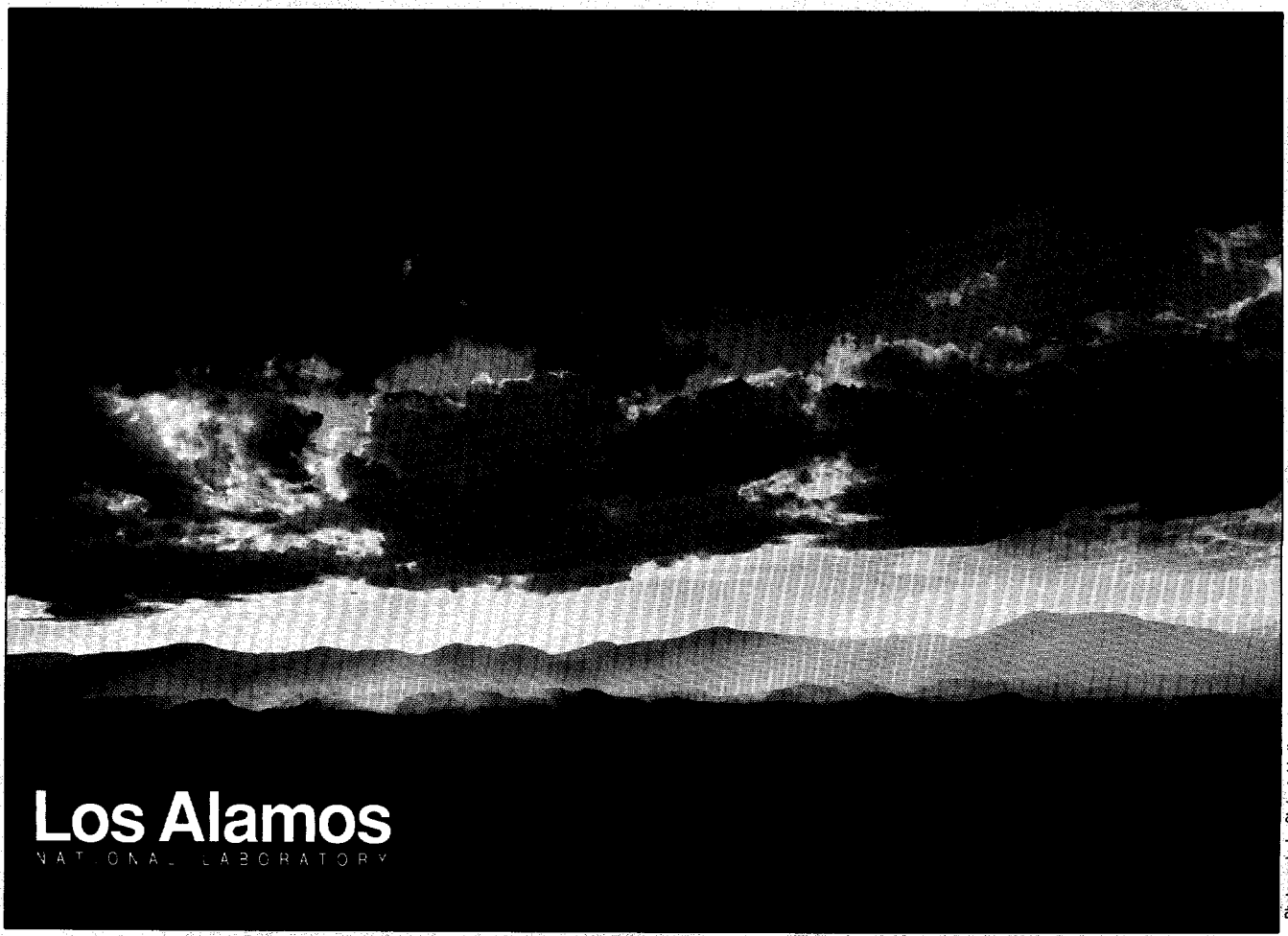
LA-UR-99-41
January 1999

USER'S INFORMATION FOR THE MONTE CARLO BURNUP CODE *MONTEBURNS*

by

Holly R. Trellue and David I. Poston



Photograph: by Chris J. Lindberg

DISCLAIMER

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

LA-UR-99-41

User's Information for the Monte Carlo Burnup Code *Monteburns*

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

Introduction

Monteburns, a burnup computer code that uses the Monte Carlo technique, was developed at Los Alamos National Laboratory to be applied to a variety of nuclear design calculations (see accompanying paper on the development of *monteburns*). It is a fully automated burnup code that incorporates multiple irradiation steps and many other options. However, two of the most important aspects of developing a code are describing how to use it and benchmarking it. Thus, the operational aspects and benchmarking results from *monteburns* are discussed in this summary.

Description

The user must generate two to four different input files to execute *monteburns*.[1] The two required input files are a MCNP input file and a general *monteburns* input file. Some of the most important input parameters for the latter file are discussed below. For complex burnup scenarios, the user also must generate a feed input file that contains detailed instructions for *monteburns* at each time step (i.e., time interval, power, addition/removal of material, etc.). One other file containing MCNP cross-section preferences (specification of default libraries desired for isotopes generated during burnup but not in the initial MCNP input file) is provided with the source code but modified by the user as necessary.

A *monteburns* run is broken into three main irradiation periods.

1. Outer burn steps (the number of times representative cross sections are obtained).
2. Internal burn steps (which additionally shorten time intervals for ORIGEN2).
3. Predictor steps. Predictor steps allow cross sections to be processed more than once for each outer burn step (material compositions halfway through each step using both initial and modified cross sections can be compared to determine if enough accuracy has been obtained).

It is also important to determine for how many isotopes cross sections should be obtained in MCNP; the more isotopes processed, the longer the run time. In *monteburns*, the user enters the isotopes for which he/she definitely wants results, and then additional ones are identified as "important" by another input parameter known as the importance fraction. If an isotope (primarily actinides and fission products) contributes to a fraction of fission or absorption interactions, mass, or atom density greater than this fraction, it is included in additional MCNP runs.

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, cross sections, flux spectrums, compositions of materials, and production rates.

Results

The benchmarking process for *monteburns* consisted of five different test cases representing a variety of burnup scenarios and calculations.[2] The broad range of these cases is useful in showing the validity and versatility of *monteburns*. These cases were:

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 pressurized water reactor lattice,
4. power distribution of pins within a small boiling water reactor lattice, and
5. activity of mixed-oxide-based spent fuel after removal from a reactor.

The errors resulting from benchmarking primarily consisted of five things:

1. the system, as modeled, was typically either subcritical or supercritical and produced a different spectrum than was seen in steady-state experimental reactors;
2. the recoverable energy per fission was unknown and thus estimated;
3. resonance self-shielding/cross section differences;
4. variances in fission yields; and/or
5. statistical errors.

The majority of the results calculated by *monteburns* fell within the range of values calculated by other codes and within a relative per cent error/difference of 5% of values found experimentally (see Table 1). The technique used in *monteburns* for generating cross sections differed from what other codes (such as SCALE[3]) use (i.e., one-group, spectrum-averaged ones obtained from continuous energy data vs multi-group ones), but the differences between the two did not appear to be too significant. Thus, *monteburns* was considered adequate for the problems presented here.

In conclusion, the code *monteburns* has now been described and benchmarked for several burnup scenarios. It produces comparable results to other well-known burnup codes, such as SCALE. *Monteburns* is a straightforward, yet versatile solution requiring little training (other than that required for MCNP). When appropriate software quality assurance requirements are met, it will be made publicly available through the Radiation Safety Information Computational Center (RSICC).

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

Isotope	*monteburns*	Published[1]	% error from *monteburns*	% error from SCALE[1]
U-235	0.00751	0.00721	4.1	1.4
U-236	0.00266	0.00274	-3.1	-2.2
U-238	0.842	0.847	-0.5	-0.6
Pu-238	7.01E-05	6.95E-05	0.8	0.9
Pu-239	0.00407	0.00402	1.3	7.7
Pu-240	0.00170	0.00167	1.6	-4.2
Pu-241	5.29E-04	5.04E-04	5.0	6.0
Np-237	2.46E-04	2.60E-04	-5.6	5.5
Tc-99*	8.76E-06	8.09E-06	8.3	8.6
Cs-137*	0.0527	0.0539	-2.2	-0.8

*The units for these are given in Curies/gram UO_2 (Ci/g) instead of g/g UO_2 like the other isotopes.

References

1. 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).

2. H. R. TRELLUE, "Development of *Monteburns*: A Code that Links MCNP and ORIGEN2 in an Automated Fashion for Burnup Calculations," Los Alamos National Laboratory report LA-T-13514 (November 1998).

3. 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, NUREG/CR-0200, Rev. 5, Vol. 2, Sec. F6 (September 1995).