LA-UR-00-5314

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Author(s): Holly R. Trellue and David I. Poston

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MONTEBURNS: A MONTE CARLO BURNUP CODE FOR ACCELERATOR APPLICATIONS

by
Holly R. Trellue and David I. Poston
Los Alamos National Laboratory

ABSTRACT

Monteburns is a fully automated tool that links the Monte Carlo transport code MCNP with the radioactive decay and burnup code ORIGEN2. *Monteburns* produces criticality and burnup results based on various material feed/removal specifications, power(s), and time intervals. The program processes the input from the user that specifies the system geometry, initial material compositions, feed/removal specifications, and other code-specific parameters. Various results from MCNP, ORIGEN2, and other calculations then are output successively as the code runs. The principal function of *monteburns* is to transfer one-group, cross-section, and flux values from MCNP to ORIGEN2 and then transfer the resulting material compositions (after irradiation and/or decay) from ORIGEN2 back to MCNP in a repeated, cyclic fashion. The basic requirement of the code is that the user have a working MCNP input file and other input parameters; all interaction with ORIGEN2 and other calculations are performed by *monteburns*. Some of the latest modifications to *monteburns* include compatibility with MCNPX, more flexibility with source terms, and the ability to set a beginning-of-life desired range of k_{eff} for each cycle and have *monteburns* perform iterations on the feed rate to achieve that range.

1.0. INTRODUCTION

The past few decades have brought significant changes in several areas, two of which include the nuclear industry and computer technology. Because the restrictions placed on and the costs associated with experimental facilities have increased (because of environmental and radiological health concerns), the value of computer modeling has increased. It has become possible to model many varieties of nuclear systems (including full reactor cores) and perform complex decay and burnup calculations in a matter of minutes. With the increase in computer technology, the number of computer codes available to perform nuclear-related calculations has increased, and often the user wants to run two or more codes concurrently. Thus, many linkage codes have been written to allow concurrent use of these primary codes in an automated fashion. Two popular codes used in the design of nuclear systems are Monte Carlo N-Particle

(MCNP™) and ORIGEN2,* and the code presented in this paper is a linkage code for these two.

MCNP is widely used to perform Monte Carlo calculations of neutron, photon, and/or electron transport[1] and is primarily used to determine how particles behave within an exact geometry and material composition. However, it cannot determine the effect that irradiation (burnup) has on the materials within the system (i.e., radioactive decay and burnup calculations). Instead, this is the function of the code ORIGEN2 [The Oak Ridge National Laboratory (ORNL) Isotope Generation and Depletion Code], which analyzes the burnup and concurrent decay of isotopes in a system over time.[2] The limitation of ORIGEN2 is that it does not take into account the geometry of a system. The geometry and materials influence the neutron energy flux spectrum and thus the cross sections in various regions in the system being analyzed. These geometry-/material-dependent parameters of the system can be determined by MCNP. Thus, it is desirable to link MCNP and ORIGEN2 to allow accurate calculations of spatial isotope generation and depletion in a physical system. The code *monteburns*[3,4] has been written in the Nuclear Systems Design and Analysis group (TSA-10) at Los Alamos National Laboratory (LANL) to perform this function. This document gives background information regarding these types of calculations, a purpose and description of the code itself, and limited benchmarking results from *monteburns*.

Monteburns initially was developed for use in the Accelerator Transmutation of Waste (ATW) project[5] at LANL because it could combine a detailed three-dimensional (3D) system model of a nonreactor system (as many other codes require) with burnup calculations in an automated fashion. The code now has been expanded so that it can be used for reactor systems as well, as was shown in the benchmarking efforts.

2.0. BACKGROUND

There are two main classes of codes that can be used to perform criticality calculations for nuclear systems: a Monte Carlo code and a deterministic code. Monte Carlo techniques typically produce a statistical approximation of an answer for the exact geometry of the system, whereas deterministic codes numerically produce an exact solution of the diffusion and/or transport equations for the problem as modeled.[6] Deterministic codes generally cannot solve such equations easily for complex geometries, so approximations on the geometry must be made. Additionally, deterministic codes generally utilize less-accurate cross-section data (i.e., grouped vs continuous). By combining a Monte Carlo transport code such as MCNP with a radioactive decay and burnup code such as ORIGEN2, better system-dependent burnup calculations can be obtained (although these calculations generally take longer).

* Radiation Safety Information Computational Center (RSICC) Code Packages CCC-660 and CCC-371.

Also, several codes have been written to link MCNP and ORIGEN2, including MOCUP,[7] COUPLE,[8] and SCAMP.[9] However, each of these codes appear to have been developed for specific purposes and thus have certain limitations. In addition, ORNL designed the SCALE (Standardized Computer Analyses for Licensing Evaluation) package, which actually incorporates the linkage code COUPLE. This package encompasses a variety of codes, including several (e.g., MORSE and KENO) that perform Monte Carlo transport calculations, and ORIGEN-S, which performs radioactive decay and burnup calculations (ORIGEN-S is a "newer" version of ORIGEN2). Unfortunately, considerable training is required to run these. Concurrently, many commercial nuclear companies (both in the United States and Europe) also have developed their own methods/codes (typically deterministic ones) for analyzing the effects of burnup on a reactor core. These codes are designed for one- or two-dimensional (1- or 2D) reactor geometries and are often large, complex programs to execute and expensive to obtain. Although deterministic codes can perform burnup calculations, they do not have the physical accuracy associated with a Monte Carlo code that models a detailed 3D geometry.

3.0. PURPOSE/DESCRIPTION

The basis for the development of *monteburns* was the need for a fully automated code that could perform accurate burnup (and other) calculations for any 3D system (e.g., accelerator driven or a full reactor). Before *monteburns*, was initially developed, the following list of desired attributes was made.

- The code should be fully automated (once the input is set up, no further user interaction is required).
- The code should allow for the irradiation of several materials concurrently (each material is evaluated collectively in MCNP and burned separately in ORIGEN2).
- The code should allow the transfer of materials between regions in MCNP (shuffling).
- The code should allow any materials to be added or removed before, during, or after each step in an automated fashion.
- The code should not require the user to provide input for ORIGEN2 and should have minimal MCNP input file requirements (other than having a working MCNP deck).
- The code should be relatively easy to use and not require several complicated input files.

Although the linkage and burnup codes discussed in the previous section perform adequate calculations for the irradiation of materials in a system, they do not provide the entire range of parameters and functions useful in advanced nuclear burnup problems. *Monteburns* was developed to be as versatile as possible so that it can be applied to many situations and give the user a variety of choices of operational parameters while simplifying required user training. All of the above features have been fully or partially developed in *monteburns*, although several improvements have yet to be implemented.

3.1. Description

Monteburns is a Perl script file that frequently interacts with a FORTRAN77 program. It also acts as a postprocessor for MCNP and a pre- and postprocessor for ORIGEN2. As shown in Fig. 1, MCNP and ORIGEN2 interact primarily through *monteburns* in that (1) MCNP provides spectrum-averaged, one-group microscopic cross sections and fluxes to ORIGEN2 and (2) ORIGEN2 provides material compositions halfway through

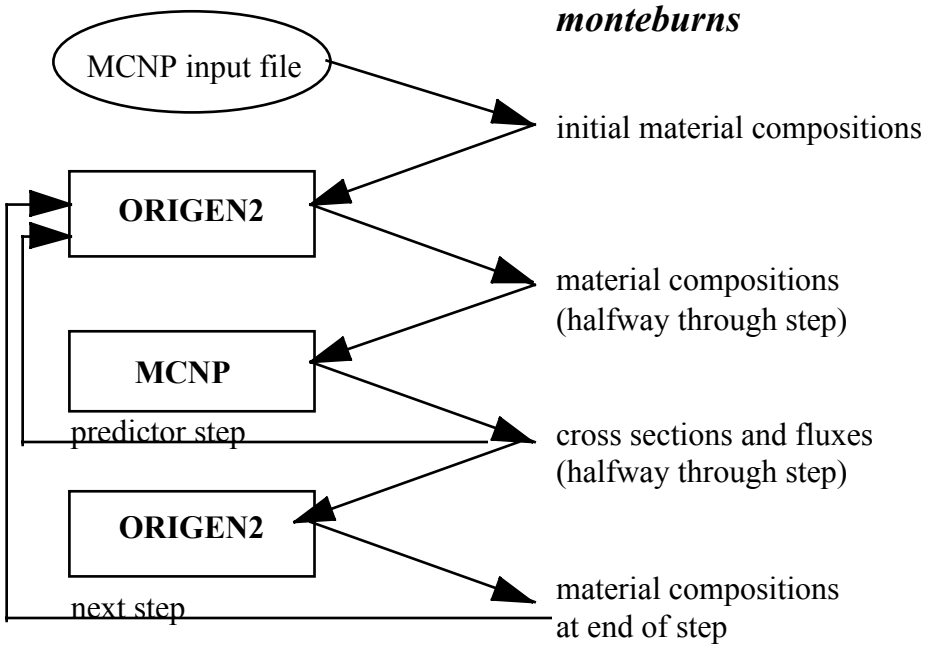

Fig. 1. Interaction of *monteburns* with MCNP and ORIGEN2.

and at the end of each irradiation step for further MCNP calculations. The "halfway" calculations are referred to as predictor steps, which may be used repeatedly to obtain the most accurate cross-section representation for a particular burn step.

When *monteburns* begins, it modifies the MCNP input file to tally the desired one-group cross sections (and other data) and generates the appropriate ORIGEN2 input files. When a material is specified to be burned in *monteburns*, the user supplies the desired MCNP material number. Each geometric region that contains this material number is burned collectively, based on the average cross sections and fluxes obtained for the entire region (the user must ensure that there are enough different regions/materials to obtain the desired accuracy). Each neutron that passes through a region contributes to the tally of the region flux and the one-group cross section of each material specified by the user.

After fluxes and one-group cross sections are calculated, *monteburns* modifies the ORIGEN2 input file and libraries to reflect these values. *Monteburns* also takes the necessary steps to add/remove materials before, during, and/or after the ORIGEN2 burn. Following irradiation by ORIGEN2, material isotopics are passed back to MCNP and the process is repeated as necessary.

3.2. Calculations

To normalize the flux to the input system power, several calculations are performed. First, the recoverable energy per fission (Q_{fis}) for each material being analyzed is determined. The value of Q_{fis} can be input explicitly by the user, or it can be calculated according to the fraction that each actinide contributes to fissions in the system and the ratio of the recoverable energy per fission of that actinide to that of ^{235}U (this value must be input by the user). This allows Q_{fis} to vary as the isotopics of the system change; however, *monteburns* does not take into account the variance in capture gamma heating as the system changes. The recoverable energy per fission in the system itself then is calculated using Eq. (1):

$$Q_{ave} = \frac{\sum_{j=1}^{m} \left(Q_{fis}{}^{j} * \varphi_n^j * \Sigma_f{}^{j} * V^j \right)}{\sum_{j=1}^{m} \left(\varphi_n^j * \Sigma_f{}^{j} * V^j \right)} \quad , \tag{1}$$

where

Q_{ave} = the average recoverable energy per fission for the entire system (MeV),

$Q_{fis}{}^{j}$ = the average recoverable energy per fission in material j (MeV),

φ_n^j = the neutron flux (n/cm^2-s) from MCNP in region containing material j,

$\Sigma_f{}^{j}$ = the macroscopic fission cross section of material j (cm^{-1}) (= $\sum_{i=1}^{n} \sigma_f(i) * n(i)$ - obtained from ORIGEN2 files), and

V^j = the volume of all cells containing material j (cm^3) (calculated by MCNP or input by user).

Once Q_{fis} for each material is determined, *monteburns* normalizes the flux in each region to reflect the total system power. This is done differently depending on whether MCNP is run in criticality ("kcode") or source ("sdef") mode. The normalization factor calculation is shown in Eq. (2):

$$C = \frac{P * 10^6 W/MW}{(1.602 * 10^{-13} J/MeV) * N * Q_{ave}} \quad , \tag{2}$$

where

P = the power (MW) input by user,

N = the source weighting term = k_{eff}/υ for "kcode" problem and *floss/src* for "nps" source definition,

k_{eff} = the effective multiplication factor (calculated by MCNP),

υ = the average number of neutrons produced per fission,

floss = the weight of neutrons lost to fission (calculated by MCNP), and

src = the weight of source neutrons (approximately equal to one) (calculated by MCNP).

From this value of the flux, the power produced in each region is

$$P^j = \frac{\left(Q_{ave} * \varphi^j * \Sigma_f{}^j * V^j * 1.60219 * 10^{-13} J/MeV\right)}{10^6 W/MW} \quad , \tag{3}$$

where

P^j = power produced by material j (MW) and

φ^j = normalized neutron flux (n/cm^2-s) in region with material j.

The equation for the neutron source term has the variable k_{eff} (or *floss/src*, which represents the fraction of neutrons lost in fission in a "nps" source definition) in the denominator because the equation modifies the value of the neutron flux of systems not modeled at critical. For a "kcode" problem, the flux calculated by MCNP is normalized per fission neutron, which assumes that the number of fissioning neutrons in the system modeled is representative of how many produce the given steady-state (critical) power level. However, if the system is subcritical, then if the flux is normalized per fission neutron, it is only a fraction (k_{eff}) of the flux produced at steady state because only that fraction (k_{eff}) of neutrons in the steady-state system is represented (the other fraction must be produced externally to make up the difference). Dividing by k_{eff} increases the value of this flux appropriately. Similarly, the relative number of fission neutrons produced in a supercritical system is greater than that in a reactor at steady-state, so the flux must be reduced to accurately reflect power production.

3.3. Input

The user must generate two to four different input files before executing *monteburns*. The two required input files are the MCNP input file and a general *monteburns* input file containing commands regarding the operation of *monteburns*. For complex burnup scenarios, the user also must generate a feed input file, which contains detailed instructions for *monteburns* at each time step (i.e., time interval, power, or material feed/removal). Finally, one other file containing cross-section identifier preferences for MCNP (specification of default libraries desired for isotopes generated during burnup but not in the initial MCNP input file) is required; a general one is provided with the source code but may be modified by the user as necessary. Some of the most important input parameters in *monteburns* include system power; recoverable energy per fission of ^{235}U; materials (and possibly volumes) for regions of interest; the number of outer,

inner, and predictor steps; the importance fraction, the number (and a listing) of isotopes being tracked; and detailed information about feed/removal of materials.

The number of outer steps represents the number of time periods for which burnup calculations are performed and representative cross sections are obtained (the burn step then uses spectrum-averaged, one-group cross sections calculated at a predictor step halfway through that step). Each outer step also can indicate the addition and/or removal of a material. The number of inner burn steps is the number of additional times into which the irradiation period is divided for ORIGEN2 calculations (if the outer burn step is relatively long, then breaking it into additional steps may increase the accuracy of the burnup calculations).

The number of predictor steps represents how many times in an outer burn step that cross sections are calculated in MCNP (they are updated automatically an additional time for the first burn step to transform the original ORIGEN2 cross-section library into one representative of the system being studied). If there is more than one predictor step, initial cross sections are calculated for that outer burn step and input into ORIGEN2, which is rerun to obtain new material compositions halfway through the step. These compositions are put back into MCNP, which is also rerun for that outer burn step. Material compositions from the initial run and the second (predictor) run can be compared halfway through this step to determine if the desired accuracy was achieved.

The next important input parameter is determining how many isotopes should be processed between ORIGEN2 and MCNP. For every additional isotope for which cross sections are obtained in MCNP, the run time increases. Thus, it is inefficient to process every isotope (not to mention the fact that MCNP does not contain cross sections for every isotope). In *monteburns*, users enter the isotopes for which they definitely want results (automatic isotopes); then additional ones are determined by another input parameter known as the importance fraction. If an isotope contributes to a fraction of the fission or absorption interactions, mass, or atom fraction greater than this importance fraction, then it is included in additional MCNP runs. This allows significant fission products and actinides to be included in further processing.

3.4. Output

Output produced by *monteburns* includes the following parameters as a function of burnup: effective multiplication factor (k_{eff}), number of neutrons per fission (υ), average recoverable energy per fission (Q_{fis}), thermal factor (η), neutron flux spectrum, macroscopic fission cross section (Σ_f), power generation, burnup, flux spectrums, production rates, cross sections, fission-to-capture ratios, compositions, activities, toxicities, and heatloads of all automatic isotopes in each material.

4.0. BENCHMARKING

One of the most important aspects of developing a new computer code is benchmarking it against existing experimental data and/or published calculations from other codes. The linkage code *monteburns* is no exception. To show that it is capable of performing burnup calculations well, a variety of test cases were run. Statistical analyses also were performed for selected input parameters and various system models to determine how the parameters affect the outcome. Limited results from initial benchmarking efforts and statistical analyses are presented here.

4.1. Benchmarking

The initial benchmarking process for *monteburns* used five different test cases, representing a variety of burnup scenarios. These test cases show the versatility of *monteburns* in performing all types of burnup calculations. First, changes in the concentration of uranium and plutonium isotopes were calculated as a function of burnup, and then both a pin in a simple-cell geometry and a full-reactor assembly were analyzed. The first three test cases examined a PWR system with low-enriched uranium fuel, the fourth involved a boiling-water-reactor (BWR) system, and the fifth incorporated mixed-oxide (MOX) fuel results. The broad range of these cases is useful in showing the validity of *monteburns* in handling a variety of parameters. All cases were modeled using temperature-dependent cross sections derived from the ENDF/B-V data set and processed by NJOY.[10] Brief descriptions of these five test cases are

1. uranium and plutonium isotopic concentrations as a function of burnup,
2. composition of isotopes in a fuel pin at fixed burnups,
3. concentrations of isotopes in a PWR lattice at fixed burnups,
4. power distribution of pins within a small BWR lattice, and
5. activity of MOX-based spent fuel after removal from a reactor.

The majority of the results calculated by *monteburns* fell within the range of values calculated by other codes and within a relative percent error/difference of 5% of values found experimentally (see Table 1 for results).

The errors resulting from this benchmarking consisted primarily of five different effects: (1) an approximate system model (typically this was either slightly subcritical or supercritical and produced a different spectrum than probably was seen in steady-state experimental reactor data), (2) estimated recoverable-energy-per-fission inputs, (3) resonance self-shielding/cross-section differences, (4) variances in fission yields, and/or (5) statistical errors.

First, the accuracy to which a system is modeled influences both the neutron flux and the energy spectrum in each region. If the model of the system is subcritical but the

actual system is critical, then the spectrum of the modeled system may not be representative of the actual one, cross sections may be inaccurate, and incorrect ratios of fission, capture, and leakage may be obtained. These three competing processes produce different nuclides (or none in the case of leakage) such that the resulting isotopic compositions of the system are affected by any misrepresentation of the

Table 1. Results for a Burnup of 23.81 GWd/MTHM (g/g UO_2)

Isotope	*Monteburns*	Published[11]	% Error from *monteburns*	% Error from SCALE[11]
^{235}U	0.00751	0.00721	4.1	1.4
^{236}U	0.00266	0.00274	-3.1	-2.2
^{238}U	0.842	0.847	-0.5	-0.6
^{238}Pu	7.01E-05	6.95E-05	0.8	0.9
^{239}Pu	0.00407	0.00402	1.3	7.7
^{240}Pu	0.00170	0.00167	1.6	-4.2
^{241}Pu	5.29E-04	5.04E-04	5.0	6.0
^{237}Np	2.46E-04	2.60E-04	-5.6	5.5
^{99}Tc[a]	8.76E-06	8.09E-06	8.3	8.6
^{137}Cs[a]	0.0527	0.0539	-2.2	-0.8

[a]The units for these are given in curies/gram (Ci/g) UO_2 instead of gram/gram (g/g) UO_2, as are the other isotopes.

spectrum. However, *monteburns* is not designed to account for such a spectrum shift in either direction. Instead, it accounts only for a linear change in the true flux as a function of $1/k_{eff}$ [see Eq. (2)]. For a system designed to be subcritical, this effect is not as dominant because it does not have to be modeled exactly at critical throughout life to be representative of the actual system. In either case, it is recommended that users model a system such that k_{eff} at all time steps is as close to true values as possible so that the correct spectrum and results are obtained. Errors observed through benchmarking may have been a result of the fact that none of the test cases, as described in the references, were exactly critical.

Second, resonance self-shielding also may have contributed to errors in cross-section values and thus final material compositions. As burnup increases, the change in isotopes caused by fission and absorption varies the overall resonance structure of the system and the effective one-group absorption cross sections (which are weighted by energy) change. Some codes use fixed cross sections throughout burnup calculations, which definitely do not account for cross-section variances due to resonances. Thus, errors are expected when *monteburns* values are compared to results from these codes and ones that change cross-section values more frequently. Additionally, variances in

MCNP continuous cross-section and resonance data compared to the behavior of resonances and neutron absorption from experimental data in actual systems may have contributed to errors.

Finally, the other errors seen when using *monteburns* probably resulted from estimations in input parameters (i.e., recoverable energy per fission), inaccuracies in ORIGEN2 and MCNP data (i.e., fission yields and cross sections), and statistical errors (cross sections and fluxes are obtained from tallies in MCNP, and the accuracy of these tallies are highly dependent on the number of neutrons per cycle, total number of cycles, placement of sources, etc.).

In particular, the errors seen in Table 1 were probably a result of the fact that the technique used in *monteburns* for generating cross sections differed from what other codes such as SCALE use (i.e., one-group, spectrum-averaged cross sections obtained from continuous energy data vs multigroup cross sections). However, the differences between the two did not appear to be too significant. Thus, *monteburns* was considered adequate for the problems presented here. Unfortunately, there are currently no readily available experimental data for a fast system, so no benchmarks were performed for one. However, it is assumed that because the code has been shown to work well for a thermal system, it can calculate decent results for a fast system as well.

4.2. Statistics

Preliminary statistical analyses revealed that the test cases studied (those involving reactor geometries) typically were well represented by eight outer burn steps (four irradiation cycles plus cooling periods after each), two inner burn steps (continuous feed cases with varying beginning and ending feed rates and cases with irradiation periods greater than 100 MW days may require additional inner burn steps), and one predictor step (again, cases involving irradiation periods greater than 100 MW days may require additional predictor steps). In addition, a value of the recoverable energy per fission for ^{235}U of 200 MeV and an importance fraction around 0.01 produced comparable results to experimental data for the cases examined.

5.0. CONCLUSION

In conclusion, the code *monteburns* now has been described and benchmarked for several reactor burnup scenarios. It produces comparable results to other well-known burnup codes, such as those in the SCALE suite of programs. *Monteburns* is a straightforward yet versatile solution requiring little training other than that required for MCNP. It is compatible with all MCNP4 versions and MCNPX with a neutron source and should work on most platforms (including PC, HP, and Sun). It is publicly available through the RSICC at ORNL as code P00455.

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