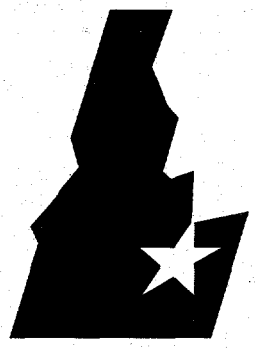

Idaho
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SUMMARY

MOCUP is a system of external processors that allow for a limited treatment of the temporal composition of the user-selected MCNP cells in a time-dependent flux environment. The ORIGEN2 code computes the time-dependent compositions of these individually selected MCNP cells. All data communication between the two codes is accomplished through the MCNP and ORIGEN2 input/output files, the MOCUP Processor Output files, and two user supplied tables. MOCUP is either command line or interactively driven. The interactive interface is based on the portable X11 window environment and the Motif tool kit. MOCUP was constructed so that no modifications to either MCNP or ORIGEN2 were necessary. *Section 4 of the writeup contains the input instructions needed to set up the MOCUP run.*

MOCUP is extremely useful for analysts who perform isotope production, material transformation, and depletion and isotope analyses on complex, non-lattice geometries, and uniform and non-uniform lattices.

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1.0 Introduction

MOCUP provides a limited treatment of the time-dependent composition of coupled nuclides in Monte Carlo particle transport by using a system of external processing functions that operate on and communicate with MCNP[1] and ORIGEN2[2] input/output files. This effort was motivated in part by a need to simulate isotope generation/depletion for the MCNP Monte Carlo models of the Advanced Test Reactor (ATR) and the Advanced Neutron Source (ANS). Prior to MOCUP, time-dependent modeling for both the ATR and ANS were performed manually, which proved to be time consuming, and probably error prone.

MOCUP was developed under the requirement that no code changes would be made to either MCNP or ORIGEN2. MOCUP is a series of processes that start with an initial MCNP input file. By means of uniquely constructed comment lines in the MCNP input file the user specifies one or more special sets of flux and reaction rate tallies that indicate which MCNP cells will be treated as time-dependent.

The MCNP Post-processor (mcnpPRO) part of MOCUP takes input from five sources including the MCNP input, output, and tally files, as well as two special user supplied files referred to as the Nuclide Correspondence and Flux Multiplier tables. Using the five input files, mcnpPRO generates MOCUP Processor Output files (MPO files). The number of processor output files generated depends on the number of sets of special flux and reaction rate tallies specified in MCNP. One processor output file is generated for each set of time-dependent tallies. The MOCUP Processor Output Files contain the time-dependent MCNP cell identifications, fluxes, nuclides, cross sections and other information for each specified set of time-dependent tallies. The next step of the process, the ORIGEN2 Pre-processor (origenPRO), operates on the MOCUP Processor Output Files as well as user supplied skeletal ORIGEN2 input files and generates modified ORIGEN2 input files. The number of supplied skeletal files corresponds to the number of MOCUP Processor Output Files that are generated by mcnpPRO. The origenPRO module will then run ORIGEN2 for all cells that have been identified as being time-dependent and keeps track of the ORIGEN2 computed number densities for the next time sequence through the process. Finally, the Composition Processor extracts the updated MCNP nuclide densities from the ORIGEN2 composition files and creates a new MCNP input file for the next time step through the process. This oversimplified explanation is expanded in the remainder of the report. Command line instructions for operating MOCUP are included in Appendix A. The Data Flow Diagram in Appendix B provides an "at a glance" view of the system. *Section 4 of the writeup contains the input instructions needed to set up the MOCUP run.*

As a final note in this introduction, MOCUP can be either command line driven or interactively driven from any point in the process as long as all the necessary files from the previous step are available. The interactive presentation was constructed with the X11 window environment[3] along with the Motif[4] tool kit for the sake of portability, appearance, and implementation.

2.0 Methods

2.1 Motivation

Previous incarnations of neutronics-depletion codes have relied almost exclusively upon diffusion theory, or some equivalent, for the neutronics portion. This has been due to the speed and simplicity inherent in the solution of the diffusion equation for large systems. This method has worked extremely well for large light-water and fast reactors, as well as for a variety of experimental reactor target applications. However, when encountered with a depletion problem involving a highly-absorbing medium, diffusion theory breaks down and produces inaccurate results. Additionally, most diffusion codes are limited to rectangular or hexagonal Cartesian, cylindrical, and/or spherical coordinate systems. This further reduces the applicability to the general class of depletion problems, many of which involve complex geometries. For these problems, a generalized-geometry transport-depletion code is desired.

This need inspired the development of the MOCUP code, which provides a path to use the MCNP generalized-geometry Monte Carlo transport code to provide the neutronics solution and the ORIGEN2 depletion and isotope generation code to perform the depletion. This allows a general material (target, fuel, control, etc.) to be depleted in a neutral particle field, with the accuracy of a transport neutronics solution. This document details the structure and use of the MOCUP code, with this section describing the external codes employed, and the methods used in the development of MOCUP.

2.2 Code Descriptions

2.2.1 MCNP

MCNP is a general purpose, generalized-geometry, continuous energy, time-dependent, coupled neutron/photon/electron Monte Carlo transport code that solves transport problems in an arbitrary three-dimensional geometry defined by first-, second-, and some special fourth-degree surfaces. The neutron energy range is from 10^{-5} eV to 20 MeV, the photon energy range is from 1 keV to 100 MeV, and the electron energy is from 1 keV to 1000 MeV, with the upper limit reduced to 100 MeV for coupled photon/electron problems. The capability to calculate the effective multiplication factor (k_{eff}) is also included in the code.

Quantities that may be tallied include particle or energy current and flux across a surface, flux or energy deposition averaged over a volume, and flux at a point for a point detector. A wide variety of multipliers are available to augment any of these tallies, ranging from dose conversion factors to any cross section defined for ENDF/B. Sources can be defined in an arbitrary fashion for all particle types. Cross section data are available for most isotopes used in nuclear applications.

2.2.2 ORIGEN2

ORIGEN2 is used for calculating the generation, decay, and processing of radioactive isotopes. Several libraries of cross section, decay, and production data are available with the code to allow the data used to be tailored to fit the application. Options are included to allow for material reprocessing, continuous isotope feed streams, modification of libraries to incorporate new reactions or isotopes, and a host of output formats and data. ORIGEN2 performs its calculations in one neutron group, and depletion can be controlled either by total power, or by the flux level within the material.

The depletion equations are solved using the matrix exponential technique. ORIGEN2 uses a unique method for storing the necessary coefficients for solution of the couple equations, and for solving the system. These techniques are described fully in the literature, and will not be reproduced here.

2.3 MOCUP Methods

As described in the introduction, the MOCUP standard execution path recursively executes MCNP and ORIGEN2 to perform the desired depletion, with the MOCUP modules serving as "format bridges" between the codes. This requires that MOCUP observe the input formats and restrictions of both codes, and reads the necessary data from both code output formats. It is this requirement of the MOCUP code which results in a seemingly bizarre sequence of operations. The tallied one-group fluxes and reaction rates from MCNP are read by MOCUP, and the resultant depletion cell spectrum-averaged one-group cross sections are then computed from the ratio. This is necessary because, even though the depletion equations are solved using the reaction rates, ORIGEN2 is not equipped to accept them directly.

Prior to formatting the MCNP flux tallies for input into the ORIGEN2 code, these flux tallies must be appropriately normalized. This entails multiplying the resultant tallies by the fission neutron source in the calculation, as all tallies from MCNP k_{eff} calculations are normalized by MCNP to be per fission neutron. This fission source normalization by MOCUP allows the correct material depletion to be carried out. A detailed description of how the fission source normalization factor is computed is given in the MCNP user manual or one can find it in Redmond[5] and Wemple[6].

2.4 Statistical Limitations

As MCNP is a Monte Carlo code, it is appropriate to discuss the anticipated propagation of errors in MOCUP. At each depletion step, an MCNP calculation is performed to determine the flux for the next time step. The resulting cell flux and important (capture, fission) reaction rate values each have an associated statistical error, which is generally about 0.5-2.0% of the tally value. These values are then fed to the ORIGEN2 code, where several time steps are taken over the defined time interval between MCNP calculations.

These ORIGEN2 calculated compositions are then used in a subsequent MCNP calculation, so the flux and cross section errors are then increased. This will further accelerate the error propagation in the ORIGEN2 calculations. It thus behooves the user to pay close attention to the flux and reaction rate convergence levels in the MCNP calculation to prevent the accumulated statistical errors from growing to the point where confidence is lost in the results. In general, a 1% or less relative error on the flux and important reaction rates should be sufficient for most anticipated cases. Additionally, enough time steps (≥ 10) should be used in each ORIGEN2 calculation to ensure that the limitations of the matrix exponential method to not come into play.

So the user does not lose all hope of getting meaningful answers from stochastic depletion, very important property of depletion calculations in general should be reiterated: depletion calculations are inherently self-correcting. If the flux is overestimated at a given timestep, then this flux will over-deplete the existing concentrations during that timestep. This will reduce the flux in the next timestep, causing the reverse to occur. The net effect is a sawtooth oscillation about the "correct" solution with the magnitude of the oscillations increasing with depletion time. **The statistical uncertainties from the MCNP flux and reaction rate calculation control the magnitude of the oscillations.** It thus truly behooves the user to reduce the "important" reaction rate and flux tally statistical uncertainties as much as practical at each timestep to control these oscillations.

3.0 Processor Modules

3.1 MCNP Post-processor (mcnpPRO)

The MCNP Post-processor provides the cell fluxes and the radiative capture, alpha production, fission, (n,2n), and (n,3n) cross sections for the ORIGEN2 calculation through the MOCUP intermediate file, which is referred to as the MCNP processor output (mpo) file. The MCNP fluxes are adjusted by the flux multiplier table. The mpo files also contain both the MCNP and ORIGEN2 nuclide identifications as well as cell volumes taken from the MCNP standard output.

Input Files:

- Initial MCNP input file with special flux and reaction rate tally edits (section 4.1.1).
- MCNP tally edit (mctal) file (section 4.1.3).
- MCNP standard output (outp) file (section 4.1.2).
- Nuclide Correspondence Table (nct) (section 4.4).
- Flux Multiplier Table (fmt) (section 4.2).

Output File:

- MCNP Processor Output (mpo) (section 4.2).

3.2 ORIGEN2 Pre-processor (origenPRO)

The ORIGEN2 Pre-processor takes the flux and cross section information from the MPO files and merges it into the skeletal ORIGEN2 input files to create modified ORIGEN2 input files for each MCNP cell to be depleated. Note that for the first time step the ORIGEN2 Pre-processor also passes through the nuclide densities. The ORIGEN2 Pre-processor can also execute ORIGEN2 for each input file and prepare the newly generated composition data for the next time sequence.

Input Files:

- MCNP processor output (MPO) (section 4.2).
- ORIGEN2 skeletal input file (section 4.3.1).

Output Files:

- Modified ORIGEN2 Input Files (MOI) (section 4.3.2).
- ORIGEN2 Composition Files (OCF) (section 4.3.3).

3.3 Composition Processor (compPRO)

The Composition Processor (compPRO) extracts the number densities from the ORIGEN2 Composition Files and merges this into the current MCNP input file to create the MCNP input file to start the next time sequence. The compPRO module uses the NCT to convert the ORIGEN2 nuclide identifications to MCNP nuclide identification. The compPRO module also requires the volumes for MPO to convert the ORIGEN2 isotopic concentration (moles) into units of atoms/bn-cm.

Input Files:

- Current MCNP Input File (section 4.1).
- ORIGEN2 Composition Files (ocf) (section 4.3.3).
- MCNP processor output (mpo) (section 4.2).
- Nuclide Correspondence Table (nct) (section 4.4).

Output File:

- MCNP input file for next time step.

4.0 MOCUP Input Instructions And Associated Files

4.1 MCNP files

MOCUP uses the MCNP standard input specification (default = inp), standard output (default = outp), and the tally output (default = mctal). See the MCNP user's manual for information pertaining to the construction, generation, and use of these files.

4.1.1 MCNP standard input specification for use with MOCUP

To use MOCUP with MCNP one needs to first alter the MCNP input deck by the use of comment cards placed in appropriate locations in the MCNP input deck. The comment cards have no effect on the MCNP run. They are only used as flags in the mcnpPRO module of MOCUP to tell mcnpPRO which flux and reaction rate tallies are to be treated as time dependent.

Appendix C contains a listing of a sample MCNP input deck. This listing correspond to a sample problem that is supplied with this release of the MOCUP code. The sample problem has no physical significance except for use as a test problem. The first MOCUP comment card the user is required to input is a card with the comment entry "**c begin_mocup_flux_tallies**" . This entry corresponds to line 198 of the sample MCNP input deck. All the special comment cards that the user is required to input are typed in lower case letters. There are four spaces separating the comment indicator "c" and the word "begin". The double quotes are not entered. This card signifies the beginning of the flux tally regions that the user has identified to be time-dependent. The user can specify as many flux tally regions as needed. In the sample problem we have specified two regions, namely, a fuel region and a clad region. Each flux tally region must begin with a comment card with the comment entry "**c time dependent flux**". There are four blanks separating comment indicator "c" and the word "time". The time-dependent flux card for the fuel region corresponds to line 199 and the time-dependent flux card for the clad region corresponds to line 206 of the sample MCNP input deck. At the end of the flux tally block the user must place a comment card with the comment entry "**c end_mocup_flux_tallies**" (line 210 of the sample MCNP input deck). Again there are four blanks separating comment indicator "c" and the word "end". The other comment cards (blank comment lines and dashed separators) are only to improve readability.

Next the user specifies the beginning of the time-dependent reaction rate tallies by placing a comment card with the comment entry "**c begin_mocup_reaction_rate_tallies**" (line 214 of the sample MCNP input deck). The regions specified for the reaction rate tallies must be the same as specified for the flux tallies. Each region must also begin with a comment card with the comment entry "**c time dependent reaction rates**". Viewing Appendix C we find for the sample MCNP input deck these cards correspond to lines 215 and 240. The last user input comment card is one identifying the end of the reaction rate tally block. This card contains the comment entry "**c end _mocup_reaction_rate_tallies**" (line 248 of the sample MCNP input deck).

The mcnpPRO module uses the above tally information to determine which cells are time-dependent, then extracts the fluxes and derives the cross sections from the tally edit file. For the first time sequence, mcnpPRO takes the initial densities for the time-dependent nuclides and passes them through to ORIGEN2 via the MOCUP Processor Output Files (mpo.x), where x can be a, b,...., z depending on the number of time-dependent tally sets indentified in the MCNP input deck.

As a result of the above use of comment cards the user can input additional tallies other than the cell flux and reaction rate tallies required for cross section evaluations. The example problem MCNP input deck listed in Appendix A shows with the time-dependent flux and reaction rate tallies, seven additional tally descriptions. These additional tally descriptions begin at line 144 and end at line 195.

There is one additional flag that can be set in the MCNP input file. This flag sends a message to origenPRO by means of the mpo file. The flag is a $ placed in the column just after the last closed parentheses of one, two, or as many of the isotopes listed in the reaction rate tally block as one wants to identify. In the example problem, a $ has been placed on line 232 and 246 of the MCNP input deck (see Appendix C).

Existing ORIGEN2 cross section libraries contain (n,2n) and (n,3n) cross sections for many heavy metals. Currently, if the $ flag is not set the origenPRO module will simply zero the (n,2n) and (n,3n) cross-section values if reaction rate data are not available from MCNP through the mpo files. If the $ flag is set, the cross sections for (n,2n) and (n,3n) from the user specified ORIGEN2 cross section library are retained for the ORIGEN2 calculation if they have not been updated by MCNP.

In addition, the ORIGEN2 cross section libraries contain branching fractions to the excited state of the product nuclide for many radiative capture and (n,2n) reactions. Suitable ENDF/B cross section evaluations are not available for many MCNP materials; thus when the $ flag is set, the ORIGEN2 branching fractions are retained even through the total capture or (n,2n) cross section is being updated using MCNP-calculated fluxes and reaction rates.

An example and discussion of the example using the $ flag will be provided in section 4.3.3.

4.1.2 MCNP standard output

Since this is an output file from MCNP, there is no required user input to this file. The mcnpPRO module searches this file for the string "print table 60" so that it can extract the cell volumes and write these volumes to the MCNP Processor Output files (mpo.x).

These volumes are required so that the MCNP density unit of atoms/bn-cm can be converted to moles for the ORIGEN2 depletion step and back to atom/bn-cm for the beginning of

the next time sequence.

4.1.3 MCNP tally output

Since this is an output file from MCNP there is no required user input to this file. The mcnpPRO module extracts the cell fluxes from this file based on the information obtained from the special flux tally edits identified by the user. The mcnpPRO module uses the special reaction rate tally edit to determine the time-dependent cross sections required by the depletion step by dividing the various reaction rates by the cell fluxes.

4.2 MCNP Processor Output File

The MCNP Processor Output Files (mpo.x) are generated by mcnpPRO. These files contain the cell fluxes and radiative capture, alpha production, fission, (n,2n), and (n,3n) cross sections for the ORIGEN2 isotope depletion/generation calculation for each region identified in the MCNP input deck. The file extension .x corresponds to a, b, c, and so on, depending on the number of flux or reaction rate sets (since they are the same) identified on the MCNP input file (see section 4.1.1). For the example problem corresponding to the MCNP input deck contained in Appendix C, two mpo output files will be generated. These two files will be named mpo.a and mpo.b and will be written to the same directory where the mcnpPRO module is executed. It should be noted that when the user specifies the mpo file on the command line script or the interactive X11 window environment no extension should be added (see Appendix A for the appropriate command line script). The mpo.a and mpo.b generated files corresponding to the example problem are shown in Appendix D. For multiple time steps the mpo files are regenerated each time step using the new information from the new MCNP input deck generated by the MOCUP module compPRO.

On line one of the mpo.a file (Appendix D) we find the number .1, which corresponds to the first time step. Additional time steps will be recorded as .2, .3, and so on depending on the number of time steps needed to solve the problem at hand. Line 2 of the mpo.a file tells us that for the sample problem there is only one cell associated with the fuel region contained on the mpo.a file. Line 3 contains the following information needed by origenPRO: (1) the cell number; (2) the material identification number for the cell; (3) the total neutron flux for the cell (neutron/cm^2-sec); (4) the density associated with the cell (atom/bn-cm); and (5) the cell volume (cm^3). The MCNP fluxes are adjusted by entries in the flux multiplier table. The cell volumes are needed for density unit conversions. Line 4 gives the number of time-dependent isotopes being considered for the cell. The first number in line 5 corresponds to the MCNP isotope identification number for the first time-dependent isotope of the cell. The second number is the corresponding ORIGEN2 identification for the same isotope. The last number is the atom density for the isotope (atom/bn-cm). The information contained on line 6 tells origenPRO that for this isotope only one reaction is being considered. The second number is a flag to tell origenPRO which option to use. This flag is set in the MCNP input deck by the use of a $ (The placement of the $ is explained in section 4.1.1). If the $ sign is present in the MCNP input deck for this isotope, the

value of the second number on line 6 will read 1, otherwise it will read 0. Looking at line 54 of the mpo.a file we find that the $ flag was set for isotope 93237.55c. In the mpo.b file we find that the $ flag was set for isotope 25055.50c. The location of this flag in the input is explained in section 4.1.1. The next line, (line 7) identifies the reaction type being considered, the reaction rate divided by the neutron flux and the statistical error on the reaction rate. The statistical error on the reaction rate has not been implemented as yet, thus the value in that location is zero. There are five reaction types which may be used. MCNP can calculate information for a sixth reaction type (n,p) usually identified as (105) in MCNP input deck; however, at this time mcnpPRO can not utilize this information. The reaction types which mcnpPRO recognizes are:

1.	SNG	radiative capture	usually identified as (102) in MCNP input deck
2.	SN2N	(n,2n) reaction	usually identified as (16) in MCNP input deck
3.	SN3N	(n,3n) reaction	usually identified as (17) in MCNP input deck
4.	SNF	fission reaction	usually identified as (18) or (19) in MCNP input deck
5.	SNA	alpha production	usually identified as (107) in MCNP input deck

Each isotope identified as being time-dependent can have one to five reaction types associated with it. Looking at line 35 of the mpo.a file we see that isotope 92235.50c has four reaction types associated with it, i.e. the 4 on line 36.

If more than one cell is specified per tally set, the generated information for each additional cell is contained on the mpo file representing that set. The information on line 2 of the mpo file states how many cells have been used to represent the region. MOCUP sets no limit on the number of cells that can be used to represent a region.

4.3 ORIGEN2 Files

Data stored in the ORIGEN2 skeletal input files as well as the MOCUP Processor Output Files (mpo.x files) are used by the ORIGEN2 Pre-processor to construct the modified ORIGEN2 input files (moi.xxxx.1.inp) for each time-dependent cell. The variable xxxx stands for the cell number. These files are written to a directory called moi_files. This directory is a subdirectory of the directory where the origenPRO module is executed and must be created by the user prior to executing MOCUP.

4.3.1 ORIGEN2 Cross Section Library

Originally the skeletal file required a complete cross section/yield specification for each time-dependent nuclide (isotope) even though each nuclide cross section is updated by the

origenPRO module. The lastest release of MOCUP has eliminated the manual placement of the complete cross section/yield specification for each time-dependent nuclide with one exception. The library identification number and the nuclide identification number of the first nuclide located on the first LPU card must be specified. The details will be discussed in section 4.3.2.

To eliminate the manual placement of the nuclide cross section information in the skeletal file, the origenPRO module must have access to the cross section library of interest. This requires copying the correct cross section library to a file called ***cross.lib***. This file must reside in the directory where the origenPRO module is executed. Note the cross section libraries used by ORIGEN2 were generated to be used with a FORTRAN code. Thus, some of the cross section values in the library are given as x.xxxxxE 05, where x.xxxxx is a number. In order for MOCUP to use the information from the cross section library, the numerical format has to be of the following form for all positive exponent numbers, x.xxxxxE+05. The change can be accomplished by doing a global change to the newly created cross section library file using a text editor such as vi. *If this is not done, MOCUP will abort.*

4.3.2 ORIGEN2 Skeletal Input

These files contain the basic depletion information required by ORIGEN2. It is assumed in this discussion that the user of MOCUP is familiar with the basic input requirements for ORIGEN2 (skeletal file). There is one skeletal file required for each time-dependent flux set defined in the MCNP input deck, i.e, the number of skeletal files match the number of mpo files generated by the mcnpPRO module. Each skeletal file is identified by a unique tag, yyyyyy.zzz.x where x can be a, b, c, ..., z. The extension a, b, c, ..., z must correspond to the mpo.x file that was generated by the mcnpPRO module for the time-dependent region of interest. The value of yyyyyy can be any file name you choose to identify your run with. This name must also have an extension zzz, which you are also free to choose. Since there were two time-dependent flux regions identified for the sample problem, there are two skeletal files that must be built. The two skeletal files for the sample problem are named skeleton.inp.a (fuel region)and skeleton.inp.b (clad region). These files are listed in Appendix E.

For the identified time-dependent fuel region (skeleton.inp.a file) we are only interested in the heavy metal and fission product isotopes as noted by the activation (minus sign in front of the library number) of the heavy metal library (-205) and the fission product library (-206) on line 16 of the skeleton.inp.a file. For the clad region (skeleton.inp.b file) we are only interested in the deplection of the light elements as noted by the activation of the light metal library (-204) on line 8 of the skeleton.inp.b file.

This skeleton input file must instruct ORIGEN2 to use the density units as moles. This requires placing a value of 2 in the second location on the INP card (line 21 in the skeleton.inp.a file for the example problem, see Appendix E).

IRF or IRP entries for the desired depletion time steps are required even though MOCUP will replace the fluxes given in these entries by the MCNP computed flux contained in the approprate mpo.x files. Multiple sets of IRF or IRP commands are supported. The sample skeleton.inp.a file listed in Appendix E shows the use of two sets of IRF cards. The first set runs from line 22 to line 31 and the second set runs from line 33 to line 60. The user is free to input as many sets as are needed. IRP cards can now can be used in place of the IRF cards; however, at this time the multiplier in the flux multiplier table must be modified such that a correct flux-to-power conversion is achieved.

As stated in section 4.3.1, the library identification number and the nuclide identification number of the first nuclide located on the first LPU card must be specified. Viewing the skeleton.inp.a input file line 46 contains this information. The complete cross section/yield specification for this nuclide as well as all other time-dependent nuclides are then generated by the origenPRO module and placed in the modified ORIGEN2 input file decussed in section 4.3.3.

4.3.3 Modified ORIGEN2 Input

These files are transparently generated by origenPRO for each cell based on the information stored in mpo.x files and the ORIGEN2 skeletal input files. The user specifies the file prefix (default = moi) and origenPRO appends a cell number/time step suffix to this file name.

The generated ORIGEN2 input files (moi.1100.1.inp and moi.1300.1.inp) contained in Appendix E will now be discussed. The first 21 lines in moi.1100.1.inp are the same as listed in the skeleton.inp.a file. The flux values on line 22 through line 42 have been changed from the input value of 1.1111E+11 to 7.742750E+13, the value calculated by MCNP. Starting on line 46 and running through line 73, we see that the complete cross section/yield specification for all nuclides listed on the LPU cards have been generated. Lines 74 through 91 contain the origenPRO generated nuclide composition cards.

As stated in section 4.1.1, an example of the use of the $ flag is discussed. For the sample problem, isotopes 93237.55c and 25055.50c have been flagged. Line 2 in Appendix F contains the cross section values of (n,γ), (n,2n), (n,3n), (n,f), (n,γ^*), and (n,2n*) obtained from the ORIGEN2 cross section library. Line 4 show the values contained in the moi.1100.1.inp input file using no $ flag. As seen, the first four cross section values have been updated using information from MCNP by way of the mpo.a file. The (n,2n*) cross section has been set to zero because MCNP does not contain the needed information to calculate correct branching fractions to the excited state of the product nuclide for many radiative capture and (n,2n) reactions. Line 6 contains the cross section value writen to the moi.1100.1.inp file using the $ flag. The first, third, and fourth cross section values listed on Line 6 are the same as listed on Line 4 of Appendix F. The second cross section value is now listed as 1.028E-04 instead of the 3.978E-04 value listed on Line 4 for the no $ flag case. However, we see that a value of 2.949E-04 now appears in the (n,2n*) cross section location. This value and the value of 1.028E-04 when added together sum to 3.978E-04. Thus, when the $ flag is used, the (n,2n) cross section is split between the (n,2n)

and the (n,2n*) cross section based on the split seen using the information from the ORIGEN2 cross section library (Line 2).

The same information for isotope 25055.50c as isotope 93237.55c is listed on lines 8, 10, and 12. Line 8 in Appendix F contains the cross section values of (n,γ), (n,2n), (n,α), (n,p), (n,γ^*), and (n,2n*) obtained from the ORIGEN2 cross section library. The information from the ORIGEN2 cross section library (line 8) shows cross section values for (n,γ), (n,α) and (n,p). The cross section values for (n,2n), (n,γ^*), and (n,2n*) are all zero. Line 10 show values contained in the moi.1300.1.inp using no $ flag. We find that all the cross section values are zero except the (n,γ) value. This means that MCNP only contained information enough to compute the (n,γ) cross section, thus the other values were set to zero. Using the $ flag for this isotope we see that cross section values now exist (see line 12 in Appendix F) for (n,γ), (n,α) and (n,p). (n,γ) is the value computed by MCNP, and the (n,α) and (n,p) values are from the ORIGEN2 cross section library. We note that the (n,2n), (n,γ^*), and (n,2n*) values are all zero in the ORIGEN2 cross section library. If these values had been non-zero then non-zero values would have been written to the moi.1300.1.inp file with the $ option invoked.

4.3.3 ORIGEN2 Composition File

Each ORIGEN2 problem will create its own composition file. The origenPRO module will uniquely rename this file with the default prefix, ocf. The ocf file is then available to the origenPRO module for the next time sequence.

The compPRO module writes a new MCNP input file (mcnp.x) using information obtained from a number of sources as shown in Figure B1 (Appendix B). There is no direct user input to this process. The x in mcnp.x stands for the next time step i.e., 2, 3, ..., n, where n is the last time step in the problem. The new MCNP input file can still be modified by the user as needed, for example control changes.

4.4 Nuclide Correspondent Table (nct)

The Nuclide Correspondence Table is a user-supplied table that provides two pieces of information that are required by the MCNP Post-processor and the composition processor. First it requires the user to specify which nuclides are potentially time-dependent. It then contains both the MCNP and ORIGEN2 charge-mass identification to resolve the differences between MCNP and ORIGEN2 for this specification. The table is free format and is arranged such that each line of the table contains the following columns, ZAID(MCNP) ZAID(ORIGEN2). The ZAID(MCNP) column identifies the nuclides as input in the MCNP input deck and the ZAID(ORIGEN2) column identifies the corresponding nuclides as used in ORIGEN2. This file is used by both the MOCUP mcnpPRO and compPRO modules.

4.5 Flux Multiplier Table (FMT)

The Flux Multiplier Table is the second user-supplied table which allows the user to adjust or normalize (as in a power normalization) the MCNP fluxes prior to the depletion step. It is used by the MCNP Post-processor and can either specify a global or cell by cell multiplier. For a global multiplier the table only contains the multiplier. If a cell by cell multiplier is desired, each line of the table will contain the cell number followed by its flux multiplier. For cells that are not specified, a unit multiplier will be assumed.

5.0 MOCUP Interface

This section describes how to use the interactive MOCUP interface, which was constructed using X11/Motif. Initially it is probably most convenient to place the MOCUP program and the resource file, Mocup, in the same directory from which the user will run MCNP. Then, set the X11 environment variable, XAPPLRESDIR, to this directory. There are a number of different ways to handle this so the user may wish to check with the local UNIX or X11 expert. Also, it is important to remember that any of the MOCUP processors may be run from the command line at any point in the run sequence as long as the requisite files are available.

Once MOCUP is properly installed, the user simply issues MOCUP from the command line and something like Figure 1 should appear. If it doesn't, it is likely that your X11 server has not found the MOCUP resource file. Notice there are six buttons (selections) on the MOCUP control panel. The button labeled "toolkit" is not implemented for this version of MOCUP, but is reserved for future user monitoring, control, and housekeeping of the MOCUP processes. If the first button (labeled "mcnp") is selected by pointing to it with the mouse and depressing the left mouse button, the MCNP control panel should appear as shown in Figure 2. This control panel is used to run the MCNP problem and allows the user to specify the MCNP files that will be needed for the MOCUP processes. The various MOCUP control panels follow the same general layout, and there is a great deal of flexibility available for specifying the file names. The left column in general contains buttons, and the right column contains the file names or time step number labels. If the user selects the button labeled "Time Step Number", the file name labels to the right of the file name buttons will be automatically filled in with default file names. The user may enter a time step number in the label box to the right of the time step button by pointing to it with the mouse, depressing the left button, then entering something to identify the time sequence from the keyboard. If the user then selects the time step button, the time sequence identification will be automatically appended to the default file names.

The user may also enter or edit the file names from the keyboard. Finally, the user may depress the file name button, and the standard Motif file selection widget will appear, and the user may select the file from a list of files in the current working directory or some other directory.

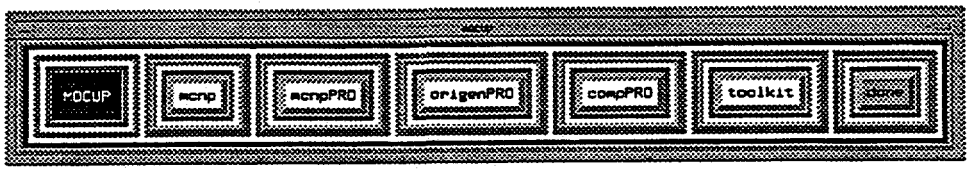

Figure 1: MOCUP Control Panel.

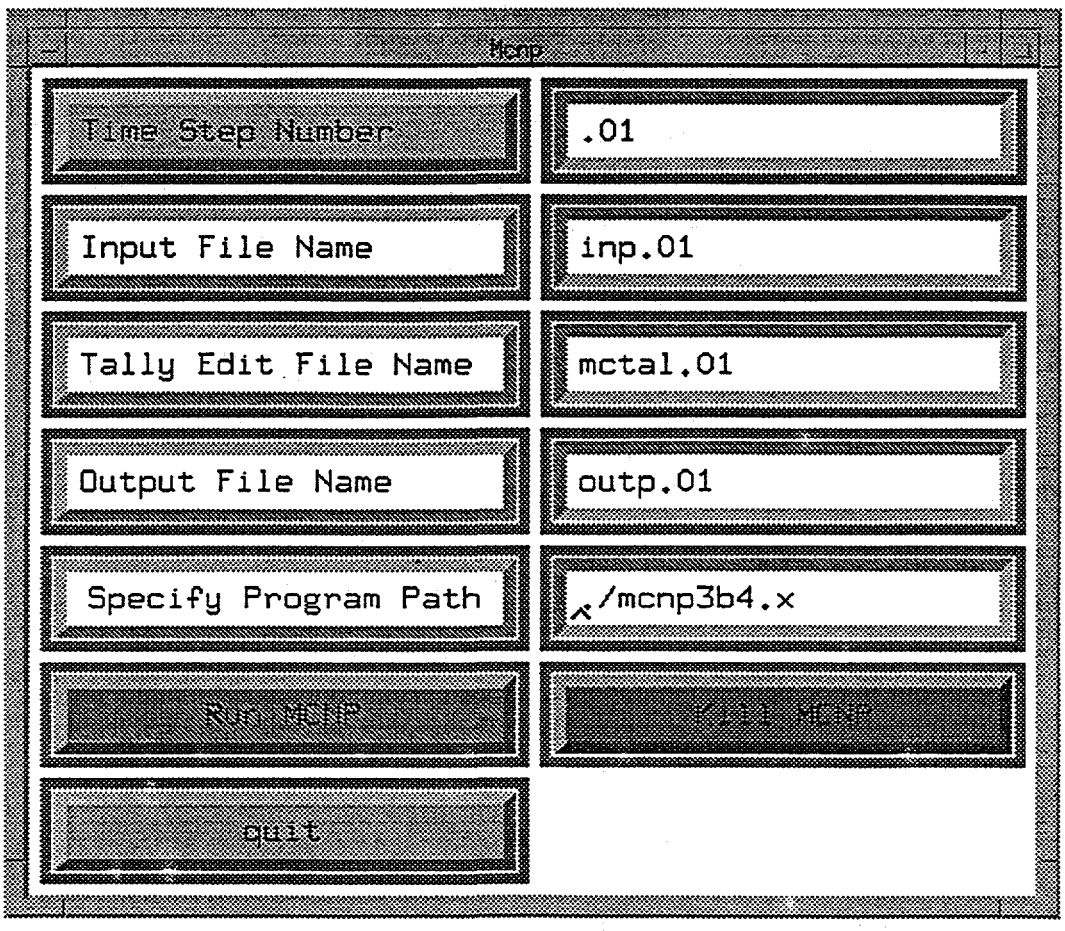

Figure 2: MCNP Control Panel.

Once the files are specified, the user may run or kill MCNP from this control panel. When the quit button from the MOCUP control panel is selected, the MCNP Post-processor (Figure 3) panel will appear. The file names can be specified as they were in the previous panel, and the MCNP Post-processor may then be run. This panel also has entries for the Nuclide Correspondence Table (section 4.4) and the search string for locating the cell volumes in the MCNP standard output file. The origenPRO selection for the MOCUP control panel brings up the control panel presented in Figure 4. The user needs to enter the file name prefix for the ORIGEN2 composition file(s). In the general case, there will be several time-dependent cells, which will be depleted separately by ORIGEN2. Each ORIGEN2 will require its own composition file, which must be uniquely identified. The MOCUP ORIGEN2 Pre-processor will automatically take care of this by appending the cell number followed by the time step sequence number to the composition file prefix. After the ORIGEN2 Pre-processor step is completed, the compPRO selection may be made from the MOCUP panel. This will display a window that looks like Figure 5. After this step is completed, the next time sequence may start with the MCNP step, which will use as the standard input, the file in the "Next MCNP File" label.

6.0 Current Restrictions

The following restrictions apply only to the MOCUP special tally edits:

- groups of cells not permitted.
- only one energy group allowed.
- no time bins
- no cosine bins.
- no detector bins.
- no user bins
- no segment bins

Users will find the restriction of only one energy group may impose hardship for the treatment of photoneutron production, which can be treated by adjusting the (n,2n) reaction in ORIGEN2. Until we remove this restriction, the user will have to manually edit the modified ORIGEN2 input files for the cases where photoneutrons are important.

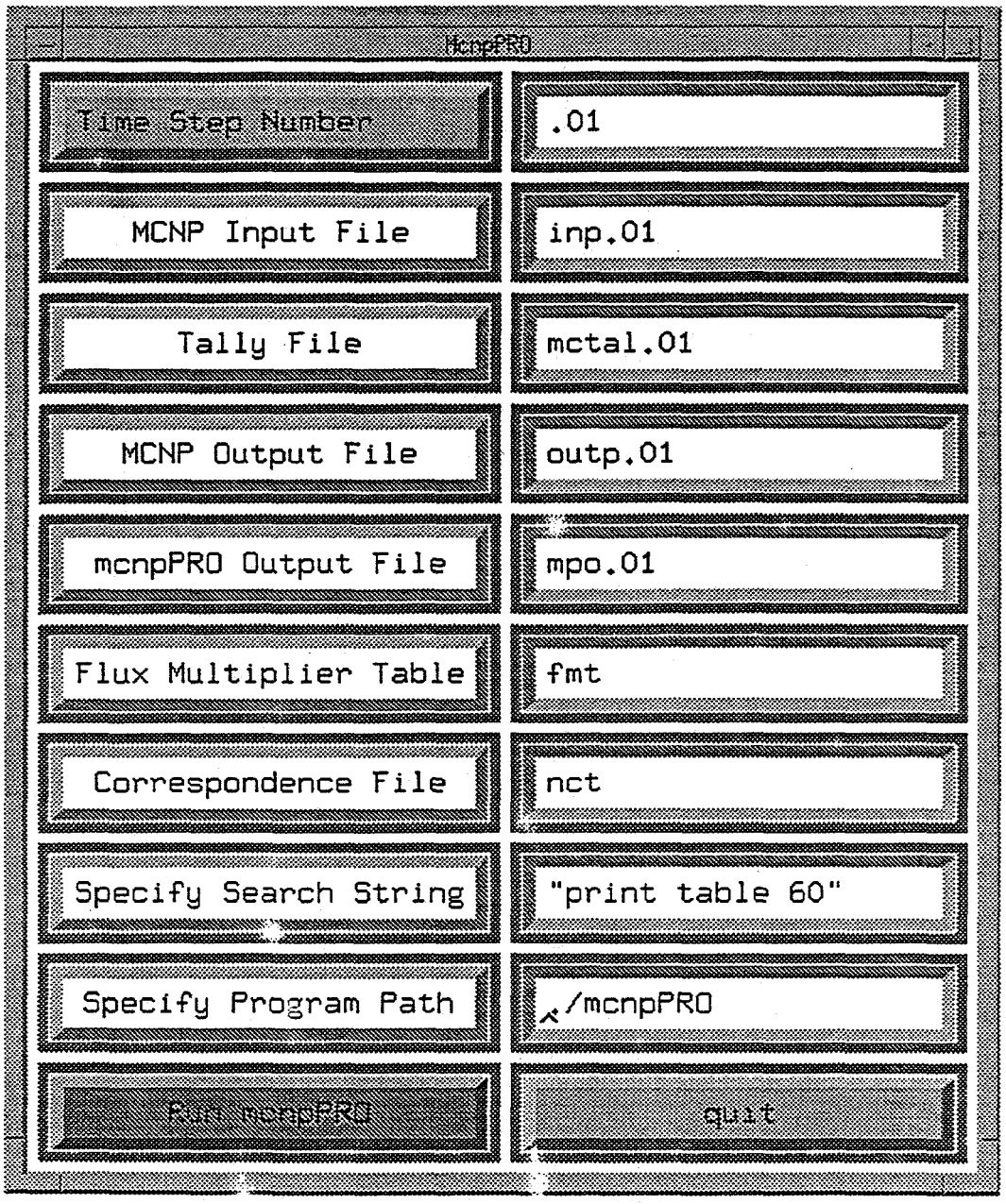

Figure 3: MCNP Post-processor Panel.

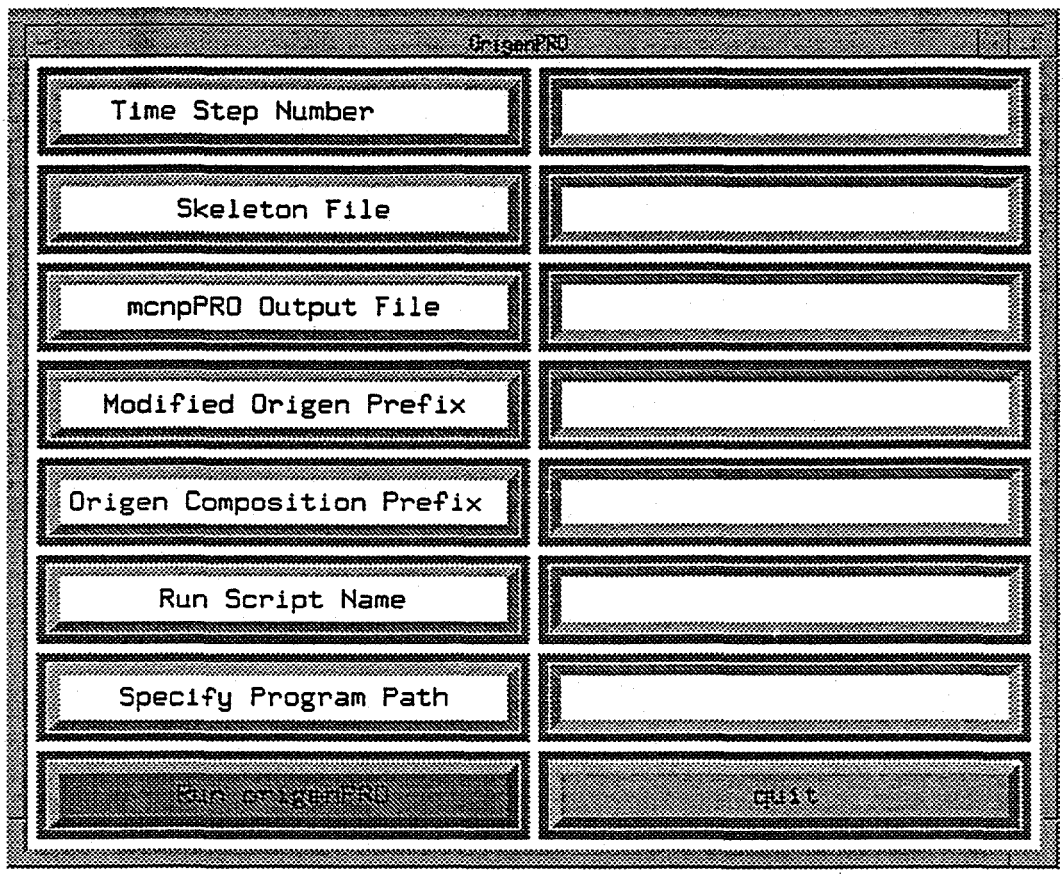

Figure 4: ORIGEN2 Pre-processor Panel.

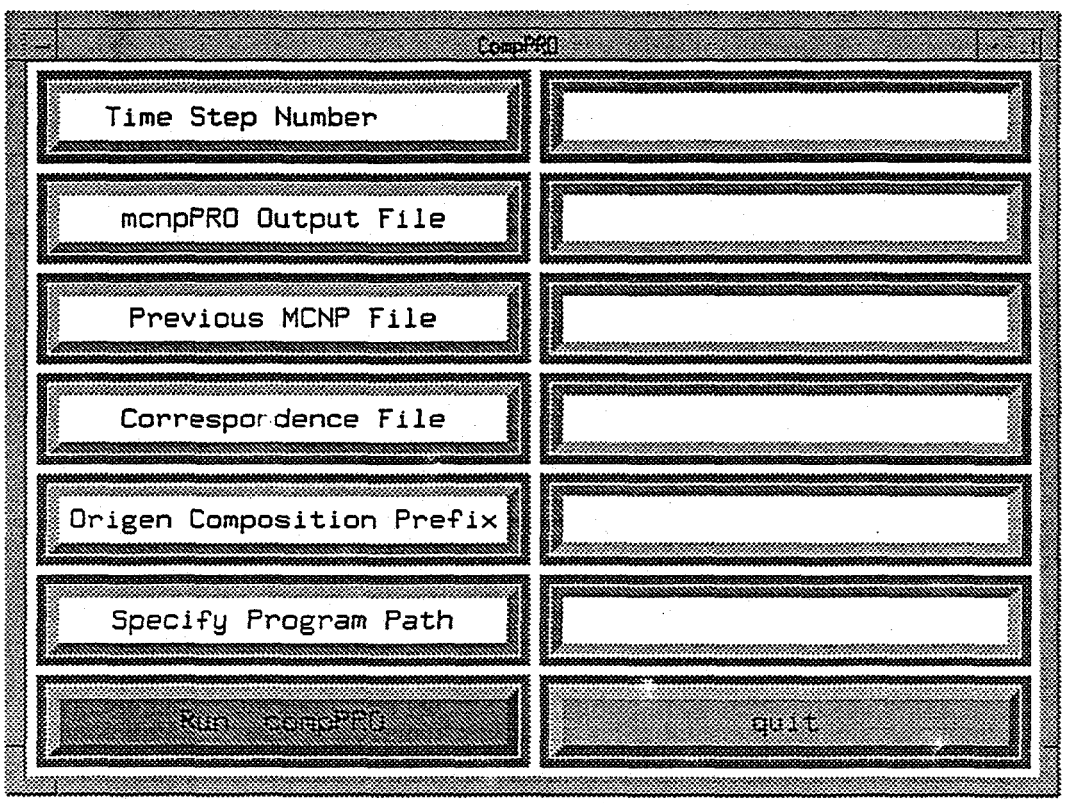

Figure 5: Composition Processor Panel.

MOCUP does not yet allow for the use of the MCNP repeated structures option. This will be implemented in a future version of the code system.

Additionally, MOCUP must have MCNP density units specified as atoms/bn-cm and ORIGEN2 density units as moles. Finally, the MCNP filenames are restricted to eight or less characters. While this may appear to the user as a MOCUP restriction, it is actually an MCNP restriction.

7.0 Future Modifications or Extensions

In the next version of MOCUP the one energy bin restriction from the special tally edits will be removed. We also plan to allow cell groupings in a later version. The use of the IRP card for constant-power depletion will be expanded. Other reactions allowed in ORIGEN2.1 (e.g., (n,p)) will be added. The use of the repeated structures option in MCNP will also be added. Finally, standalone operation will be implemented, whereby an entire multistep depletion calculation can be run with just a single user interaction. Comments from MOCUP users will be incorporated as funding permits. We also hope to improve the MOCUP interface and allow various user-monitoring of the MOCUP process.

8.0 References

[1] "MCNP - A General Monte Carlo Code for Neutron and Photon Transport Version 4a," LA-12625-M, J. F. Briesmeister, Ed., Los Alamos National Laboratory, November 1993.

[2] A. G. Croff, "ORIGEN 2.1 - Isotope Generation and Depletion Code Matrix Exponential Method," ORNL/TM-7175 (CCC-371), Oak Ridge National Laboratory, July 1980.

[3] Robert W. Scheifler, James Gettys, and Ron Newman, *X Windows System: C Library and Protocol Reference,* Digital Press, 1988.

[4] *OSF/Motif Programmers Reference*, Open Software Foundation, Prentice Hall, 1991.

[5] E. L. Redmond II, "Monte Carlo Methods, Models, and Applications for the Advanced Neutron Source," MIT Master's Thesis, Cambridge, MA (1990).

[6] C. A. Wemple, "Detailed Heat Load Calculations for the Conceptial Design of the Advanced Neutron Source Reactor," 1994 Topical Meeting on Advances in Reactor Physics, Knoxville, TN, April 11-15, 1994, Vol. III, p. 343.

APPENDIX A: Command Line Instructions

A General Comments

To allow for greater user flexibility in execution of the MOCUP modules, each module may be run from the command line. This section lists and explains the various command line instructions and arguments needed to correctly execute each module.

A.1 MCNP

The generic MCNP command line appears as:

mcnp inp=***inp*** outp=***outp*** mctal=***mctal***

where:

inp	=	input file name
outp	=	code standard output file name
mctal	=	tally output file name

Further details of the meanings, formats, and contents of these files are available in the MCNP documentation (Ref. 1), and are not reproduced here.

A.2 mcnpPRO

The following command line will execute the mcnpPRO module:

mcnpPRO timestep=***tn*** inp=***inp*** mctal=***mctal*** outp=***outp*** mpo=***mpo*** fmt=***fmt*** nct=***nct***

where:

tn	=	number of the depletion timestep (optionally appended to all filenames)
inp	=	MCNP input file name (from execution of MCNP)
mctal	=	MCNP tally output file name (from execution of MCNP)
outp	=	MCNP standard output file name (from execution of MCNP)
mpo	=	output file from mcnpPRO execution.
fmt	=	flux multiplier table (supplied by user)
nct	=	nuclide correspondence table (supplied by user)

The mpo, fmt, and nct files are explained in Chapter 4 of this document.

Following is the mcnpPRO command line used to run the example problem included with the source code.

./mcnpPRO timestep=*.1* inp=***mcnp.inp*** mctal=***mcnp.tal*** outp=***mcnp.out*** mpo=***mpo*** fmt=***mcnp.fmt*** nct=***mcnp.nct*** "'print table 60"'

The mcnpPRO command line must be one continuous line.

A.3 origenPRO

The following command line will execute the origenPRO module:

origenPRO timestep=***tn*** skeleton=***skeleton*** mpo=***mpo*** moi=***moi*** ocf=***ocf*** run=***run***

where:

tn	=	number of the depletion timestep (see A.2)
skeleton	=	name of the skeletal ORIGEN2 input file
mpo	=	output file from mcnpPRO execution
moi	=	prefix for the modified ORIGEN2 input files
ocf	=	prefix for the ORIGEN composition files created by origenPRO
run	=	name of the script used to run the ORIGEN2 cases

The mpo, moi, and ocf files are described in Chapter 4 of this document.

Following is the origenPRO command line used to run the example problem included with the source code.

./origenPRO timestep=*.1* skeleton=**skeleton.inp** mpo=***mpo*** moi=***moi*** ocf=***ocf*** run=***run***

The origenPRO command line must be one continuous line.

A.4 compPRO

The following command line will execute the compPRO module:

compPRO timestep=***tn*** mpo=***mpo*** inp=***inp*** nct=***nct*** ocf=***ocf***

where:

tn	=	number of the depletion timestep (see A.2)
mpo	=	output file from mcnpPRO execution (MOCUP Processor Output File)
inp	=	MCNP input file name (from execution of MCNP)
nct	=	nuclide correspondence table (supplied by user)
ocf	=	prefix for the ORIGEN composition files created by origenPRO

The mpo, nct, and ocf files are described in Chapter 4 of this document.

Following is the compPRO command line used to run the example problem included with the source code.

./compPRO timestep=*.1* mpo=***mpo*** inp=***mcnp.inp*** nct=***mcnp.nct*** ocf=***ocf***

The compPRO command line must be one continuous line.

APPENDIX B: MOCUP Data Flow Diagram

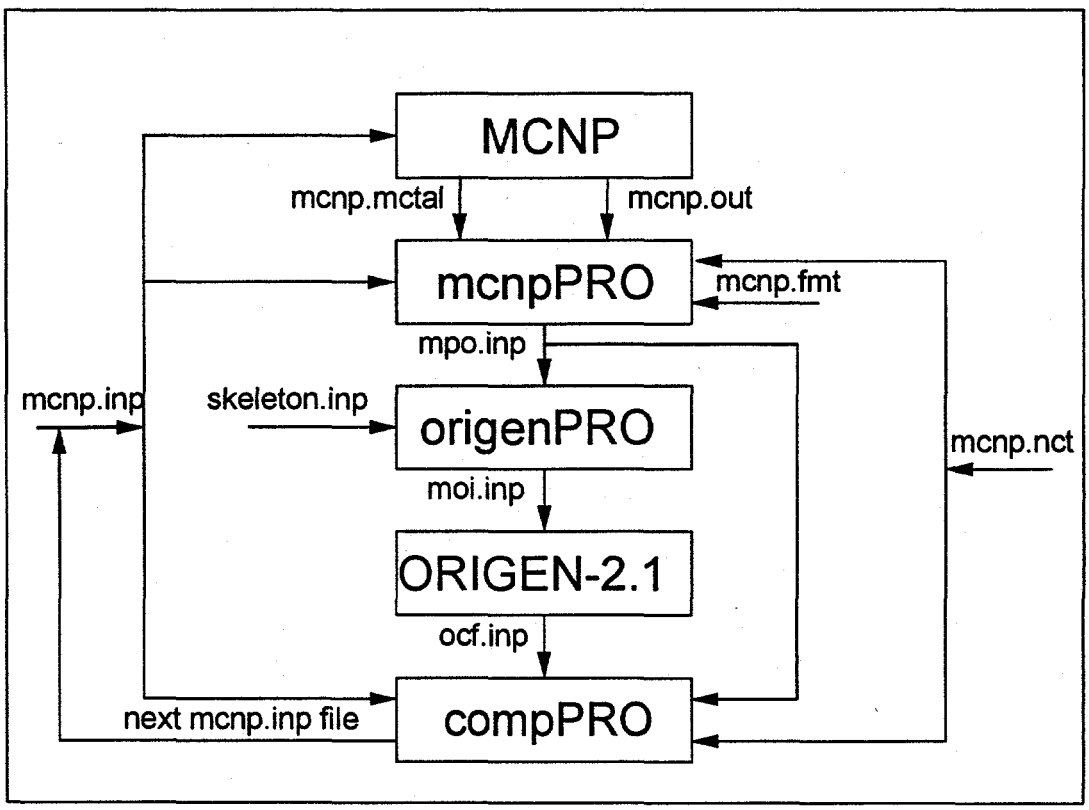

Figure B1 Linking MCNP and ORIGEN2-2.1 Using MOCUP

APPENDIX C: MCNP Input Deck For Sample Problem

```
 MTC-004/MOCUP TEST CASE/LIGHT ELEMENT DEPLETION/MULTIPLE MOCUP TALLIES
c     ------------------------------------------------------------------
c
c     SINGLE FUEL PIN FROM CE 16 X 16 BUNDLE WITH 236 FUELED LOCATIONS
c     3800 MW TOTAL THERMAL POWER IN 56,876 PINS
c     1810.957 GRAMS TOTAL URANIUM (3.0 WEIGHT PERCENT U-235)
c     66.402 KW PIN POWER FOR 300 DAYS FOR 11000 MWD/MTU
c     2 LIGHT ELEMENTS PLUS 10 FISSION PRODUCTS PLUS 8 HEAVY METALS
c
c     ------------------------------------------------------------------
c
  100  10  6.92964-2    98  -100   300  -400   500  -600    $ Lower Water
       imp:n=1   imp:p=1          vol=0.0000  tmp=2.53e-8
  200  10  6.92964-2   200  -202   300  -400   500  -600    $ Upper Water
       imp:n=1   imp:p=1          vol=0.0000  tmp=2.53e-8
 1000  10  6.92964-2               1300                      $ Unit Cell Water
                      500  -600    300  -400   100  -200    $ Unit Cell Water
       imp:n=1   imp:p=1          vol=342.795 tmp=2.53e-8
 1100  11  6.75077-2                     -1100   100  -200    $ Fuel Pin
       imp:n=1   imp:p=1          vol=0.0000  tmp=2.53e-8
 1200  12  1.00000-4               1100 -1200   100  -200    $ Gap
       imp:n=1   imp:p=1          vol=0.0000  tmp=2.53e-8
 1300  13  4.34907-2               1200 -1300   100  -200    $ Clad
       imp:n=1   imp:p=1          vol=0.0000  tmp=2.53e-8
 9999   0              (-98:202:-300:400:-500:600)            $ External Void
       imp:n=0   imp:p=0          vol=0.0000  tmp=2.53e-8
c
c      BLANK LINE MUST FOLLOW
c
c          SURFACE DEFINITIONS
c
    98   pz  -220.500                    $ bottom of water reflector
   100   pz  -190.500                    $ bottom of active core
   200   pz   190.500                    $ top of active core
   202   pz   220.500                    $ top of water reflector
  *300   px    -0.640                    $ low-x edge of unit cell
  *400   px     0.640                    $ high-x edge of unit cell
  *500   py    -0.640                    $ low-y edge of unit cell
  *600   py     0.640                    $ high-y edge of unit cell
  1100   cz     0.41250                  $ Fuel Pin
  1200   cz     0.42140                  $ Gap
  1300   cz     0.48490                  $ Clad
c
c       MATERIALS
c
awtab   44103 102.022000    45105 104.005000   53129 127.797997
        54133 131.764008    55134 132.757004   56140 138.709000
        57140 138.707993    58141 139.697998   58143 141.684998
        59143 141.682999    60147 145.654000   61147 145.653000
```

```
          61148 146.647000    61149 147.639000   61151 149.625000
          62151 149.623000    62153 151.608002   63155 153.592000
          63156 154.585007
c
c
c     H2O (2200 PSI at 600 F)      (6.92964e-2)
m10      8016.50c   2.30988e-2
          1001.50c   4.61976e-2
mt10      lwtr.04t
c
c     3.0 wt% U-235                (6.75077e-2)
m11     1001.50c  1.0000e-24   5010.50c  2.0000e-09   5011.56c   8.0000e-09
         8016.50c  4.50051e-02   45105.50c  1.0000e-24   54133.60c  1.0000e-24
         43099.50c  1.0000e-24   54135.50c  1.0000e-24   55133.50c  1.0000e-24
         59143.60c  1.0000e-24   61147.50c  1.0000e-24   62149.50c  1.0000e-24
         62151.50c  1.0000e-24   62152.50c  1.0000e-24   92235.50c  6.83451e-04
         92238.50c  2.18191e-02   93236.35c  1.0000e-24   93237.55c  1.0000e-24
         93238.35c  1.0000e-24   94238.50c  1.0000e-24   94239.55c  1.0000e-24
         94240.50c  1.0000e-24
mt11     lwtr.04t
c
c     Helium                       (1.00000e-4)
m12      2004.50c   1.00000e-4
c
c     Zircaloy-4                   (4.34907-2)
m13     40000.50c   4.34907-2
          1001.50c   5.08762-5
          5010.50c   2.39624-8
          5011.56c   9.64516-8
          6000.50c   3.94087-5
          7014.50c   2.25294-5
          8016.50c   2.34213-4
         13027.50c   3.50863-6
         16032.50c   4.30621-6
         22000.50c   1.64699-6
         23000.50c   1.54865-6
         24000.50c   9.48258-5
         25055.50c   1.43600-6
         26000.55c   1.58920-4
         27059.50c   6.69303-7
         28000.50c   1.34397-6
         29000.50c   1.24145-6
         48000.50c   8.77257-9
         50000.35c   5.31719-4
         72000.50c   1.72375-6
         74000.55c   4.29083-7
c
c      Tally Materials
c
m701     5010.50c  1.00000
m702     5011.56c  1.00000
```

```
m703     25055.50c  1.00000
m704     27059.50c  1.00000
m801     43099.50c  1.00000
m802     45105.50c  1.00000
m803     54133.60c  1.00000
m804     54135.50c  1.00000
m805     55133.50c  1.00000
m806     59143.60c  1.00000
m807     61147.50c  1.00000
m808     62149.50c  1.00000
m809     62151.50c  1.00000
m810     62152.50c  1.00000
m901     92235.50c  1.00000
m902     92238.50c  1.00000
m903     93236.35c  1.00000
m904     93237.55c  1.00000
m905     93238.35c  1.00000
m906     94238.50c  1.00000
m907     94239.55c  1.00000
m908     94240.50c  1.00000
c
ksrc   0.000     0.000   -175.0
       0.000     0.000   -150.0
       0.000     0.000   -125.0
       0.000     0.000   -100.0
       0.000     0.000    -75.0
       0.000     0.000    -50.0
       0.000     0.000    -25.0
       0.000     0.000      0.0
       0.000     0.000     25.0
       0.000     0.000     50.0
       0.000     0.000     75.0
       0.000     0.000    100.0
       0.000     0.000    125.0
       0.000     0.000    150.0
       0.000     0.000    175.0
c
c      ********** TALLY DESCRIPTIONS******************************
c      defaults
c
fq0    e f
c
c      ------------------------------------------------------------
c
fc14  Cell-Averaged Neutron Flux (neutrons/cm**2 per source neutron)
e14    5.32-7   5.53-3   0.821   6.8   10.0   20.0
f14:n
        1100   1300                          $ FUEL AND CLAD ZONES
c
c      ------------------------------------------------------------
c
```

```
fc24  Cell-Averaged Photon Flux (photons/cm**2 per source neutron)
e24   6.75  7.0  8.0  9.0  10.0  11.0  12.0  20.0
f24:p
        1100   1300                              $ FUEL AND CLAD ZONES
c
c     ---------------------------------------------------------------
c
fc16   Cell-Averaged Neutron Energy Deposition (Mev/gram per source neutron)
e16    5.32-7   5.53-3   0.821   6.8   10.0   20.0
f16:n
        1100   1300                              $ FUEL AND CLAD ZONES
c
c     ---------------------------------------------------------------
c
fc26   Cell-Averaged Photon Energy Deposition (Mev/gram per source neutron)
e26   6.75  7.0  8.0  9.0  10.0  11.0  12.0  20.0
f26:p
        1100   1300                              $ FUEL AND CLAD ZONES
c
c     ---------------------------------------------------------------
c
fc36   Cell-Averaged N-P Energy Deposition (Mev/gram per source neutron)
e36    5.32-7   5.53-3   0.821   6.8   10.0   20.0
f36:n,p
        1100   1300                              $ FUEL AND CLAD ZONES
c
c
---------------------------------------------------------------------
c
fc47   Cell-Averaged Fission Energy Deposition (Mev/gram per source neutron)
e47    5.32-7   5.53-3   0.821   6.8   10.0   20.0
f47:n
        1100                                          $ FUEL ZONE
c
c     ---------------------------------------------------------------
c
c      (total fuel volume = 67566.03 cm*3)
fc54    Total Fissions        Total Fission Neutrons
fm54   (-67566.03    11  (-6)  (-6 -7))
e54    5.32-7   5.53-3   0.821   6.8   10.0   20.0
f54:n
        1100                                          $ FUEL ZONE
      t
c
c     ---------------------------------------------------------------
c
c    begin_mocup_flux_tallies
c    time dependent flux
fc84  Cell-Averaged Neutron Flux (neutrons/cm**2 per source neutron)
f84:n
        1100                                        $ FUEL ZONE
```

```
c
c     ---------------------------------------------------------------------
c
c    time dependent flux
fc94  Cell-Averaged Neutron Flux (neutrons/cm**2 per source neutron)
f94:n
       1300                                                  $ CLAD ZONE
c    end_mocup_flux_tallies
c
c    ---------------------------------------------------------------------
c
c    begin_mocup_reaction_rate_tallies
c    time dependent reaction rates
fc804  (n,2n)/(n,f)/(n,gamma) for heavy metals; (n,gamma) for fission products
f804:n
       1100                                                  $ FUEL ZONE
fm804   (1.0  801                      (102))
        (1.0  802                      (102))
        (1.0  803                      (102))
        (1.0  804                      (102))
        (1.0  805                      (102))
        (1.0  806                      (102))
        (1.0  807                      (102))
        (1.0  808                      (102))
        (1.0  809                      (102))
        (1.0  810                      (102))
        (1.0  901  (16)(17)    (19:20)(102))
        (1.0  902  (16)(17)    (19:20)(102))
        (1.0  903  (16)(17)    (19)   (102))
        (1.0  904  (16)(17)(18)       (102))$
        (1.0  905  (16)(17)    (19)   (102))
        (1.0  906  (16)(17)    (19:20)(102))
        (1.0  907  (16)(17)(18)       (102))
        (1.0  908  (16)(17)    (19:20)(102))
c
c     ---------------------------------------------------------------------
c
c    time dependent reaction rates
fc904  (n,2n)/(n,f)/(n,gamma) for heavy metals; (n,gamma) for fission products
f904:n
       1300                                                  $ CLAD ZONE
fm904   (1.0  701            (107)    (102))
        (1.0  702                      (102))
        (1.0  703                      (102))$
        (1.0  704                      (102))
c    end_mocup_reaction_rate_tallies
c
c     ---------------------------------------------------------------------
```

```
c
mode    n p
kcode   1000    1.0     5   55
prdmp   55 55 55
print  -60 -85 -130 -140
```

APPENDIX D: Mpo.a and Mpo.b Output Files From Sample Problem

mpo.a file

```
1    .1
2    1
3     1100  11  7.742750E+13  6.750770E-02  2.036680E+02
4      18
5      43099.50c 430990 1.000000E-24
6       1  0
7       SNG 9.131381E+00 0.000000
8      45105.50c 451050 1.000000E-24
9       1  0
10      SNG 1.594601E+03 0.000000
11     54133.60c 541330 1.000000E-24
12      1  0
13      SNG 2.329663E+01 0.000000
14     54135.50c 541350 1.000000E-24
15      1  0
16      SNG 2.189532E+05 0.000000
17     55133.50c 551330 1.000000E-24
18      1  0
19      SNG 1.093679E+01 0.000000
20     59143.60c 591430 1.000000E-24
21      1  0
22      SNG 1.157516E+01 0.000000
23     61147.50c 611470 1.000000E-24
24      1  0
25      SNG 6.171671E+01 0.000000
26     62149.50c 621490 1.000000E-24
27      1  0
28      SNG 6.881470E+03 0.000000
29     62151.50c 621510 1.000000E-24
30      1  0
31      SNG 6.344025E+02 0.000000
32     62152.50c 621520 1.000000E-24
33      1  0
34      SNG 9.494805E+01 0.000000
35     92235.50c 922350 6.834510E-04
36      4  0
37      SN2N 2.307836E-03 0.000000
38      SN3N 3.018256E-06 0.000000
39      SNF 4.703962E+01 0.000000
40      SNG 1.044616E+01 0.000000
41     92238.50c 922380 2.181910E-02
42      4  0
43      SN2N 4.378302E-03 0.000000
44      SN3N 3.985044E-05 0.000000
45      SNF 9.456511E-02 0.000000
46      SNG 8.409221E-01 0.000000
47     93236.35c 932360 1.000000E-24
```

```
 4  0
 SN2N 3.694824E-03 0.000000
 SN3N 1.630816E-05 0.000000
 SNF 2.467573E+02 0.000000
 SNG 9.258662E+00 0.000000
93237.55c 932370 1.000000E-24
 4 1
 SN2N 3.977605E-04 0.000000
 SN3N 6.623422E-06 0.000000
 SNF 4.963559E-01 0.000000
 SNG 3.715230E+01 0.000000
93238.35c 932380 1.000000E-24
 4  0
 SN2N 4.332750E-03 0.000000
 SN3N 3.019986E-05 0.000000
 SNF 2.037287E+02 0.000000
 SNG 9.258662E+00 0.000000
94238.50c 942380 1.000000E-24
 4  0
 SN2N 1.176752E-03 0.000000
 SN3N 4.673727E-05 0.000000
 SNF 2.413083E+00 0.000000
 SNG 3.562882E+01 0.000000
94239.55c 942390 1.000000E-24
 4  0
 SN2N 9.621763E-04 0.000000
 SN3N 2.408008E-06 0.000000
 SNF 1.238030E+02 0.000000
 SNG 7.122405E+01 0.000000
94240.50c 942400 1.000000E-24
 4  0
 SN2N 4.056298E-04 0.000000
 SN3N 6.413690E-06 0.000000
 SNF 5.675296E-01 0.000000
 SNG 2.339750E+02 0.000000
```

mpo.b file

```
.1
1
 1300  13  7.752930E+13  4.349070E-02  6.888430E+01
  4
 5010.50c 50100 2.396240E-08
  2  0
  SNA 3.525403E+02 0.000000
  SNG 4.585647E-02 0.000000
 5011.56c 50110 9.645160E-08
  1  0
```

```
11          SNG 4.698920E-04 0.000000
12         25055.50c 250550 1.436000E-06
13          1  1
14          SNG 1.491668E+00 0.000000
15         27059.50c 270590 6.693030E-07
16          1  0
17          SNG 5.246714E+00 0.000000
```

APPENDIX E: Skeletal Input Files And Modified ORIGEN2 Input Files For Sample Problem

skeleton.inp.a

```
1       -1
2       -1
3       -1
4       TIT   PWR FUEL PIN/0 TO 60 DAYS IRRADIATION
5       BAS   PWR FUEL PIN (CE 16 X 16 BUNDLE) 1810.957 G U 3 WT% U-235
6       LIP   0 0 0
7       LPU           922350                  922380
8                     932360  932370  932380
9                     942380  942390  942400                          -1
10      LPU   430990                                        451050
11                                                          541330
12            551330          541350
13                            591430                        611470
14                                          621490
15            621510  621520                                          -1
16      LIB   0 0 2 3     0 -205 -206 9 50 0 4 0
17      OPTL  8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
18      OPTA  8 8 7 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
19      OPTF  8 8 7 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
20      CUT   3 1.0E-24  28 1.0E-75          -1
21      INP   1  2  -1  -1  1  1
22      IRF      3.0     1.1111E+11     1    2   4   2
23      IRF      6.0     1.1111E+11     2    3   4   0
24      IRF      9.0     1.1111E+11     3    4   4   0
25      IRF     12.0     1.1111E+11     4    5   4   0
26      IRF     15.0     1.1111E+11     5    6   4   0
27      IRF     18.0     1.1111E+11     6    7   4   0
28      IRF     21.0     1.1111E+11     7    8   4   0
29      IRF     24.0     1.1111E+11     8    9   4   0
30      IRF     27.0     1.1111E+11     9   10   4   0
31      IRF     30.0     1.1111E+11    10   11   4   0
32      OUT     11   1  0   0
33      IRF     33.0     1.1111E+11    11    1   4   0
34      IRF     36.0     1.1111E+11     1    2   4   0
35      IRF     39.0     1.1111E+11     2    3   4   0
36      IRF     42.0     1.1111E+11     3    4   4   0
37      IRF     45.0     1.1111E+11     4    5   4   0
38      IRF     48.0     1.1111E+11     5    6   4   0
39      IRF     51.0     1.1111E+11     6    7   4   0
40      IRF     54.0     1.1111E+11     7    8   4   0
41      IRF     57.0     1.1111E+11     8    9   4   0
42      IRF     60.0     1.1111E+11     9   10   4   0
43      PCH      0   10  10
44      OUT     10   1  0   0
45      STP   4
```

```
46      205  922350
47      2   922350
48      0
```

moi.1100.1.inp file

```
 1      -1
 2      -1
 3      -1
 4      TIT   PWR FUEL PIN/0 TO 60 DAYS IRRADIATION
 5      BAS   PWR FUEL PIN (CE 16 X 16 BUNDLE) 1810.957 G U 3 WT% U-235
 6      LIP   0 0 0
 7      LPU           922350                  922380
 8                    932360  932370  932380
 9                    942380  942390  942400                          -1
10      LPU   430990                                        451050
11                                                          541330
12            551330          541350
13                            591430                        611470
14                                            621490
15            621510  621520                                -1
16      LIB   0 0 2 3     0 -205 -206 9 50 0 4 0
17      OPTL  8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
18      OPTA  8 8 7 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
19      OPTF  8 8 7 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
20      CUT   3 1.0E-24  28 1.0E-75          -1
21      INP   1  2  -1  -1  1  1
22      IRF  3.000000 7.742750E+13 1 2 4 2
23      IRF  6.000000 7.742750E+13 2 3 4 0
24      IRF  9.000000 7.742750E+13 3 4 4 0
25      IRF  12.000000 7.742750E+13 4 5 4 0
26      IRF  15.000000 7.742750E+13 5 6 4 0
27      IRF  18.000000 7.742750E+13 6 7 4 0
28      IRF  21.000000 7.742750E+13 7 8 4 0
29      IRF  24.000000 7.742750E+13 8 9 4 0
30      IRF  27.000000 7.742750E+13 9 10 4 0
31      IRF  30.000000 7.742750E+13 10 11 4 0
32      OUT     11   1  0   0
33      IRF  33.000000 7.742750E+13 11 1 4 0
34      IRF  36.000000 7.742750E+13 1 2 4 0
35      IRF  39.000000 7.742750E+13 2 3 4 0
36      IRF  42.000000 7.742750E+13 3 4 4 0
37      IRF  45.000000 7.742750E+13 4 5 4 0
38      IRF  48.000000 7.742750E+13 5 6 4 0
39      IRF  51.000000 7.742750E+13 6 7 4 0
40      IRF  54.000000 7.742750E+13 7 8 4 0
41      IRF  57.000000 7.742750E+13 8 9 4 0
42      IRF  60.000000 7.742750E+13 9 10 4 0
43      PCH     0   10  10
44      OUT     10   1  0   0
```

```
  STP   4
205 922350 1.045E+01 2.308E-03 3.018E-06 4.704E+01 0.000E+00 0.000E+00 -1.000000
205 922380 8.409E-01 4.378E-03 3.985E-05 9.457E-02 0.000E+00 0.000E+00 -1.000000
205 932360 9.259E+00 3.695E-03 1.631E-05 2.468E+02 0.000E+00 0.000E+00 -1.000000
205 932370 3.715E+01 1.028E-04 6.623E-06 4.964E-01 0.000E+00 2.949E-04 -1.000000
205 932380 9.259E+00 4.333E-03 3.020E-05 2.037E+02 0.000E+00 0.000E+00 -1.000000
205 942380 3.563E+01 1.177E-03 4.674E-05 2.413E+00 0.000E+00 0.000E+00 -1.000000
205 942390 7.122E+01 9.622E-04 2.408E-06 1.238E+02 0.000E+00 0.000E+00 -1.000000
205 942400 2.340E+02 4.056E-04 6.414E-06 5.675E-01 0.000E+00 0.000E+00 -1.000000
206 430990 9.131E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     2.98E-09 8.61E-06 4.16E-05 3.24E-09 6.23E-06 2.04E-07 2.03E-07 2.03E-07
206 451050 1.595E+03 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     4.09E-10 3.45E-07 5.20E-03 4.41E-06 6.55E-05 1.75E-06 1.78E-06 1.78E-06
206 541330 2.330E+01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     5.43E-05 1.53E-02 8.79E-04 3.32E-03 1.02E-02 1.06E-03 1.06E-03 1.06E-03
206 551330 1.094E+01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     7.46E-09 3.69E-05 4.46E-05 1.68E-05 1.52E-05 4.27E-07 4.26E-07 4.26E-07
206 541350 2.190E+05 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     2.01E-02 5.38E-01 9.78E-02 7.85E-02 4.61E-01 9.46E-02 9.44E-02 9.44E-02
206 591430 1.158E+01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     3.99E-07 1.51E-04 2.95E-06 2.80E-07 9.17E-06 2.69E-06 2.69E-06 2.69E-06
206 611470 6.172E+01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     7.78E-10 3.33E-06 2.73E-07 9.06E-05 2.10E-07 2.35E-08 2.35E-08 2.35E-08
206 621490 6.881E+03 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     3.62E-11 2.98E-07 6.53E-09 4.18E-10 1.91E-08 3.48E-09 3.48E-09 3.48E-09
206 621510 6.344E+02 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     3.75E-08 8.39E-05 3.80E-06 3.22E-04 2.47E-05 6.19E-06 6.18E-06 6.18E-06
206 621520 9.495E+01 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.000000
 206     5.69E-07 6.41E-04 4.65E-05 1.45E-05 3.29E-04 8.19E-05 8.17E-05 8.17E-05
3 430990 3.381989E-22 0 0.0
3 451050 3.381989E-22 0 0.0
3 541330 3.381989E-22 0 0.0
3 541350 3.381989E-22 0 0.0
3 551330 3.381989E-22 0 0.0
3 591430 3.381989E-22 0 0.0
3 611470 3.381989E-22 0 0.0
3 621490 3.381989E-22 0 0.0
3 621510 3.381989E-22 0 0.0
3 621520 3.381989E-22 0 0.0
2 922350 2.311424E-01 0 0.0
2 922380 7.379196E+00 0 0.0
2 932360 3.381989E-22 0 0.0
2 932370 3.381989E-22 0 0.0
2 932380 3.381989E-22 0 0.0
2 942380 3.381989E-22 0 0.0
2 942390 3.381989E-22 0 0.0
2 942400 3.381989E-22 0 0.0
0
```

Skeleton.inp.b

```
 1       -1
 2       -1
 3       -1
 4       TIT   PWR FUEL PIN CLAD/0 TO 60 DAYS IRRADIATION
 5       BAS   PWR FUEL PIN CLAD (CE 16 X 16 BUNDLE) 1810.957 G U 3 WT% U-235
 6       LIP   0 0 0
 7       LPU    50100   50110   250550   270590                          -1
 8       LIB   0 1 2 3  -204 205 206 9 50 0 4 0
 9       OPTL  8 8 7 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
10       OPTA  8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
11       OPTF  8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
12       CUT   3 1.0E-24  28 1.0E-75          -1
13       INP   1  2  -1  -1  1  1
14       IRF      3.0    1.1111E+11     1    2   4   2
15       IRF      6.0    1.1111E+11     2    3   4   0
16       IRF      9.0    1.1111E+11     3    4   4   0
17       IRF     12.0    1.1111E+11     4    5   4   0
18       IRF     15.0    1.1111E+11     5    6   4   0
19       IRF     18.0    1.1111E+11     6    7   4   0
20       IRF     21.0    1.1111E+11     7    8   4   0
21       IRF     24.0    1.1111E+11     8    9   4   0
22       IRF     27.0    1.1111E+11     9   10   4   0
23       IRF     30.0    1.1111E+11    10   11   4   0
24       OUT     11   1  0   0
25       IRF     33.0    1.1111E+11    11    1   4   0
26       IRF     36.0    1.1111E+11     1    2   4   0
27       IRF     39.0    1.1111E+11     2    3   4   0
28       IRF     42.0    1.1111E+11     3    4   4   0
29       IRF     45.0    1.1111E+11     4    5   4   0
30       IRF     48.0    1.1111E+11     5    6   4   0
31       IRF     51.0    1.1111E+11     6    7   4   0
32       IRF     54.0    1.1111E+11     7    8   4   0
33       IRF     57.0    1.1111E+11     8    9   4   0
34       IRF     60.0    1.1111E+11     9   10   4   0
35       PCH     10   10  10
36       OUT     10   1  0   0
37       STP   4
38      204   50100
39      1    50100
40      0
```

moi.1300.1.inp file

```
-1
-1
-1
TIT   PWR FUEL PIN CLAD/0 TO 60 DAYS IRRADIATION
BAS   PWR FUEL PIN CLAD (CE 16 X 16 BUNDLE) 1810.957 G U 3 WT% U-235
LIP   0 0 0
LPU    50100   50110   250550   270590                          -1
LIB   0 1 2 3  -204 205 206 9 50 0 4 0
OPTL  8 8 7 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
OPTA  8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
OPTF  8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8 8   8 8 8 8
CUT   3 1.0E-24  28 1.0E-75          -1
INP   1  2  -1  -1  1  1
IRF  3.000000 7.752930E+13 1 2 4 2
IRF  6.000000 7.752930E+13 2 3 4 0
IRF  9.000000 7.752930E+13 3 4 4 0
IRF  12.000000 7.752930E+13 4 5 4 0
IRF  15.000000 7.752930E+13 5 6 4 0
IRF  18.000000 7.752930E+13 6 7 4 0
IRF  21.000000 7.752930E+13 7 8 4 0
IRF  24.000000 7.752930E+13 8 9 4 0
IRF  27.000000 7.752930E+13 9 10 4 0
IRF  30.000000 7.752930E+13 10 11 4 0
OUT     11   1  0   0
IRF  33.000000 7.752930E+13 11 1 4 0
IRF  36.000000 7.752930E+13 1 2 4 0
IRF  39.000000 7.752930E+13 2 3 4 0
IRF  42.000000 7.752930E+13 3 4 4 0
IRF  45.000000 7.752930E+13 4 5 4 0
IRF  48.000000 7.752930E+13 5 6 4 0
IRF  51.000000 7.752930E+13 6 7 4 0
IRF  54.000000 7.752930E+13 7 8 4 0
IRF  57.000000 7.752930E+13 8 9 4 0
IRF  60.000000 7.752930E+13 9 10 4 0
PCH     10   10  10
OUT     10   1  0   0
STP   4
204 50100 4.586E-02 0.000E+00 3.525E+02 0.000E+00 0.000E+00 0.000E+00 -1.000000
204 50110 4.699E-04 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 -1.000000
204 250550 1.492E+00 0.000E+00 3.210E-05 3.698E-04 0.000E+00 0.000E+00 -1.000000
204 270590 5.247E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 -1.000000
1 50100 2.740943E-06 0 0.0
1 50110 1.103263E-05 0 0.0
1 250550 1.642571E-04 0 0.0
1 270590 7.655832E-05 0 0.0
0
```

APPENDIX F: Data Showing Differences In The Use Of The $ Flag In The MCNP Input Deck

1 Values from ORIGEN library for nuclide 932370

2 205 932370 3.212E+01 2.746E-04 2.912E-06 5.244E-01 0.000E+00 7.877E-04 -1.000000

3 Values using no $ flag for nuclide 932370 cell 1100

4 205 932370 3.715E+01 3.978E-04 6.623E-06 4.964E-01 0.000E+00 0.000E+00 -1.000000

5 Values using $ flag for nuclide 932370 cell 1100

6 205 932370 3.715E+01 1.028E-04 6.623E-06 4.964E-01 0.000E+00 2.949E-04 -1.000000

7 Values from ORIGEN library for nuclide 250550

8 204 250550 1.523E+00 0.000E+00 3.210E-05 3.698E-04 0.000E+00 0.000E+00 -1.000000

9 Values using no $ flag for nuclide 250550 cell 1300

10 204 250550 1.492E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 -1.000000

11 Values using $ flag for nuclide 250550 cell 1300

12 204 250550 1.492E+00 0.000E+00 3.210E-05 3.698E-04 0.000E+00 0.000E+00 -1.000000