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The Status of Nuclear Data for Transmutation Calculations

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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 CSIRS 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^{8,24-30} 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.

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