

LA-UR- 95 - 3431

CONF-960415--4

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

RECEIVED

NOV 27 1995

OSTI

TITLE: THE STATUS OF NUCLEAR DATA FOR TRANSMUTATION
CALCULATIONS

AUTHOR(S): Wilson, W.B., T-2
England, T. R., T-2
MacFarlane, R. E., T-2
Muir, D. W., T-2
Young, P. G., T-2

SUBMITTED TO: Submitted for presentation at the ANS RP&S Topical Meeting
on Advancements and Applications in Radiation Protection and
Shielding, April 21-25, SEACREST, North Falmouth,
Massachusetts.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO. 836 R4
ST. NO. 2629 5/81

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

at

DISCLAIMER

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

The Status of Nuclear Data for Transmutation Calculations

W. B. Wilson, T. R. England, R. E. MacFarlane, D. W. Muir, and P. G. Young

Theoretical Division
Los Alamos National Laboratory
Los Alamos, New Mexico 87545 USA

Submitted for presentation at the ANS RP&S Topical Meeting on
Advancements and Applications in Radiation Protection and Shielding,
April 21-25, SEACREST, North Falmouth, Massachusetts

ABSTRACT

At this point, the accurate description of transmutation products in a radiation environment is more a nuclear data problem than a code development effort.

We have used versions of the CINDER code for over three decades to describe the transmutation of nuclear reactor fuels in radiation environments. The need for the accurate description of reactor neutron-absorption, decay-power, and decay-spectra properties have driven many AEC, ERDA, and DOE supported nuclear data development efforts in this period. The level of cross-section, decay, and fission-yield data has evolved from rudimentary to a comprehensive ENDF/B-VI library¹⁻⁵ permitting great precision in reactor calculations.

The precision of the data supporting reactor simulations provides a sturdy foundation for the data base required for the wide range of transmutation problems currently studied. However, such reactor problems are typically limited to neutron energies below 10 MeV or so; reaction and decay data are required for actinides of, say, $90 \leq Z \leq 96$ and neutron-rich fission products of $22 \leq Z \leq 72$. The expansion into reactor structural materials and fusion systems extends these ranges in energy and Z somewhat.

Recent applications involving medium- and high-energy accelerators have greatly expanded the range of data required for transmutation studies in that

- ion reactions must be described;
- neutron reactions up to the accelerator beam energy are important; and,
- the Z - A range of nuclides for which reaction and decay data are required now extends over the entire chart of the nuclides and beyond.

During the past five or so years we have developed a code for the description of nuclide inventories in transmutation problems. This code, CINDER'90^{6,7}, evolved from earlier versions of CINDER⁸⁻¹⁰ and REAC¹¹, uses the algorithm of CINDER with modifications to accommodate the input of additional constant destruction and production rates associated with reactions outside of the code's particle or energy domain. In reactor problems, these additional terms are typically zero. In medium-energy accelerator problems, these terms are produced in the radiation transport calculations with the LAHET Code System. LAHET uses online reaction models to describe all ion reactions and neutron reactions above some cutoff energy — typically 20 MeV. The code follows neutrons down to this cutoff and passes all surviving neutrons to MCNP for transport with evaluated data. The neutron fluxes calculated in MCNP are used in the CINDER'90 calculation to calculate neutron transmutation below 20 MeV. Products of the CINDER'90 calculation include nuclide densities, activities, decay power, gamma spectra, and radiological hazard associated with environmental release in air or water.

The range of nuclides for which transmutation data are needed for accelerator problems expands to include spallation products far from stability. The scarcity of data for these nuclides has been observed elsewhere.¹²⁻¹⁵ We have relied greatly on data from international associates for data describing decay,^{16,17} radiological hazard,¹⁸ and cross-section¹⁹ properties. The data accumulated have been subjected to validation studies of data²⁰ and aggregate results²¹⁻²³ where available. Unfortunately, the availability of such benchmarks is severely limited; for example, measured cross section data exist in the CSISRS experimental data file at one or more energies for only 2279 of the over 15000 reactions of the library.

The library of nuclear data, constantly growing in breadth and quality with international cooperation, is now described in the following table.

Content of Present CINDER'90 Data Library

Value	Quantity
25	Maximum Neutron Energy, MeV
63	Neutron-Group Cross Sections
25	Photon-Group Spectra
3400	Total Nuclides
259	Stable Nuclides
3141	Unstable Nuclides
2762	Ground State Nuclides
583	1st. Isomeric State Nuclides
55	2nd. Isomeric State Nuclides
55	Nuclides Decaying by Spontaneous Fission
736	Nuclides Having Reaction Paths
66	Nuclides Having (n,f) Paths
15269	Total Non-fission Reaction Paths
4041	Total Non-fission Decay Paths

Validation of specific calculated results is currently approached in the following sequence:

1. identify the major contributors to a significant calculated result;
2. identify the paths leading to each major contributor;
3. compare the major data contributing to the calculation of each path with any available measured data to estimate data uncertainties; and,
4. trace the impact back through the significant paths and major contributors to estimate an uncertainty in each significant calculated result.

This sequence suggests a more consistent, automated uncertainty evaluation requiring the evaluation of uncertainties in all data. This approach is highly recommended by the authors.

To date the data and code have been applied to a variety of interesting accelerator problems^{6,24-30} that will be briefly described.

The data improvement effort continues with the cooperation of international evaluators. For example, the MENDL-2³¹ and WIND³² libraries are in hand to be validated and incorporated into the cross-section data.

REFERENCES

1. Evaluated Nuclear Data Files, ENDF/B, Version VI, developed for and maintained by the National Nuclear Data Center (NNDC) at the Brookhaven National Laboratory (BNL), Upton, NY.
2. T. R. England, J. Katakura, F. M. Mann, C. W. Reich, R. E. Schenter and W. B. Wilson, "Decay Data Evaluation for ENDF/B-VI," Proceedings of the Symposium on Nuclear Data Evaluation Methodology, October 12-16, 1992, Brookhaven National Laboratory; World Scientific (Hong Kong) 1993, pp. 611-622.
3. W. B. Wilson and T. R. England, "Development and Status of Fission-Product Yield Data and Applications to Calculations of Decay Properties," Trans. Am. Nucl. Soc. 66, 152 (1992).
4. T. R. England and B. F. Rider, "Evaluation and Compilation of Fission Product Yields," Los Alamos National Laboratory report LA-UR-94-3106 (October 1994).
5. W. B. Wilson, T. R. England and D. C. George "Sensitivity of Fission-Product Neutron Absorption to ENDF/B-IV, -V, and -VI Nuclear Data Parameters," Proceedings of the Specialists' Meeting on Fission Product Nuclear Data, May 25-27, 1992, JAERI, Tokai, Japan; Organization for Economic Co-Operation and Development Nuclear Energy Agency report NEA/NSC/DOC(92)9, pp.450 - 457.
6. W. B. Wilson, T. R. England, E. D. Arthur, C. A. Beard, C. D. Bowman, L. N. Engel, A. Gavron, D. C. George, L. L. Daemen, H. G. Hughes, III, W. W. Kinnison, R. J. LaBauve, D. M. Lee, H. Lichtenstein, P. W. Lisowski, D. W. Muir, A. P. Palounek, R. T. Perry, E. J. Pitcher, R. E. Prael, G. J. Russell, G. Sanders, L. S. Waters, P. G. Young and H.-J. Ziocck, "Accelerator Transmutation Studies at Los Alamos with LAHET, MCNP, and CINDER'90," Proceedings of the Workshop on Simulation of Accelerator Radiation Environments, January 11-15, 1993, Santa Fe, New Mexico; Los Alamos National Laboratory conference proceedings LA-12835-C (October 1994) pp.115-133; also available as Los Alamos National Laboratory informal document LA-UR-93-3080 (January 11, 1993).
7. W. B. Wilson, T. R. England, D. C. George, D. W. Muir and P. G. Young, "Recent Development of the CINDER'90 Transmutation Code and Data Library for Actinide Transmutation Studies," accepted for presentation at the GLOBAL'95 meeting, Versailles, France, September, 1995.
8. T. R. England, "CINDER — A One-Point Depletion and Fission Product Program," Bettis Atomic Power Laboratory report WAPD-TM-334 (August 1962; Rev. June 1964).
9. W. B. Wilson, T. R. England, R. J. LaBauve and D. C. George, "CINDER-3: Depletion Code for Class VI Computers," Trans. Am. Nucl. Soc. 46, 724 (1984).
10. T. R. England, "CINDER10 Code for DNA Use at Los Alamos," Los Alamos National Laboratory informal report LA-UR-93-2930 (August 1993).
11. F. M. Mann, "Transmutation of Alloys in MFE Facilities as Calculated by REAC," Hanford Engineering Development Laboratory report HEDL-TME 81-37 (August 1982).
12. W. B. Wilson and T. R. England, "Nuclear Data Needs for Studies of Accelerator Induced Neutron Transmutation of Nuclear Waste," Proceedings of the Specialists' Meeting on Fission Product Nuclear Data, May 25-27, 1992, JAERI, Tokai, Japan; Organization for Economic Co-Operation and Development Nuclear Energy Agency

13. W. B. Wilson and T. R. England, "Nuclear Data Needs for Studies of Accelerator Induced Neutron Transmutation of Nuclear Waste," Proceedings of the Specialists' Meeting on Fission Product Nuclear Data, May 25-27, 1992, JAERI, Tokai, Japan; Organization for Economic Co-Operation and Development Nuclear Energy Agency report NEA/NSC/DOC(92)9, pp.475 - 481.
14. E. D. Arthur, W. B. Wilson and P. G. Young, "Nuclear Data Needs for Accelerator-Driven Transmutation Systems," (invited), Proc. OECD Nuclear Energy Agency Specialists' Meeting on Intermediate Energy Nuclear Data, May 30-June 1, 1994, Issy-les-Moulineaux, France.
15. P. G. Young, W. B. Wilson and M. B. Chadwick, "Nuclear Data Requirements for Accelerator-Driven Transmutation Systems," presented at the 1st Int. Conf. on Accelerator-Driven Transmutation Technologies and Applications, July 25-29, 1994, Las Vegas, Nevada; Los Alamos National Laboratory preprint LA-UR-94-1565.
16. F. M. Mann, F. Schmittroth, T. R. England and C. W. Reich, "Master Decay Library," in Reports to the DOE Nuclear Data Committee,
17. J. Blachot and C. Nordborg, "Decay Data Evaluation for JEF-2," Proceedings of the Symposium on Nuclear Data Evaluation Methodology, October 12-16, 1992, Brookhaven National Laboratory; World Scientific (Hong Kong) 1993, pp. 623-632.
18. T. R. England, W. B. Wilson and A. J. Martinez, "Radiation Protection Data to be Used in Assessing the Relative Ionization Toxicity of Calculated Mixtures of Radionuclides," Los Alamos National Laboratory informal document LA-UR 92-392 (January 23, 1992).
19. J. Kopecky, H. A. J. van der Kamp, H. Gruppelaar and D. Nierop, "The European Activation File EAF-3 with Neutron Activation and Transmutation Cross-Sections," Netherlands Energy Research Foundation (ECN) report ECN-C-92-058 (September 1992).
20. D. W. Muir and W. B. Wilson, "Validation of a Large Activation Cross-Section Library," Proceedings of the International Conference on Nuclear Data for Science and Technology, May 9-13, 1994, Gatlinburg, Tennessee; American Nuclear Society, La Grange Park, Illinois, pp. 772-776.
21. T. O. Brun, C. A. Beard, L. L. Daemen, E. J. Pitcher, G. J. Russell, and W. B. Wilson, "LAHET Code System/CINDER'90 Validation Calculations and Comparison With Experimental Data," Proceedings of the Twelfth Meeting of the International Collaboration on Advanced Neutron Sources, May 24-28, 1993, The Cosener's House, Abingdon, Oxfordshire, U. K.
22. J. L. Ullmann, A. Gavron, L. King, J. Koster, P. W. Lisowski, D. Mayo, R. O. Nelson, L. Waters, S. A. Wender, C. Zoeller, D. Jagnow, R. Laird, G. Butler, M. Fowler, R. Gritzko, J. Wilhelmy, M. A. Yates, and W. Wilson, "APT Radionuclide Production Experiment," Los Alamos National Laboratory informal report LA-UR-93-3448 (September 28, 1993).
23. J. L. Ullmann, P. Staples, G. Butler, M. Fowler, A. Gavron, R. Gritzko, D. Jagnow, J. D. King, R. Laird, P. W. Lisowski, D. Mayo, R. O. Nelson, L. Waters, S. A. Wender, J. Wilhelmy, W. Wilson, M. A. Yates, and C. Zoeller, "Thick Target Spallation Product Yields from 800 MeV Protons on Tungsten," Proceedings of the International Conference on Nuclear Data for Science and Technology, May 9-13, 1994, Gatlinburg, Tennessee; American Nuclear Society, La Grange Park, Illinois (1994) pp. 374-376.
24. W. B. Wilson, T. R. England and A. Gavron, "Preliminary Calculations of Radionuclide Inventories and Aggregate Decay Properties of Sample Coupons in a Tungsten Target to be Irradiated at WNR," Los Alamos National Laboratory informal report T-2-IR-93-1 (January 4, 1993).
25. A. P. T. Palounek, L. S. Waters, T. R. England, H. G. Hughes, H. Lichtenstein, R. E. Prael, W. B. Wilson, and H. J. Ziock, "Calculation of Neutron Backgrounds and the Production and Decay of Radionuclides in the SDC Detector," Solenoidal Detector Collaboration Note SDC-93-467 (March 1993).

26. M. Diwan, Y. Fisyak, N. Mokhov, D. Lee, L. Waters, W. Wilson, Y. Efremenko, B. Moore, M. Marx, C. Wuest, J. Rutherford and V. Morgunov, "*Radiation Environment and Shielding for the GEM Experiment at the SSC*" Superconducting Super Collider Laboratory report SSCL-SR-1223 (July 1993).
27. R. S. Waters, R. E. Prael and W. B. Wilson, "*Accelerator Applications of the Los Alamos High Energy Transport Code System*," presented at the Specialists' Meeting on Shielding Aspects of Accelerators, Targets and Irradiation Facilities, April 28-29, 1994, Arlington, Texas.
28. L. S. Waters and W. B. Wilson, "*LAHET/MCNP/CINDER'90 Activation Calculations for the Atlas Integrated Forward Calorimeter Concept*," Los Alamos National Laboratory informal report LA-UR-94-2137 (June 25, 1994).
29. S. K. Lee, C. A. Beard, W. B. Wilson, L. L. Daemen, D. J. Liska and M. L. Adams, "*Structural Activation Calculations Due To 20-1000 MeV Proton Beam Loss In The APT Accelerator Design*," presented at the 1st Int. Conf. on Accelerator-Driven Transmutation Technologies and Applications, July 25-29, 1994, Las Vegas, Nevada.
30. J. Balderas, M. Cappiello, C. E. Cummings, Rj. Davidson, L. A. Domingueq, J. S. Elson, J. Garcia, A. Gavron, M. Hall, S. Howe, P. W. Keaton, R. Kidman, C. F. Lebeda, P. W. Lisowski, W. P. Lysenko, J. Martin, R. Nelson, J. Park, D. B. Pelowitz, R. T. Perry, E. Pitcher, D. A. Poling, G. Russell, E. Schwegler, T. Stratton, J. Teel, D. Trujillo, E. A. Wadlinger, R. B. Walton, and W. B. Wilson, "*Accelerator Driven Assembly: Final Report to the Defense Nuclear Agency — Development of Accelerator Technology for Defense Applications*," Los Alamos National Laboratory informal report LA-UR-94-3305 (April, 1995).
31. Yu. N. Shubin, V. P. Lunev, A. Yu. Konobeyev, and A. I. Dityuk, "*Cross-Section Data Library MENDL-2 to Study Activation and Transmutation of Materials Irradiated by Nucleons of Intermediate Energies, Part 1: Neutron Data*," draft Obninsk report (1994).
32. A. Yu. Konobeyev, Yu. A. Korovin, P. E. Pereslavytsev, V. I. Plyaskin, and A. Yu. Stankovsky, "*Nuclear Cross-Section Data Library for Actinides up to 100 MeV*," summary documentation by A. B. Pashchenko, International Atomic Energy Agency Nuclear Data Services document IAEA-NDS-143 (February 1995).

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.