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Analysis of the MZA/MZB benchmarks with modern nuclear data sets

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ABSTRACT

For fast reactor design and analysis, our laboratory uses, amongst others, the ERANOS code system. Unfortunately, the publicly available version of ERANOS does not have the most recent nuclear data. Therefore, it was decided to implement an integrated processing system to generate cross sections libraries for the ECCO cell code, as well as covariance data. Cross sections are generated from the original ENDF files. For our purposes, it is important to ascertain that the ECCO cross section libraries are of adequate quality to allow design and analysis of advanced fast reactors in an academic context. In this paper, we present an analysis of the MZA/MZB benchmarks with nuclear data from JENDL-4.0, JEFF-3.1.2 and ENDF/B-VII.1. Results are that reactivity is generally well predicted, with an uncertainty of about 1% due to covariances of the nuclear data. Reaction rate ratios are satisfactorily calculated, as well as the flux spectrum and reaction rate traverses. Some problems remain: the magnitude of the void effect is not satisfactorily calculated, and reaction rate traverses are not always satisfactorily calculated. On the whole, the ECCO libraries are sufficient for design and analysis tasks in an academic context. For high-precision calculations, such as required for licensing tasks and detailed design calculations, data adjustment is still necessary as the "native" covariance data in the ENDF files is not accurate enough.

1. Introduction

In a recent M.Sc. Thesis (Tamagno, 2011) the MZA and MZB benchmarks documented in the IRPhEP handbook were analyzed with the ERANOS code system, which includes the ECCO cell code, in an effort to validate cross section libraries based on JENDL-4.0. While the work presented in Tamagno (2011) shows consistent results between JENDL-4.0 and other nuclear data sets, the calculations showed quite large biases with respect to the benchmark values for reactivity. It is not immediately clear whether this bias is due to the cross sections, a modeling error, or limitations of the ERANOS code system.

Recently, several sets of nuclear data have had a new release or an update: JENDL-4.0 was updated in September 2012, JEFF-3.1.2 was released in February 2012, and ENDF/B-VII.1 was released in 2011. As a result of the work presented in Tamagno (2011) and Tamagno and van Rooijen (2013), we had obtained some experience in the generation of ECCO libraries. Therefore it was decided to make ECCO libraries based on JENDL-4.0, JEFF-3.1.2, and ENDF/B-VII.1. The MOZART benchmarks were analyzed to assess the performance of these new libraries. The main goals of the present work are twofold: (1) give an insight of how to produce cross section libraries and uncertainty libraries for ERANOS, and (2) evaluate the performance of the ERANOS libraries we produced. We are well aware that one benchmark is a small basis to judge the quality of a nuclear data library. The most important goal is to ascertain that the ERANOS libraries have a sufficient performance for design calculations on fast reactors in an academic setting, and our main system of interest is the prototype FBR Monju and similar systems. Specifically, it is not our goal to assess the overall quality of the evaluated nuclear data sets, nor is it our goal to evaluate the performance of the ERANOS code system. To our knowledge, there are very few places in the world where ERANOS libraries are made, and the MZA/MZB benchmarks are not often analyzed. Therefore we think that our results are of interest to the community at large.

A complete cross section processing system was implemented in Python, focusing on consistency and uniformity, parallelization, as well as targeting a minimum of "outside input", i.e. necessary data for the processing is taken as much as possible from the ENDF files directly. Several utility codes to extract information from ENDF files were developed. In this paper, we present an analysis of many of the measurements described in the MOZART benchmarks. This work serves to assess the quality of the evaluated nuclear data sets and to assess the associated uncertainties.

This paper is organized as follows: in Section 2 we give a brief overview of how to generate cross sections for the ECCO cell code, as well as uncertainty data for ERANOS. In Sections 3–5 we introduce the MOZART cores (MZA, MZB/1, MZB/2 and MZB/3), and in Section 6 we give the results of our analyses. The paper finishes with a set of Conclusions.

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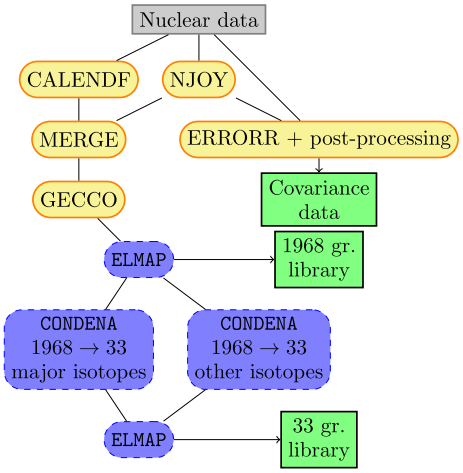

Fig. 1. Flow chart for the generation of an ECCO library. = nuclear data (ENDF format), = code, = ERANOS module, = output library.

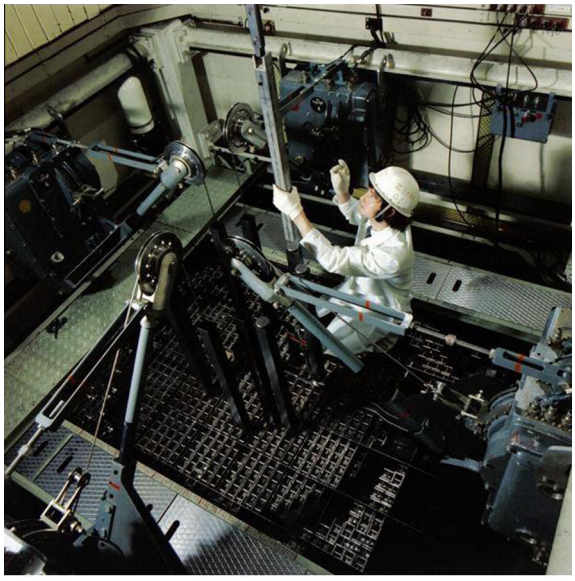

Fig. 2. View of the ZEBRA facility, reproduced from Briggs and Gulliford (2011). A fuel element (rectangular) is being loaded into the core. Note the 5 × 5 super lattice.

2. Computational infrastructure

This section concerns the details of the generation of an ECCO library, the details of the generation of covariance data for ERANOS, an explanation of the nuclear data evaluations used in this study, and some notes about the modeling options of ERANOS. The reader who is already familiar with these subjects may skip this section.

2.1. Cross sections for ECCO

The cell code in ERANOS is ECCO. The ECCO cell code uses a subgroup method to calculate effective group cross sections. Furthermore, ECCO uses two or more energy group structures in one calculation (typically 1968 groups and 33 groups, but one may use as many group structures as desired, as long as the group structures have common energy boundaries). This feature of ECCO makes it necessary to produce at least two cross section libraries (one library with 1968 groups and one library with 33 groups). In the following, isotopes which are included in the 1968-group library are referred to as *major isotopes*; isotopes which are present in the 33-group library only are referred to as *minor* isotopes. See Table A.1 for a list of major and minor isotopes. The production of an ECCO library takes several steps (see Fig. 1):

- A utility program was created to read an ENDF file and determine several parameters for the subsequent calculation: atomic mass, radioactive half-life, presence or absence of a fission cross section and delayed neutron parameters, presence or absence of covariance data. If information about the half-life is missing in the ENDF file of a given isotope, the half-life is taken from the decay files of JEFF-3.1.1 or ENDF/B-VII.1.
- NJOY (MacFarlane and Muir, 1994): the first step is a calculation with NJOY to generate a 1968-group GENDF file for an individual isotope. In the present work, we have chosen to use five temperatures for all isotopes (274 K, 574 K, 974 K, 1474 K, 2974 K). Since the subgroup method does not rely on the concept of dilution (background cross section), only infinitely dilute group cross sections are calculated. Anisotropy of scatter is developed up to P1, because ECCO only transfers P1 anisotropic scattering cross sections for heterogeneous cells (Rimpault, 2012). NJOY v99.393 was used.
- CALENDF (Jean-Christophe et al., 2011): the second step is to use CALENDF for each isotope. The major task of CALENDF is to generate the probability tables used in the ECCO subgroup calculation. In this step the same temperatures and dilution are used as in NJOY. CALENDF prepares probability tables using the so-called *Ribon-method* in which the subgroup parameters are determined in a strictly mathematical framework. In both the resolved and unresolved resonance range, CALENDF ignores the instructions on the ENDF file about the resonance formalism, but instead relies on its own heuristics to do an optimal calculation with the resonance parameters on the ENDF file. This treatment may fail for certain isotopes. In those cases, an input parameter is used to force CALENDF to follow the instructions on the ENDF file for the resonance treatment. In the unresolved resonance range (URR), CALENDF uses a probabilistic approach, which allows to treat the unresolved resonances in

Table 1
Convergence settings in BISTRO and TGV-VARIANT. Note: the simplified spherical harmonics option is used in TGV because nonsensical results were obtained when using the full spherical harmonics option.

BISTRO	
Outer iterations	
Maximum number	150
Integral convergence	10^{-6}
Local convergence	10^{-5}
Inner iterations	
Maximum number	75
Integral convergence	10^{-5}
Local convergence	10^{-4}
S_N quadrature set	S_8 symmetric
TGV-VARIANT	
Spatial approximation	
Interior flux expansion order	4
Interface flux expansion order	2
Source expansion order	3
Angular approximation	
Flux expansion order	P_5
Leakage expansion oder	P_3
Harmonics set	Simplified
Max. outer iterations	100
Convergence	
k_{eff}	5×10^{-6}
Point fission source	5×10^{-4}
Average fission source	5×10^{-5}