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Validation of the burn-up code EVOLCODE 2.0 with PWR experimental data and with a Sensitivity/Uncertainty analysis



F. Álvarez-Velarde*, E.M. González-Romero, I. Merino Rodríguez

CIEMAT, Centro de Investigaciones Científicas, Medioambientales y Tecnológicas, Avda. Complutense, 40 Ed. 17, 28040 Madrid, Spain

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ABSTRACT

A validation of the burn-up simulation system EVOLCODE 2.0 is presented here, involving the experimental measurement of U and Pu isotopes and some fission fragments production ratios after a burn-up of around 30 GWd/tU in a Pressurized Light Water Reactor (PWR). This work provides an in-depth analysis of the validation results, including the possible sources of the uncertainties. An uncertainty analysis based on the sensitivity methodology has been also performed, providing the uncertainties in the isotopic content propagated from the cross sections uncertainties. An improvement of the classical Sensitivity/ Uncertainty (S/U) model has been developed to take into account the implicit dependence of the neutron flux normalization, that is, the effect of the constant power of the reactor. The improved S/U methodology, neglected in this kind of studies, has proven to be an important contribution to the explanation of some simulation-experiment discrepancies for which, in general, the cross section uncertainties are, for the most relevant actinides, an important contributor to the simulation uncertainties, of the same order of magnitude and sometimes even larger than the experimental uncertainties and the experiment-simulation differences. Additionally, some hints for the improvement of the JEFF3.1.1 fission yield library and for the correction of some errata in the experimental data are presented.

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1. Introduction

Computer codes with the burn-up capability to simulate irradiation history have been extensively used on the one hand for understanding the behaviour of current reactors fuel pins under irradiation, especially when dealing with high burn-up simulations achievable in the current nuclear concepts mainly for economic reasons (extending the cycle length). On the other hand, concerning advanced nuclear concepts such as Generation IV fast reactors (and even some Generation III reactors), still without worldwide implementation, the computer simulation has been the most widely used tool to model and evaluate their properties, including reactivity, safety and waste management issues.

The EVOLCODE 2.0 simulation system (Álvarez-Velarde et al., 2007) was developed at CIEMAT with the aim of providing a computer code able of making simulations of current and future reactors in any range of operation and to provide detailed spatial distribution and time evolution of the isotopic composition of fuels and activated materials. Particularly, the capability of making simulations of isotopic evolution in the fuel for nuclear systems with

very diverse characteristics and reaching long fuel burn-ups was focused. For these reasons, the present version of the EVOLCODE system is based upon the MCNPX code (Pelowitz et al., 2009) for the neutronic transport simulation and the ORIGEN code (Croff, 1980) for the depletion calculations. Any version of these codes can be implemented in EVOLCODE 2.0. Alternatively, the user has the option of using MCNP5 code (Brown et al., 2010) for transport and the ACAB code (Sanz et al., 2008) for depletion instead of the base codes to gain additional capabilities.

The code has been validated (mainly for fast neutron systems) up to now by the participation in international code benchmarks (Janczyszyn et al., 2011; Broeders et al., 2010). However, recently an experimental data set focused on Pressurized Light Water Reactors (PWRs) discharge composition has become available. This experiment, the Isotopic Correlation Experiment (ICE) (Koch and Schoof, 1981), was intended for the measure of some actinides and fission products generated after burn-up.

The ICE experimental measurements have been used by different institutions to validate several burn-up codes (with generally high degree of success) (Koch and Schoof, 1981; Cao et al., 2010; Send, 2005), which is the case of MCNPX with the integration of CINDER (Fensin et al., 2006), the deterministic code KAPROS and its burn-up module KARBUS (Broeders et al., 2004) or preliminarily with EVOLCODE 2.0 (Álvarez-Velarde and González-Romero,



^{*} Corresponding author. Tel.: +34 91 346 6731; fax: +34 346 6576. *E-mail address:* francisco.alvarez@ciemat.es (F. Álvarez-Velarde).

2011). This work was accomplished in the frame of the IAEA Coordinated Research Project on *Analytical and Experimental Benchmark Analyses of Accelerator Driven Systems* (Broeders et al., 2010). Nevertheless, in these studies only a direct comparison between experimental and simulation data was performed without extensive analysis of the sources of the discrepancies.

In this paper, a Sensitivity/Uncertainty analysis (S/U) has been performed to investigate the sources of the differences between the experimental data and the simulations results, possibly caused by the propagation of the cross sections uncertainties, or by other uncertainty sources that must be taken into account. A detailed description of the results found from the validation of EVOLCODE 2.0 using the ICE measurements has also been included.

This work is framed within the ANDES project (ANDES, 2010) (Accurate Nuclear Data for nuclear Energy Sustainability, 7th Framework Programme of the European Union). Its results will allow providing some guidelines in order to advise additional strategies for cross section uncertainty reduction.

2. Methodology

2.1. Description of EVOLCODE 2.0

EVOLCODE 2.0 is a combined neutronics and burn-up evolution simulation code aimed for the description of the burn-up evolution of either critical or subcritical reactors operating in any neutron spectrum regime. The code is able to estimate a great variety of nuclear reactor parameters, in particular, the isotopic composition evolution of the fuel in a nuclear reactor.

Burn-up problems are solved by EVOLCODE 2.0 using an timeinterval method consisting in the successive calculation of first the neutron flux for fixed material densities at a given time and later the depletion of these densities, using the hypothesis of constant neutron flux. Given that the validity of the hypotheses of constant properties is limited in the irradiation time, several calculations are needed to solve the system for the whole irradiation period. Each iteration, corresponding to a partial irradiation period, is called an EVOLCODE cycle. The cycle data flow of the EVOLCODE procedure is shown in Fig. 1.

In the present version of the code (Álvarez-Velarde et al., 2007), the neutron transport calculations are implemented by the general Monte Carlo N-Particle Transport Code MCNPX or alternatively by the MCNP5 code. The Isotope Generation and Depletion Code ORI-GEN currently implements the depletion of the geometry zones, requested by the user, although the code ACAB has also been implemented in the EVOLCODE 2.0 system to provide results uncertainties and to enlarge the number of nuclear reactions taken into account by the irradiation calculations. Both ORIGEN and ACAB are point-depletion and radioactive decay computer codes, and share the main computational mechanism called the transition matrix method (Croff, 1983). The user chooses which depletion code or version of MCNP/X is used in the simulations.

As it will be shown in the following, many of the characteristics of the programming of EVOLCODE 2.0 are aimed to deal with the proper implementation of the applied hypotheses so that the precision in the calculation is optimized.

The space dependence of the neutron flux is determined by the MCNPX cell definition, together with the entire geometry definition, allowing an important degree of the heterogeneity description in the reactor core model. The energy dependence is obtained by means of the energy spectrum of the neutron flux for each of these cells. On the one hand, the neutron flux is normalized so that the depletion is simulated using the proper value of the system thermal power. On the other hand, the neutron flux energy spectra are used for creating (outside MCNPX) one-group effective cross-section libraries for ORIGEN. Even using a largely detailed number of energy groups (around 30,000), EVOLCODE 2.0 performances reduce the computer time by one-two dozens while providing results with the same accuracy (Álvarez-Velarde, 2011) as if the simulation was made using the MCNPX burn-up capability. This fact has also been observed in other burn-up codes using this methodology (Haeck and Verboomen, 2007).

EVOLCODE is pushed to use the same basic libraries that MCNP does, so that the consistency in the data treatment is ensured. From these basic libraries, the information of those reactions suitable for ORIGEN and available in the database is selected, disregarding the information about elastic collisions. Additionally, since isomers may have very different half-lives and reaction cross sections compared with the ground state isotope (leading to different transmutation chains), the information of the isomer producing reactions is provided to the code by a separated file, ENDF File 9, containing the information of the branching ratios, i.e.,



Fig. 1. EVOLCODE2 cycle data flow scheme.

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