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Abstract: Nuclear data uncertainties and their impact on a very wide range of reactor systems, including their associated fuel cycles, have to be assessed in order to consolidate preliminary design studies for new innovative systems. One specific class of systems is the so-called "dedicated waste transmuters", that are fast neutron systems (critical or sub-critical, i.e. ADS), loaded with a Minor Actinide (MA) dominated fuel and potentially uranium-free. The availability of very general tools for sensitivity and uncertainty analysis together with new variance-covariance matrix data, produced in a joint effort under the auspices of the OECD-NEA by the world leading nuclear data evaluation groups, makes that endeavor particularly significant. In this report major results of interest for dedicated ADS are discussed and the most important fields and data types are pointed out, where priority improvements are required.

Introduction

The potential impact of nuclear data uncertainties on a large number of performance parameters of an ADS dedicated to the transmutation of radioactive wastes was presented in [1,2]. An uncertainty study was performed based on sensitivity analyses, which did underline the cross-sections, the energy range, and the isotopes that were responsible for the most significant uncertainties. In particular, in [2], the uncertainty assessment was performed with the use of the new covariance data recently developed within the WPEC Subgroup 26 [3] by joint efforts of several laboratories. The new set of uncertainties [4 to 13] is called BOLNA (standing for BNL, ORNL, LANL, NRG, ANL, from the Labs where the covariances were produced). The integral parameters analyzed in [2] were all the ADS parameters potentially most sensitive to nuclear data uncertainties: multiplication factor, power peak, defined as the point maximum power value normalized to the total power, burnup $\Delta k/k$, coolant void reactivity coefficient, nuclide density at end of cycle (transmutation potential), the ratio φ^* of the average external source importance to the average fission neutron importance, the values of the displacements per atom (dpa), He production, H production and the ratio (He production)/dpa at the spatial point where they reach their maximum value (Max dpa, Max (n,α), Max (n,p), Max (n,α)/dpa). The Doppler reactivity coefficient has not been considered due to its small calculated value.

The uncertainty analysis carried out in [2] lead to the following conclusions. The overall uncertainties on the selected integral parameters are quite significant. Pu-241 and some of the higher Pu isotopes contribute to the uncertainties, while the Pu-239 contribution is always very small, in agreement with what was already pointed out in [1]. However, the major contributions are due to MA data and in particular to Cm-244 data uncertainties. Am-241, Am-243, Cm-245 give also some noteworthy contributions. As for structural materials, Fe-56 and Bi-209 show non-negligible effects. Concerning the isotope reactions that are the most important contributors to the uncertainties, the role of fission cross-section uncertainties is found remarkable for most parameters. In fact, uncertainties in the fission cross-sections have an effect both on the reactivity and in the hardness of the spectrum. This last effect can be seen both on the power peak and on the Max (n,α)/dpa ratio. With respect to the previous study [1], there is much less impact of (n,2n) cross-sections, due to lower values of uncertainty in the present variance-covariance data (~10%, to be compared to the 100% value used in [1]). On the contrary, the significant impact of the Fe-56 inelastic cross-section is confirmed, in particular on the void reactivity coefficient.

To provide guidelines on priorities for new evaluations or experimental validations, in the present paper required accuracies on specific nuclear data have been derived. This analysis is similar to the work performed in [1]. However, the present results account for the target accuracies on major design parameters, recently established within the NEA WPEC Subgroup 26, and are consistent with the uncertainty assessment carried out with the BOLNA covariance matrix. Additionally, the present study involves the use of more sophisticated computational tools.

Data target accuracies

To be consistent wit the target accuracy study presented in [14], the guidelines that will be provided in the present paper for data improvements are based on the analysis of the following parameters: multiplication factor, power peak, coolant void reactivity coefficient, burn up Δk/k, nuclide density at end of cycle. Within the Subgroup 26, a preliminary list of design target accuracies for fast reactor systems (at first, independently of the coolant and fuel type) has been established as presented in Table 1. These target accuracies reflect the perceived state of the art, even if they are not yet the result of a systematic analysis, which should necessarily involve industrial partners. Moreover, it has to be kept in mind that no final, well defined "images" for any of the dedicated transmuter (critical or sub critical) systems exist at present. This means that the target accuracies shown in Table 1 reflect the current hypothesis for transmutation systems with innovative fuels and core configurations as described in [15,16] (i.e. fast spectrum sodium (Na) -cooled "burner" systems), and are applied to the Lead Bismuth Eutectic (LBE) -cooled ADS under study as well.

Table 1. *Fast Burner Reactor and ADS Target Accuracies (1σ)*

Multiplication factor (BOL)	300 pcm	Reactivity coefficients (Coolant void and Doppler)	7%
Power peak (BOL)	2%	Major nuclide density at end of irradiation cycle	2%
Burnup reactivity swing	300 pcm	Other nuclide density at end of irradiation cycle	10%

Theoretical approach and reference calculations

The chosen ADS system has some general features (e.g., the mass ratio between plutonium and MA, the americium-to-curium ratio, etc.) that are representative of the class of MA transmuters with a fast neutron spectrum and a uranium-free fuel. The target and the coolant material of the core consist of LBE, and the model is very close to the sub-critical core, which has been analyzed in the framework of an international OECD-NEA benchmark [17].

Sensitivity and uncertainty coefficients are consistent with the results presented in [2] and calculated at ANL with the ERANOS code system [18].

As reminder, once the sensitivity coefficient matrix S_R for each integral parameter R and the covariance matrix D are available, the uncertainty on the integral parameter can be evaluated as follows:

$$\Delta R_0^2 = S_R^+ D S_R \qquad \text{Eq. 1}$$

A successive step is the assessment of target accuracy requirements. To establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted by defining target accuracy on design parameters and finding out the required accuracy on the nuclear data σ_i. In fact, the unknown uncertainty data requirements d_i can be obtained (e.g. for parameters i not correlated among themselves), by solving the following minimization problem:

$$\sum_i \lambda_i / d_i^2 = \min \qquad (i = 1…I, I: \text{total number of parameters}) \qquad \text{Eq. 2}$$

with the following constraints:

$$\sum_i S_{R_n i}^2 d_i^2 < \left(R_n^T\right)^2 \quad (n = 1…N, N: \text{total number of integral design parameters}),$$

where $S_{R_n i}$ are the sensitivity coefficients for the integral parameter R_n, and R_n^T are the target accuracies on the N integral parameters; λ_i are "cost" parameters related to each σ_i and should give a relative figure of merit of the difficulty of improving that parameter (e.g., reducing uncertainties with an appropriate experiment).

The cross-sections uncertainties required for satisfying the target accuracies have been calculated by a minimization process that satisfies the nonlinear constraints with bounded parameters. The SNOPT code [19] has been used for this purpose. To avoid the introduction of meaningless parameters, as unknown "d" parameters (i.e., as cross-sections for which target accuracies are required), only those which globally account at least for 98% of the overall uncertainty for each integral parameter have been chosen. Concerning the cost parameters, as already done in previous work [15], a constant value of one for all λ_i is initially taken. Additionally, at the first stage it was decided not to account for correlations between data. This assumption is of course rather arbitrary, but it is consistent with standard requirements for reactor designs in early phases of development.

Results

The most relevant cross-section accuracy requirements are presented in Table 2. It can be observed that tight requirements are found for MA cross-sections, in particular for σ_{fiss} of Cm-244, Am241, Cm-245, Am-243, Cm-242, Am-242m, for σ_{inel} of Am-243 and for v of Cm-244. For these reactions, the required accuracies are an order of magnitude below the present uncertainties. Concerning the major actinides, improvements are required for σ_{fiss} of Pu-241 (again ~factor 10), for σ_{fiss} of Pu-238 (~factor 5) and for v of Pu-238 (~factor 3). Finally, important requirements are also found for structural materials, particularly for σ_{inel} of Fe-56, Bi-209, Pb and Zr-90.

Table 2. *Uncertainty Reduction Requirements Needed to Meet Integral Parameter Target Accuracies*

Isotope	Cross-Section	Energy Range	Uncert. (%) Initial	Uncert. (%) Target	Isotope	Cross-Section	Energy Range	Uncert. (%) Initial	Uncert. (%) Target
Cm244	σ_{fiss}	6.07 - 2.23 MeV	31.3	3.0	Bi209	σ_{inel}	2.23 - 1.35 MeV	34.1	2.8
		2.23 - 1.35 MeV	43.8	2.6			1.35 - 0.498 MeV	41.8	4.2
		1.35 - 0.498 MeV	50.0	1.5	Am243	σ_{fiss}	6.07 - 2.23 MeV	11.0	2.3
Fe56	σ_{inel}	6.07 - 2.23 MeV	7.2	2.5			1.35 - 0.498 MeV	9.2	1.6
		2.23 - 1.35 MeV	25.4	1.6	Cm244	v	6.07 - 2.23 MeV	11.1	2.5
		1.35 - 0.498 MeV	16.1	1.5			1.35 - 0.498 MeV	5.5	1.3
Am243	σ_{inel}	1.35 - 0.498 MeV	42.2	2.3	N15	σ_{el}	1.35 - 0.498 MeV	5.0	1.2
		498 - 183 keV	41.0	3.6	Pb	σ_{inel}	6.07 - 2.23 MeV	5.4	2.9
		183 - 67.4 keV	79.5	3.7	Zr90	σ_{inel}	6.07 - 2.23 MeV	18.0	3.3
Pu241	σ_{fiss}	1.35 - 0.498 MeV	16.6	2.1	Pu238	σ_{fiss}	2.23 - 1.35 MeV	33.8	6.0
		498 - 183 keV	13.5	1.7			1.35 - 0.498 MeV	17.1	3.4
		183 - 67.4 keV	19.9	1.7			498 - 183 keV	17.1	3.9
Am241	σ_{fiss}	6.07 - 2.23 MeV	11.7	1.7	Cm242	σ_{fiss}	6.07 - 2.23 MeV	52.6	26
		2.23 - 1.35 MeV	9.8	1.4			498 - 183 keV	66.0	28.4
		1.35 - 0.498 MeV	8.3	1.2	Pu238	v	1.35 - 0.498 MeV	7.0	2.8
Cm245	σ_{fiss}	1.35 - 0.498 MeV	49.4	3.3			498 - 183 keV	7.0	3.4
		498 - 183 keV	37.2	2.9	Am242m	σ_{fiss}	498 - 183 keV	16.6	4.8
		183 - 67.4 keV	47.5	2.9			183 - 67.4 keV	16.6	4.8
		67.4 - 24.8 keV	26.5	3.2					

The required nuclear data accuracies, obtained from the optimization procedures, are such that the design target accuracies are fulfilled in most cases. Table 3 shows the initial integral parameter uncertainties (using the "BOLNA diagonal" covariance matrix) and the calculated uncertainties with the required cross-section uncertainties, as obtained with the minimization procedure. Note that the required parameter accuracies are not exactly met because of the cross-sections not accounted in the minimization procedures which give as consequence a residual uncertainty to be added to the specified accuracy. In Table 3, in italic font are the initial parameter uncertainties out of the required accuracies summarized in Table 1. Besides the parameters listed in Table 1 (e.g. the parameters for which accuracy requirements have been defined),

uncertainties on the additional integral quantities investigated in [2] have been recalculated. Uncertainties on nuclide densities at end of irradiation have not been reported because low values are found in general due to the short burn up.

Table 3. Integral Parameter Uncertainties (%) with Initial and Required σ Uncertainties

	k_{eff} [pcm]	Power Peak	Void	Burnup [pcm]	φ^*	Max dpa	Max (n,α)	Max (n,p)	Max (n,α)/ dpa
Initial	*1882*	*14.2*	*13.1*	*603*	1.43	20.53	9.71	16.29	13.12
With required uncertainties	283	2.2	3.5	216	0.34	3.18	5.29	3.47	5.16

Acknowledgments

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