LA-UR-99-42
January 1999

DEVELOPMENT OF A FULLY-AUTOMATED MONTE CARLO BURNUP CODE *MONTEBURNS*

by

David I. Poston and Holly R. Trellue

Photograph: by Chris J. Lindberg

DISCLAIMER

LA-UR-99-42

Development of the Fully Automated Monte Carlo Burnup Code *Monteburns*

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

Introduction

Several computer codes have been developed to perform nuclear burnup calculations over the past few decades.[1,2] In addition, because of advances in computer technology, it recently has become more desirable to use Monte Carlo techniques for such problems. Monte Carlo techniques generally offer two distinct advantages over discrete ordinate methods: (1) the use of continuous energy cross sections and (2) the ability to model detailed, complex, three-dimensional (3-D) geometries. These advantages allow more accurate burnup results to be obtained, provided that the user possesses the required computing power (which is required for discrete ordinate methods as well).

Several linkage codes have been written that combine a Monte Carlo N-Particle transport code (such as MCNP™)[3] with a radioactive decay and burnup code.[2,4] This paper describes one such code that was written at Los Alamos National Laboratory: *monteburns*.[5] *Monteburns* links MCNP with the isotope generation and depletion code ORIGEN2.[6] 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 3-D system (accelerator-driven or a full reactor core). Before the initial development of *monteburns*, a list of desired attributes was made and is given below.

- The code should be fully automated (that is, after 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 (shuffling) between regions in MCNP.
- 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 a working MCNP deck).
- The code should be relatively easy to use and not require several complicated input files.

All of these features have been developed fully or partially in *monteburns*, although several improvements have yet to be implemented.

Description

As shown in Fig. 1, the primary way in which MCNP and ORIGEN2 interact through *monteburns* is that MCNP provides spectrum-averaged, one-group microscopic cross sections and fluxes to ORIGEN2 and ORIGEN2 provides material compositions to MCNP halfway through and at the end of each irradiation step for further calculations. The "halfway" calculations are referred to as predictor steps, which may be used repeatedly to obtain the most accurate representation for a particular burn step (extra predictor steps usually are required only for long burn steps over which material isotopics change substantially).

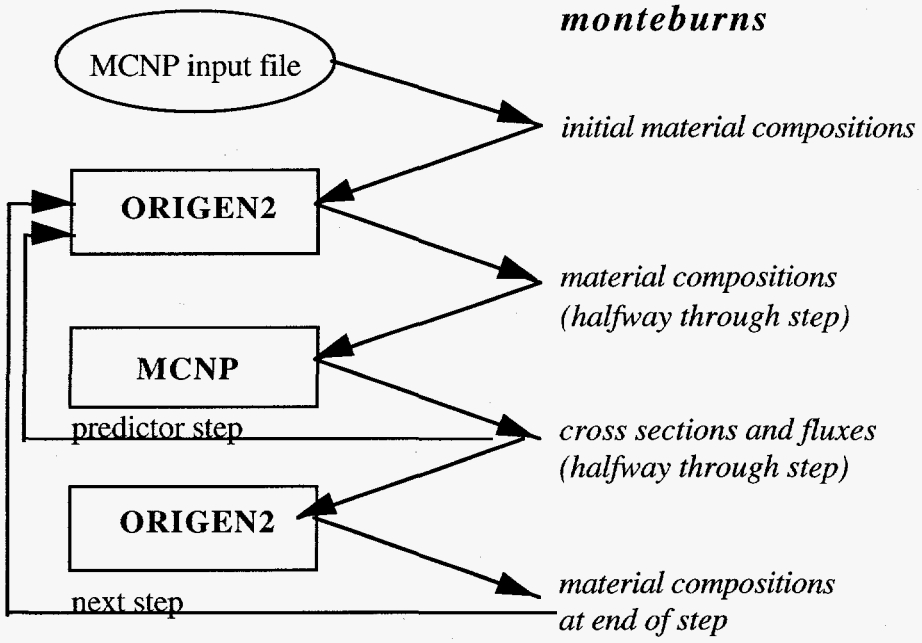

Fig. 1. Interaction of *monteburns* with MCNP and ORIGEN2.

When *monteburns* begins execution, it first modifies the MCNP input file to tally the desired one-group cross sections (and other data), then it generates the appropriate ORIGEN2 input files. When a material is specified to be burned, the user supplies the desired MCNP material number. Each MCNP region that contains this material number is burned collectively based on the average cross sections and fluxes obtained for the entire region. (It is up to the user to ensure that there are enough different regions/materials to obtain the desired accuracy.) Several calculations are performed to normalize the flux to

the input system power. First, the recoverable energy per fission (Q_{fis}) is determined. The value of Q_{fis} can be input explicitly by the user, or it can be calculated according to the fission fraction of each actinide in the system. 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. When Q_{fis} is determined, *monteburns* normalizes the flux in each region to correspond to the total system power. This is done differently depending on whether MCNP is run in criticality (KCODE) or source (SDEF) mode. 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 the irradiation step in ORIGEN2, material isotopics are passed back to MCNP, and the process is repeated as necessary.

Conclusion

Monteburns has proven to be a very useful and versatile burnup code for both reactor and accelerator-driven systems. Initial benchmarking efforts have been successful, although additional work is still required. Several enhancements to *monteburns* currently are being considered, including expanding the number of platforms on which the code operates, modifying the burnup/depletion and fission product yield calculations currently performed by ORIGEN2, improving the calculation of Q_{fis} (particularly with respect to capture gamma heating), and expanding the output (material activities, neutrons/gamma sources, etc.).

References

1. O. W. HERMANN, "COUPLE: Scale System Module to Process Problem-Dependent Cross Sections and Neutron Spectral Data for ORIGEN-S Analyses," Oak Ridge National Laboratory/US Nuclear Regulatory Commission report NUREG/CR-0200, Rev. 5, Vol. 2, Sec. F6 (September 1995).

2. R. L. MOORE, B. G. SCHNITZLER, C. A. WEMPLE, R. S. BABCOCK, and D. E. WESSOL, "MOCUP: MCNP/ORIGEN Coupling Utility Programs," Idaho National Engineering and Environmental Laboratory report INEL-95/0523 RSICC Code PSR-365 (October 1997).

3. J.F. BRIESMEISTER, "MCNP™—A General Monte Carlo N-Particle Transport Code," Los Alamos National Laboratory report LA-12625-M, Version 4B (March 1997).

4. D. BOWEN and R. D. BUSCH, "Using ORIGEN and MCNP to Calculate Reactor Criticals and Burnup Effects," *Trans. Am. Nucl. Soc.* 77, 223 (1997).

5. D. I. POSTON and H. R. TRELLUE, "User's Manual, Version 1.00, for *Monteburns*, Version 3.01," Los Alamos National Laboratory report LA-UR-98-2718 (June 1998).

6. A. G. CROFF, "A User's Manual for ORIGEN2 Computer Code," Oak Ridge National Laboratory report ORNL/TM-7175 (July 1980).