OFFSCALE: A PC Input Processor for the SCALE Code System

The ORIGNATE Processor for ORIGEN-S

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ABSTRACT

OFFSCALE is a suite of personal computer input processor programs developed at Oak Ridge National Laboratory to provide an easy-to-use interface for modules in the SCALE-4 code system. ORIGNATE is a program in the OFFSCALE suite that serves as a user-friendly interface for the ORIGEN-S isotopic generation and depletion code. It is designed to assist an ORIGEN-S user in preparing an input file for execution of light-water-reactor (LWR) fuel depletion and decay cases. ORIGNATE generates an input file that may be used to execute ORIGEN-S in SCALE-4. ORIGNATE features a pulldown menu system that accesses sophisticated data entry screens. The program allows the user to quickly set up an ORIGEN-S input file and perform error checking. This capability increases productivity and decreases the chance of user error.

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1 INTRODUCTION

ORIGEN-S¹ is a powerful and flexible computer code for performing isotopic generation and depletion for many applications, including light-water-reactor (LWR) spent fuel analyses. ORIGEN-S computes time-dependent concentrations and source terms of a large number of isotopes, which are simultaneously generated or depleted through neutronic transmutation, fission, and radioactive decay. Input requirements include initial nuclide compositions, irradiation and/or decay history, and an appropriate cross-section library. Its design is general in nature. The number of input parameters and options can be overwhelming, which contributes not only to its flexibility, but also to its difficulty to use. In order to provide a user-friendly interface program to a wide range of users that would be easy to learn and useful for most applications, a personal computer (PC) input processor named ORIGNATE has been developed.

ORIGNATE is a program designed to assist an ORIGEN-S user in preparing an input file for execution of LWR fuel depletion and decay cases within the SCALE-4 code system² and is part of the OFFSCALE suite of PC input processors. The purpose of OFFSCALE is to provide updated easy-to-use interfaces to a wide range of SCALE users. Development of OFFSCALE separate from SCALE-4 prevented the need for major changes to the established and tested input routines currently used by SCALE-4. The most significant limitation in ORIGNATE is that it is restricted to the use of binary libraries only. The ability to use card-image libraries was not incorporated because these libraries currently contain data

that are only appropriate for very general scoping calculations.

The ORIGNATE program is written in Microsoft BASIC 7.1 (Ref. 3) and runs on an MS-DOS-based PC. ORIGNATE generates a card-image input file that may be used to execute ORIGEN-S in SCALE-4. ORIGNATE features a pulldown menu system similar to the type used in many commercial PC software products. The menu system organizes the major command categories as menu titles and pulldown commands and may be used with either a keyboard or a mouse.

When an option is selected from the menu system, a sophisticated data entry screen or series of screens is displayed. Each field on a screen has a help message associated with it which may be displayed by pressing a function key. The message gives a brief description of the input parameter and occasionally refers to a section in the SCALE-4 manual² for more detailed information. This feature minimizes the amount of time that might be used searching through the documentation when setting up an ORIGEN-S input file. Some fields have a multiple-choice menu associated with them. These menus minimize the possibility of input errors by providing a complete list of valid choices for given parameters. Depending on input options selected, the program protects other fields that are not needed for those options. ORIGNATE performs extensive error checking for each input screen and displays appropriate warning and error message boxes when applicable.

2 GETTING STARTED

To install ORIGNATE, first make a directory on your hard disk where ORIGNATE will reside by using the DOS MKDIR command:

```
MKDIR \ORIGNATE
```

Next, change to that directory:

```
CHDIR \ORIGNATE
```

Then place the ORIGNATE distribution diskette into drive A or B:

```
COPY A:\ORIGNATE\*.*
```

This will install all the ORIGNATE files. To execute the program, enter the program name:

```
ORIGNATE
```

The easiest way to learn how to use ORIGNATE is to read through the rest of the documentation while running the program so you can use the options and keys as you read about them. The following two sections, "Using the Menu System" and "Using the Input Screens," give an overview of how to use the program. Following these sections is a detailed description of how to use each of the menu options.

3 USING THE MENU SYSTEM

After paging through the introductory screen, you reach the ORIGNATE pulldown menu system. The menu system contains a menu bar across the top of the screen. Under each menu bar option there is a unique pulldown menu. The menu bar options are summarized below.

Files	Options to retrieve files, save files and exit the program
Initial Input	Options to input compositions and energy group edit structure
Case Types	Options to input depletion cases and decay cases
Modifying Cases	Options to insert cases and delete cases

When ORIGNATE begins, it presents the **Files** pulldown menu. You may scan across the menu bar by using the left and right arrow keys. You may select an option from a pulldown menu by using the up and down arrow keys. A description of the highlighted option will appear on the bottom line of the screen. To execute the option, simply press the <Enter> key

or the highlighted letter (known as the "hot key") of the desired option.

The mouse may also be used to select an option by moving it left or right along the menu bar or up and down on a pulldown menu. To choose a pulldown menu command, simply move the mouse cursor over the desired option and click the left mouse button. Some users may prefer to "drag" the mouse (holding the left mouse button) over the menus and then release the left button when the cursor is over the desired command. One difference between the two methods of using the mouse is that dragging the mouse will cause the description of the highlighted option to be displayed on the bottom of the screen as when using the keyboard.

Some pulldown menu commands are black with a hot key, while others are gray. The black commands are active; the gray commands are inactive and will produce no effect if selected. Commands will be activated as necessary data are entered. For example, once the Initial Input data are entered, the Case Types options are active. Most of the options will become active when ORIGNATE files are retrieved.

4 USING THE INPUT SCREENS

Once an option is selected, an input screen or series of input screens will be displayed. The cursor will appear at the first data field on the screen that is not protected. Fields may be protected by the program, depending on the input options selected. For example, on the Compositions screen, if "Input" is "Dataset," the nuclide fields for card input are protected. To move from one field to the next, press <Enter> or <Tab>. To move backward to the previous field, press <Shift+Tab> or <Backspace>. The cursor must be at the beginning of the field for <Backspace> to move to the previous field, because within a data field it moves back one space and deletes the previous character. You may also change fields with the arrow keys, but the movement will be somewhat erratic because the cursor skips fields if there is more than one field per screen line. <Home> moves the cursor to the beginning of the field, and <End> moves to the end of the field. The <Ins> and keys perform their normal functions for editing a field. <Ctrl+Home> moves the cursor to the first field on the screen, and <Ctrl+End> moves the cursor to the last field. <PgUp> and <PgDn> may perform the same respective functions, if they are not active functions listed on the bottom of the current input screen.

Some fields have a multiple-choice menu associated with them. Pressing <Enter> or the Space Bar at one of these fields will activate the multiple-choice menu. When this menu is displayed, all other processing and function keys are disabled until a choice is selected and the menu disappears from the

screen. Pressing a letter on the keyboard will move the cursor to the next choice that begins with that letter. If there is not a choice that begins with that letter, the cursor moves to the beginning of the list. The up and down arrow keys, <PgUp>, <PgDn>, or the mouse may be used to make a selection. <Home> moves the cursor to the first choice, and <End> moves the cursor to the last choice. Once the desired choice is highlighted, press <Enter> to select it and remove the menu.

Logical (YES or NO) fields use "Y" and "N" or "X" and ". No other values will be accepted. You may toggle between the two choices with the space bar.

Most fields have a help message associated with them. Pressing <F1> displays the message. Often the message will refer to a section of the SCALE manual for more detailed information. Press <Enter> or <Esc> to remove the message from the screen. If there is no message for a particular field and it is one of several identical fields on a screen, try moving the cursor to the first of these fields on the screen and pressing <F1>. For the Compositions screens, the help messages are only active for the first screen and the first occurrence of each field on subsequent screens.

Title and comment fields must be entered whenever they appear on an input screen. Delimiters are automatically provided by ORIGNATE and should not be input by the user.

5 MENU SYSTEM OPTIONS

The purpose of this section is to present an overview of the menu system commands. Menu bar options are presented next to square bullets; corresponding pull-down commands are listed next to round bullets. The underlined letter in commands discussed below represents the hot key for the command; these hot keys appear on the screen as bright letters, and they allow immediate access to an item by pressing the highlighted key.

■ Files

The Files menu allows you to retrieve and save files and to exit the program.

● Retrieve Files

This option allows you to retrieve random-access files that you have previously saved with ORIGNATE. A random-access file is saved for each pull-down menu option for which data are entered. Each random access file for a problem has the same file name as specified by the user but a different file extension designated by ORIGNATE. A listing of these file extensions is given in Table 5.1. ORIGNATE presents a list of all files in the current directory that have the ".CMP" file extension (this random-access file is always required). When you select the desired file name, ORIGNATE loads all files with that file name and one of the extensions listed in Table 5.1. The program copies the files to a set of temporary files, ORIGTEMP.* (i.e., file extensions remain the same). If you wish to retrieve only a portion of the ORIGNATE files associated with an ORIGIN-S input file you have previously generated (e.g., the Compositions data), rename or copy those files using the same file extensions. Two sets of sample files have been provided on the distribution diskette. The naming conventions are BWR.* and PWR.* and represent actual boiling-water-reactor (BWR) and pressurized-water-reactor (PWR) fuel assembly depletions, respectively. These sample problems are discussed in detail in Sect. 6 of this document.

● Save Files / Input Deck

This option saves the data you have entered in random-access files, which can later be retrieved by the program for modification. A card image ORIGIN-S input file is also generated. ORIGNATE will not save files in this option unless sufficient data have been

entered to generate a meaningful ORIGIN-S input file. A random-access file will be saved for each menu option used to input data, up to a maximum of four files. ORIGNATE will prompt you for the file name for the ORIGNATE files. In addition to the random-access files, ORIGNATE also writes a card-image ORIGIN-S input file and a MS-DOS batch file to execute the ORIGIN-S case using SCALE-PC. The ORIGIN-S input file has the file extension .IN and the MS-DOS batch file has the file extension .BAT. If files with these names already exist, ORIGNATE will ask if you want to overwrite these files.

Table 5.1 ORIGNATE random-access files

ORIGNATE	
file extensions	Contents
.CMP	Compositions input
.DCY	Decay cases
.DPL	Depletion cases
.GRP	Energy group structures

● Save Partial Files

This option saves ORIGNATE random-access files, regardless of the amount of data entered. It does not generate a card-image ORIGIN-S input file. This option is designed to allow you to occasionally save input data so that they will not be lost if the program terminates abnormally. Note that if ORIGNATE does fail, the data entered still exist in the ORIGTEMP.* files. When ORIGNATE is restored, it will notify you that it has detected these files and will give you an opportunity to rename and save them.

● Quit

This option terminates the program. If you have selected any option other than retrieving or saving files immediately prior to this option, the program will verify if this is what you want to do. Since this option does not save files, you may also use this option to cancel any changes you have made since the last time you saved files.

Options

■ **Initial Input**

The **Initial Input** menu provides you with selections to input the case independent initial data required by ORIGIN-S.

● **Compositions**

Nuclide compositions are required input for ORIGIN-S to define the initial configuration of the system being analyzed. This is the only active option other than **Retrieve Files** when you enter the program. Select either "Cards" or "Dataset" as your source of input in the first field. If "Cards" is selected, the second field gives you a choice of input units. You specify each nuclide by element from an alphabetized menu and then type the isotope [e.g., "U(92)" and "235" for U-235 and "Xe(54)" and "135m" for Xe-135 metastable]. The program checks the isotope number to ensure it is valid for the element selected. A complete list of valid isotopes is given in Sect. F7.B of the SCALE manual.² To obtain the natural abundances of an element in the ORIGIN-S light-element library (NEX1=4 in the ORIGIN-S 75\$ array), input "Nat1" for the isotope. If the specified nuclide appears in more than one of the ORIGIN-S master libraries (light element, actinide, or fission product), a menu is provided of the available libraries. Select a library based on the origin of the nuclide and the desired edit grouping. If only one library is valid, the program automatically fills the field with the appropriate library. Then input the concentration in the units previously selected. The concentration that is input for each nuclide determines the "basis" of the problem (e.g., fuel assembly, metric ton of uranium, etc.). Note that the problem basis is important because it determines the limits of other input parameters such as power for depletion cases and the units of output parameters such as nuclide concentrations or source terms.

This option displays a maximum of three screens. Each screen contains 10 nuclides, for a maximum of 30 nuclides. The <PgDn> and <PgUp> keys are used to move forward and backward, respectively, between screens. To change an element selection, simply select a new one from the multiple-choice menu. To erase an element that has been selected, press <Ctrl+E> while the cursor is on that element field.

If you want ORIGIN-S to read the nuclides from a dataset written by a previous ORIGIN-S job, select "Dataset" as the source of input in the first field. All nuclide fields are then blanked and protected. The second field then represents the input/output (I/O) unit number of the dataset and the position of the concentrations in the dataset. For example, "71+2" specifies I/O unit number 71 and the second position in the file. Note that ORIGIN-S prints the position in the file when it writes the data. If you omit the position number from this field, ORIGIN-S assumes that you want to read from the first position in the file. You must specify the appropriate restart dataset in the script or job control language that executes the ORIGIN-S case. For example, if executing ORIGIN-S on a PC or UNIX workstation, and the I/O unit number is specified as 71 in ORIGIN-S, the restart dataset should be named ft71f001.

IMPORTANT NOTE: If you read and write restart data in the same job, ORIGIN-S begins writing data in the file position immediately following the one from which it read. It does not search for the end of file. If you are reading from a position prior to the last one in the file, the data that follow may be overwritten if new restart data are saved.

Use <F4> to cancel or <F10> to save the data and return to the main menu.

● **Neutron/Gamma Groups**

This option displays two screens, one each for the energy group structure for neutron spectra edits and gamma spectra edits. These edits are for individually selected time steps in the decay cases for which source terms are desired to perform shielding calculations. The first field on each screen gives a multiple-choice list of energy group structures corresponding to commonly used neutron or gamma cross-section libraries. You may choose one of these or input your own group structure by selecting "Other." If you are running only depletion cases or you do not want these edits, you may select "None".

If you select one of the standard group structures or "None," ORIGIN-S protects the remaining fields on the screen and advances to the next screen. <PgUp> and <PgDn> may be used to move from one screen to the other. If you select "Other," specify the number

of energy groups. ORIGNATE requires you to input the maximum energy cutoff in eV for each group, beginning with group 1 (the highest energy group). The field following the maximum energy cutoff for the lowest energy group must contain the minimum energy cutoff for that group. The remaining fields on the page remain protected. ORIGNATE verifies that the energies are entered in order from highest to lowest.

■ Case Types

The **Case Types** menu provides you with selections to enter depletion and/or decay case data. (A "case" in ORIGNATE is equivalent to a "subcase" in ORIGEN-S.) Each case is limited to ten time steps, because this is the maximum number which fit across a page of the ORIGEN-S output. Each case has a title card and a basis card. The basis card is a subtitle in the ORIGEN-S output that describes the basis for the calculations performed as determined by the concentrations input (e.g., a fuel assembly or a metric ton of uranium). All depletion cases are entered via one option, and all decay cases are entered via another option. The order in which they are entered determines the order in which they appear in the ORIGEN-S input file and is reflected by the case number that is displayed in ORIGNATE.

● Depletion Cases

A depletion case consists of a series of time steps where nuclear fuel is irradiated. The power at which the fuel is irradiated and the time duration are required for each time step. This option displays three screens: (1) the depletion case input, (2) the depletion case I/O options, and (3) the depletion case library specifications. The screen initially displayed is the depletion case input for a new case with a case number one greater than the last case saved. The data for a case are saved by pressing <F10> to advance to the next case, or <F9> to go back to the previous case. To avoid saving changes on the screen, press <F4> to return to the main menu system. ORIGNATE asks you if you want to save the changes on the screen before returning. To review existing cases, press <Ctrl+R>. This displays a list of case numbers, types, and titles.

Each depletion case consists of a series of time steps. The beginning time, which is defaulted to zero, and the ending time for the case are specified first. Then

the power (MW / basis unit) and the cumulative time from the case beginning time are input for each time step.

IMPORTANT NOTE: The power must be consistent with the basis for the calculation (e.g., fuel assembly, MTU, etc.) in order for the calculated results to be correct.

To specify downtime during or at the end of the case, input 0 for the power. (ORIGNATE automatically resets it to 1.0E-20.) For periods greater than 100 days, a separate decay case is recommended. The time entered for the last time step must match the "ending time" field. In addition, the program checks that the cumulative time for each step is greater than the previous step. The maximum recommended increment per time step is 100 days, or 0.3 years, and the recommended minimum number of steps is three per case. If the time-step increments are larger or the number of time steps is less, ORIGNATE prints a message on the screen and automatically inserts additional steps up to the maximum of ten steps per case. The intent of this feature is to allow you to specify only the times at which you want to change power level or to obtain output and let ORIGNATE determine any remaining steps needed to ensure accurate results. You can modify the steps generated by ORIGNATE by simply editing the fields. ORIGNATE only checks the data once per edit of each case. If you later return to a case and edit any of the data, ORIGNATE checks the length and number of time steps again.

The option to write restart data for a time step is set by typing an "X" in the appropriate field. These data may be written for as many time steps as desired. If the compositions input specified reading from a dataset, these data are written to the same unit, immediately following the input data read. As noted previously, **this will result in a loss of any data following the input data in that dataset.** If the compositions input was specified on cards, the restart data are written to I/O unit 71.

The I/O options screen is accessed by pressing <Ctrl+O>. This screen only controls the I/O options for depletion cases. This screen must be edited and saved for the first depletion case. ORIGNATE automatically displays it with a set of default values when you press <F10> to initially save the first case. The options stay in effect until they are changed in a sub-

Options

sequent case. The time units that are displayed on the depletion case input screen are selected on this screen.

The library options screen is used to specify the binary depletion library for each case. Note that ORIGNATE is not designed for use with card-image libraries, but only binary libraries. The ORIGEN-S card-image libraries contain data that are only suitable for general scoping calculations. Such scoping calculations for LWR depletion analyses may be performed using the PRLIMLWR binary library available in SCALE-4 (see Sect. M6.7.3 of the SCALE-4 manual). This library is a modified version of the ORIGEN-S card-image libraries updated with cross sections from all nuclides in the SCALE 27-group burnup library. More appropriate burnup-dependent libraries that account for the assembly and reactor type, initial enrichment, and power history may be created by the SAS2H sequence of SCALE.

The library options screen is accessed by pressing <Ctrl+L>. ORIGNATE automatically displays the library options screen with the values from the previous case when you press <F9> or <F10> to initially save a new case. It is very important that you choose an appropriate library for each case. In order to ensure that this is done, ORIGNATE requires that you edit this screen for each case. If you use the same library for consecutive cases, the program prints a dialog box to verify that you want to do that. Specify the I/O unit number for a user-supplied library that has been previously generated with SAS2H or select one of the SCALE-supplied libraries (available in SCALE-4.1 or later). The SCALE-supplied libraries are categorized by:

- (1) reactor type,
- (2) enrichment / maximum burnup,
- (3) power, and
- (4) cycle number / burnup range.

The selections available for each of these categories are shown in Table 5.2. The nearest enrichment should be the criterion for choosing the enrichment / maximum burnup. The maximum burnup is simply an upper bound for which cross sections are available. The burnup range is the criterion for selecting the cycle number / burnup range. The cycle number is an arbitrary indexing for the libraries generated for a particular enrichment and does not necessarily correspond to the number of cycles in which the fuel being modeled has been burned. An ORIGNATE case that

exceeds the lower or upper burnup limit by 5 or 10% is acceptable. For some fuel cycles, it may be necessary to break up the cycle into two or more cases to match the burnup ranges of the depletion libraries.

An example would be a 3.6 wt % PWR fuel assembly that accumulates 18 GWd/MTU of burnup in its first cycle. From Table 5.2 it can be seen that a library set exists with an enrichment of 3.6 wt % and burnup increments of 10 GWd/MTU. The problem input would require one case from 0 to 10 GWd/MTU and a second from 10 to 18 GWd/MTU. The first case would use the Cycle 1 / 0-10 GWd/MTU library, and the second would use the Cycle 2 / 10-20 GWd/MTU library.

The I/O unit numbers for the SCALE-supplied libraries are automatically assigned beginning with unit 51. For user-supplied libraries, unit numbers between 31 and 50 may be used. These numbers were selected in order to avoid conflicts with other SCALE datasets. The PRLIMLWR library can be used by specifying a user-supplied library on unit 31 and then assigning the PRLIMLWR library to unit 31 in the script or job control language that executes the ORIGEN-S case. An example of this is included in the ORIGEN-S sample problem 1 included with ORIGNATE as SAMPLE1. You must ensure that your job control language specifies the correct dataset names and unit numbers for the libraries you use, whether they are SCALE- or user-supplied libraries. For more information on executing ORIGEN-S on an MS-DOS PC, refer to Sect. 6.

• Decay Cases

A decay case consists of a series of time steps where irradiated material undergoes radioactive decay. This option displays three screens: (1) the decay case input, (2) the decay case I/O options, and (3) element fractions. The screen initially displayed is the decay case input for a new case with a case number one greater than the last case saved. The <F4>, <F9>, <F10>, and <Ctrl+R> keys function the same as on the depletion case input screen.

Like a depletion case, each decay case consists of a series of time steps. The beginning time, which is defaulted to zero, and the ending time for the case are specified first. The time entered for the last time step must match the "ending time" field. In addition, the

Table 5.2 SCALE-supplied library parameters

Reactor Type: PWR		Power (MW/MTU)	
		18	
		28	
		40	
Enrichment/maximum burnup (wt % U-235) (GWd/MTU)	Number of cycles	Burnup per cycle (GWd/MTU)	
2.4 wt% / 25	3	8.333	
2.8 wt% / 30	3	10.000	
3.2 wt% / 35	4	8.750	
3.6 wt% / 40	4	10.000	
3.9 wt% / 45	5	9.000	
4.2 wt% / 50	5	10.000	

Reactor Type: BWR		Power (MW/MTU)	
		12	
		20	
		30	
Enrichment/maximum burnup (wt% U-235) (GWd/MTU)	Number of cycles	Burnup per cycle (GWd/MTU)	
1.9 wt% / 20	3	6.667	
2.3 wt% / 25	3	8.333	
2.7 wt% / 30	4	7.500	
3.1 wt% / 35	4	8.750	
3.4 wt% / 40	5	8.000	
3.8 wt% / 45	5	9.000	

program checks that the cumulative time for each step is greater than the previous step. The recommended maximum initial time step is 100 days, or 0.3 years, and the cumulative time for subsequent steps should be ≤ 3.3 times the cumulative time for the previous time step. Because the nuclides decay exponentially, this factor ensures accurate results. This is commonly known as the "Rule of 3's." If the time-step

increments are larger, ORIGNATE prints a message on the screen and automatically inserts additional steps up to the maximum of ten steps per case. For a cumulative time of 3 raised to a power of 10 (0.3, 3, 30, 300, etc.), ORIGNATE sets the time for the next step to 10 raised to the same power of 10 (1, 10, 100, 1000, etc.). The intent of this feature is to allow you to specify only the times at which you want to obtain

output and let ORIGNATE determine any remaining steps needed to ensure accurate results. You can modify the steps generated by ORIGNATE by simply editing the fields. ORIGNATE only checks the data once per edit of each case. If you later return to a case and edit any of the data, ORIGNATE checks the length and number of time steps again.

The decay case input screen allows you to save restart file data in the same manner as the depletion case input screen. In addition, it allows you to request neutron and gamma source spectra output edits for any time step. These are printed by ORIGEN-S according to the energy group structures designated in the Neutron/Gamma Groups option. If "None" is selected for both group structures, requesting an edit on this screen has no effect.

The I/O options screen is accessed by pressing <Ctrl+O>. This screen only controls the I/O options for decay cases. This screen must be edited and saved for the first decay case. ORIGNATE automatically displays it with a set of default values when you press <F10> to initially save the first case. The options stay in effect until they are changed in a subsequent case. The time units that are displayed on the decay case input screen are selected on this screen. The (α, n) source is typically UO_2 , unless you are modeling high-level waste in borosilicate glass. See Sects. F7.2.8 and F7.2.9 of the SCALE manual for details. ORIGN-S allows the cutoff for the decay output edits to be in the units of the edit or % of the total. The latter is designated by typing "%" at the end of the cutoff value. In order to simplify the output edits menu, the 63 choices possible in the ORIGEN-S 65\$ array (Sect. F7.6.10 of the SCALE manual) have been reduced by grouping according to the three dimensions of the array. This procedure may result in more output than desired in some cases (e.g., if you wanted only grams of light elements but grams and curies of fission products). The ORIGEN-S card-image input generated by ORIGNATE has been formatted and labeled by subgroups so that an experienced ORIGEN-S user can easily modify the input by turning on or off individual edit options in the 65\$ array.

The element fractions screen is an optional screen that allows you to keep or remove all or part of a maximum of ten elements from the previous case. This allows you to isolate part of the problem being modeled, such as the endfittings of a fuel assembly. To access this screen, type "Y" for the element

fractions field on the decay case input screen and press <Ctrl+F>. Select whether to keep or remove the elements, then select the elements from a multiple-choice menu, and specify the fractions of each to be kept or removed.

● Review Cases

This option displays a list of case numbers, types, and titles for all cases that have been created. This function may also be performed by pressing <Ctrl+R> at the main menu or while using screens that require case numbers: Depletion Cases (screen 1) and Decay Cases. To remove the list from the screen, press <Enter> or <Esc>.

■ *Modifying Cases*

The **Modifying Cases** menu contains options for inserting or deleting cases, so that you can retrieve an existing set of cases and modify them to model different scenarios, such as adding or deleting a cycle from a fuel assembly's burnup history.

● Insert Cases

This option presents a dialog box with two fields: the type of case to be inserted (depletion or decay), and where to insert it (the new case goes before the case selected). Use the <Tab> and <Shift+Tab> keys to move between the two fields and the up and down arrow keys to select the choice for each field. The mouse may also be used in the dialog box. Selecting the <Cancel> button at the bottom of the box or pressing <Esc> returns you the main menu system without inserting a case. When you press <Enter> or click the mouse to accept the choices made, ORIGNATE automatically adjusts the case numbers and moves directly to the depletion or decay input screen to enter the data for the new case.

● Delete Cases

This option presents a dialog box with a list of all cases. Select the case to delete by using the up and down arrow keys or the mouse. The case numbers for the remaining cases will be automatically adjusted. Selecting the <Cancel> button at the bottom of the box or pressing <Esc> returns you to the main menu system without deleting a case.

6 EXECUTING ORIGIN-S IN SCALE-PC

For SCALE-PC users, ORIGNATE writes an MS-DOS batch file to execute the ORIGIN-S case. The batch file has the same DOS eight-character file name as the other ORIGNATE files followed by the .BAT extension. As an example, the PWR.BAT file included with ORIGNATE is shown in Table 6.1.

The first line of the batch file contains the DOS command to copy the selected SCALE-supplied binary depletion library to the correct I/O unit dataset name in the SCALE-PC working subdirectory. If more than one SCALE-supplied library (i.e., different enrichment or power) is specified in the input, there will be an additional line in the .BAT file for each additional library. If a user-supplied library is specified in ORIGNATE, "____LIB" is written as the library name. The correct library name must be substituted by the user. For example, to use the PRLIMLWR library for the SAMPLE1 problem, FT21F001 should be substituted for ____LIB, because that is the standard file name for the PRLIMLWR library in SCALE-PC.

The second line in the batch file calls SCALE-PC to execute using the appropriate input and output files. The third line copies the optional ORIGIN-S restart file written to I/O unit 71 to the current directory with the same eight-character file name as the ORIGNATE files followed by the .F71 extension. The last two lines delete the restart file and the copy of the binary depletion library in the SCALE-PC working subdirectory in order to keep free as much disk space as possible.

If the path names in the batch file written by ORIGNATE are correct, the SCALE-PC case can be executed immediately after exiting ORIGNATE by simply typing the file name for the case at the DOS prompt. For example, to execute PWR.BAT, type "PWR" and press the enter key.

To execute ORIGIN-S on a UNIX workstation, the user must construct a script file containing similar commands to those in the batch file.

Table 6.1 PWR.BAT sample file

```

COPY \SCALE41\DATA\LIB\P3028LIB \SCALE41\WORK\FT51F001
CALL SCALE4 PWR.IN PWR.OUT
COPY \SCALE41\WORK\FT71F001 PWR.F71
DEL \SCALE41\WORK\FT71F001
DEL \SCALE41\WORK\FT51F001

```

7 FILES ON THE DISTRIBUTION DISKETTE

ORIGNATE is available as part of the OFFSCALE package from the Energy, Science, Technology Software Center (ESTSC) and from the Radiation Shielding Information Center (RSIC) at ORNL. It is also distributed with the SCALE code package from RSIC.

Files included on the ORIGNATE distribution diskette which are necessary for running the program are listed in Table 7.1. ORIGNATE.EXE is the executable program. ORIGNATE.QLS is the ORIGNATE QuickScreen library developed with Crescent Software's QuickScreen program⁴ and contains all the input screens displayed by ORIGNATE. In addition, ORIGNATE contains several routines from Crescent Software's QuickPak Professional Library.⁵ The files with the ".FRM" extension contain the form definition for each of the screens in the ORIGNATE QuickScreen library. The files with the ".BSV" extension were written with Microsoft BASIC's BSAVE command³ and contain the following data: nuclides, elements, neutron energy group boundaries, and gamma group energy group boundaries.

In addition to these files, ORIGNATE files for three sample problems are included on the diskette. These files are listed in Table 7.2 and may be retrieved in ORIGNATE. The card image ORIGEN-S input files which were generated with these files have the extension ".IN". The BWR case models assembly CZ205 from Cooper Nuclear Station. This assembly was in core for three cycles, out of core for two cycles, and in core for two more cycles. The PWR case models assembly D-15 from Turkey Point Unit 3. This assembly was used for three consecutive cycles and then discharged. The power histories and other pertinent data for these two assemblies used in setting up the ORIGNATE input data are presented in Tables 7.3, 7.4, and 7.5. These two assemblies have been used for decay heat measurements which have served as benchmarks for ORIGEN-S calculations. For more information, see Ref. 6.

Finally, a copy of this document is included on the diskette in the README.DOC file.

Table 7.1 Files required by ORIGNATE

<u>File name</u>	<u>Extension</u>
COMPNUC1	.FRM
COMPNUC2	.FRM
DECACAS1	.FRM
DECACAS2	.FRM
DECACAS3	.FRM
DEPLCAS1	.FRM
DEPLCAS2	.FRM
DEPLCAS3	.FRM
G18ORIG2	.BSV
G18SCALE	.BSV
G20	.BSV
G44	.BSV
GROUP1	.FRM
GROUP2	.FRM
N218	.BSV
N22	.BSV
N227	.BSV
N238	.BSV
N27	.BSV
N47	.BSV
ORIGCOMP	.BSV
ORIGELEM	.BSV
ORIGNATE	.EXE
ORIGNATE	.QLS
RENAMFIL	.FRM
SAVEFIL	.FRM
SAVEPART	.FRM

Table 7.2 ORIGNATE sample problem files

<u>File names</u>	
BWR.BAT	} BWR sample problem
BWR.CMP	
BWR.DCY	
BWR.DPL	
BWR.GRP	
BWR.IN	
PWR.BAT	} PWR sample problem
PWR.CMP	
PWR.DCY	
PWR.DPL	
PWR.GRP	
PWR.IN	
SAMPLE1.BAT	} ORIGEN-S sample problem 1
SAMPLE1.CMP	
SAMPLE1.DCY	
SAMPLE1.DPL	
SAMPLE1.GRP	
SAMPLE1.IN	

Table 7.3 Data for Cooper BWR assembly CZ205

Burnup history data ^a				
Cycle No.	Power (MW/assembly)	Burnup (MWd/MTU)	Cycle length (days)	Outage length (days)
1	2.427	10,298	807	59
2	4.608	7,414	306	31
3	3.464	2,987	164	35
4 ^b	0.0	0	370	—
5 ^b	0.0	0	394	—
6	1.118	1,864	317	48
7	1.520	2,781	348	—
Total		25,344	1942	

^aAverage power = 25,344 MWd/MTU / 1942 days = 13.05 MW/MTU

Fuel loading = 0.1902 MTU

Initial uranium isotopics: ^{234}U wt % = 0.022 ^{235}U wt % = 2.500
 ^{236}U wt % = 0.012 ^{238}U wt % = 97.466

Cooling times (days): 857 871 886 892 899 946
 Measured heat (watts): 324.0 343.5 331.8 327.5 311.4 317.1

^bAssembly was out of core during this cycle.

Table 7.4 Data for Turkey Point 3 PWR assembly D-15

Burnup history data				
Cycle No.	Power (MW/assembly)	Burnup (MWd/MTU)	Cycle length (days)	Outage length (days)
2	13.771	9,480	314	58
3	13.603	9,752	327	62
4	13.040	8,920	312	—
Total		28,152	953	

^aAverage power = 28,152 MWd/MTU / 953 days = 29.54 MW/MTU

Fuel loading = 0.4561 MTU

Initial uranium isotopics: ^{234}U wt % = 0.023 ^{235}U wt % = 2.557
 ^{236}U wt % = 0.012 ^{238}U wt % = 97.408

Cooling times (days): 962 1144 2077
 Measured heat (watts): 1423 1126 625

Table 7.5 Fuel assembly light-element contents

Element	Cooper Station (kg/assembly)	Turkey Point (kg/assembly)
H	3.1000	—
B	0.0130	—
O	50.5000	62.000
Cr	0.4500	2.700
Mn	0.0290	0.150
Fe	1.2000	5.900
Co	0.0046	0.034
Ni	0.4500	4.500
Zr	98.2000	101.000
Nb	—	0.320
Sn	1.6000	1.600
Gd	0.5440	—

8 REFERENCES

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