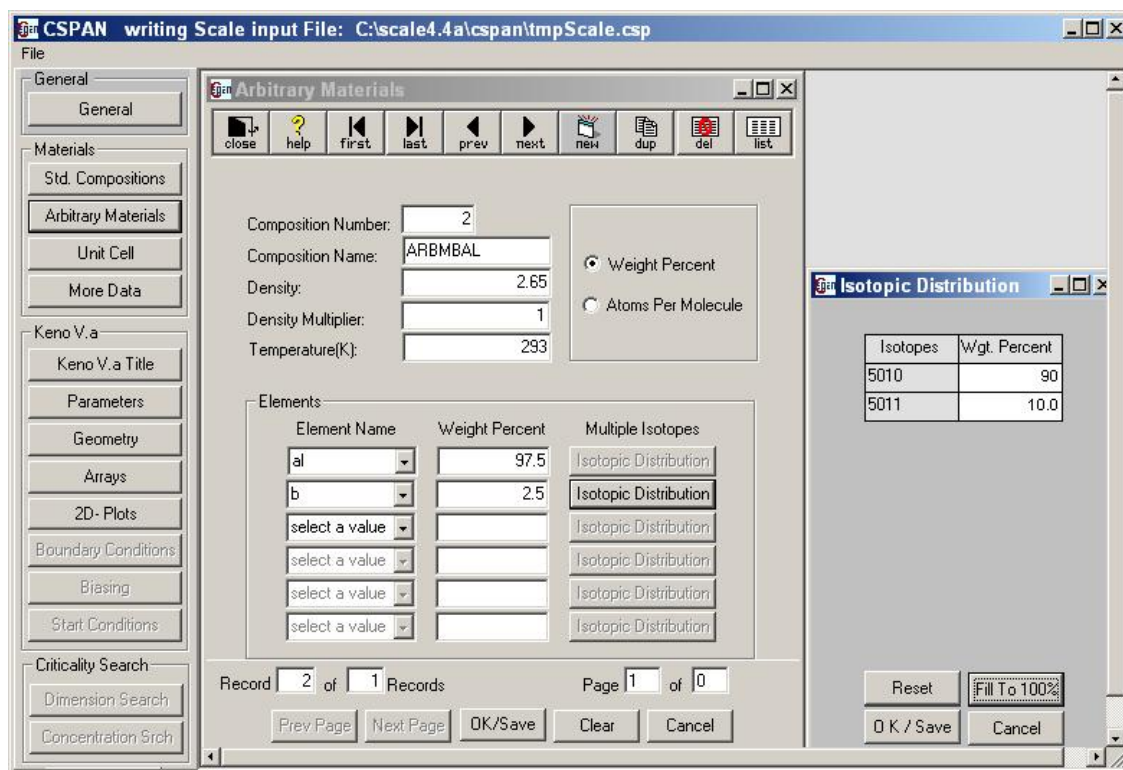
### 6.2.2. Description of an Arbitrary Material with Weight Percents and Isotopic Abundance

For this example, we will enter the material information for borated aluminum, density of 2.65 g/cc, that is 2.5 wt % boron. The boron is 90 wt % B-10 and 10 wt % B-11. For **Composition name** enter arbmbal. Now enter the **Density** of 2.65 g/cc, and leave the **Density Multiplier** and **Temperature** at the default values. For this material, we know the weight percents so we want to enter information in terms of weight percent. Select the **Weight Percent** box. Now for each element, select the element name and then enter the weight percent. To start, select al for the **Element Name** and enter 97.5 for **Weight Percent**. Then enter the information for boron with a weight percent of 2.5. Note that after selecting b, the isotopic distribution box is highlighted. Selecting this box will give the isotopic composition of the element, in this case boron. For this material we need to change the composition to 90 wt % B-10 and 10 wt % B-11. After doing this, select **Save/OK** on the **Isotopic Distribution** form. The completed form should look like Fig. 81. Click **OK/Save** on the **Arbitrary Materials** form.

Note that you can not mix atom per molecule entries with elemental 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 elements and use the isotopic distribution box to enter the proper isotopic weight percents.

### 6.2.3. Combinations of Basic Standard Compositions and Arbitrary Materials to Define a Mixture

For this example, we will enter the material information for a burnable poison, density of 3.7 g/cc, that 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 an arbitrary material for Al<sub>2</sub>O<sub>3</sub> and a basic standard composition for the B<sub>4</sub>C. Open the **Arbitrary Materials** window. For **Composition Name** enter arbmalox. Again, the first 4 characters of the **Composition Name** must be arbm for an arbitrary material. 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.



**Fig. 81. Arbitrary material for borated aluminum.**

For this material, we know the chemical composition so we want to enter information in terms of atoms per molecule. So select the **Atoms Per Molecule** box. Now for each element, select the element name and then enter the atoms per molecule. To start, select **al** for the **Element Name** and enter 2 for **Atoms/Molecule**. Continue with oxygen. The completed form should look like Fig. 82. After doing this, select **Save/OK**.

Now for the  $B_4C$ , click on the **Std. Compositions** button. For **Composition Number** change it to be the same as the mixture number for  $Al_2O_3$ , so that it will be part of the same mixture. For **Composition Name** select **b4c** and specify 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). Selecting 5000 gives the weight percents of the two isotopes in natural boron as shown in Fig. 83. Click **OK** and then enter **User Specified** under the **Density** box. Then enter the mixture density of 3.7 g/cc. The completed information should look like Fig. 83. (If you have closed the **Isotopic Distribution** window, then it will not appear on the screen.)



CSPAN writing Scale input File: C:\SCALE4.4A\CSPAN\tmpScale.csp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

Geometry

Arrays

2D- Plots

Boundary Conditions

Biasing

Start Conditions

Criticality Search

Dimension Search

Concentration Srch

Help

Arbitrary Materials

close help first last prev next new dup del list

Composition Number: 1

Composition Name: ARBMalox

Density: 3.7

Density Multiplier: 0.98605

Temperature(K): 293

☐ Weight Percent

☒ Atoms Per Molecule

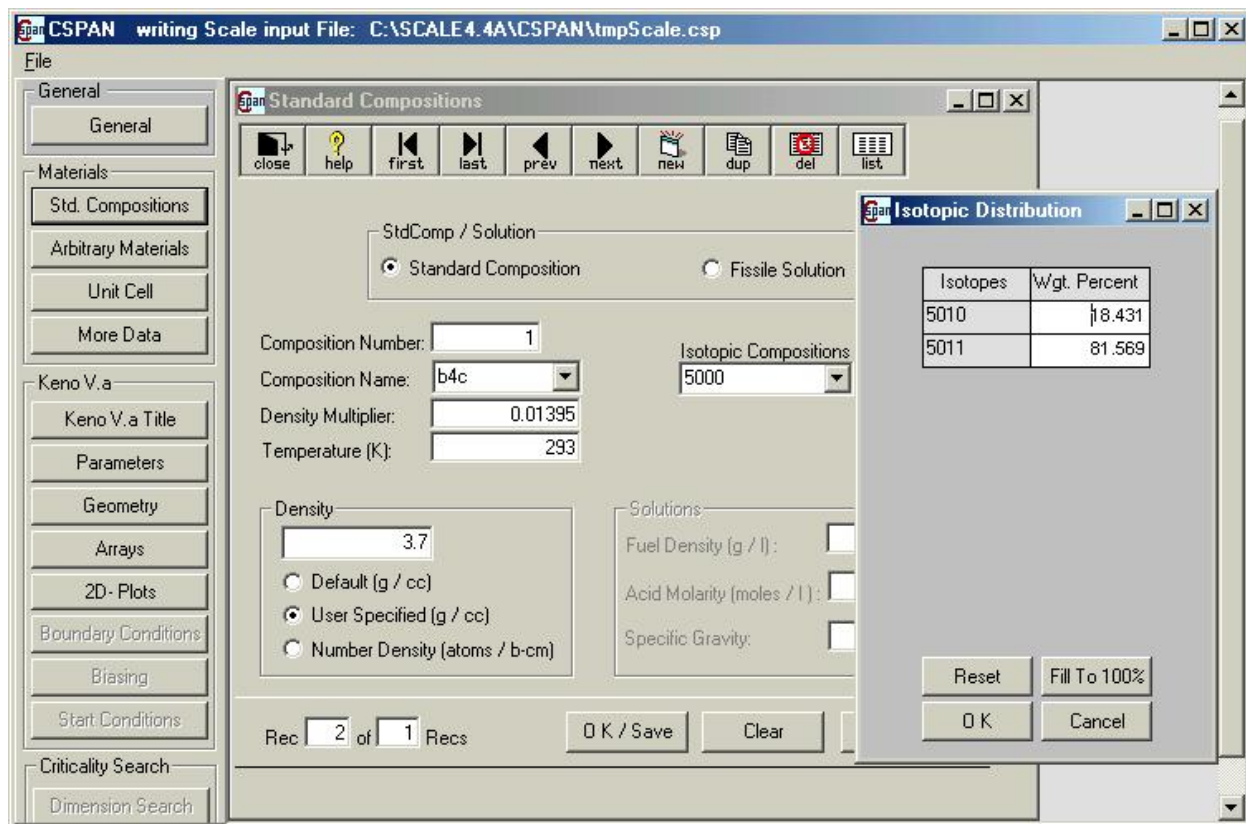
Elements

Element Name	Atoms/Molecule	Multiple Isotopes
al	2	Isotopic Distribution
o	3	Isotopic Distribution
select a value		Isotopic Distribution
select a value		Isotopic Distribution
select a value		Isotopic Distribution
select a value		Isotopic Distribution

Record 1 of 0 Records Page 1 of 0

Prev Page Next Page OK/Save Clear Cancel

Fig. 82. Arbitrary material description for  $\text{Al}_2\text{O}_3$  in burnable poison mixture.



**Fig. 83. Standard composition part of burnable poison mixture.**

This completes the description of the burnable poison mixture using an arbitrary 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 percent of each material.

## 6.3. SUMMARY

This section has shown you how to:

- Define an arbitrary material and use CSPAN to enter data for it.
- Define a mixture by using a combination of an arbitrary material and a basic standard composition.

## 7. UNIT CELLS AND CROSS-SECTION PROCESSING

The examples we have used thus far have been limited to relatively large homogeneous systems where the 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 CSPAN 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.

### 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. The unit cell is typically a portion of the system that can be used to define the neutron spectrum characteristics of the problem.

### 7.3. UNIT CELL TYPES

The Material Information Processor offers three types of unit cell calculations: INFHOMMEDIUM, LATTICECELL, and MULTIREGION.

#### 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.

When the infinite homogeneous medium treatment is specified, every material specified in the problem is treated as an infinite 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. When the LATTICECELL treatment is used, 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. Unless the appropriate resonance and Dancoff data are explicitly entered in the optional parameter data, all other mixtures and their nuclides are treated as INFHOMMEDIUM. Limitations of the LATTICECELL treatment include:

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.
2. Only one cell description is allowed in a problem. This limitation can be circumvented by entering the appropriate Dancoff factors data and cell geometry/mixture data in the **More Data** window of CSPAN.
3. 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 can become important.

### 7.3.3. MULTIREGION

The MULTIREGION treatment is appropriate for 1-D geometric regions where the geometry effects may be important, but the lattice cell treatment is inappropriate. 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). 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.
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. The cross-section treatment then uses an interlump (i.e., lump-to-lump) Dancoff factor of zero in the geometric correction calculations.
5. If the outer boundary of a MULTIREGION cell has a boundary condition other than vacuum, 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.
6. The intralump (i.e., within the lump) Dancoff factor is determined using homogenized interior zones.

**NOTE:** If you want to apply boundary conditions other than the default conditions supplied for INFHOMMEDIUM or LATTICECELL to your unit cell model, then you must use the MULTIREGION cell treatment.

## 7.4. UNIT CELL SPECIFICATIONS

Unit cell data are not required for INFHOMMEDIUM. With the LATTICECELL and MULTIREGION treatments, you must specify the unit cell dimensions and materials to be used in the resonance self-shielding process. Only one unit cell can be defined in a problem. The unit cell is always 1-D: infinitely long cylinders, infinite slabs, or spheres. 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 (CSAS1X, CSAS2X, and CSAS4X sequences).

### 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 directly account for lattice effects, so it is best used for problems where lattice effects are not important.

## 7.5. PROBLEM DESCRIPTIONS

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

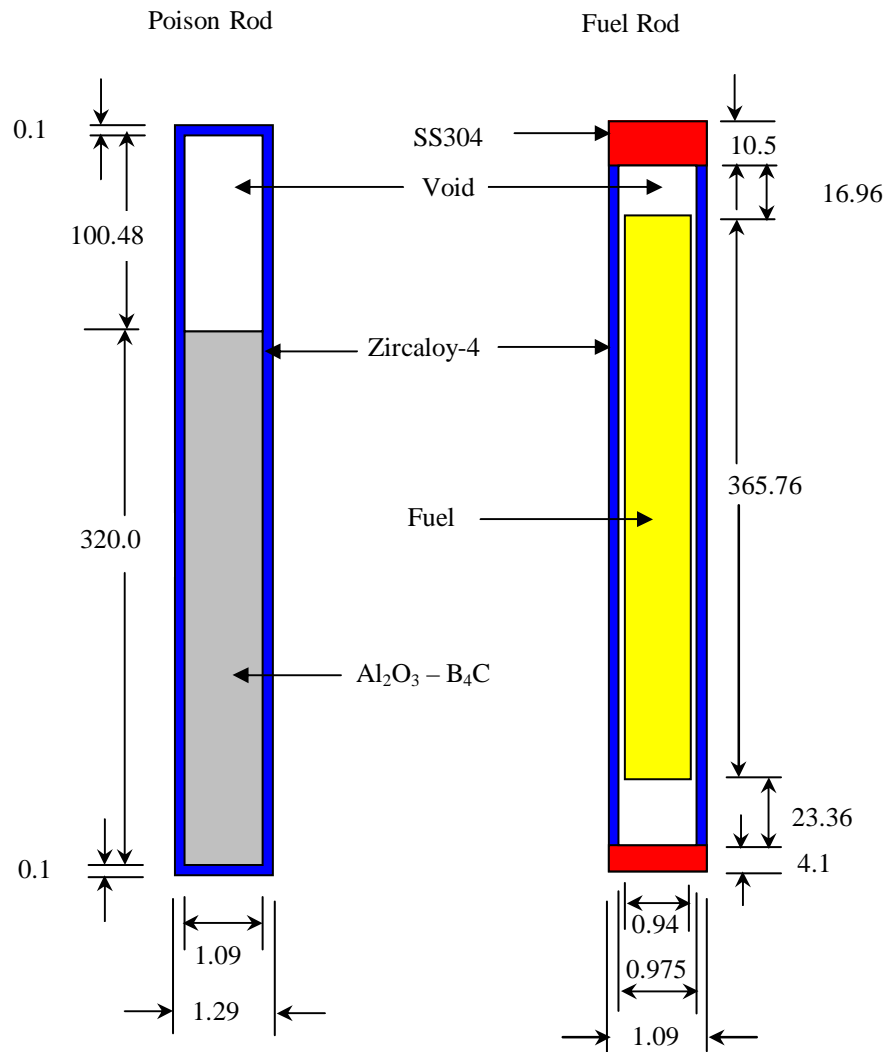
### 7.5.1. Lattice Cell Example: 9×9 Fuel Assembly

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 UO<sub>2</sub> 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. 84.

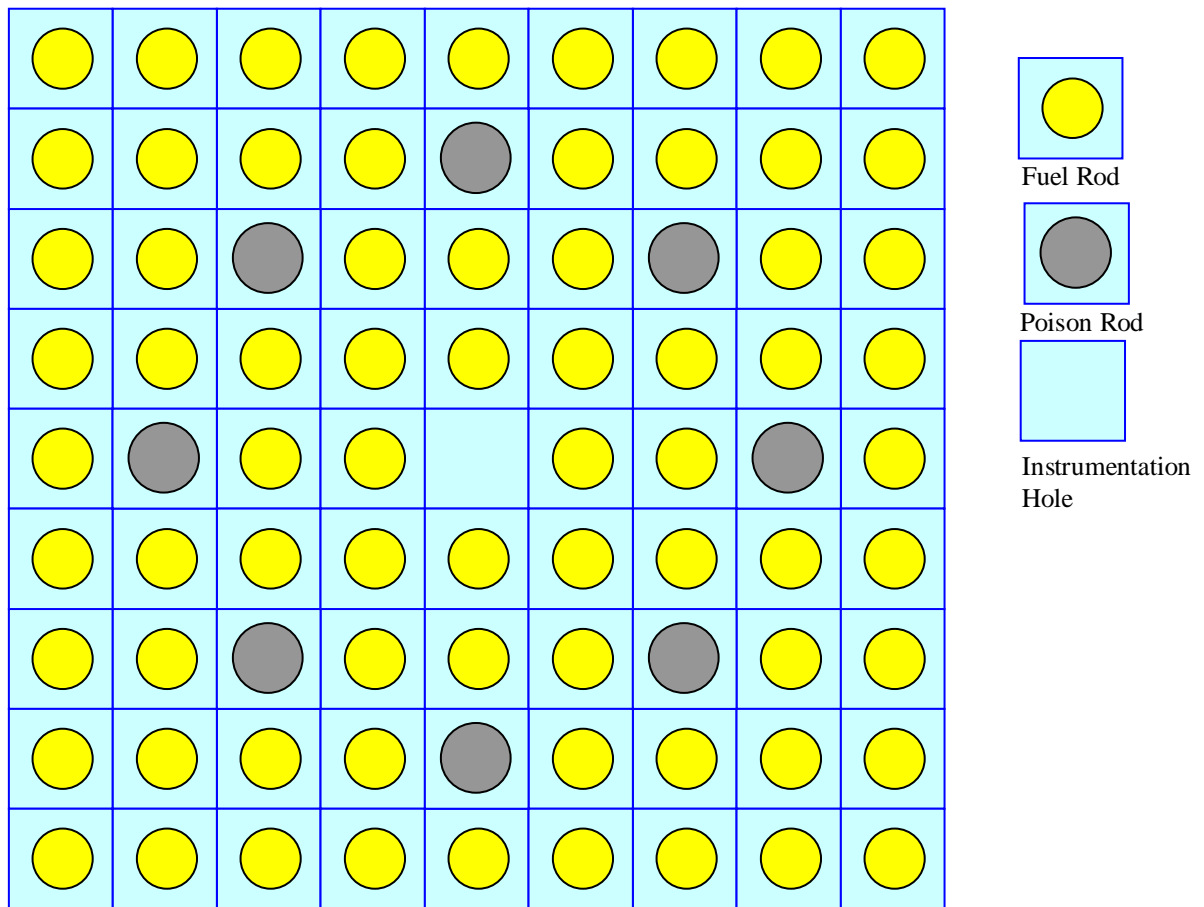
The fuel assembly has a water-filled central instrumentation hole with eight burnable poison rods in various lattice positions as shown in Fig. 85. The burnable poison rods are composed of Al<sub>2</sub>O<sub>3</sub>-B<sub>4</sub>C, having a density of 3.7 gm/cc and are 1.260 wt % B<sub>4</sub>C. The boron in the B<sub>4</sub>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. 84. Axial layout of assembly rods.**



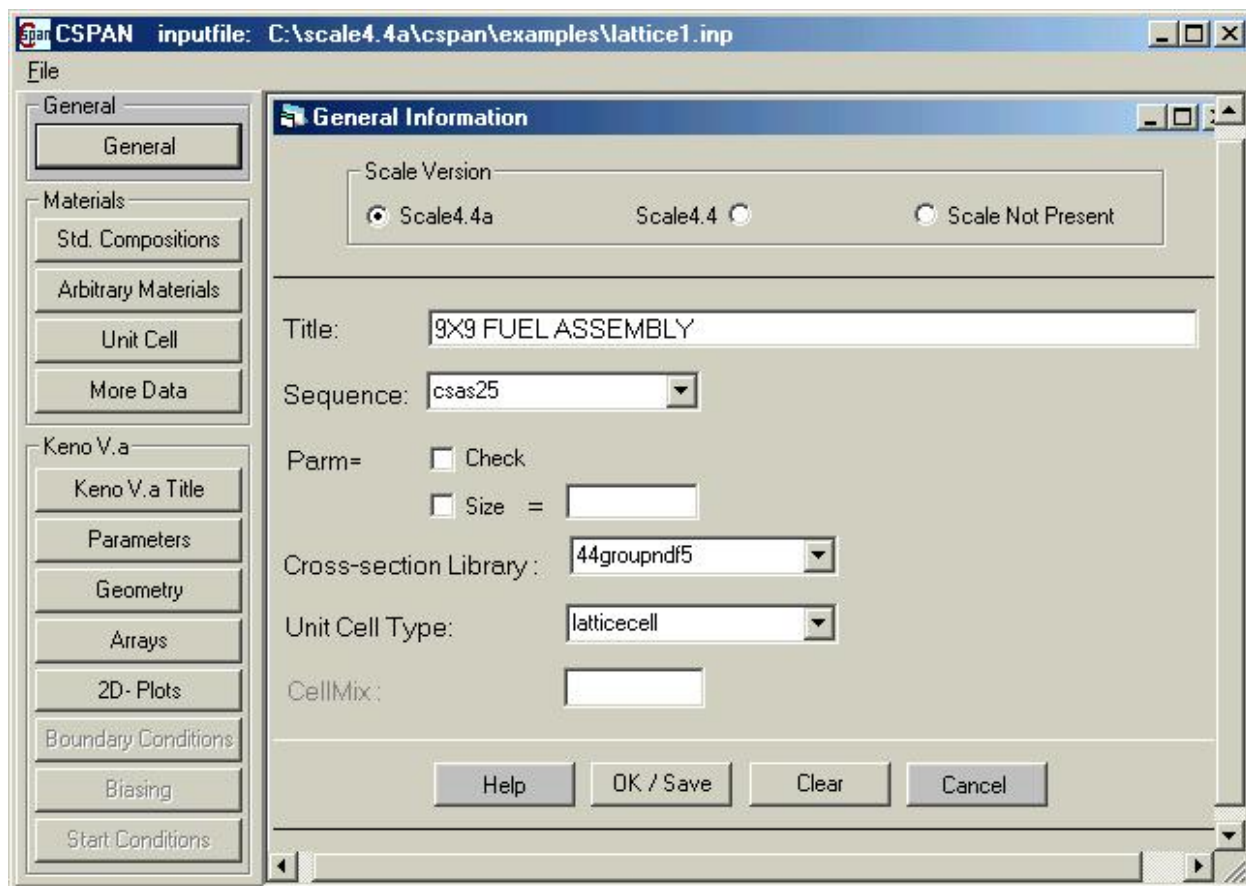
**Fig. 85. Plan view of rod positions in 9×9 assembly.**

#### 7.5.1.1. General and material data

The initial data entry for this example is the same as previous problems. Start the CSPAN input processor and then select **File** and **New Problem**. Select the **General** button on the left hand side and enter the problem **Title**, the **SCALE Sequence**, the **Cross-section Library**, and the **Unit Cell Type** information. The only change for this problem is that the **Unit Cell** is `latticecell` rather than `INFHOMMEDIUM`. The **General Information** window should look like that in Fig. 86.

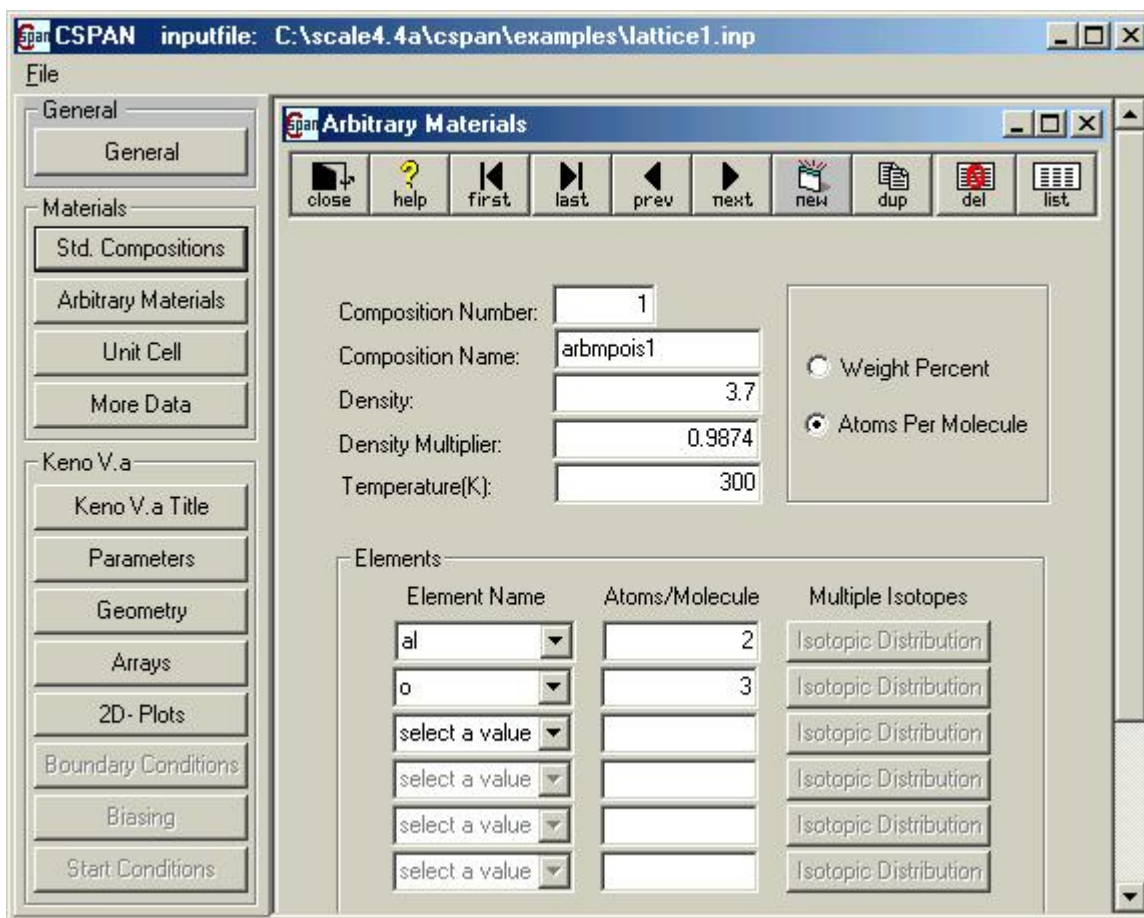
Now we need to enter the **Materials** information. For four of the materials, Standard Compositions can be used: `h2o` (Composition No. 2); `uo2` (Composition No. 3), `zirc2` (Composition No. 4); and `ss304` (Composition No. 5). You should be able to enter the information for these from the problem 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 `uo2` is 3.44 wt %  $^{235}\text{U}$ , so the isotopics need to be entered for this material.





**Fig. 86. 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  $B_4C$  and  $Al_2O_3$ . The material is 1.260 wt %  $B_4C$  with natural boron. As before we will specify this mixture using an arbitrary material for  $Al_2O_3$  and standard composition for the  $B_4C$ . Select the **Arbitrary Materials** screen. For **Composition Number** enter 1 as we will call this mixture composition 1. For **Composition Name** enter arbmpois1. Now for the **Density**, enter the mixture density of 3.7 g/cc with a **Density Multiplier** of  $(1-0.0126) = 0.9874$ . The data entry screen should look like Fig. 87.



**Fig. 87. Data for  $\text{Al}_2\text{O}_3$  portion of burnable poison mixture.**

For the  $\text{B}_4\text{C}$ , click the **Std. Compositions** button. Change the **Composition 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 Compositions**. Enter the mixture **Density** of 3.7 g/cc. The completed information should look like Fig. 88.

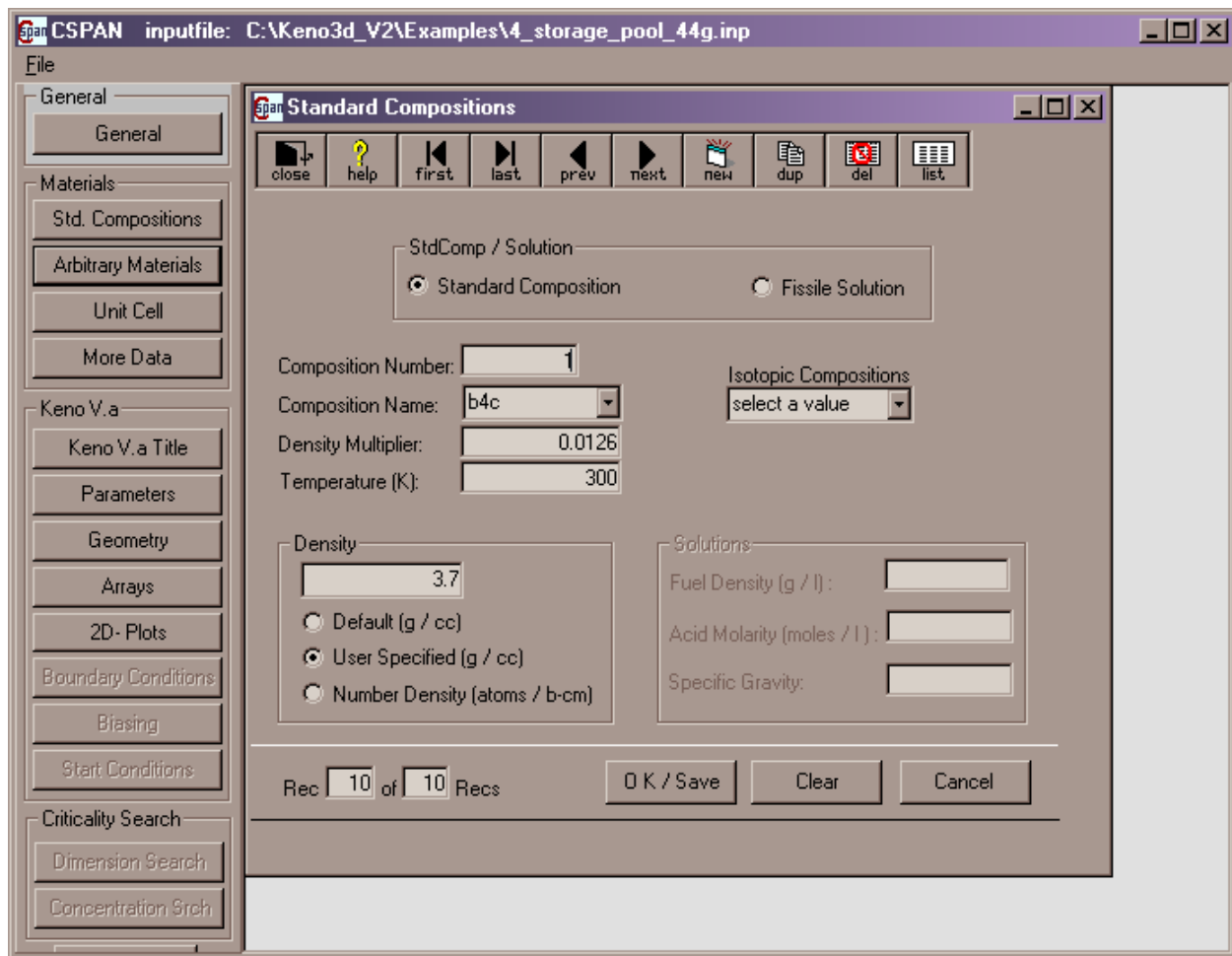


Fig. 88. B<sub>4</sub>C portion of burnable poison mixture.

#### 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 **Unit Cell** button on the left hand side menu will bring up the window shown in Fig. 89 where you enter the unit cell description. 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 1.64 for the **Pitch (cm)** and 0.94 for the **Fuel Outer Diam. (cm)**. Select the uo2 material from the menu for **Fuel Mixture Number**. The **Moderator** is water, so select the h2o material from the menu for **Moderator Mix. Number**. Now, our fuel rods have both a gap and a clad so we need to check those two boxes in the middle of the screen. Checking these boxes activates data entry for the **Clad Description** and the **Gap Description**.

For the **Clad Description**, enter 1.09 for the **Clad Outer Diam. (cm)** and select material **zirc2** for the **Clad Mixture Number**. For the **Gap Description**, enter 0.975 for the **Clad Inner Diam. (cm)** and select material **void** for the **Gap Mixture Number**. The completed Unit Cell screen should look like Fig. 89.

**Unit Cell Specifications**

**UNIT CELL SPECIFICATION FOR A LATTICE CELL**

*Unit Cell Description*

Type of Lattice: squarepitch  
 Pitch (cm): 1.64  
 Fuel Outer Diam. (cm): 0.94  
 Fuel Mixture Number: 3 uo2  
 Moderator Mix. Number: 2 h2o  
 2nd Moderator Diam. (cm):  
 2nd Moderator Mix Number:

☒ Clad Material Present      ☒ Gap Between Fuel and Clad

*Clad Description*

Clad Outer Diam. (cm): 1.09      Clad Mixture Number: 4 zirc2

*Gap Description*

Clad Inner Diam. (cm): 0.975      Gap Mixture Number: 0 void

Help    OK / Save    Clear    Cancel

**Fig. 89. Unit cell description.**

### 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. It is entered in the geometry specification using the menu under **Geom Type**. When selected, it replicates the shape just above it but extends its dimensions by a specified thickness. The required information for the **REPLICATE** command is: the material in the new, outer

region; and the delta dimensions beyond the previous region. 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 thickness and delta above the rod height. Then the clad would replicate the gap cylinder with a clad thickness and a delta above the gap height. 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 data, select the **Geometry** buttons. In this problem, we will define four units as follows. Unit 1 will be a fuel rod; Unit 2 will be a burnable poison rod; Unit 3 will be the instrumentation hole filled with water; 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. 84. Now the fuel rod has end caps made from SS304, so these require a fourth cylinder enclosing the previous three cylinders. The radial dimensions of this cylinder are the same as those 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 they touch 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  $\pm 0.5 \cdot \text{pitch}$  while the Z-dimensions are the same as those for the SS304 end caps. When the data have been entered, the screen should look like Fig. 90.

CSPAN writing Scale input File: C:\SCALE4.4A\CSPAN\tmpScale.csp

File

General

Materials

Std. Compositions

Arbitrary Materials

Unit Cell

More Data

Keno V.a

Keno V.a Title

Parameters

Geometry

Arrays

2D-Plots

Boundary Conditions

KENO GEOMETRY -- Labels will change when Geom Type is selected

Form Toolbar

Unit Toolbar

Region Toolbar

Global Unit

Go To Unit select a value

Unit Displayed = 1

COM = 3.44% enr. fuel rod

Unit Colors:

Geom Type	Mixture	BiasID	Radius	H-Max	H-Min	X-coord	Y-coord	Chord
cylinder	3 uo2	1	0.47	182.88	-182.88			
cylinder	0 void	1	0.4875	199.84	-206.24			
cylinder	4 zirc2	1	0.545	199.84	-206.24			
cylinder	5 ss304	1	0.545	210.34	-210.34			
Geom Type	Mixture	BiasID	X-Max	X-Min	Y-Max	Y-min	Z-Max	Z-Min
cuboid	2 h2o	1	0.82	-0.82	0.82	-0.82	210.34	-210.34

Fig. 90. Geometry information for a fuel rod.



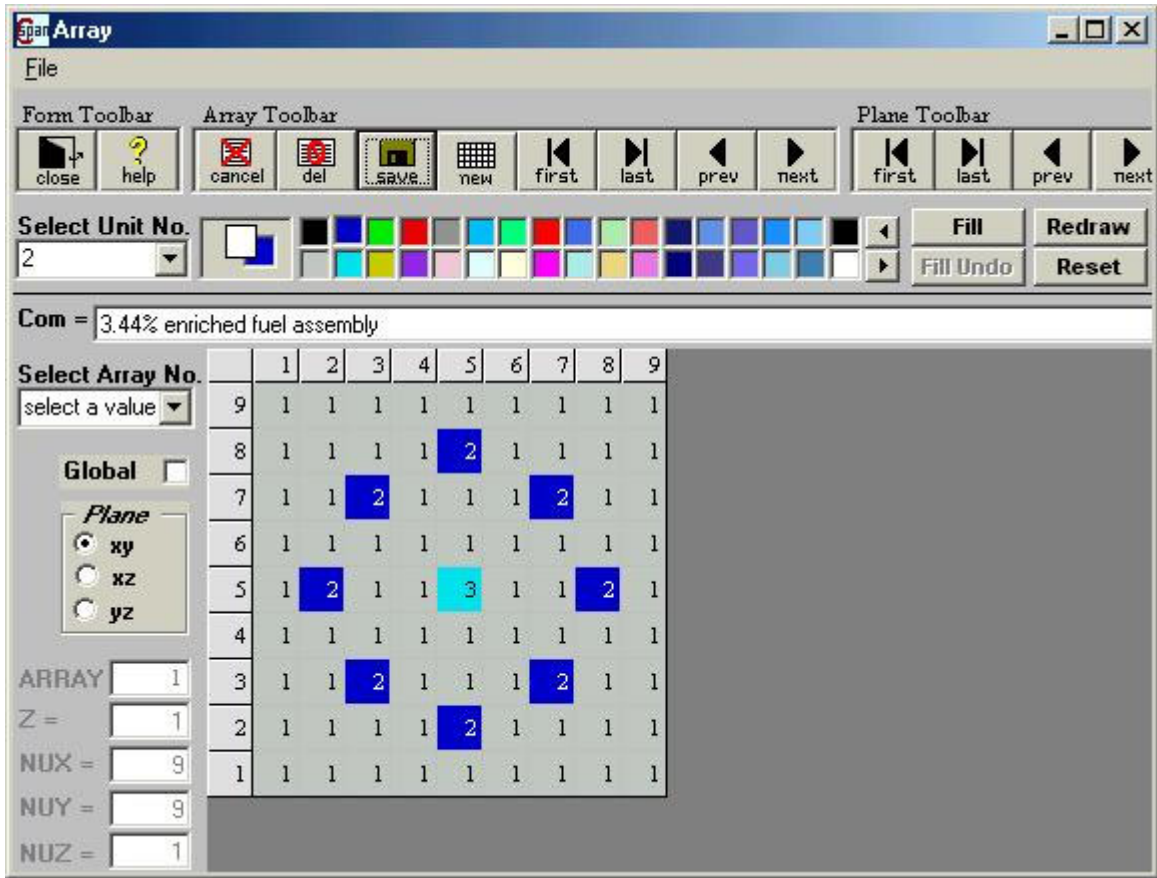
UNIT 2 is the burnable poison rod. This unit is handled just like UNIT 1 but with three cylindrical shapes instead of four. (The end caps are made of the same material as the cladding.) Enter the data using the dimensions from Fig. 84. Now enclose the cylinders in a cuboid containing the moderator. The X- and Y-dimensions are again  $\pm 0.5 \times \text{pitch}$  while the Z-dimensions are the same as those for the zirc2 cylinder. When the data have been entered, the screen should look like Fig. 91.

The screenshot shows the CSPAN KENO GEOMETRY software interface. The title bar indicates the input file is C:\scale4.4a\cspan\examples\lattice1.inp. The left sidebar contains a 'File' menu and a list of buttons: General, Materials, Std. Compositions, Arbitrary Materials, Unit Cell, More Data, Keno V.a, Keno V.a Title, Parameters, Geometry, Arrays, 2D-Plots, Boundary Conditions, Biasing, Start Conditions, Criticality Search, Dimension Search, Concentration Search, and Help. The main window is titled 'KENO GEOMETRY -- Labels will change when Geom Type is selected'. It features three toolbars: Form, Unit, and Region. Below the toolbars, there are fields for 'Global Unit' (checkbox), 'Go To Unit' (dropdown), 'Unit Displayed' (input field with value 2), and 'Unit Colors' (a color palette). The main area contains a table with columns for Geom Type, Mixture, BiasID, Radius, H-Max, H-Min, X-coord, Y-coord, and Chord. The table has four rows of data: 1. cylinder, 1 arbmpois1.b, 1, 0.545, 160, -160, -160, -160, -160; 2. cylinder, 0 void, 1, 0.545, 260.48, -160, -160, -160, -160; 3. cylinder, 4 zirc2, 1, 0.645, 260.58, -160.1, -160.1, -160.1, -160.1; 4. cuboid, 2 h2o, 1, 0.82, -0.82, 0.82, -0.82, 260.58, -1. Below the table, there are several rows of 'select a value' dropdowns for Geom Type, Mixture, BiasID, X-max, X-min, Y-max, Y-min, Z-max, and Z-min. At the bottom, there are buttons for 'RecNo 2 of 4', 'PrevPage', 'NextPage', 'O K / Save', 'Clear', 'Cancel', and 'Pag'.

Geom Type	Mixture	BiasID	Radius	H-Max	H-Min	X-coord	Y-coord	Chord
cylinder	1 arbmpois1.b	1	0.545	160	-160	-160	-160	-160
cylinder	0 void	1	0.545	260.48	-160	-160	-160	-160
cylinder	4 zirc2	1	0.645	260.58	-160.1	-160.1	-160.1	-160.1
cuboid	2 h2o	1	0.82	-0.82	0.82	-0.82	260.58	-1

Fig. 91. Geometry information for burnable poison rod.

For UNIT 3, the geometry is quite simple. We have a cuboid containing h2o and with the same dimensions as the cuboid from UNIT 2. Before defining UNIT 4, which is the Global Unit, it is easiest to define the array first. In this case, the array is 9 units in the X-, 9 units in the Y-, and 1 unit in the Z-directions. Open the **Array** window and set up a new array with **NUX** = 9, **NUY** = 9, and **NUZ** = 1. Using Fig. 85 as a guide, place the appropriate units into each position using a double click of the mouse at each location. Provide a comment for the array and then save the information. The screen should look like Fig. 92.



**Fig. 92. Array layout for 9×9 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-Min, Y-Min, and Z-Min coordinates of the lower left hand corner. For this problem, the **Array No.** is 1, and the lower left hand corner is located at  $(-7.38, -7.38, -10.1)$ . The **X-Min** is  $(9 \times 0.5 \times \text{the pitch})$ , the **Y-Min** is  $(9 \times 0.5 \times \text{the pitch})$ , and the **Z-Min** is the bottom of UNIT 1. These values place the origin at the center of the bottom of the fuel assembly.

The next region is the cuboid containing the water inside the shroud. The shroud is 14.96 cm in width so the X- and Y-dimensions will be  $\pm 7.48$  while the Z-dimensions are  $\pm 210.34$ . Now the SS304 shroud is also a cuboid whose thickness is 0.16 cm greater than the cuboid just entered. For this we will use the REPLICATE command. We select replicate from the **Geom Type** menu and then select the ss304 mixture. 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 even for the -X, -Y, and -Z deltas. The **No. Regions** entry is 1.



The last entry handles the water outside the shroud. Again, this is a cuboid shape so we will use REPLICATE. Select replicate from the **Geom Type** menu and then select the h2o mixture. Now we have different thicknesses so we enter the delta thicknesses of 7.62 in the +X, -X, +Y, and -Y direction and 15.24 in the +Z, and -Z-directions. This is the global unit so we need to check the **Global Unit** box and provide a comment for this UNIT. The completed geometry screen should look like Fig. 93.

**KENO GEOMETRY -- Labels will change when Geom Type is selected**

Form Toolbar: close, help  
Unit Toolbar: first, last, prev, next, dup, list, del  
Region Toolbar: insert, copy, paste, del

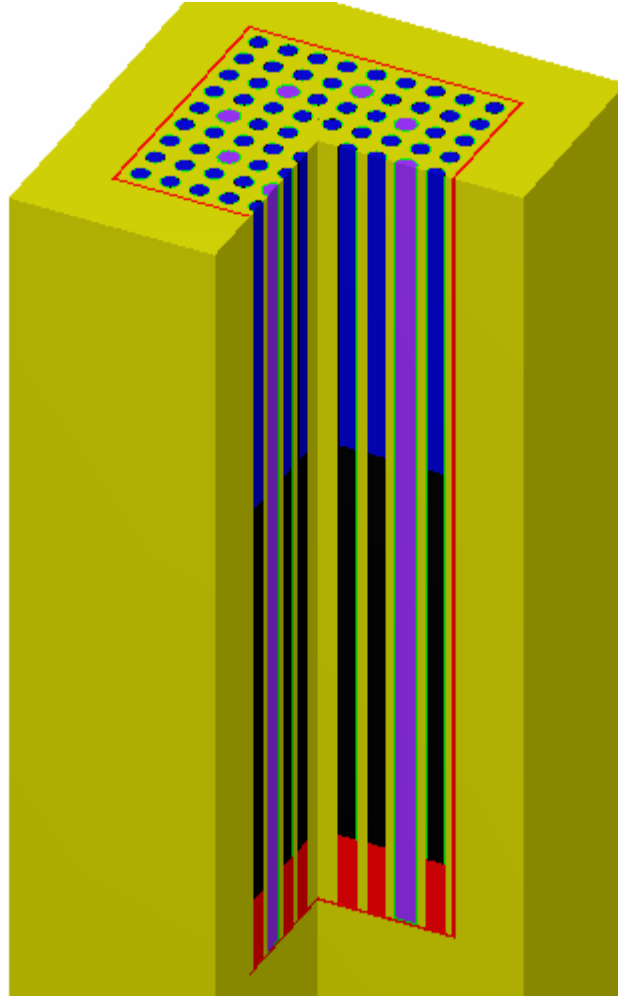
Global Unit: ☒ COM = 3.44% enriched fuel assembly  
Go To Unit: select a value  
Unit Displayed = 4  
Unit Colors: [Color palette]

Geom Type	Mixture	BiasID	ArrayNo	X-min	Y-min	Z-min	Z-max	Z-min	Chord
array			1	-7.38	-7.38	-210.34			
Geom Type	Mixture	BiasID	X-Max	X-Min	Y-Max	Y-min	Z-Max	Z-Min	Chord
cuboid	2 h2o	1	7.48	-7.48	7.48	-7.48	210.34	-210.34	
Geom Type	Mixture	BiasID	Delta X-Max	Delta X-Min	Delta Y-Max	Delta Y-min	Delta Z-Max	Delta Z-Min	No.Regions
replicate	5 ss304	1	0.16	0.16	0.16	0.16	0.16	0.16	1
Geom Type	Mixture	BiasID	Delta X-Max	Delta X-Min	Delta Y-Max	Delta Y-min	Delta Z-Max	Delta Z-Min	No.Regions
replicate	2 h2o	1	3.81	3.81	3.81	3.81	15.24	15.24	1
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							

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**Fig. 93. Global unit for 9x9 fuel assembly.**

A cutaway view of the bottom portion of the assembly is shown in Fig. 94.

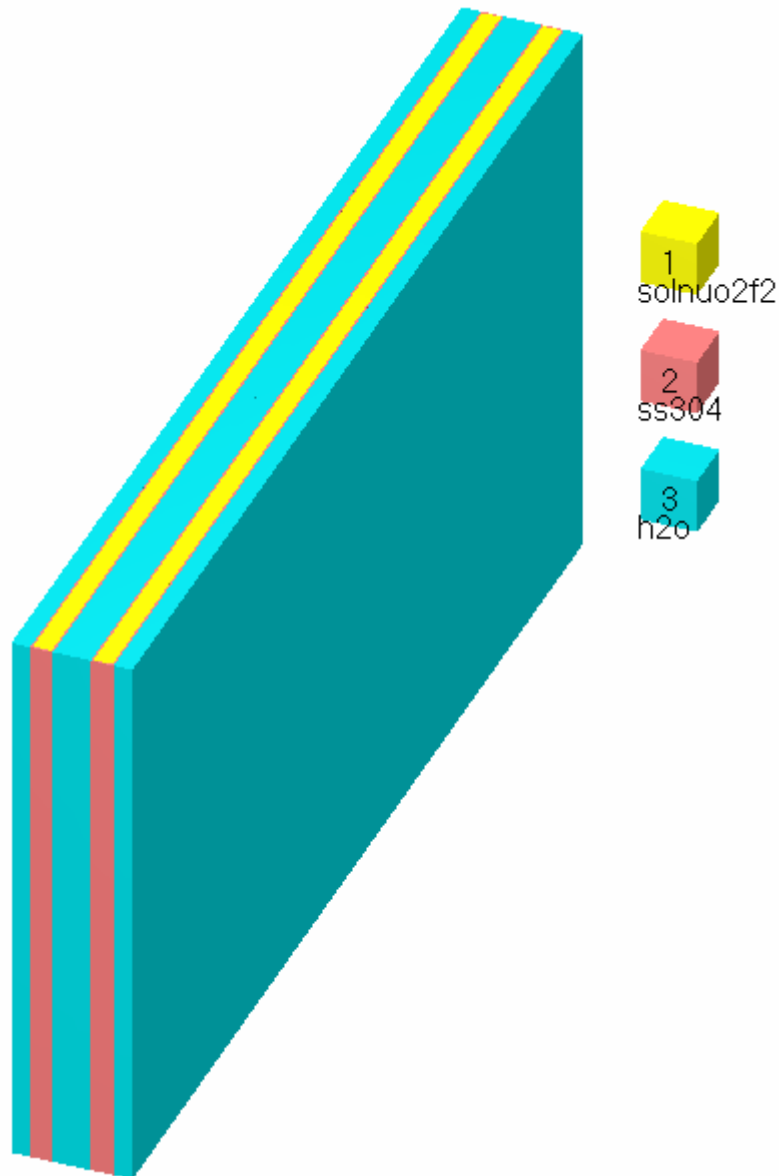


**Fig. 94. 3-D view of bottom part of 9×9 array.**

Save the changes in a new input file and execute CSAS. For this problem, 1003 generations were run to stabilize the  $k_{eff}$ . The calculated  $k_{eff}$  with 1003 generations was  $0.56340 \pm 0.00077$  for 58 generations skipped while for 203 generations, it was  $0.56092 \pm 0.00192$  for 22 generations skipped.

### 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  $\text{U}(93)\text{O}_2\text{F}_2$  with a fuel density of 0.459 gm/cc and a solution density of 1.566 gm/cc. The slab tank inner dimensions are: 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. 95.



**Fig. 95. 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 the CSPAN input processor and then select **File** and **New Problem**. Select the **General** button on the left hand side and enter the problem **Title**, the SCALE **Sequence**, the **Cross-section Library**, and the **Unit Cell Type** information. Other than the title, the only change for this problem is that the **Unit Cell** is multiregion rather than latticecell. The **General Information** window should look like that in Fig. 96.

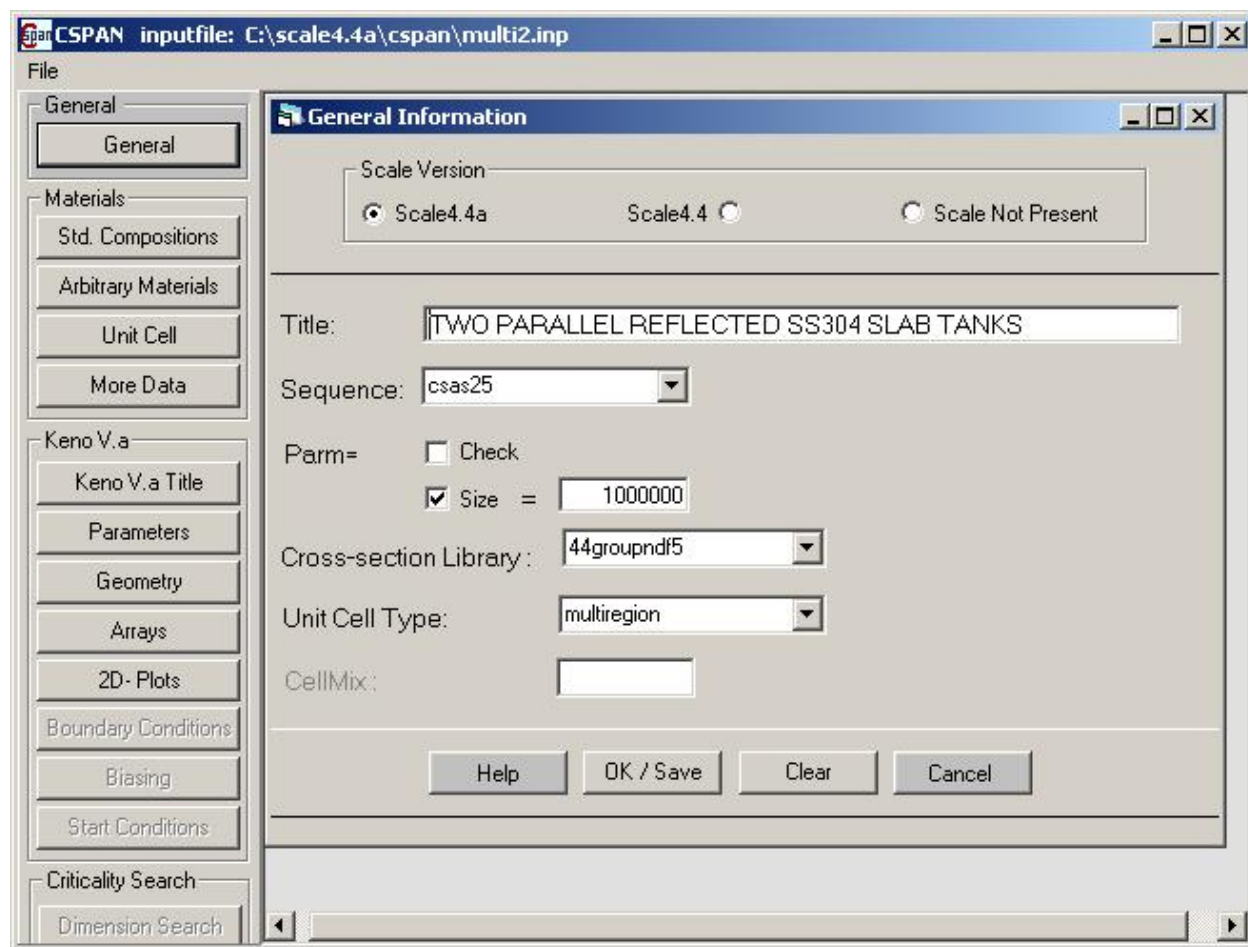


Fig. 96. General information for multiregion problem.

Now we need to enter the **Materials** information. For the three materials, Standard Compositions can be used:  $\text{uO}_2\text{F}_2$  (Composition No. 1);  $\text{ss304}$  (Composition No. 2), and  $\text{h}_2\text{o}$  (Composition No. 3). You should be able to enter the information for these from the problem statement. Remember that the  $\text{uO}_2\text{F}_2$  is a solution with 93 wt %  $^{235}\text{U}$ , so the isotopics need to be entered for this material. The solution has a fuel density of 459 g/l and a specific gravity of 1.566. The default theoretical densities are used for the other two materials.

### 7.5.2.2. 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 **Unit Cell** button on the left hand side menu will bring up the window shown in Fig. 97 where you enter the unit cell description. The first entry is **Type of Geometry**. The menu has the three standard 1-D geometry choices and then choices for a cylinder or a slab with leakage (buckledcyl, buckledslab). As a slab tank is similar to an infinite slab in leakage, we will select Slab for the geometry. For the **Left (inner) Boundary Condition** there are four choices: Periodic Reflected Vacuum, or white. For this problem, we will use the Reflected boundary condition on the inside to utilize the symmetry of the slab tank. Thus, we create a model that starts at the center of the tank and goes to the right. A description of the various boundary conditions is given in Section 7.5.2.3. For the **Right (outer) Boundary Condition**, select Vacuum.

For the **Zone** information, you need to enter the mixture and position starting from the left or innermost and moving towards the right or outermost material. Remember 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 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 water + 0.5 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 Unit Cell screen should look like Fig. 97.

**MULTIREGION UNIT CELL**

Type of Geometry:  Dy:   
Left (inner) Boundary Condition:  Dz:   
Right (outer) Boundary Condition:  Origin:

Zone	Mixture No.	Outside Cumulative Radius or Thickness (cm)	Zone	Mixture No.	Outside Cumulative Radius or Thickness (cm)
1	3 h2o	5	6	select a value	
2	2 ss304	5.5	7	select a value	
3	1 solnuo2f2	10.5	8	select a value	
4	2 ss304	11	9	select a value	
5	3 h2o	16	10	select a value	

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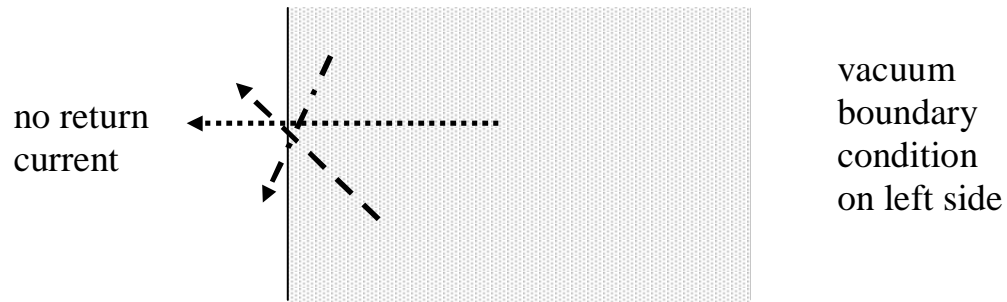
**Fig. 97. Multiregion unit cell description.**

### 7.5.2.3. 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), while the default for the right or outer boundary is *Vacuum*.

#### 7.5.2.3.1. Vacuum boundary condition

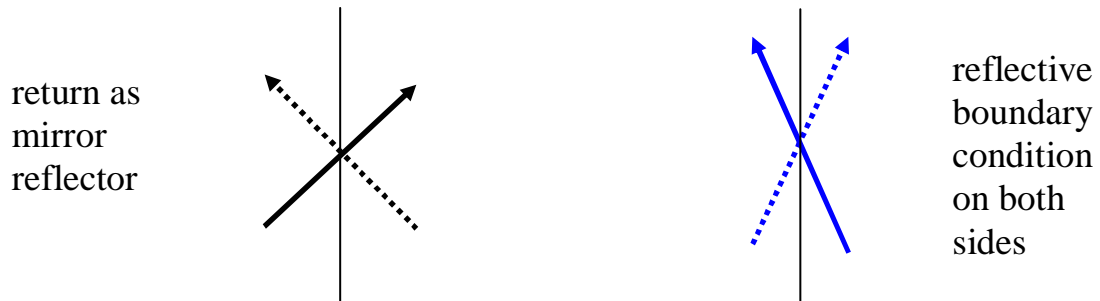
A vacuum boundary condition means that no neutrons will re-enter the boundary. Thus, any neutron exiting the system through a vacuum boundary is permanently lost to the system. This condition is shown in Fig. 98. (**NOTE:** *In the following figures, a dashed arrow indicates neutrons leaving the system while 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. 98. Vacuum boundary condition.**

### 7.5.2.3.2. Reflective boundary condition

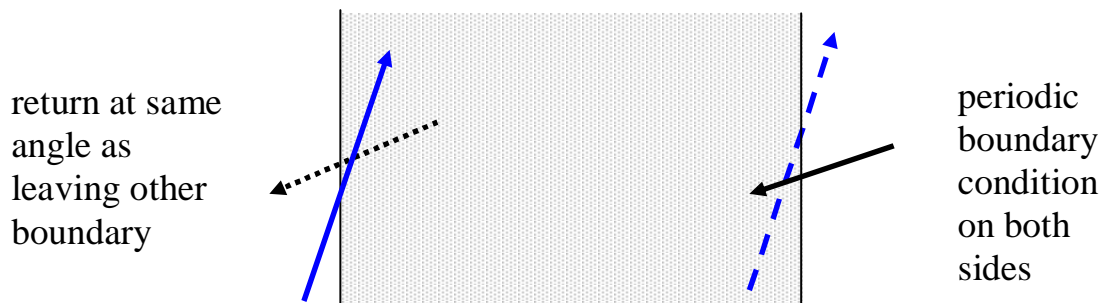
For the reflective boundary condition, the incoming angular flux is set equal to the outgoing angular flux in the direction corresponding to mirror or specular reflection. The reflective boundary should not be used on curved surfaces, that is, the outer boundary of a cylinder or sphere. It is the default for the left or inner boundary of a cylindrical or spherical system. As shown in Fig. 99, 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. 99. Reflective boundary condition.**

### 7.5.2.3.3. 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. 100 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. 100. Periodic boundary condition.**

#### 7.5.2.3.4. 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. 101) and is suitable for all geometries. Although the white boundary condition is in a sense non-physical on a curved surface, it is the best possible approximation of a reflective or repeating boundary condition, such as a lattice cell.

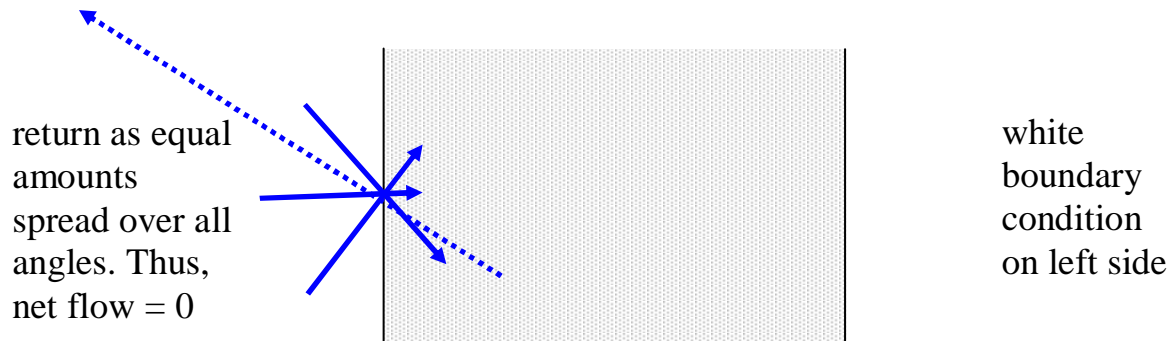


Fig. 101. White boundary condition.

#### 7.5.2.4. KENO V.a data

For the KENO input data, select the **Geometry** button. In this problem, we will define one unit and one array as follows. UNIT 1 will be a slab tank with fuel, stainless steel container, and water reflection. The array will be a global array containing the two slab tanks, side by side.

We will start with UNIT 1. The first shape is the cuboid of fuel ( $5\text{ cm} \times 300\text{ cm} \times 150\text{ cm}$ ), which is then enclosed by the SS304 tank (0.5-cm-thick) on five sides (not including the top), and then 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 **Delta Z-Max** 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 **No. Regions** for both the SS304 tank and the water reflector as 1. For the water reflector, the REPLICATE command is again used, but only the **Delta X-Max**, and **Delta X-Min** values are greater than zero. The geometry for the completed unit should look like Fig. 102.



**KENO GEOMETRY** -- Labels will change when Geom Type is selected

Form Toolbar: close, help

Unit Toolbar: first, last, prev, next, dup, list, del

Region Toolbar: insert, copy, paste, del

Global Unit: ☐ COM = 2

Go To Unit: select a value

Unit Displayed = 1

Unit Colors:

Geom Type	Mixture	BiasID	X-Max	X-Min	Y-Max	Y-Min	Z-Max	Z-Min	Chord
cuboid	1 solnuo2f2	1	2.5	-2.5	150	-150	75	-75	
Geom Type	Mixture	BiasID	Delta X-Max	Delta X-Min	Delta Y-Max	Delta Y-Min	Delta Z-Max	Delta Z-Min	No.Regions
replicate	2 ss304	1	0.5	0.5	0.5	0.5	0	0.5	1
replicate	3 h2o	1	5	5	0	0	0	0	1
Geom Type	Mixture	BiasID	X-max	X-min	Y-max	Y-min	Z-max	Z-min	Chord
select a value	select a value	1							
select a value	select a value	1							
select a value	select a value	1							
select a value	select a value	1							
select a value	select a value	1							
select a value	select a value	1							

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**Fig. 102. Geometry information for slab tank.**

For the array, the geometry is quite simple. It is simply a  $2 \times 1 \times 1$  array with UNIT 1 in both positions. Open the **Array** window and set up a new array with **NUX** = 2, **NUY** = 1, and **NUZ** = 1 and fill both locations with UNIT 1. Provide a comment for the array, mark it as Global, and then save the information. The screen should look like Fig. 103.

Save the changes in a new input file and execute CSAS. The calculated  $k_{eff}$  was  $0.95732 \pm 0.00202$  for six generations skipped.

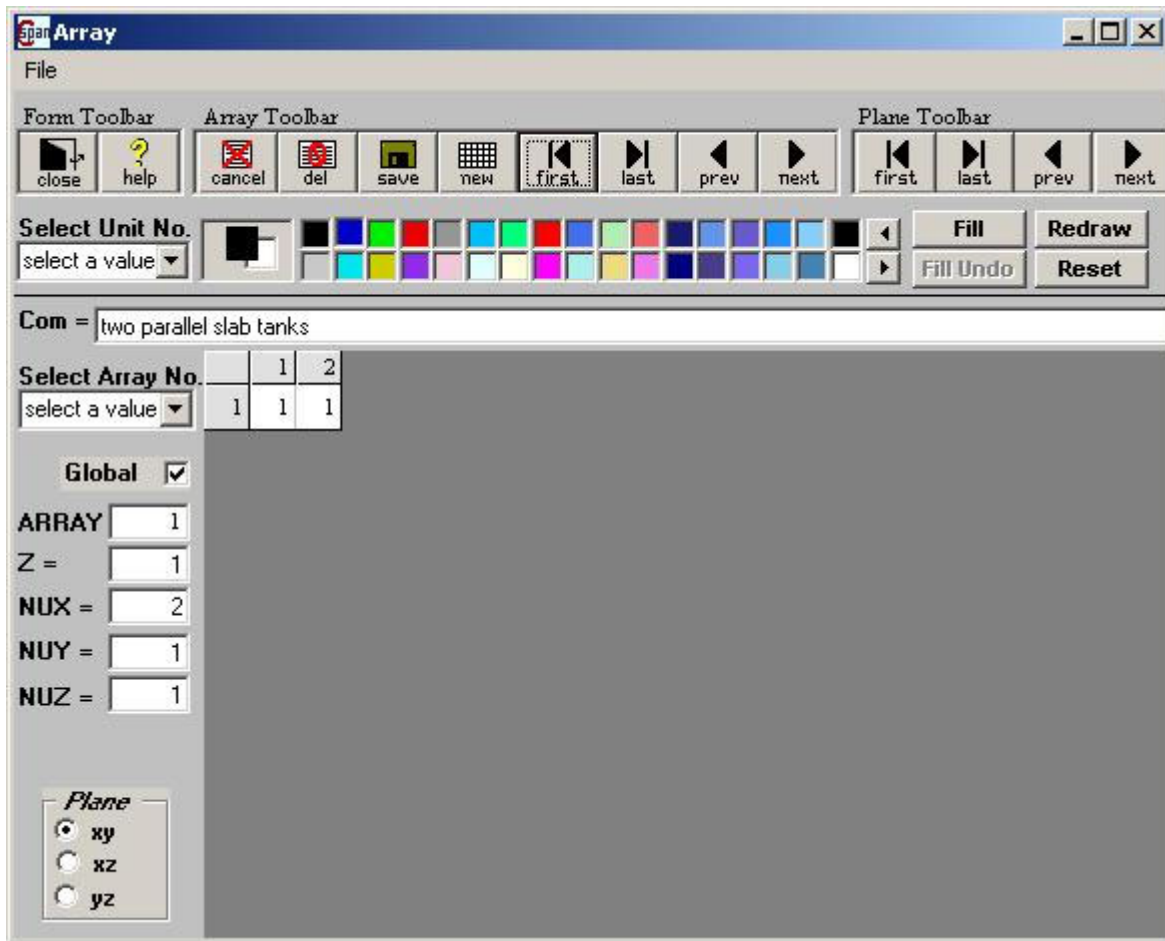


Fig. 103. Array information for two parallel slab tanks.

## 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 CSPAN 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.

## 8. 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 CSPAN input processor to create and run SCALE/KENO V.a input files to model criticality problems.
- Find and interpret  $k_{eff}$  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/scale](http://www.ornl.gov/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/scale/keno3d](http://www.ornl.gov/scale/keno3d).

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



## 9. REFERENCES

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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," CD-ROM, NEA/NSC/DOC(95)03, September 2001 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 a number of references to sections of the SCALE 4.4a manual in the form of “[see Section Mx.x.x].” There are nine cross-section libraries distributed with SCALE, eight of which are automatically available in the SCALE system. Six of these libraries were designed primarily for criticality analysis. The 218-group library is a fine-group library derived from ENDF/B-IV data. The library contains 140 fast groups and 78 thermal groups and includes explicit resonance data in the resolved resonance range. No unresolved resonance data are available in the library. The 27-group library (27GROUPNDF4) is the broad-group library collapsed from the 218-group library and has 14 fast and 13 thermal groups. This library has been extensively validated against critical experiments. The 27-group depletion library (27BURNUPLIB) contains the same data as 27GROUPNDF4 plus pre-release ENDF/B-V data for a large number of fission products. This was the first library designed for use with the SAS2 depletion/decay sequence. The 238-group library (238GROUPNDF5) is the most complete library in SCALE. 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. 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.

### 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 [Sect. M4, Tables M4.2.1 and M4.2.2].

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

### **A.2.1. THE 218-GROUP ENDF/B-IV LIBRARY (218GROUPNDF4)**

The 218-group ENDF/B-IV library is one of the more complete libraries available in SCALE. The source of the data was ENDF/B-IV, and the processing of the cross sections by XLACS in the AMPX system is well documented. The weighting function used in the  $P_3$  cross-section generation was a fission- $1/E$   $\sigma_t$ -Maxwellian weighting (except for resonance nuclides, which were weighted  $1/E$  instead of  $1/E \sigma_t$ ). One of the features of the library is that explicit resonance data carried with it can be used to generate problem-dependent, resonance-region group cross sections using NITAWL-II. This capability allows great flexibility in the use of the library as a general-purpose criticality analysis library. The library has 140 fast groups and 78 thermal groups (below 3.05 eV). The group structure was designed to fit the cross-section variation and reaction thresholds of the light and intermediate nuclides and to fit the major resonances of the intermediate and heavy nuclides. The unresolved resonance region was processed at a  $\sigma_p = 50,000$ . Because no unresolved resonance data are carried in the library there is no problem dependence over this region.

The 218-group library has not been routinely validated because of its size and the related costs. However, the 27-group ENDF/B-IV library was derived directly from the 218-group library and has been validated against a large number of critical experiments [see Sect. M4.2.2]. The 218-fine-group structure of the library generally will give either the same or more precise results than its companion 27-broad-group library. An obvious advantage of a fine-group library over a broad-group library is that the library is less sensitive to the weighting spectrum used to generate the library. The cross sections more closely represent the base data, and the group structure allows a more detailed determination of the energy dependence of the flux. In past validations, it has been found useful to compare a fine-group calculation against a broad-group calculation when bias is observed. [Tables M4.2.4 and M4.2.5 show 218-group nuclides that have resonance data and thermal scattering data, respectively.]

### **A.2.2. THE 27-GROUP ENDF/B-IV LIBRARY (27GROUPNDF4)**

The 27-group ENDF/B-IV library is the broad-group companion library to the 218-group ENDF/B-IV library. The 218-group library was flux collapsed using MALOCS and the MT 1099 flux file carried with the fine-group cross sections. (This flux file is the group representation of the original weighting spectrum used to generate the 218-group cross sections from ENDF/B-IV data.) The library has 14 fast groups and 13 thermal groups (below 3 eV). The group structure was chosen to match the 16-group Hansen-Roach structure with two additional fast groups and seven additional thermal groups. The additional groups were chosen such that, for the systems considered, the broad-group calculations meet an acceptance criterion of  $\Delta k_{eff}/k_{eff} < 0.3\%$  when compared with the reference 218-group calculation using the XSDRN code.<sup>A.1</sup> This criterion was relaxed to 1% for  $^{238}\text{U}$  in systems where the median fission energy was greater than 1 eV and less than 100 eV. The resonance data and the thermal scattering data carried with the 27-group library and the 218-group library are the same and are processed by NITAWL-II. The library was conceived as a general-purpose criticality analysis library with a special interest in applicability toward shipping cask analysis and thermal neutron systems.

The 27-group library has been extensively validated against critical experiments.<sup>A.2-A.10</sup> Areas of validation include highly enriched uranium-metal, compound and solution systems, moderated low-enriched uranium, heterogeneous and homogeneous systems, and plutonium metal and solution systems. The 27-group ENDF/B-IV cross-section set is known to have a 1 to 2% positive bias for highly thermal <sup>239</sup>Pu systems. Negative bias of 1 to 2% has been observed for LWR fuel lattice depending on the degree of lattice moderation. 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). Refer to the SCALE manual [Sect. M4.B] for more information on ORNL experience with the 27-group ENDF/B-IV library.

### A.2.3. 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.11</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, as listed below:

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  $k_{eff}$  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.2.4. 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 15 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 experiments. The experiments primarily consisted of various configurations of light-water-reactor-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 light-water-reactor-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 mixed-oxide 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.2.5. 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.12</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 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 highly enriched uranium-metal, compounds and solutions, moderated low-enriched uranium 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.13.

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 verbal 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	27-group ENDF/B-IV	218-group ENDF/B-IV	44-group ENDF/B-V	238-group ENDF/B-V
Fast HEU	Very good $0.995 \pm 1\%$	Very good $0.995 \pm 1\%$	Very good $1.00 \pm 1\%$	Very good $1.00 \pm 1\%$	Very good $0.995 \pm 1\%$
Thermal HEU	Very poor 2% high to 4% low	Poor 3% high to 2% low	Poor $1.00 \pm 2\%$	Poor $1.00 \pm 3\%$	Poor $1.00 \pm 2\%$
LWR lattices	Fair $\pm 1.5\%$ bias vs energy	Good $0.995 \pm 1\%$ small bias vs energy	Good $0.99 \pm 1\%$ small bias vs energy	Very good $1.00 \pm 1\%$	Very good $0.995 \pm 1\%$
Homogeneous LEU	Poor $\pm 2\%$ bias vs energy	Fair $1.00 \pm 1.5\%$	Fair $0.995 \pm 1.5\%$	Fair $1.01 \pm 1.5\%$	Fair $1.005 \pm 1.5\%$
<sup>239</sup> Pu	Very poor up to 5% high bias vs energy	Poor up to 5% high bias vs energy	Poor up to 5% high bias vs energy	Fair $1.01 \pm 1.5\%$	Fair $1.005 \pm 1.5\%$
MOX lattices	Very poor 3% high to 1% low	Fair $1.00 \pm 1.5\%$ bias vs energy	Fair 1% high to 2% low bias vs energy	Excellent $1.003 \pm 0.6\%$	Very good $1.00 \pm 1\%$ small bias vs energy
<sup>233</sup> U	Poor thermal - $0.99 \pm 2\%$ fast - $1.0 \pm 1\%$	Poor thermal - $1.02 \pm 1.5\%$ fast - $0.97 \pm 1\%$	Poor thermal - $1.015 \pm 1.5\%$ fast - $0.97 \pm 1\%$	Good thermal - $1.00 \pm 1.5\%$ fast - $0.997 \pm 0.5\%$	Good thermal - $0.995 \pm 1.5\%$ fast - $0.999 \pm 0.4\%$

Use of hafnium and gadolinium data not recommended for ENDF/B-IV libraries (27-group and 238-group).

<sup>a</sup> This table is taken from Table 8.1 of Ref. A.13.



### 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.14–A.16</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  $k_{eff}$ . 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  $k_{eff}$  by 2 to 3%.

### A.3.2. SCALE 218-GROUP ENDF/B-IV LIBRARY

1. How the library was generated or collapsed:

This library was generated from ENDF/B-IV data using  $\chi(E)-1/(E\sigma_t)$ -Maxwellian weighting. The base weighting allowed the library to be successfully collapsed using the weighting spectrum to a broad-group structure that could reproduce the behavior of the fine-group library. The unresolved resonance region was processed with an extremely high-background cross section of 50,000 barns, resulting in infinite-dilution cross sections in this region. Only the  $s$ -wave resonances were carried on the library, and any  $p$ -wave and  $d$ -wave resonances were integrated into the background cross section. The processing of the unresolved resonances with the extremely high-background cross section and the integration of the higher angular momentum  $p$ - and  $d$ -wave resolved resonances into the background cross section resulted in too much absorption in the intermediate-energy range.

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

The  $^{238}\text{U}$  base data had too much capture in the epithermal range, leading to the underprediction of  $k_{eff}$  for low-enriched systems, particularly for harder thermal systems. The graphite thermal kernel is deficient, with unknown results. There may be a problem with the thermal plutonium cross sections.

3. Application areas where the library performs well:

This library performs well for most realistic criticality safety problems. Fast, small metal units, highly-enriched thermal systems, and very thermal low-enriched systems are generally well predicted.

4. Application areas where the library performs poorly:

Low-enriched systems with a hard thermal spectrum underpredict by approximately 1% and sometimes more. Plutonium thermal systems overpredict  $k_{eff}$  by 1.5 to 3%. The 218-group library overpredicts thermal  $^{233}\text{U}$  systems by about 2%, while it underpredicts fast  $^{233}\text{U}$  systems by 2 to 4%. Intermediate-energy systems can be wrong by large amounts.

### **A.3.3. SCALE 27-GROUP ENDF/B-IV LIBRARY**

1. How the library was generated or collapsed:

The 27-group library was collapsed from the 218-group library, using the weighting spectra with which the nuclides were originally generated. Because of the  $1/(E\sigma_i)$  weighting in the resonance range, the broad-group library calculates many systems nearly as well as the fine-group library does. Trends and biases in the fine-group library were preserved in the broad-group library.

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

Same as the 218-group library.

3. Application areas where the library performs well:

Generally the same as the 218-group library. Some trends and biases may be slightly more pronounced in the broad-group library, but most results are fairly equivalent.

4. Application areas where the library performs poorly:

Same as the 218-group library.

### A.3.4. 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 mixed-oxide 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.3.5. 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 mixed-oxide lattices are the library's strong point, 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.

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## **APPENDIX B**

### **WARNING MESSAGES AND ERROR MESSAGES**





## **APPENDIX B**

### **WARNING MESSAGES AND ERROR MESSAGES**

KENO V.a prints warning and error messages that are identified by K5- followed by a unique number (i.e., K5-1 is the identifier of the first message). For additional information concerning the message, simply look up the identifier number in this section.

Warning messages appear when a possible error is encountered. If the code alters data, that fact is stated in the message. It is the responsibility of the user to verify correct usage whenever a warning message is printed.

When an error is encountered, the error flag MFLAG is set true and an error message is printed. The code stops if the error is too severe to continue. The warning and error messages in this section may show an underscore or a numbered underscore (1) where data will be printed by the code. The explanation of the message will show an underscore or a numbered underscore to indicate the corresponding data.

A complete list of messages is found in the SCALE/KENO V.a manual [Sect. F11.7]. Most of the messages indicate format problems that should not occur if you are using CSPAN. Those messages that might show up even with the use of CSPAN are given here with an indication of how you might fix the problem.

#### **B.1. MESSAGES**

##### **K5-15 MIXING TABLE TOO BIG**

This message is from subroutine MIXIT. It indicates that additional core space is necessary to allow entry of the existing mixing table. A STOP 114 is executed in conjunction with this message and a traceback may be printed from subroutine STOP.

##### **K5-17 UNRECOGNIZABLE GEOMETRY WORD**

This message is from subroutine KENOG. In the process of reading the geometry data, the word was encountered when a geometry word was expected. Several of these messages may be generated. A message is generated for each word of data that is read, until a valid geometry word is found. The data are out of phase or the geometry word is misspelled. Check the previous geometry card for a mixture ID, a bias ID, and the proper number of dimensions. [See Sect. F11.4.4 for a list of accepted geometry words.]

K5-19 AN ERROR WAS FOUND IN THE HEMISPHERE DESIGNATION

This message from subroutine KENOG indicates that the direction in which the hemisphere exists was incorrectly specified. [See Sect. F11.4.4 to determine the correct specification.]

K5-33 UNIT \_\_\_\_\_ IS INVALID AT X INDEX=\_\_\_\_\_ Y INDEX=\_\_\_\_\_ Z  
INDEX=\_\_\_\_\_

This message comes from subroutine SORTA. It is printed for each position in the unit orientation array that is in error. The message is printed a maximum of 10 times. [Refer to Sect. F11.4.5 for assistance in correcting the error(s).]

K5-35 \*\*\*\*\* ERROR \*\*\*\*\* IN THE ALBEDO INPUT DATA IS AN INVALID  
FACE CODE NAME.

This message is from subroutine RDREF. It occurs if an invalid face code name was entered in the albedo data. [See Table F11.4.3 in Sect. F11.4.6 for a list of acceptable face code names.]

K5-36 A PERIODIC BOUNDARY CONDITION WAS SPECIFIED WITH A NON-  
COMPATIBLE BOUNDARY CONDITION ON THE OPPOSING FACE. THE PROBLEM  
WILL NOT BE RUN.

This self-explanatory message is from subroutine RDREF. If a periodic boundary condition is specified on one X face, it must also be specified on the other X face, etc.

K5-53 NOT ENOUGH STORAGE TO MIX

This message from subroutine MIXER indicates that more storage is necessary in order to do the cross-section mixing operations. A STOP 112 is executed in conjunction with this message, and a traceback may be printed from subroutine STOP.

K5-55 \*\*\*\*\* ERROR FOUND IN MIXING CROSS SECTIONS \*\*\*\*\*  
THE FOLLOWING NUCLIDE(S) SPECIFIED IN THE MIXING TABLE WERE  
NOT FOUND ON THE CROSS SECTION LIBRARY.

ENTRY NUCLIDE ID

. .  
. .  
. .

This self-explanatory message is from subroutine MIXMIX. Either a nuclide ID was misspelled or was not in the cross-section library.

K5-79 THIS PROBLEM IS TOO LARGE FOR THE AMOUNT OF CORE THAT WAS ALLOCATED.

This message is from subroutine NSUPG. It occurs during the process of determining the number of supergroups, if the amount of storage is found to be insufficient to contain the energy-dependent information associated with one of the energy groups. Change the job control language to allow more storage. A STOP 116 is executed in conjunction with this message and a traceback may be printed from subroutine STOP.

K5-80 \_\_\_\_\_ WORDS OF STORAGE WERE ALLOCATED, BUT AT LEAST \_\_\_\_\_ ADDITIONAL WORDS ARE NEEDED TO HOLD THE INPUT DATA. EVEN MORE SPACE WILL BE NECESSARY TO RUN THE PROBLEM.

This message from subroutine NSUPG is printed if the available storage is too small to hold the input data. Change the job control language to allow more storage.

K5-83 \*\*\*\*\* FOR ARRAY \_\_\_\_\_ THE \_\_\_\_\_ DIMENSIONS OF UNIT \_\_\_\_\_ AT ( \_\_\_\_\_ , \_\_\_\_\_ , \_\_\_\_\_ ) DO NOT MATCH THOSE OF UNIT \_\_\_\_\_ AT ( \_\_\_\_\_ , \_\_\_\_\_ , \_\_\_\_\_ ) \*\*\*\*\*  
FOR UNIT \_\_\_\_\_ + \_\_\_\_\_ = \_\_\_\_\_ AND - \_\_\_\_\_ = \_\_\_\_\_ WHILE FOR UNIT \_\_\_\_\_ + \_\_\_\_\_ = \_\_\_\_\_ AND - \_\_\_\_\_ = \_\_\_\_\_ .

This message is from subroutine ARASIZ. The common faces of adjacent units or box types must be the same size and shape. This message occurs whenever this requirement is not met. One or more of the dimensions of the units or box types specified in the message may be incorrect, or the array definition data may be incorrect. [Carefully check the input data relating to the geometry region data and the array definition data as described in Sects. F11.4.4 and F11.4.5.]

K5-85 UNIT \_\_\_\_\_ IS INVALID AT POSITION X=\_\_\_\_\_ Y=\_\_\_\_\_ Z= \_\_\_\_\_ IN UNIT ORIENTATION ARRAY NUMBER \_\_\_\_\_ .

This message from subroutine ARASIZ occurs if the unit number named in the message is less than or equal to zero or greater than NBOX (the number of different box types). The position of the offending unit is also given. This error usually results from leaving some positions undefined in the unit orientation array or from erroneous data in the unit orientation data. (This includes extra data, misspunched data and omitted data.) [See Sect. F11.4.5 for additional information.]

K5-91       \*\*\*\*\*       UNIT       CONTAINS       THE       FOLLOWING       GEOMETRY  
INCONSISTENCIES.       \*\*\*\*\*

This message from subroutines JOMCHK, HOLEXT or HOLHOL indicates that one or more intersecting geometry regions were encountered in unit or box type. K5-92 is the companion message from subroutine JOMCHK and specifies the regions that intersect. K5-166 is the companion message from subroutine HOLEXT. K5-169 and K5-179 are the companion messages from subroutine HOLHOL. Correct the geometry region data and resubmit the problem. [Section F11.4.4 may provide assistance in correctly specifying the data.]

K5-92 REGION NUMBER \_\_\_\_\_ INTERSECTS REGION NUMBER \_\_\_\_\_

This message from subroutine JOMCHK is a companion message to K5-91 and K5-94. It specifies the intersecting regions. The user must determine which region is incorrectly specified or if the data are out of order. KENO V.a REQUIRES THAT EACH SUCCESSIVE GEOMETRY REGION MUST COMPLETELY ENCLOSE THE PREVIOUS REGION. THIS DOES ALLOW COMMON FACES AND TANGENCY.

K5-94       \*\*\*\*\* THE REFLECTOR DIMENSIONS ARE INCONSISTENT       \*\*\*\*\*

This message is from subroutine JOMCHK. It is a companion to message K5-95 and is printed whenever one or more intersecting geometry regions are encountered in the external reflector.

K5-95 REGION NUMBER IN UNIT NUMBER CONTAINS AN ERROR IN THE  
DIMENSIONS.

This message from subroutine VOLUME indicates an error in the geometry input data such that the negative dimension specification for a cube or cuboid is larger than the positive dimension specification (i.e., the  $-X$  dimension is greater than the  $+X$  dimension, or the  $-Y$  dimension is greater than the  $+Y$  dimension or the  $-Z$  dimension is greater than the  $+Z$  dimension). This message is also printed if the magnitude of the chord for a hemicylinder or hemisphere is larger than the radius. [See Sect. F11.4.4 for assistance in specifying the geometry correctly.]

K5-96 THE VOLUME DEFINED BY GEOMETRY CARD IS NEGATIVE.

This message from subroutine VOLUME is printed whenever a negative volume is calculated. This can be caused by the positive dimension being smaller than the negative dimension on a face of a geometry region. It can also be caused by having intersecting regions, or be the result of roundoff when the volumes are calculated. Either the geometry regions are incorrectly specified, or the data are out of order, or the dimensions are so tight fitting that

roundoff causes the net volume of the region to be negative. If the error is caused by roundoff, adjust the appropriate dimensions slightly. [See Sect. F11.4.4.]

K5-97 ERROR ERROR. THE VOLUME FOR UNIT IS NEGATIVE.

This message is from subroutine VOLUME. A negative volume for a unit or box type can be caused by having intersecting regions within the unit, or by having a unit or box type consisting of one region and having a positive dimension smaller than the negative dimension on one or more faces. Message K5-95 or K5-96 may accompany this message. [See Sect. F11.4.4 for assistance in specifying the geometry data correctly.]

K5-99 \*\*\* ERROR IN UNIT \*\*\* THE LAST GEOMETRY REGION OF A UNIT UTILIZED IN THE UNIT ORIENTATION DESCRIPTION OF THE ARRAY DATA MUST BE A CUBE OR CUBOID.

This message is from subroutine ARASIZ. It can occur when a single unit problem whose outer region is not a cube or cuboid is specified as a  $1 \times 1 \times 1$  array. To eliminate this message, add a cuboidal outer region containing void, or remove the array data. If the problem is an array problem, be sure each unit used in the unit orientation description ends with a cube or cuboid. [See Sects. F11.4.4 and F11.4.5.]

K5-100 THIS PROBLEM WILL NOT BE RUN BECAUSE ERRORS WERE ENCOUNTERED IN THE INPUT DATA.

This message is from subroutine MASTER and indicates that other error messages were printed in the problem output. Find these messages and correct the data accordingly. A STOP 129 is executed when this message is printed.

K5-101 \*\*\* ERROR \*\*\* NO FISSILE MATERIAL WAS FOUND IN SUBROUTINE START.

This message is from subroutine START. It indicates that none of the mixtures utilized in this problem have a fission spectrum associated with them. Either the geometry data did not specify a fissionable mixture number, the mixing table is incorrect, the wrong mixed cross-section data set was mounted, or the mixed cross-section data set was incorrectly or incompletely made. A STOP 128 is executed in conjunction with this message, and a traceback may be printed from subroutine STOP.

K5-105 \*\*\*\*\* WARNING, ONLY \_\_\_\_\_ INDEPENDENT STARTING POSITIONS WERE GENERATED. \*\*\*\*\*

This message is from subroutine START. KENO V.a must have npb [NPG= in Sect. F11.4.3] starting positions. This message is to inform the user that fewer than npb starting positions were generated. The remaining starting positions are randomly selected from those that were generated, thus giving duplicate starting positions. If the number of independent starting positions is nearly npb, the starting distribution is probably acceptable. If it is much smaller than npb, a different start type should be used to give a better starting distribution [see Sect. F11.4.8]. The amount of time allowed to generate the starting positions is controlled by parameter TBA= [see Sect. F11.4.3]. If the start data are appropriate, it may be necessary to increase the value of TBA to ensure generating npb starting positions.

K5-132 WARNING....ONLY \_\_\_\_\_ INDEPENDENT FISSION POINTS WERE GENERATED

This message from subroutine NSTART indicates that fewer than npb [NPG= in Sect. F11.4.3] fission points were generated during the previous generation. Because npb fission points are required by the code, the remaining fission points are randomly selected from those that were generated, thus utilizing duplicate fission points. If the  $k_{eff}$  of the system is significantly less than 1.0, several of these messages should be expected in the first few generations. The code attempts to set RAKBAR so the message can be expected to occur about once every 100 generations. The message may occur more frequently in a correctly modeled problem. However, if the number of fission points is considerably less than npb for most of the generations, the answer can be affected.

K5-150 \*\*\* ERROR \*\*\*\*\* ERROR \*\*\* TOO FEW ENTRIES WERE SUPPLIED IN THE REFLECTOR GEOMETRY DESCRIPTION.

This message from subroutine KENOG indicates that too few data entries were supplied for the geometry word REFLECTOR. The mixture ID, bias ID, one of the thickness/region specifications or the number of regions to be generated was omitted or incorrectly specified. Each REFLECTOR entry requires (1) a mixture ID, (2) a bias ID, (3) N entries for the thickness/region specifications, and (4) the number of regions to be generated. [The thickness/region can be obtained from the Increment Thickness column of Table F11.4.5 for the material to be used in the regions generated by the REFLECTOR specification.] N is the number of thickness/region specifications required by the geometry shape: N=1 for spheres or hemispheres, N=3 for cylinders and hemicylinders, and N=6 for cubes, cuboids, and cores. A flag is set to terminate the problem when the input data reading is completed.

K5-157 \*\*\* ERROR \*\*\* THE FIRST HOLE IN A UNIT MUST FOLLOW A VALID GEOMETRY REGION.

A STOP 141 accompanies this message from subroutine READGM. If HOLES are to be utilized in the geometry region data [Sect. F11.4.4], they must follow the region in which they are to be placed. This message indicates that HOLE was the first geometry description in a unit or was placed inside a CORE or ARRAY description. Correct the geometry region data and resubmit the problem.

K5-160 THE HOLES ARE RECURSIVELY NESTED.

This message from subroutine HOLE indicates that the geometry region data description [Sect. F11.4.4] specifies HOLES that are recursively nested. This can happen if a unit contains a HOLE whose definition traces back to the same unit or are defined in terms of each other. A simple example of recursive nesting is

```
UNIT 1 CUBE 0 1 2PI0.0 HOLE 2 3*0.0
```

```
UNIT 2 CUBE 0 1 2PI0.0 HOLE 1 3*0.0
```

Thus unit 1 contains unit 2 and unit 2 contains unit 1. Check the geometry region data for recursive nesting. In the absence of recursive nesting, a code error is the probable cause of this message. A STOP 143 is executed when this message occurs and a traceback is printed.

K5-166 HOLE NUMBER \_\_\_\_\_ INTERSECTS REGION NUMBER \_\_\_\_\_

This form of message K5-166 is from subroutine HOLEXT. It indicates that the specified HOLE intersects the region in which the HOLE was placed. A flag is set to terminate execution when the data reading is completed. Correct the geometry data [Sect. F11.4.4] and resubmit the problem.

K5-169 HOLE NUMBER \_\_\_\_\_ INTERSECTS REGION NUMBER \_\_\_\_\_

This message from subroutine HOLHOL occurs if a HOLE intersects the first region interior to the region in which the HOLE is emplaced. This may be a real intersection or it may be due to roundoff in processing the HOLES. If it is due to roundoff, adjust *xhole*, *yhole* and/or *zhole* and/or the dimensions as appropriate. This message indicates that the problem will be terminated when the data reading is completed.

K5-179 HOLE NUMBER \_\_\_\_\_ INTERSECTS HOLE NUMBER \_\_\_\_\_ IN REGION  
NUMBER \_\_\_\_\_

This message from subroutine HOLHOL indicates that the specified HOLES intersect. Check the dimensions and origins of the units being placed in the region.

K5-197 \*\*\* ERROR IN UNIT \*\*\* A VALID GEOMETRY REGION MUST  
PRECEDE A REPLICATE REGION.

This message from subroutine KENOG indicates that a replicate specification follows an invalid geometry specification (for example, REPLICATE immediately follows a UNIT specification).

K5-205 \*\*\*\*\* ERROR \*\*\*\*\* A GLOBAL UNIT MUST BE SPECIFIED FOR A  
SINGLE UNIT PROBLEM

This message from subroutine FLDATA is printed if a global unit is not specified for a single unit problem. A STOP 164 is executed when the message is printed. If the input data do not specify the global unit, it is defaulted to unit 1. If several units are described in a problem that does not use array data, the user must specify which unit to use to run the calculation. This is done by entering the word GLOBAL before the UNIT, BOX TYPE, or BOXTYPE of that unit.

K5-223 \*\*\* THE PLUS CUBE FACE IS NOT GREATER THAN THE MINUS CUBE  
FACE PLUS FACE = \_\_\_\_\_ MINUS FACE = \_\_\_\_\_

This message from subroutine KENOG is printed if the data for a CUBE has the positive face not greater than the negative face. This will lead to negative thicknesses in each dimension for a CUBE. Correct the data making sure that the positive face is greater than the negative face.

K5-224 \*\*\* THE PLUS FACES OF A CUBOID ARE NOT GREATER THAN THE  
MINUS FACES +X= \_\_\_\_\_ -X = \_\_\_\_\_ +Y = \_\_\_\_\_ -Y = \_\_\_\_\_ +Z =  
\_\_\_\_\_ -Z

This message from subroutine KENOG is printed if the data for one or more pairs of faces for a cuboid are out of order (i.e., the positive face is not greater than the negative face). Correct the data making sure the positive face is greater than the negative face.



K5-225 \*\*\* THE CYLINDER RADIUS IS NOT GREATER THAN ZERO, OR THE  
+ HEIGHT IS NOT GREATER THAN THE % HEIGHT RADIUS = \_\_\_\_\_ +H =  
\_\_\_\_\_ -H = \_\_\_\_\_

This message from subroutine KENOG is printed if the data for a cylinder has a radius that is not greater than zero, or the top of the cylinder is not specified as greater than the bottom of the cylinder. Correct the data making sure the radius is positive, and the top is greater than the bottom.

K5-226 \*\*\* THE SPHERE RADIUS IS NOT GREATER THAN ZERO % RADIUS =  
\_\_\_\_\_

This message from subroutine KENOG is printed if a sphere is specified with a radius that is not greater than zero. Correct making sure the radius is greater than zero.

K5-227 \*\*\* A REPLICATE THICKNESS IS LESS THAN ZERO  
SURFACE NUMBER = \_\_\_\_\_ THICKNESS = \_\_\_\_\_

This message from subroutine KENOG is printed if a REPLICATE is specified with a negative thickness. Correct making sure that none of the thicknesses are less than zero.

## B.2. STOP CODES

The STOP codes that are encountered in KENO V.a are listed in tabular form below, indicating the subroutine where they occur and the associated error message. A STOP is executed whenever a fatal error is recognized. Look up the associated message number to determine the appropriate corrective measures. A traceback may be generated whenever subroutine STOP is called to print a message. If no traceback is indicated in the STOP CODE table, a STOP is executed as soon as the associated message is printed.

STOP NUMBER	SUBROUTINE	TRACEBACK	ASSOCIATED MESSAGE
20			See Sect. B.3
100	ARAYIN	Yes	K5-25
101	ARAYIN	No	K5-31
102	CRMAX	Yes	K5-135
103	CROS	No	K5-126
104	CROS	No	K5-127
105	WRTALB	No	K5-71
106	ICEMIX	No	K5-68

STOP NUMBER	SUBROUTINE	TRACEBACK	ASSOCIATED MESSAGE
107	INDX	No	K5-124
108	INITAL	No	K5-2
109	INITAL	No	K5-2
110	MAKANG	Yes	K5-57
111	MIXCRS	Yes	K5-52
112	MIXER	Yes	K5-53
113	MIXER	Yes	K5-54
114	MIXIT	Yes	K5-15
115	NORM1D	No	K5-56
116	NSUPG	Yes	K5-79
117	NSUPG	No	K5-81
118	PARAM	No	K5-7 or K5-8
119	PRTLBA	No	K5-89
120	RDALB	No	K5-49
121	RDCALC	No	K5-116 or K5-146 or K5-147 or K5-177 or K5-178
122	RDICE	No	K5-50
123	RDRST	No	K5-48
124	RDTAPE	No	K5-69
125	READGM	No	K5-20
126	SAVST6	Yes	K5-140
127	SRMAX	Yes	K5-136
128	START	Yes	K5-101
129	MASTER	No	K5-100
130	MASTER	No	K5-117 or K5-128
131	VOLFIS	No	K5-110
132	WRTICE	No	K5-72
133	WRTRST	No	K5-70
134	TRACK	No	K5-62
135	DATAIN	Yes	K5-142
136	DATAIN	Yes	K5-143
137	ARAYIN	No	K5-151
138	SORTA	Yes	K5-153
139	SORTA	No	K5-154
140	LODARA	No	K5-155
141	READGM	No	K5-157
142	SORTA	No	K5-159
143	HOLE	No	K5-160
144	FLDATA	No	K5-161
145	CRMIN	Yes	K5-167

STOP NUMBER	SUBROUTINE	TRACEBACK	ASSOCIATED MESSAGE
146	SRMIN	Yes	K5-168
147	MASTER	Yes	K5-182
148	WAITIN	No	K5-185
149	WAITIN	No	K5-186
150	WATES	Yes	K5-22
151	RDBIAS	No	K5-184
152	DATAIN	No	K5-46
153	RCHRS	Yes	K5-195
154	RDCALC	No	K5-196
155	GEOMIN	Yes	K5-25
156	SORTA	Yes	K5-25
157	START	No	K5-202
158	START	No	K5-206
159	START	No	K5-207
160	START	No	K5-210
161	WAITIN	No	K5-211
162	KENO V.a	Yes	K5-213
163	RDCALC	No	K5-215

### B.3. “LMP” ERROR MESSAGES

The error messages that are associated with a STOP 20 in KENO V.a are listed below in numerical order. Look up the appropriate message number to determine corrective measures.

LMP001 DA ERROR – INVALID UNIT NUMBER. THE LOGICAL UNIT NUMBER IS \_\_\_\_.

This message from the subroutine library direct-access routines indicates that an invalid unit number was specified as a direct-access device. In KENO V.a, this message is indicative of a code error.

LMP002 DA ERROR – FORTRAN USING THIS UNIT. THE LOGICAL UNIT NUMBER IS \_\_\_\_.

This message from the subroutine library direct-access routines indicates that the specified unit number is open as a sequential dataset rather than a direct-access dataset. In KENO V.a, this error may be caused by entering a direct-access unit number for LIB= or XSC=.

LMP003 DA ERROR – DCB NOT OPEN. THE LOGICAL UNIT NUMBER IS \_\_\_\_.

This message from the subroutine library direct-access routines indicates that the program attempted to read or write on a direct-access device but the data control block was not open. In KENO V.a this message is indicative of a code error.

LMP004 DA ERROR – UNABLE TO OPEN DCB. THE LOGICAL UNIT NUMBER IS \_\_\_\_.

This message from the subroutine library direct-access routines indicates that the program is unable to open the data control block for the direct-access device. This message indicates that the job control language did not include proper specification of the above named unit.

LMP005 DA ERROR – RELATIVE BLOCK NOT IN DATA SET. RELATIVE BLOCK NUMBER IS \_\_\_\_.

This message from the subroutine library direct-access routines indicates that the number of direct-access blocks is too small for the problem. Increase the number of direct-access blocks in the KENO V.a parameter data by entering the parameter NB8=nnn where nnn is larger. For example, if the relative block number is 201, try increasing the number of direct-access blocks to 300 or more.

LMP006 DA ERROR – INVALID BLOCK LENGTH. THE BLOCK LENGTH IS \_\_\_\_.

This message from the subroutine library direct-access routines indicates that the length of the direct-access blocks is invalid. A valid block length must be positive. This message is indicative of a code error.

LMP007 DA ERROR – DCB ALREADY OPEN. THE LOGICAL UNIT NUMBER IS \_\_\_\_.

This message from the subroutine library direct-access routines indicates that the data control block for the above named unit was previously opened and not closed.

LMP008 DA ERROR – PERMANENT I/O ERROR.

This message from the subroutine library direct-access routines indicates that a permanent input/output error has occurred.

**APPENDIX C**

**INPUT FILES FOR EXAMPLE PROBLEMS**



## APPENDIX C

### INPUT FILES FOR EXAMPLE PROBLEMS

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

##### 2.3.1. Jezebel

```
=csas25      parm=size=1500000
JEZEBEL PROBLEM, bare plutonium sphere with nickel shell
44groupndf5 multiregion
pu-239      1 0    3.7047E-2      293.0      end
pu-240      1 0    1.751E-3      293.0      end
pu-241      1 0    1.17E-4      293.0      end
gallium     1 0    1.375E-3      293.0      end
nickel      2 0    9.1322E-2      293.0      end
  end comp
Spherical  end
1 6.38493
2 6.39763
  end zone
JEZEBEL PROBLEM, bare plutonium sphere with nickel shell as multiregion
read geom
'
global unit 1
com='jezebel core with nickel plating'
sphere     1    1 6.38493
sphere     2    1 6.39763
  end geom
end data
end
```

## SECTION 3 – MATERIAL INFORMATION INPUT

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

```
=csas25      parm=size=1000000
EXAMPLE PROBLEM 1
44groupndf5 infhommedium
u-235        1  den=18.742  1      293.      end
      end comp

read geom
'
unit 1
com='bare cylinder'
cylinder  1 1 7.82 7.82 -7.82
      end geom
end data
end
```

### 3.5.2. Bare U(93.7) Metal Cylinder

```
=csas25      parm=size=1000000
Ch. 3 EXAMPLE PROBLEM 2
44groupndf5 infhommedium
u            1  den=18.7  1      293.  92235 93.71  92238 6.29
      end
      end comp

read geom
'
unit 1
com='bare cylinder'
cylinder  1 1 7.82 7.82 -7.82
      end geom
end data
end
```



### 3.5.3. Bare U(93.7)O<sub>2</sub> Metal Cylinder

```
=csas25      parm=size=1000000
Ch. 3 EXAMPLE PROBLEM 3
44groupndf5 infhommedium
uo2          1  0.95      293.  92235 93.71  92238 6.29      end
      end comp

read geom
'
unit 1
com='bare cylinder'
cylinder 1 1 12.8 12.8 -12.8
      end geom
end data
end
```

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

```
=csas25      parm=size=1000000
Ch. 3 EXAMPLE PROBLEM 4
44groupndf5 infhommedium
u            1  0    1.8439E-3    293.  92235 30.3  92238 69.7      end
fluorine     1  0    3.6844E-3    293.      end
h            1  0    5.97522E-2    293.      end
o            1  0    3.35605E-2    293.      end
      end comp

read geom
'
global unit 1
com='uo2f2 (30.3) cylinder'
cylinder 1 1 15.225 15.225 -15.225
      end geom
end data
end
```

## SECTION 4 – GEOMETRY INPUT

### 4.2.2. Z-Cylinder

```
=csas25      parm=size=1000000
SINGLE MATERIAL, Z-AXIS Cylinder
44groupndf5 infhommedium
u-235          1  den=18.742 1      293.0      end
  end comp
Z-Axis Cylinder Example with U235 metal
read geom
'
global unit 1
com='single z axis cylinder'
cylinder  1 1 7.82 7.82 -7.82
  end geom
end data
end
```

### 4.2.3. Z-Cylinder Offset 2 cm from Origin

```
=csas25      parm=size=1000000
SINGLE MATERIAL, Z-AXIS Cylinder
44groupndf5 infhommedium
u-235          1  den=18.742 1      293.0      end
  end comp
Z-Axis Cylinder Example with U235 metal
read geom
'
global unit 1
com='single z axis cylinder with origin 2cm above bottom'
zcylinder  1 1 7.82 13.64 -2
  end geom
end data
end
```

## 4.2.4. X-Cylinder

```
=csas25      parm=size=1000000
SINGLE MATERIAL, Z-AXIS Cylinder
44groupndf5 infhommedium
u-235          1  den=18.742 1      293.0      end
    end comp
Z-Axis Cylinder Example with U235 metal
read geom
'
global unit 1
com='single x axis cylinder with origin at bottom'
xcylinder 1 1 7.82 15.64 0
    end geom
end data
end
```

### 4.5.1. Reflected Pu Metal Cylinder

```
=csas25      parm=size=1000000
REFLECTED PU(5) CYLINDER H/D=7.1/5.7
238groupndf5 infhommedium
c              2  den=1.6 1      293.0      end
pu              1  den=15.44 1      293.0      94239 95
                                           94240 5      end

      end comp
reflected pu(5) cylinder h/d=7.1/5.7
read geom
'
global unit 1
com='reflected cylinder'
cylinder 1 1 2.86 40.96 0
cylinder 2 1 20.64 58.74 -17.78
      end geom
end data
end
```

### 4.5.2. <sup>235</sup>U Sphere with Graphite and Water Reflectors

```
=csas25
NESTED SHAPE EXAMPLE
44groupndf5 infhommedium
u-235          1  den=18.74 1      293.0      end
c              2  den=1.65 1      293.0      end
h2o            3      end

      end comp
nested shape example
read geom
'
global unit 1
com='nested shapes, sphere inside cylinder inside cube'
sphere 1 1 7
cylinder 2 1 10 10 -10
cube 3 1 12 -10
      end geom
end data
end
```

### 4.6.1. 2×2×2 Array of U(93.2) Metal Cylinders

```
=csas25
2c8 array
44groupndf5 infhommedium
u          1 den=18.76 1          293.0          92234 1    92235 93.2
          92238 5.6
          92236 0.2
          end
      end comp
2c8 array, u metal cylinders
read geom
'
unit 1
com='unit cell'
cylinder  1 1 5.748 10.765 0
cuboid    0 1 6.87 -6.87 6.87 -6.87 11.8875 -1.1225
  end geom

read array
ara=1 gbl=1 nux=2 nuy=2 nuz=2
com='2x2x2 array of U(93.2) metal cylinders'
fill 8r1
  end fill
  end array
end data
end
```

## 4.6.2. Stack of Six Disks and Flat Plate

```
=csas25
Array of disks and plates
44groupndf5 infhommedium
u          1 den=18.74 1          293.0          92234 1  92235 93.2
          92238 5.6
          92236 0.2
          end
c          2 den=1.65 1          293.0          end
al         3      end
      end comp
Array of disks and plates
read geom
'
unit 1
com='Disk 1'
cylinder  2 1 10 1.25 -1.25
cuboid    0 1 15 -15 15 -15 1.25 -1.25
'
unit 2
com='Disk 2'
cylinder  1 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 geom

read array
ara=1 gbl=1 nux=1 nuy=1 nuz=7
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

```
=csas25
flat bottom sphere
44groupndf5 infhommedium
solnpu(no3)4    1 39 0.4 spg=1.103 1 293. 94239 95.4 94240 4.6
  end
ss316           2    end
  end comp
flat bottom sphere
read geom
'
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 geom
end data
end
```

### 5.3.1. Simple HOLE

```
=csas25    parm=size=1000000
Ch 5 Holes Example
44groupndf5 infhommedium
u-235      1  den=18.7    1      293.    end
ss316      2    end
c          3    end
  end comp

read geom
'
unit 1
com='u-235 cylinder'
cylinder   1 1 6.85 10 -10
'
global unit 2
com='steel cylinder'
cuboid     3 1 -2 -14 14 2 10 -10
cylinder   0 1 20 10 -10
hole       1 6 -6 0
cylinder   2 1 20.2 10.2 -10.2
  end geom
end data
end
```

### 5.4.1. Shipping Container with Five Cylinders

```
=csas25
HOLES AND ARRAYS
44groupndf5 infhommedium
uc          1 1      293.0      92235 93.2      92238 6.8
                                end
h2o         2      end
ss316       3      end
    end comp

read geom
'
unit 1
com='cruciform'
cuboid      1 1 5 -5 0.5 -0.5 10 -10
cylinder    2 1 6 10 -10
hole        2 0 2.75 0
hole        2 0 -2.75 0
cylinder    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
cylinder    0 1 20 10.1 -10.1
hole        1 0 12.4 0
hole        1 0 -12.4 0
cylinder    3 1 20.2 10.2 -10.2
    end geom

read array
ara=1 nux=3 nuy=1 nuz=1
com='array central'
fill 3r1
    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

```
=csas25
9X9 FUEL ASSEMBLY
44groupndf5 latticecell
uo2          3  0.925  300.  92235 3.44  92238 96.56  end
arbmipois1   3.7 2 0 1 0 13027 2.0  8016 3.0  1 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
squarepitch  1.64  0.94  3  2  1.09  4  0.975  0  end
9x9 fuel assembly
read param  gen=1003 end param
read geom
'
unit 1
com='3.44% enr. fuel rod'
cylinder  3 1 0.47 182.88 -182.88
cylinder  0 1 0.4875 199.84 -206.24
cylinder  4 1 0.545 199.84 -206.24
cylinder  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'
cylinder  1 1 0.545 160 -160
cylinder  0 1 0.545 260.48 -160
cylinder  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 3.81 3.81 3.81 3.81 15.24 15.24 1
  end geom

read array
ara=1 nux=9 nuy=9 nuz=1
com='3.44% enriched fuel assembly'
fill 13r1 2 6r1 2 3r1 2 12r1 2 2r1 3 2r1 2 12r1 2 3r1 2 6r1 2 13r1
  end fill
  end array
end data
end
```

## 7.5.2. Two Parallel Slab Tanks

```
=csas25
Two slab tanks
44groupndf5 multiregion
ss304          2    end
solnuo2f2      1 459 0 spg=1.566 1 293. 92235 93 92238 7  end
h2o            3    end
    end comp
Slab  end
3 5
2 5.5
1 10.5
2 11
3 16
    end zone

read geom
'
unit 1
com='2'
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 geom

read array
ara=1 gbl=1 nux=2 nuy=1 nuz=1
com='two parallel slab tanks'
fill 2r1
    end fill
    end array
end data
end
```



## **APPENDIX D**

### **KMART**



## APPENDIX D

### KMART

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.]

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 is identified 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. As an example, if it is desired to model the SHEBA solution reactor, a simple KENO V.a. file might look like:

```
#csas25      parm=(size=500000)
sheba II
44group      infhom
solnuo2f2 1 978 0.25 den=2.1092 1 293 92234 .027 92235 4.998
                                         92236 .049 92238 94.926 end

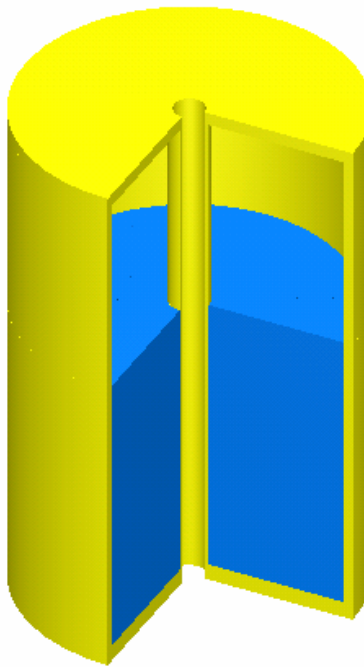
ss304s      2 den=7.8419 1 293 end
end comp
sheba
read parm   res=100 wrs=35 npg=2000 nb8=600 mku=yes fmu=yes
           mkp=yes fmp=yes flx=yes fdn=yes end parm
read geom
unit 1
com='section 0 - 5.0 of solution in the tank'
cylinder 0 1 2.54 44.8 0.0
cylinder 2 1 3.175 44.8 0.0
cylinder 1 1 24.4475 44.8 0.0
cylinder 2 1 25.4 44.8 0.0
cuboid 0 1 4p25.4 44.8 0.0
unit 10
com='bottom of tank'
cylinder 0 1 2.54 2.8575 0.0
cylinder 2 1 25.4 2.8575 0.0
cuboid 0 1 4p25.4 2.8575 0.0
unit 11
com='void section of tank'
cylinder 0 1 2.54 76.5175 44.8
cylinder 2 1 3.175 76.5175 44.8
cylinder 0 1 24.4475 76.5175 44.8
cylinder 2 1 25.4 76.5175 44.8
cuboid 0 1 4p25.4 76.5175 44.8
unit 12
com='top of tank'
cylinder 0 1 2.54 1.905 0.0
cylinder 2 1 25.4 1.905 0.0
cuboid 0 1 4p25.4 1.905 0.0
end geom
```

```

read array
  com='array putting the sheba tank together - stacked from bottom to top'
  gbl=1 ara=1 nux=1 nuy=1 nuz=4
  fill 10 1 11 12 end fill
end array
' suppress k5-60 & k5-64 messages, use p5 scattering
read mixt  eps=1.0 sct=3  end mixt
end data
end

```

This creates a model as shown in Fig. D.1.



**Fig. D.1. 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 associated KMART input is given below.

```

#csas25      parm=(size=500000)
sheba II
238group    infhom
solnuo2f2 1 978 0.25 den=2.1092 1 293 92234 .027 92235 4.998
                                         92236 .049 92238 94.926 end
ss304s     2 den=7.8419 1 293 end
end comp

```



```

sheba
read parm  res=100 wrs=35 npg=2000 nb8=600 mku=yes fmu=yes
      mkp=yes fmp=yes flx=yes fdn=yes  end parm
read geom
unit 1
com='section 0 - 5.0 of solution in the tank'
cylinder  0 1  2.54   5.0  0.0
cylinder  2 1  3.175  5.0  0.0
cylinder  1 1  6.5    5.0  0.0
cylinder  1 1  9.5    5.0  0.0
cylinder  1 1 12.5    5.0  0.0
cylinder  1 1 15.5    5.0  0.0
cylinder  1 1 18.5    5.0  0.0
cylinder  1 1 21.5    5.0  0.0
cylinder  1 1 24.4475 5.0  0.0
cylinder  2 1 25.4    5.0  0.0
cuboid    0 1 4p25.4  5.0  0.0
unit 2
com='section 5 - 10 of solution in the tank'
cylinder  0 1  2.54  10.0  5.0
cylinder  2 1  3.175 10.0  5.0
cylinder  1 1  6.5   10.0  5.0
cylinder  1 1  9.5   10.0  5.0
cylinder  1 1 12.5   10.0  5.0
cylinder  1 1 15.5   10.0  5.0
cylinder  1 1 18.5   10.0  5.0
cylinder  1 1 21.5   10.0  5.0
cylinder  1 1 24.4475 10.0  5.0
cylinder  2 1 25.4   10.0  5.0
cuboid    0 1 4p25.4 10.0  5.0
unit 3
com='section 10 - 15 of solution in the tank'
cylinder  0 1  2.54  15.0 10.0
cylinder  2 1  3.175 15.0 10.0
cylinder  1 1  6.5   15.0 10.0
cylinder  1 1  9.5   15.0 10.0
cylinder  1 1 12.5   15.0 10.0
cylinder  1 1 15.5   15.0 10.0
cylinder  1 1 18.5   15.0 10.0
cylinder  1 1 21.5   15.0 10.0
cylinder  1 1 24.4475 15.0 10.0
cylinder  2 1 25.4   15.0 10.0
cuboid    0 1 4p25.4 15.0 10.0
unit 4
com='section 15 - 20 of solution in the tank'
cylinder  0 1  2.54  20.0 15.0
cylinder  2 1  3.175 20.0 15.0
cylinder  1 1  6.5   20.0 15.0
cylinder  1 1  9.5   20.0 15.0
cylinder  1 1 12.5   20.0 15.0
cylinder  1 1 15.5   20.0 15.0
cylinder  1 1 18.5   20.0 15.0
cylinder  1 1 21.5   20.0 15.0
cylinder  1 1 24.4475 20.0 15.0
cylinder  2 1 25.4   20.0 15.0
cuboid    0 1 4p25.4 20.0 15.0
unit 5
com='section 20 - 25 of solution in the tank'
cylinder  0 1  2.54  25.0 20.0
cylinder  2 1  3.175 25.0 20.0
cylinder  1 1  6.5   25.0 20.0
cylinder  1 1  9.5   25.0 20.0
cylinder  1 1 12.5   25.0 20.0
cylinder  1 1 15.5   25.0 20.0

```

```

cylinder 1 1 18.5    25.0  20.0
cylinder 1 1 21.5    25.0  20.0
cylinder 1 1 24.4475 25.0  20.0
cylinder 2 1 25.4    25.0  20.0
cuboid   0 1 4p25.4  25.0  20.0
unit 6
com='section 25 - 30 of solution in the tank'
cylinder 0 1  2.54    30.0  25.0
cylinder 2 1  3.175   30.0  25.0
cylinder 1 1  6.5     30.0  25.0
cylinder 1 1  9.5     30.0  25.0
cylinder 1 1 12.5     30.0  25.0
cylinder 1 1 15.5     30.0  25.0
cylinder 1 1 18.5     30.0  25.0
cylinder 1 1 21.5     30.0  25.0
cylinder 1 1 24.4475  30.0  25.0
cylinder 2 1 25.4     30.0  25.0
cuboid   0 1 4p25.4   30.0  25.0
unit 7
com='section 30 - 35 of solution in the tank'
cylinder 0 1  2.54    35.0  30.0
cylinder 2 1  3.175   35.0  30.0
cylinder 1 1  6.5     35.0  30.0
cylinder 1 1  9.5     35.0  30.0
cylinder 1 1 12.5     35.0  30.0
cylinder 1 1 15.5     35.0  30.0
cylinder 1 1 18.5     35.0  30.0
cylinder 1 1 21.5     35.0  30.0
cylinder 1 1 24.4475  35.0  30.0
cylinder 2 1 25.4     35.0  30.0
cuboid   0 1 4p25.4   35.0  30.0
unit 8
com='section 35 - 40 of solution in the tank'
cylinder 0 1  2.54    40.0  35.0
cylinder 2 1  3.175   40.0  35.0
cylinder 1 1  6.5     40.0  35.0
cylinder 1 1  9.5     40.0  35.0
cylinder 1 1 12.5     40.0  35.0
cylinder 1 1 15.5     40.0  35.0
cylinder 1 1 18.5     40.0  35.0
cylinder 1 1 21.5     40.0  35.0
cylinder 1 1 24.4475  40.0  35.0
cylinder 2 1 25.4     40.0  35.0
cuboid   0 1 4p25.4   40.0  35.0
unit 9
com='section 40 - 44.8 of solution in the tank'
cylinder 0 1  2.54    44.8  40.0
cylinder 2 1  3.175   44.8  40.0
cylinder 1 1  6.5     44.8  40.0
cylinder 1 1  9.5     44.8  40.0
cylinder 1 1 12.5     44.8  40.0
cylinder 1 1 15.5     44.8  40.0
cylinder 1 1 18.5     44.8  40.0
cylinder 1 1 21.5     44.8  40.0
cylinder 1 1 24.4475  44.8  40.0
cylinder 2 1 25.4     44.8  40.0
cuboid   0 1 4p25.4   44.8  40.0
unit 10
com='bottom of tank'
cylinder 0 1 2.54     2.8575 0.0
cylinder 2 1 25.4     2.8575 0.0
cuboid   0 1 4p25.4   2.8575 0.0
unit 11
com='void section of tank'

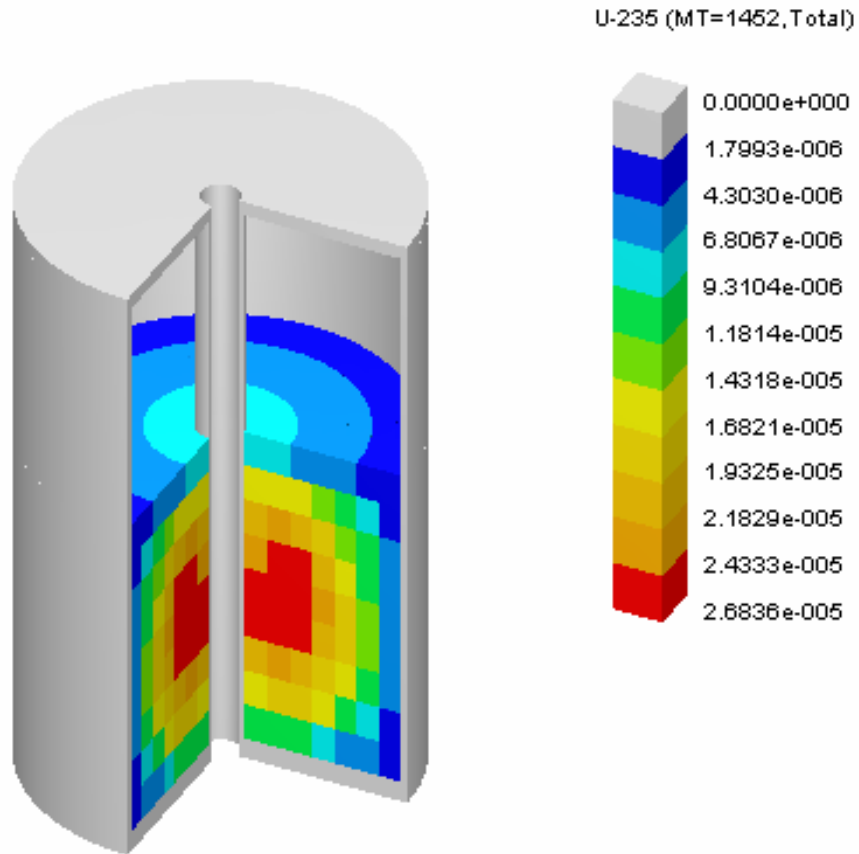
```

```

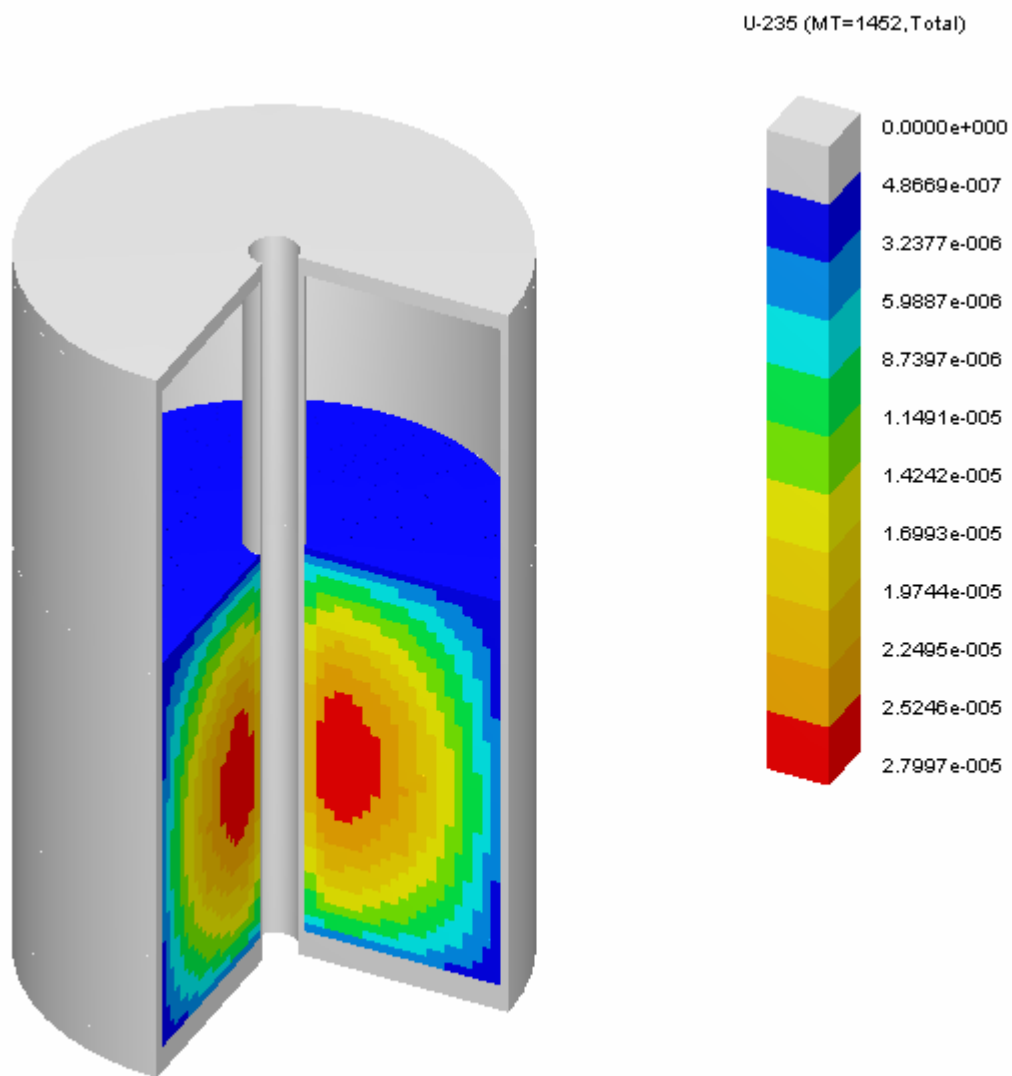
cylinder 0 1 2.54 76.5175 44.8
cylinder 2 1 3.175 76.5175 44.8
cylinder 0 1 24.4475 76.5175 44.8
cylinder 2 1 25.4 76.5175 44.8
cuboid 0 1 4p25.4 76.5175 44.8
unit 12
com='top of tank'
cylinder 0 1 2.54 1.905 0.0
cylinder 2 1 25.4 1.905 0.0
cuboid 0 1 4p25.4 1.905 0.0
end geom
read array
com='array putting the sheba tank together - stacked from bottom to top'
gbl=1 ara=1 nux=1 nuy=1 nuz=12
fill 10 1 2 3 4 5 6 7 8 9 11 12 end fill
end array
' suppress k5-60 & k5-64 messages, use p5 scattering
read mixt eps=1.0 sct=3 end mixt
end data
end
#kmart
read initial
kunit=35 xunit=4 actbygrp rrpvol keno3d 40 sheba
end initial
read collapse
lastg=44 lastg=199 lastg=238
end collapse
read activity
92234 18
92234 27
92235 18
92235 1452
92235 27
92236 18
92236 27
92238 18
92238 27
1001 27
8016 27
9019 27
end activity
end
#shell
copy sheba.kmt c:\examples
end

```

Note that the KENO3D view of the model appears the same as the simple model in Fig. D.1, but dividing it into smaller segments allows KMART to produce neutron production plots like Fig. D.2. Dividing the model into even smaller segments can result in a much higher resolution plot as shown in Fig. D.3.



**Fig. D.2. SHEBA-II neutron production.**



**Fig. D.3. Higher resolution plot of SHEBA-II neutron production.**



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70. W. W. Tippl, Framatome-ANP GmbH, Department NDM3, Postfach 10 10 63, Berliner Strasse 295-303, D-63010 Offenbach am Main / Germany
71. H. Toffer, Fluor Daniel Northwest, Inc., PO Box 1050, MSIN B4-44, 1100 Jadwin Ave., Richland, WA 99352-1050
72. E. F. Trumble, Westinghouse Safety Management Solutions, PO Box 5388, 1993 South Centennial Dr., Aiken, SC 29803
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Internet: www.ornl.gov/scale

January 21, 2003

Distribution

Dear Associates:

**Availability of Oak Ridge National Laboratory Report, ORNL/TM-2002/155, *KENO V.a Primer: A Primer for Criticality Calculations with SCALE/KENO V.a Using CSPAN for Input*, R. D. Busch and S. M. Bowman**

This note provides you with notification of the availability of the subject report. The abstract from the report follows.

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 4.4a, which includes the Criticality Safety Processor for Aalysis (CSPAN) input processor for Windows personal computers (PCs). A second edition of the primer, which uses the new KENO Visual Editor, is currently under development at ORNL and is planned for publication in late 2003. Each example in this first edition of the primer uses CSPAN 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 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 which are covered in detail in the example problems in that section. Upon completion of the primer, a new user

should be comfortable using CSPAN to set up criticality problems in SCALE/KENO V.a.

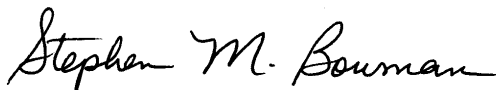
The primer provides a starting point for the criticality safety analyst using SCALE/KENO V.a. Complete descriptions are provided in the SCALE/KENO V.a manual. Although the primer is self-contained, it is intended as a companion volume to the SCALE/KENO V.a documentation. (The SCALE manual is provided 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. The information is provided in appendices so as not to obscure the basic information illustrated in each example.

The 182-page publication contains over 100 figures, most of them in color. You may obtain a copy of the report in one of three forms:

1. printed copy in black and white,
2. electronic copy on CD-ROM in PDF format (nearly 9 MB with color figures), or
3. downloaded electronic copy in PDF format (same as on CD-ROM) from [http://www.ornl.gov/scale/pubs/tm2002\\_155.pdf](http://www.ornl.gov/scale/pubs/tm2002_155.pdf).

Please notify Ms. Willena Carter by e-mail ([carterwc@ornl.gov](mailto:carterwc@ornl.gov)) or fax (865-576-3513) if you would like to receive either a printed copy or an electronic copy on CD. No notification is necessary to download the copy from the SCALE website.

Sincerely,



Stephen M. Bowman  
SCALE Project Leader  
Nuclear Analysis Methods & Applications Group  
Nuclear Science and Technology Division (94)

SMB:wcc

cc: R. D. Busch    C. V. Parks    File – RC