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Simultaneous Nuclear Data Target Accuracy Study for Innovative Fast Reactors

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Abstract: The present paper summarizes the major outcomes of a study conducted within a Nuclear Energy Agency Working Party on Evaluation Cooperation (NEA WPEC) initiative aiming to investigate data needs for future innovative nuclear systems, to quantify them and to propose a strategy to meet them

Introduction

Within the NEA WPEC Subgroup 26 an uncertainty assessment has been carried out [1] using covariance data recently processed by joint efforts of several US and European Labs. In general, the uncertainty analysis shows that for the wide selection of fast reactor concepts considered, the present integral parameters uncertainties resulting from the assumed uncertainties on nuclear data are probably acceptable in the early phases of design feasibility studies. However, in the successive phase of preliminary conceptual designs and in later design phases of selected reactor and fuel cycle concepts, there will be the need for improved data and methods, in order to reduce margins, both for economic and safety reasons. It is then important to define as soon as possible priority issues, i.e. which are the nuclear data (isotope, reaction type, energy range) that need improvement, in order to quantify target accuracies and to select a strategy to meet the requirements needed (e.g. by some selected new differential measurements and by the use of integral experiments). In this context one should account for the wide range of high accuracy integral experiments already performed and available in national or, better, international data basis, in order to indicate new integral experiments that will be needed to account for new requirements due to innovative design features, and to provide the necessary full integral data base to be used for validation of the design simulation tools.

In previous studies [2,3], a target accuracy assessment was performed separately for selected Gen-IV systems. In the present study, a simultaneous target accuracy study has been performed over an ensemble of fast neutron systems, with different coolants (sodium (Na), gas, lead, lead bismuth eutectic), different fuel types (oxides, metals, carbides, nitrides) and different Pu/TRU compositions, in different core volumes. These systems (ABTR, SFR, EFR, GFR, LFR and ADS), have been defined in [2,4,5,6] and their characteristics are summarized in Table 1.

Table 1. Features of the Investigated Systems

| System | Fuel | Coolant | TRU/(U+TRU) | MA ^(a) /(U+TRU) | Power (MWth) |
|--------|---------|---------|-------------|----------------------------|--------------|
| ABTR | Metal | Na | 0.162 | ~0 | 250 |
| SFR | Metal | Na | 0.605 | 0.106 | 840 |
| EFR | MOX | Na | 0.237 | 0.012 | 3600 |
| GFR | Carbide | He | 0.217 | 0.050 | 2400 |
| LFR | Metal | Pb | 0.233 | 0.024 | 900 |
| ADS | Nitride | Pb-Bi | 1.0 | 0.680 | 380 |

^(a) Minor Actinides

Data target accuracies

To be consistent with the target accuracy study presented in [3], the guidelines that will be provided in the present paper for data improvements will refer to the analysis of the following parameters: multiplication factor, power peak, Doppler and coolant void reactivity coefficient, burnup $\Delta k/k$, and 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 2. 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. The target accuracy requirements presented in Table 2 have also been extended to the ADS system.

Table 2. 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 ^(a) density at end of irradiation cycle | 2% |
| Burnup reactivity swing | 300 pcm | Other nuclide density at end of irradiation cycle | 10% |

^(a) U-235, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242

Moreover, the same covariance data have been used as in [3]. These data have been produced by a major joint effort within Subgroup 26 by BNL, LANL, ORNL and NRG [7 to 16]

Theoretical approach and reference calculations

As already discussed in the introduction, in addition to the selected fast systems analyzed in [2,4], the ADS system investigated in [5,6] has been also considered.

Sensitivity and uncertainty coefficients are consistent with the results presented in [1,6] and calculated at ANL with the ERANOS code system [17].

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: $\Delta R_0^2 = S_R^+ D S_R$.

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 minimization problem:

$\sum_i \lambda_i / d_i^2 = \min$, ($i = 1 \dots I$, I : total number of parameters), with the following constraints:

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

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 [18] 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 [2,3], 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.

Uncertainty results

The uncertainties on the major integral parameters due to diagonal values of the BOLNA covariance matrix are provided in Table 3 (see values only associated to the label “With initial uncertainties”). For the ADS, the Doppler reactivity coefficient has not been considered due to its small calculated value. In Table 3, in italic font are the initial parameter uncertainties larger than the required accuracies summarized in Table 2. In general, it can be observed that the power peak, the Doppler and void reactivity coefficients, meet the accuracy requirements in all cases with the only exception of the ADS for the three parameters and of the SFR for the void coefficient. The worst situation is represented by the ADS, where all integral parameter uncertainties (with the only exception of the nuclide densities at end of irradiation, due to the short burn up) do not meet the accuracy requirements. As for the nuclei densities at the end of irradiation, most of the target accuracies are already met.

Table 3. *Integral Parameter Uncertainties (%) with Initial and Required Cross-Section Uncertainties*

| | | ABTR | SFR | EFR | GFR | LFR | ADS |
|--|------------------------------------|------------|-------------|-------------|-------------|------------|-------------|
| k_{eff} BOC [pcm] | With initial uncertainties | <i>643</i> | <i>1108</i> | <i>877</i> | <i>1270</i> | <i>890</i> | <i>1882</i> |
| | With required uncertainties | 291 | 348 | 322 | 326 | 320 | 279 |
| Power Peak BOC | With initial uncertainties | 0.3 | 0.3 | 0.8 | 1.2 | 0.4 | <i>14.2</i> |
| | With required uncertainties | 0.2 | 0.1 | 0.3 | 0.3 | 0.2 | 2.2 |
| Doppler BOC | With initial uncertainties | 2.9 | 3.6 | 2.5 | 3.6 | 2.8 | - |
| | With required uncertainties | 1.4 | 1.7 | 1.1 | 1.4 | 1.4 | - |
| Void | With initial uncertainties | 5.1 | <i>15.7</i> | 6.7 | 5.5 | 5.0 | <i>13.1</i> |
| | With required uncertainties | 2.8 | 6.0 | 3.3 | 3.1 | 1.9 | 3.5 |
| Burnup [pcm] | With initial uncertainties | -37 | -152 | <i>-584</i> | 254 | -128 | <i>-603</i> |
| | With required uncertainties | -14 | -45 | -201 | 92 | -45 | -207 |

Target accuracy results

Tables 4 and 5 show the relevant target accuracy results for the ensemble of only Na-cooled and all fast systems respectively. The required nuclear data accuracies, obtained from the optimization procedures, are such that the design target accuracies are fulfilled in most cases. Besides the initial integral parameter uncertainties, Table 3 shows the calculated residual uncertainties on the major integral parameters when one uses the required cross-section uncertainties, as obtained with the minimization procedure applied to all fast systems. 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 going to be added to the specified accuracy.

In the two cases (i.e. only Na-cooled or all fast reactor types), the major requirements are related to the same type of data (Pu-241 fission, U-238 inelastic and capture, Pu-240 fission) and to approximately the same level of accuracy. Specific requirements can show up in the two cases according to the cooling type or to the specific structural materials. Minor actinide data needs become more evident if the ADS case (i.e. with MA dominated fuel) is considered. There are however some general requirements, whatever is the type of system, as e.g. for Cm-244 and Am-242m fission data.

Table 4. ABTR, SFR, EFR: Uncertainty Reduction Requirements to Meet Integral Parameter Target Accuracies

| Isotope Cross-Section | Energy Range | Uncertainty (%) | | Isotope Cross-Section | Energy Range | Uncertainty (%) | | Isotope Cross-Section | Energy Range | Uncertainty (%) | |
|--|------------------|-----------------|--------|--|------------------|-----------------|--------|---|------------------|-----------------|--------|
| | | Initial | Target | | | Initial | Target | | | Initial | Target |
| U238 σ_{inel} | 19.6 - 6.07 MeV | 29.3 | 20.1 | Fe56 σ_{inel} | 19.6 - 6.07 MeV | 13.0 | 8.9 | Am242m σ_{fiss} | 6.07 - 2.23 MeV | 23.4 | 8.0 |
| | 6.07 - 2.23 MeV | 19.8 | 4.6 | | 6.07 - 2.23 MeV | 7.2 | 4.1 | | 2.23 - 1.35 MeV | 19.7 | 8.2 |
| | 2.23 - 1.35 MeV | 20.6 | 4.5 | | 2.23 - 1.35 MeV | 25.4 | 3.3 | | 1.35 - 0.498 MeV | 16.5 | 4.3 |
| | 1.35 - 0.498 MeV | 11.6 | 5.5 | | 1.35 - 0.498 MeV | 16.1 | 3.2 | | 498 - 183 keV | 16.6 | 3.1 |
| Pu241 σ_{fiss} | 6.07 - 2.23 MeV | 14.2 | 6.5 | Pu239 σ_{capt} | 1.35 - 0.498 MeV | 18.2 | 10.1 | | 183 - 67.4 keV | 16.6 | 3.1 |
| | 2.23 - 1.35 MeV | 21.3 | 5.8 | | 498 - 183 keV | 11.6 | 6.5 | | 67.4 - 24.8 keV | 14.4 | 4.1 |
| | 1.35 - 0.498 MeV | 16.6 | 3.4 | | 183 - 67.4 keV | 9.0 | 5.6 | | 24.8 - 9.12 keV | 11.8 | 4.3 |
| | 498 - 183 keV | 13.5 | 2.6 | | 67.4 - 24.8 keV | 10.1 | 6.3 | | 9.12 - 2.03 keV | 12.4 | 6.5 |
| | 183 - 67.4 keV | 19.9 | 2.6 | | 24.8 - 9.12 keV | 7.4 | 5.5 | | 2.03 - 0.454 keV | 12.2 | 5.2 |
| | 67.4 - 24.8 keV | 8.7 | 3.3 | | 9.12 - 2.03 keV | 15.5 | 6.7 | Pu240 σ_{fiss} | 19.6 - 6.07 MeV | 9.6 | 8.6 |
| | 24.8 - 9.12 keV | 11.3 | 3.5 | O16 σ_{capt} | 19.6 - 6.07 MeV | 100.0 | 62.3 | | 6.07 - 2.23 MeV | 4.8 | 2.8 |
| | 9.12 - 2.03 keV | 10.4 | 5.4 | | 6.07 - 2.23 MeV | 100.0 | 39.5 | | 2.23 - 1.35 MeV | 5.7 | 2.6 |
| | 2.03 - 0.454 keV | 12.7 | 4.4 | Na23 σ_{inel} | 2.23 - 1.35 MeV | 12.6 | 9.3 | | 1.35 - 0.498 MeV | 5.8 | 1.8 |
| | 454 - 22.6 eV | 19.4 | 8.6 | | 1.35 - 0.498 MeV | 28.0 | 4.0 | | 498 - 183 keV | 3.9 | 3.9 |
| U238 σ_{capt} | 24.8 - 9.12 keV | 9.4 | 3.8 | Cm244 σ_{fiss} | 6.07 - 2.23 MeV | 31.3 | 8.2 | | 2.03 - 0.454 keV | 21.6 | 12.4 |
| | | | | | 2.23 - 1.35 MeV | 43.8 | 8.2 | | | | |
| | | | | | 1.35 - 0.498 MeV | 50.0 | 5.1 | | | | |
| | | | | | 498 - 183 keV | 36.5 | 12.1 | | | | |

Table 5. ABTR, SFR, EFR, GFR, LFR, ADMAB: Uncertainty Reduction Requirements to Meet Integral Parameter Target Accuracies

| Isotope Cross-Section | Energy Range | Uncertainty (%) | | Isotope Cross-Section | Energy Range | Uncertainty (%) | | Isotope Cross-Section | Energy Range | Uncertainty (%) | |
|--|------------------|-----------------|--------|---|------------------|-----------------|--------|--|------------------|-----------------|--------|
| | | Initial | Target | | | Initial | Target | | | Initial | Target |
| U238 σ_{inel} | 19.6 - 6.07 MeV | 29.3 | 9.0 | B10 σ_{capt} | 498 - 183 keV | 15.0 | 2.9 | Pu240 σ_{fiss} | 6.07 - 2.23 MeV | 4.8 | 2.9 |
| | 6.07 - 2.23 MeV | 19.8 | 2.0 | | 183 - 67.4 keV | 10.0 | 2.7 | | 2.23 - 1.35 MeV | 5.7 | 2.6 |
| | 2.23 - 1.35 MeV | 20.6 | 2.1 | | 67.4 - 24.8 keV | 10.0 | 3.3 | | 1.35 - 0.498 MeV | 5.8 | 1.6 |
| | 1.35 - 0.498 MeV | 11.6 | 2.3 | | 24.8 - 9.12 keV | 8.0 | 3.9 | | 498 - 183 keV | 3.9 | 3.7 |
| | 498 - 183 keV | 4.2 | 3.8 | | 9.12 - 2.03 keV | 8.0 | 6.0 | | 2.03 - 0.454 keV | 21.6 | 11.8 |
| | 183 - 67.4 keV | 11.0 | 4.2 | Pu239 σ_{capt} | 1.35 - 0.498 MeV | 18.2 | 6.6 | Si28 σ_{capt} | 19.6 - 6.07 MeV | 52.9 | 7.2 |
| Pu241 σ_{fiss} | 6.07 - 2.23 MeV | 14.2 | 5.0 | | 498 - 183 keV | 11.6 | 4.4 | | | | |
| | 2.23 - 1.35 MeV | 21.3 | 3.9 | | 183 - 67.4 keV | 9.0 | 4.0 | Si28 σ_{inel} | 6.07 - 2.23 MeV | 13.5 | 3.9 |
| | 1.35 - 0.498 MeV | 16.6 | 2.1 | | 67.4 - 24.8 keV | 10.1 | 4.2 | | 2.23 - 1.35 MeV | 50.0 | 7.4 |
| | 498 - 183 keV | 13.5 | 1.7 | | 24.8 - 9.12 keV | 7.4 | 3.8 | Pb206 σ_{inel} | 6.07 - 2.23 MeV | 5.5 | 4.2 |
| | 183 - 67.4 keV | 19.9 | 1.7 | | 9.12 - 2.03 keV | 15.5 | 3.2 | | 2.23 - 1.35 MeV | 14.2 | 4.0 |
| | 67.4 - 24.8 keV | 8.7 | 1.9 | O16 σ_{capt} | 19.6 - 6.07 MeV | 100.0 | 37.9 | | 1.35 - 0.498 MeV | 9.2 | 4.7 |
| | 24.8 - 9.12 keV | 11.3 | 2.0 | | 6.07 - 2.23 MeV | 100.0 | 37.9 | Pb207 σ_{inel} | 6.07 - 2.23 MeV | 5.0 | 4.9 |
| | 9.12 - 2.03 keV | 10.4 | 2.1 | Am243 σ_{inel} | 6.07 - 2.23 MeV | 17.9 | 4.9 | | 2.23 - 1.35 MeV | 13.8 | 6.0 |
| | 2.03 - 0.454 keV | 12.7 | 2.7 | | 2.23 - 1.35 MeV | 35.3 | 3.9 | Pb σ_{inel} | 1.35 - 0.498 MeV | 11.3 | 3.6 |
| Cm244 σ_{fiss} | 454 - 22.6 eV | 19.4 | 5.4 | | 1.35 - 0.498 MeV | 42.2 | 2.3 | | 6.07 - 2.23 MeV | 5.4 | 3.0 |
| | 6.07 - 2.23 MeV | 31.3 | 3.0 | | 498 - 183 keV | 41.0 | 3.7 | Am243 σ_{fiss} | 6.07 - 2.23 MeV | 11.0 | 2.3 |
| | 2.23 - 1.35 MeV | 43.8 | 2.6 | | 183 - 67.4 keV | 79.5 | 3.7 | | 2.23 - 1.35 MeV | 6.0 | 1.9 |
| | 1.35 - 0.498 MeV | 50.0 | 1.5 | | 67.4 - 24.8 keV | 80.8 | 12.4 | | 1.35 - 0.498 MeV | 9.2 | 1.7 |
| | 498 - 183 keV | 36.5 | 4.0 | Am242m σ_{fiss} | 1.35 - 0.498 MeV | 23.4 | 21.4 | Bi209 σ_{inel} | 2.23 - 1.35 MeV | 34.1 | 2.8 |
| U238 σ_{capt} | 183 - 67.4 keV | 47.6 | 7.3 | | 498 - 183 keV | 16.5 | 6.3 | | 1.35 - 0.498 MeV | 41.8 | 4.3 |
| | 24.8 - 9.12 keV | 9.4 | 1.8 | | 183 - 67.4 keV | 16.6 | 4.7 | | 2.23 - 1.35 MeV | 5.0 | 3.1 |
| | 9.12 - 2.03 keV | 3.1 | 1.8 | | 67.4 - 24.8 keV | 16.6 | 4.8 | N15 σ_{el} | 1.35 - 0.498 MeV | 5.0 | 1.2 |
| Fe56 σ_{inel} | 6.07 - 2.23 MeV | 7.2 | 2.6 | Na23 σ_{inel} | 24.8 - 9.12 keV | 14.4 | 5.6 | | 498 - 183 keV | 5.0 | 1.9 |
| | 2.23 - 1.35 MeV | 25.4 | 1.7 | | 2.04 - 0.454 keV | 11.8 | 5.9 | | 183 - 67.4 keV | 5.0 | 2.3 |
| | 1.35 - 0.498 MeV | 16.1 | 1.5 | | 1.35 - 0.498 MeV | 28.0 | 10.5 | Zr90 σ_{inel} | 6.07 - 2.23 MeV | 18.0 | 3.3 |

These results should be used with precaution. They indicate trends and general priority needs. In fact, these quantitative values have been obtained considering only diagonal (variance) uncertainty values that represent an underestimation of the real uncertainty. Moreover, and

certainly more important, the accuracy requirements and priorities are strongly dependent on the assumed initial uncertainty variance-covariance data, and in particular on the very low initial uncertainty values on the fission cross-section of Pu-239. This work however provides a clear indication for future work: a) Improvement of the present covariance data: b) Selection of a few priority differential measurements, where the expected experimental uncertainties can match the data required uncertainty; c) Definition of a strategy of combined use of high quality integral experiments, sophisticated analysis tools, scientifically based covariance data within a statistical data adjustment, in order to fully validate calculation tools for the design of future innovative systems. This approach is discussed in a companion paper at this workshop [19].

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