Nuclear data for sustainable nuclear energy

Coordinated action on nuclear data for industrial development in Europe
CANDIDE

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Nuclear data for sustainable nuclear energy

Final report of a

Coordinated Action on Nuclear Data for Industrial Development in Europe (CANDIDE)

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Executive summary

The successful development of advanced nuclear systems for sustainable energy production depends on high-level modelling capabilities for the reliable and cost-effective design and safety assessment of such systems, and for the interpretation of key benchmark experiments needed for performance and safety evaluations. High-quality nuclear data, in particular complete and accurate information about the nuclear reactions taking place in advanced reactors and the fuel cycle, are an essential component of such modelling capabilities. A primary benefit of improved nuclear data lies in the perspective of cost reductions in developing and operating nuclear reactors; with precise nuclear data, nuclear systems can be designed to reach high efficiencies whilst maintaining adequate safety standards in a cost-effective manner.

In the CANDIDE project, nuclear data needs for sustainable nuclear energy production and waste management have been analyzed and categorized, on the basis of preliminary design studies of innovative systems. Meeting those needs will require that the quality of nuclear data files be considerably improved. Remarkably, the required know-how and instruments for a significant step forward are generally available in Europe and, in many cases, are world-leading. Tremendous progress could be made if these were properly mobilized, enlarged and organized. Therefore, setting up a coherent framework and initiating a sequence of well-directed actions to improve nuclear data, with adequate support and funding, will result in significant benefits to future nuclear system developments in Europe.

The CANDIDE project has produced a set of recommendations, or roadmap, for sustainable nuclear data development. A significant part of the required progress in nuclear data is independent of the actual design that will eventually be implemented. Therefore, a distinction is made between horizontal issues, i.e. general nuclear data development required for any system, and vertical issues, i.e. more specific issues per nuclear system. The most important conclusions and recommendations for horizontal nuclear data development are:

- **A long term commitment to modern nuclear data evaluation should be provided in Europe.** This concerns nuclear data evaluation that implements the latest advances in nuclear physics into high-quality nuclear data libraries for applied use, such as the JEFF-3 library. This should include a complete assessment of the uncertainties and uncertainty correlations in nuclear data (covariance matrices). If accomplished, this will allow better determination of safety and economical margins of both existing and future nuclear systems. It will also make it possible to relate advances in experimental and theoretical nuclear physics to the needs of industrial applications. A special European targeted action for the production of high quality nuclear data libraries, including covariance data, for materials for advanced reactor design is needed, to ensure that Europe’s position remains at par with our competitors, who have recently taken such measures. This special effort should go well beyond the basic work performed as part of the OECD/NEA JEFF Project. Specific high-priority recommendations include:
  - Production of complete nuclear data libraries, including a comprehensive set of reliable covariance matrices, using both theoretical and experimental nuclear data information.
• Development of systematic quality-assured data evaluation and validation methods, which guarantee consistent nuclear data libraries in which new experimental and theoretical information becomes directly and correctly available, for subsequent library updates.

The production of covariance matrices is an extremely important task, which calls for a dedicated specially-funded action on the part of nuclear and reactor physics experts in close collaboration, rather than a broad collaborative FP project spanning the entire spectrum of nuclear data research. This is an area where targeted support from the EC could help bridge the current gap.

• **Provide and support the facilities that are capable to produce the required nuclear measurements and stimulate high-level measurements on key reactions of interest to advanced reactor development**, especially those measurements that demand higher accuracy than available from nuclear modelling, and critical data that serve as standards for large classes of other measurements. Specific high-priority recommendations include:
  - The stimulation of selected measurements that answer generally accepted high-precision nuclear data needs, such as those identified by the recent NEA SG-26 working group on nuclear data needs for advanced reactors and ADS, as categorized in the High-Priority Request List for nuclear data.
  - Insistence on a “culture change” in experimental nuclear physics, to deliver systematically to the international databases complete documentation of the experiments and all covariance information.
  - The stimulation of new integral measurements to test nuclear data in well-defined reactor-type spectra and to decrease the nuclear data uncertainties in cases where differential measurements do not suffice.

• **Provide the capability for advanced nuclear model development** to address the priority needs that cannot be met due to the lack of experimental facilities or because model calculations can provide certain important data in a more cost effective way. Specific high-priority recommendations include:
  - Bring the predictive power of nuclear models for actinides to the same level as that for non-fissile nuclides. For this, consistent nuclear fission models and parameters for all important actinides need to be developed and made generally available. This will give the possibility to produce complete covariance data for actinides as well.
  - Development of consistent statistical methods to produce reliable covariance information from both theory and experiment.

• **Ensure flexible implementation of improved nuclear data libraries in nuclear technology and design.** Those companies or institutions that can assure and reduce the cycle time for innovations and quality improvements in nuclear data have a distinct advantage in either research or the industrial markets. This requires a modern approach to reactor software development, in particular regarding the handling of nuclear data. Obviously, the nuclear data community will benefit from rapid and flexible application of their results in actual reactor calculations, and the associated feedback will allow further improvements to be made. Specific high-priority recommendations include:
  - Assist reactor code developers in developing easy upgradeable nuclear data library interfaces, for both static and dynamic system analyses. This should be pursued into the area of full-core coupled neutronic and thermo-hydraulic reactor calculations.
Develop systematic approaches to integral validation and sensitivity studies, to ensure that improved nuclear data (e.g. better covariance matrices) can directly be tested on relevant integral measurements.

In addition to these transverse or cross-cutting issues, contemporary analyses of current reactors, GEN-IV reactors and ADS also give rise to specific issues. The most important recommendations for vertical nuclear data development are:

- **Fast neutron actinide cross-sections for both critical and sub-critical reactors.** There are strongly motivated requests for improvement of the nuclear data for $^{238}$U (capture and inelastic) and the $^{238-242}$Pu isotopes (capture and fission). More precise measurements, fission model development, and careful data library evaluation including covariance data are called for.

- **Cross-sections for transmutation and target design in accelerator-driven systems.** Transmutation with sub-critical reactors, loaded with minor actinides, coupled with an accelerator are characterized by some specific nuclear data concerns:
  - Specific capture and fission measurements in the 1 eV to 1 MeV range for Am and Cm isotopes.
  - Well-chosen integral measurements for neutrons above 20 MeV.
  - Assessment of uncertainties of high-energy data (>20 MeV).

- **High burn-up systems.** Increased burn-up scenarios will put a larger emphasis on the quality of fission product evaluations. In order to better assess the neutron absorption rate of the fission products, their cross sections, fission yields and radioactive decay properties need to be improved. Therefore, decay data and fission yield data need to be critically examined and future evaluations be accompanied by both uncertainty and covariance data.

- **Fast neutron cross sections for structural materials and coolants.** Modern nuclear data evaluations and precision measurements of inelastic scattering cross sections are required for important (system-dependent) structural materials, coolants and inert fuel elements (Na, Mg, Si, Fe, Mo, Zr, Pb, Bi). In particular, an accurate determination of the sodium void coefficient of an SFR requires improvements in the inelastic scattering cross sections for $^{23}$Na and a complete covariance treatment.

In conclusion, a substantial long-term investment in an integrated European nuclear data development program is called for, complemented by some dedicated actions targeting specific issues. It can be expected that, as nuclear analysis and design methods improve, reactor designers will become more demanding in the targeted plant performance, which will result in more stringent requests on nuclear data evaluations, measurements, and validation. To be responsive, it is necessary to retain a critical mass of scientists in a variety of nuclear data related fields to maintain, develop and pass on their skills to the next generation of specialists. There are indications that, over the last few years, we have lost some of our expertise in the area of evaluation and data testing. There is also concern that the situation in this and other areas could rapidly deteriorate if no corrective action is taken. This deterioration will result from experienced people retiring or taking better career opportunities outside of their current research fields, and inadequate funding available to train replacements. As the situation appears to be fragile, it should be regularly reviewed. It is noted that significant enhancements in the nuclear data field...
can be generated through doctoral level student projects and postdoctoral research. Nuclear data students can additionally be a source for well-educated staff for the nuclear power industry and regulatory bodies, provided these positions are seen as good long-term career options.
1. Introduction

The potential benefits of advanced nuclear reactors are many and varied, including improved levels of efficiency in the use of fuel, a reduction in the amount of waste, and the ability to recycle at least part of the present reactor waste as energy-producing materials, the kinds of benefits that are encouraging authorities to look again at nuclear energy.

The road towards so-called sustainable nuclear energy production requires an ambitious research program over the entire breadth of nuclear science. The main reason for this is that there is, in contrast with current nuclear power reactors, obviously limited practical experience for the advanced systems under consideration for the coming decades. Yet, future systems will be asked to achieve comparable or even better performance than existing ones, which represents a challenge in view of the considerable feedback and optimization that benefited the latter. Therefore, the viability of new designs will depend more than ever on the quality of the underlying physics: experiments and computational simulations of high quality are needed before we can convince ourselves that the boundary conditions of sustainability can indeed be met. This difficult task can directly be translated into (i) large challenges in basic nuclear data, neutronics, material science, thermohydraulics, fuel fabrication, reprocessing and partitioning, the coupling of all these aspects (multi-physics), and modern quality-assured software that will replace the current suite of reactor simulation codes in both research and industry; (ii) many requirements in terms of “missing” experimental data, facilities and demonstration plants. As this represents a major undertaking, large consortiums such as the Generation IV (GEN-IV) International Forum (GIF) and Sustainable Nuclear Energy Technology Platform (SNETP) have been launched to agree on a limited number of most-promising systems, assess and prioritize the corresponding needs and, to all possible extent, share the associated R&D effort.

The first crucial ingredient of reactor and fuel cycle analysis is nuclear data. When designing or assessing the safety of a reactor system, nuclear data for a wide range of reactions and materials have to be known. Energy production, radiation damage, radioactivity and related matters all result from interactions between particles (usually neutrons) and nuclei; a precise simulation of these nuclear reactions is necessary to predict the system characteristics with sufficient accuracy. Therefore, in contemporary simulations, a major role is played by the uncertainty of nuclear data, which in a reactor system analysis can be propagated through the entire simulation scheme and eventually lead to uncertainties of key performance parameters of the simulated designs and the associated fuel cycle. The lack of complete and accurate nuclear data for technical design and development can lead to inefficiencies, lack of reliability, and design problems, all of which translate into larger operating margins and excess conservatism, which can be very costly. It should be emphasized that the main use of improved nuclear data in connection with future system studies will not simply be to provide proofs of principle, but to make it possible to go from laboratory to competitive industrial application with the minimum of building and operating prototype stations, i.e., accelerating development of commercial advanced reactor systems that can be operated safely at an acceptable cost. Thus, the main role of nuclear data is to improve the economy of future advanced reactors whilst maintaining safety.
A central question for the next generation of nuclear power development is: In view of the nuclear data uncertainties, how precisely can we predict the relevant reactor and fuel cycle parameters of advanced reactor systems, and is this acceptable in terms of performance, safety and sustainable operation? Next, if we can not determine these parameters with enough precision, what nuclear data developments are needed to improve this and how do we accomplish that? And finally, can we produce a validated and qualified nuclear data library, including the latest experimental and theoretical developments and covariance data, meeting the needs of both nuclear research organizations and industry, for reliable design of advanced nuclear systems? The present report addresses these questions.

1.1. Scope

Nuclear data are required for the following three fields within nuclear fission energy:
1. Optimization of existing power plants:
   - Plant lifetime extension
   - Increased performance by margin reduction (safety, economy)
   - Reduction of fuel cycle cost (high burn-up, lower enrichment,…)
2. Design and operation of new nuclear reactors
3. Specific back-end of the fuel cycle aspects and waste minimization

The CANDIDE project is restricted to Items 2 and 3, and in particular restricted to fast systems. The reason is that although the views on the future of nuclear energy may differ widely among European governments, the waste aspect of sustainability is of undisputed concern to any European country, and fast-spectrum systems have the best characteristics for waste minimization. However, the underpinning nature of nuclear data in design issues suggests that a similar status report should be produced for other nuclear applications, such as the optimization of existing power plants, or fusion.

1.2. Nuclear data

The primary objective of the nuclear data community is to produce high quality nuclear data libraries for existing and future nuclear energy systems. This rather straightforward objective requires a complex interplay between various working fields: commercial reactor operation, reactor and fuel cycle physics for either existing or future reactor and transmutation systems, data library processing and validation, data file evaluation, and theoretical and experimental nuclear physics. Worldwide, organizations and infrastructures such as measurement facilities, theoretical and computational nuclear physics groups, nuclear data centers, and reactor physics groups all contribute to provide nuclear data that enable efficient development of nuclear technology. Estimates of the total invested resources, including facilities, are difficult to make, but an indication of the size of the field is perhaps the tri-annual nuclear data conference for science technology, which hosts about 400 participants. Possibly 3000-5000 scientists worldwide are involved in the production or direct use of nuclear data for applications.

Experimental nuclear physics is a core element of nuclear data development, and for a long time has been the only credible information source that could contribute to the
understanding of processes taking place in nuclear systems. Indeed, during the heydays of nuclear power development a large worldwide nuclear data campaign was launched which resulted in about 3 million experimental nuclear data points, which are accessible in experimental databases and still in use today. In the past decades, theoretical nuclear physics has been put into practice, thanks to the huge increase in computer power, and now contributes significantly to nuclear data development by means of nuclear model software. Both experiment and theory are indispensable for nuclear data development: In general, a nuclear model code provides complete nuclear data sets, and relies on existing experimental data; these measurements provide the high precision information that can not be achieved by nuclear model codes alone. Delivering the required nuclear data for applications does not stop here however. The next stage in the process is nuclear data evaluation. The optimal combination of experimental data and nuclear model codes is used to create nuclear data libraries for all required materials. In the computational analysis of nuclear systems, two main classes of nuclear data are required: (1) data for describing the transport of neutrons and photons (and sometimes other particles) interacting with the nuclei making up the system, and (2) data for describing nuclear changes in the system constituents, as a result of fuel depletion (often called burn-up), transmutation, activation or decay reactions. For (1), so-called general purpose data files are required which contain all cross sections, resonance parameters and other nuclear reaction information entering particle balance calculations. For (2), fission yield and decay data libraries are required, as well as activation data. An essential ingredient of all these libraries is covariance data, which is a measure of the confidence we have in the quality of the nuclear data that come from measurement or theory. Similar to experiment and theory, nuclear data evaluation is a core element. Without it, nuclear data measurements and nuclear theory developments will not be put into practice. Equally important is the successful processing of basic data libraries into application libraries for the major reactor and fuel cycle codes.

It is important that the validation of nuclear data libraries with transport and reactor and fuel inventory codes, through comparison with integral measurements, remains closely connected to the rest of the nuclear data field. Large benchmark collections of integral measurements for criticality, shielding and more complex reactor experiments are already available and Monte Carlo and deterministic reactor software can readily be used to test the performance of nuclear data libraries. Finally, if nuclear covariance data are available, sensitivity analyses applied to reactor parameters can give direct insight in the required precision of nuclear data. Recently, there has been some effort in that direction for ADS and GEN-IV systems.

1.3. This report

Various cross-cuts through nuclear science can be made to assess the importance of nuclear data. For example, one could categorize nuclear data per foreseen nuclear system, or go systematically through an entire fuel cycle and address the nuclear data issues at each operation stage. Although these approaches would have their advantages, for this report we opted for a top-down-top approach: First, the important performance parameters for future nuclear energy systems are related to the current status of nuclear data. Next, the challenges for nuclear data development to meet the required quality improvement are identified and discussed. Finally, a strategy for global and specific nuclear data improvement is proposed and the possible impact of
such improvements on advanced nuclear energy systems will be outlined. We will thus go from nuclear energy to nuclear physics and back. All aspects of the nuclear fuel cycle and the various reactor systems will then automatically enter the picture.

In chapter 2 the nuclear data needs for advanced reactor development are discussed. In chapter 3 the current performance of nuclear data libraries for reactor simulation is described. Chapter 4 discusses the present nuclear data methodologies in the world, which have led to the current nuclear data libraries. Chapter 5 contains a roadmap for nuclear data development, describing the required steps forward to ensure high-quality analyses for advanced nuclear energy systems. Finally, the conclusions are given in chapter 6. A more detailed description of several nuclear data issues is provided in a collection of CANDIDE working documents [CANDIDE 2008].
2. Nuclear data needs for advanced reactor systems

2.1. Importance of nuclear data for energy production

Nuclear data are an integral part of reactor codes. Such codes are used by many in the research, development and plant operations fields, often with little awareness of the impact of nuclear data on the final results. That impacts are large is manifestly demonstrated by sensitivity studies that relate the uncertainties of calculated system parameters to the uncertainties of the underlying nuclear data. This chapter summarizes the outcomes of recent sensitivity studies for advanced reactors together with the employed methodology. This evidence for the importance of nuclear data is combined with, and corroborated by, feedback from comparisons between measured and calculated results for representative integral experiments. The final result of these analyses is presented as well: a list of requirements for nuclear data improvements.

Table 1. Target uncertainty (one sigma) for “viability” and “performance”

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Viability</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{en}(BOL)$</td>
<td>0.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>Peak core power</td>
<td>5%</td>
<td>3%</td>
</tr>
<tr>
<td>Breeding Gain</td>
<td>± 0.06</td>
<td>± 0.04 or better</td>
</tr>
<tr>
<td>Reactivity swing / cycle</td>
<td>1%</td>
<td>0.5%</td>
</tr>
<tr>
<td>Damage to Structures</td>
<td>15%</td>
<td>9%</td>
</tr>
<tr>
<td>Void effect</td>
<td>16%</td>
<td>7-10%</td>
</tr>
<tr>
<td>Doppler Effect</td>
<td>16%</td>
<td>10%</td>
</tr>
<tr>
<td>Control rod worth and absorbers</td>
<td>16%</td>
<td>10%</td>
</tr>
<tr>
<td>$\gamma$ Heating</td>
<td>16%</td>
<td>10%</td>
</tr>
<tr>
<td>$\beta$-eff</td>
<td>13%</td>
<td>7%</td>
</tr>
<tr>
<td>Decay heat in core and of spent fuel</td>
<td>10% (greater than 10s)</td>
<td>5%</td>
</tr>
<tr>
<td></td>
<td>20% (less than 10s)</td>
<td>10%</td>
</tr>
<tr>
<td>Radiation dose of spent fuel (neutrons)</td>
<td>20%</td>
<td>15%</td>
</tr>
<tr>
<td>Radiation dose of spent fuel ($\gamma$-Rays)</td>
<td>40%</td>
<td>30%</td>
</tr>
<tr>
<td>Criticality of spent fuel</td>
<td>10%</td>
<td>5%</td>
</tr>
</tbody>
</table>

A key question in cost-effective development of sustainable nuclear energy is how much time and effort may be saved by high quality modelling capabilities. Limiting the question to the neutronics and reactor physics domain: which quantities should be predicted and with what uncertainty? Recent sensitivity studies for advanced reactors [Salvatores 2008] considered simple models of a sodium-cooled fast reactor (SFR), a gas-cooled fast reactor (GFR), a lead-cooled fast reactor (LFR), a very high temperature reactor (VHTR, four of the six Generation-IV systems), an accelerator driven minor actinide burner (ADMAB), the European Fast Reactor (EFR) and a UOx-fuelled pressurized water reactor (PWR) with extended burn-up. Within international collaborations the main targets for model calculations and their uncertainties were agreed upon, see Table 1 for the requirements of fast reactors. It should be noted that the selected models represent a few particular core concepts among many possible variants for a given coolant (different fuel forms, fissile
content, subassembly geometries, core constituents and arrangements, etc.), most of which are still at a very early development stage today; therefore, it is expected that additional requirements will arise when more specific and detailed design studies will be completed.

A distinction is made between targets for viability studies and for performance analyses, the latter being considerably more tight in order to meet more stringent economic and safety margins.

**Sensitivity studies and target uncertainties for nuclear data**

Two questions may now be asked about the relevance of nuclear data when it comes to achieving the system target uncertainties of Table 1: 1) Given an initial estimate of nuclear data uncertainties, what is the estimated uncertainty of the system parameters (forward propagation) and how do they compare to the target uncertainties, and 2) Given the target uncertainties, what are the constraints on the uncertainties of the nuclear data (backward propagation)? Both questions were investigated and answered.

A particularly comprehensive work in this respect was that of Aliberti et al that was contributed to SG26 [Salvatores, 2008]. The results of the forward study was based on the BOLNA\(^1\) set of nuclear data covariance matrices, which comprise a total of 52 materials with covariance data that have all been produced in 15- and 187-group representations. Various labs produced data for different energy ranges, different nuclides and different covariance methods. Therefore, the resulting BOLNA set of covariance data is arguably of uneven quality. Nevertheless, it was considered sufficient to perform a first sensitivity study of advanced reactor systems.

Since it is clear from the forward propagation of uncertainties that currently precise nuclear data are lacking when it comes to meeting the targets of Table 1, the next question is which nuclear data should be improved and to what degree, in order to meet the targets. To answer this question, a backward propagation study was performed for each of the systems mentioned above. Such a backward propagation study translates the systems parameter target uncertainties into requirements on nuclear data covariances by means of computed sensitivity coefficients. Within these constraints, a cost function is minimized that weights the required uncertainty improvements by their perceived relative difficulty. Obviously different cost functions will lead to different requirements. In the end, a quantified set of nuclear data requirements is established by comparing the nuclear data target uncertainties with the currently achieved uncertainties (the BOLNA covariance matrices in this case).

Below the results of these studies are presented first for SG26 and then for the ADS-specific work of NUDATRA [CANDIDE 2008:5]. A much larger inventory of nuclear data needs, arising from testing the JEFF-3 library against many integral experiments is available [CANDIDE 2008:1].

### 2.2. Nuclear data issues identified by SG26

The list of nuclear data requirements from the work of SG26 is rather long due to the minor actinides and the fact that some of the systems differ in non-actinide content:

- fission cross sections of \(^{234}\text{U},^{235}\text{Np},^{238,240-242}\text{Pu},^{241,242m,243}\text{Am},^{242-246}\text{Cm},\)
- fission nu-bar of \(^{238,240}\text{Pu},^{241}\text{Am}\) and \(^{244}\text{Cm},\)

\(^1\) BOLNA: the Brookhaven, Oak Ridge, Los Alamos and Argonne National Laboratories together with the Nuclear Research consultancy Group, Petten
This longer list is however further prioritized considering the fact that for sustainable nuclear energy, fast systems are most important and by further limiting the list to the outstanding issues that are of common interest to more than one system. This reduced list of priority needs is presented in Table 2.

Several general features can be pointed out. Very tight requirements are shown for the $\sigma_{\text{inel}}$ of $^{238}\text{U}$ (2-3%), $^{239}\text{Pu}$ (6-15%), $^{56}\text{Fe}$ (3-6%), $^{23}\text{Na}$ (4-10%) and $^{90}\text{Zr}$ (4-10%) and even for Pb isotopes. In system specific cases Si, $^{209}\text{Bi}$, $^{241}$, $^{243}\text{Am}$ and even $^{240,242}\text{Pu}$ inelastic scattering shows up. Some of the required accuracies are probably beyond achievable limits with current differential experimental techniques. There are little margins to relax the requirements on $\sigma_{\text{inel}}$ if one does not want to produce equally difficult requirements on $\sigma_{\text{fiss}}$ and $\sigma_{\text{capt}}$ of some of the Pu isotopes. On the other hand, these margins need to be exploited to eliminate the requirements of Pu and Am inelastic scattering for which only improved theoretical estimates may be expected and the accuracy will thus not be significantly below 10%

Table 2. Summary of the SG26 Highest Priority Target Accuracies for Fast Reactors

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$\sigma_{\text{fiss}}$</th>
<th>Energy Range</th>
<th>Current Accuracy (%)</th>
<th>Target Accuracy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{238}\text{U}$</td>
<td>6.07 $\div$ 0.498 MeV</td>
<td>10 $\div$ 20</td>
<td>2 $\div$ 3</td>
<td></td>
</tr>
<tr>
<td>$^{239}\text{Pu}$</td>
<td>2.23 $\div$ 0.498 MeV</td>
<td>16 $\div$ 25</td>
<td>3 $\div$ 6</td>
<td></td>
</tr>
<tr>
<td>$^{240}\text{Pu}$</td>
<td>1.35 $\div$ 0.498 MeV</td>
<td>2.7 $\div$ 9</td>
<td>1.5 $\div$ 2</td>
<td></td>
</tr>
<tr>
<td>$^{241}\text{Pu}$</td>
<td>6.07 $\div$ 2.23 MeV</td>
<td>14 $\div$ 21</td>
<td>3 $\div$ 5</td>
<td></td>
</tr>
<tr>
<td>$^{242}\text{Pu}$</td>
<td>1.35 $\div$ 0.183 MeV</td>
<td>17</td>
<td>3 $\div$ 5</td>
<td></td>
</tr>
<tr>
<td>$^{243}\text{Am}$</td>
<td>1.35 $\div$ 0.498 MeV</td>
<td>50</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>$^{244}\text{Cm}$</td>
<td>6.07 $\div$ 1.35 MeV</td>
<td>14 $\div$ 25</td>
<td>3 $\div$ 6</td>
<td></td>
</tr>
<tr>
<td>$^{245}\text{Cm}$</td>
<td>1.35 $\div$ 0.498 MeV</td>
<td>11</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$^{56}\text{Fe}$</td>
<td>1.35 $\div$ 0.498 MeV</td>
<td>14</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$^{90}\text{Zr}$</td>
<td>1.35 $\div$ 0.498 MeV</td>
<td>11</td>
<td>3</td>
<td></td>
</tr>
</tbody>
</table>

Under the assumptions made for the SG26 study, further major actinide requirements are few. The main other requirement concerns neutron capture by $^{239}\text{Pu}$ (3-6%), a case which could be aggravated by putting a large cost parameter for inelastic scattering. Accuracy requirements for other Pu isotopes predominantly concern the fission cross section (2-4%) and for $^{238,240}\text{Pu}$ also nu-bar (1-3%). The high content of Pu in the fuel
and the relatively clean Pu vector are at the origin of this. The requirement for improved accuracy of the higher Pu isotopes, and in particular the fission of $^{241}$Pu, is more stringent for the EFR, GFR and LFR cases.

For MA, the needed uncertainty improvements for selected isotopes and reactions are very significant in some cases. However, this is the case when MA play an important role in the neutron balance, as for a MA dedicated burner with a fuel heavily loaded with MA (SFR and ADMAB, but to a lesser degree LFR). For these very specific cases, the accuracy requirement for $\sigma_{\text{fiss}}$ of selected MA isotopes can range from 3-7%.

It may be noted, finally, that a few requirements concern elastic scattering ($^{238}$U, C, $^{15}$N, O, $^{52}$Cr, $^{56}$Fe, Pb). Except for $^{52}$Cr and $^{56}$Fe, these are system specific.

A summary of the main data requirements related to thermal neutron systems, i.e. the VHTR and the extended burn-up PWR indicates some relevant requirements. In the case of the VHTR, it is required to improve $^{241}$Pu $\sigma_{\text{fiss}}$ below ~400 eV. Very tight $\sigma_{\text{capt}}$ requirements for $^{239}$Pu and $^{241}$Pu below ~0.5 eV are also identified, together with C data improvements (both capture and inelastic) with respect to current uncertainty estimates. For the PWR with extended burn-up, the requirements to improve $^{241}$Pu and some O data can be stressed.

One other important point seems to be the shift of priority from the three major actinide fission data to their inelastic (in particular for $^{238}$U) and capture data (for $^{239}$Pu, and, to a lesser extent, for $^{238}$U; the case of $^{235}$U capture data in the keV region is presently under investigation). This shift of priority is obviously related to the relatively small $a$ priori uncertainty values associated to the fission cross-sections of $^{239}$Pu. This shows the importance of a careful uncertainty assessment of leading nuclides and reactions. Higher priority should also be given to higher Pu isotopes (and in particular to their fission data) and to selected coolant/structural material inelastic cross-sections (e.g., $^{56}$Fe and $^{23}$Na). Minor actinide data play a significant role only for dedicated burner reactors (ADMAB or SFR).

A target accuracy assessment has been performed to provide a quantitative evaluation of nuclear data improvement requirements by isotope, nuclear reaction and energy range. First priorities were formulated on the basis of common needs for fast reactors and, separately, thermal systems.

The results of the assessment indicate that a careful analysis is needed in order to define the most appropriate and effective strategy for data uncertainty reduction.

It should be stressed that not all nuclear data that can play an important role in advanced reactor systems have been subjected to the SG-26 sensitivity studies. Examples are fission product cross sections, fission yield and radioactive decay data, fission neutron spectrum, and thermal scattering data. One reason for this is either the lack of covariance data or that the sensitivity codes are not yet able to handle such data in a perturbation analyses. Both issues can and must be solved in the coming decade.

### 2.3. Nuclear data issues of ADS

The results [CANDIDE 2008:5] obtained for the EFIT prototype indicate that there are 21 isotopes which are relevant for the determination of the transmutation efficiency, the decay heat, the neutron emission and the radiotoxicity.
The evaluation has concluded that there are 51 important cross sections involved in the calculation of the inventory. Furthermore, 31 cross sections are critical since they introduce already uncertainties in the final concentrations larger than the 5% target accuracy requested:

- The neutron capture cross sections \((n,\gamma)\) of \(^{242-244-245-246-247-248}\text{Cm}\) and \(^{237}\text{Np},^{241}\text{Am},^{249}\text{Bk},^{230-231}\text{Cf}\) have a very large impact. The neutron capture cross sections \((n,\gamma)\) of \(^{234}\text{U},^{238-240-242}\text{Pu},^{242m}\text{Am},^{243}\text{Cm}\) and \((n,\gamma-M)\) of \(^{234}\text{U},^{241-243}\text{Am}\) are less relevant.

- The neutron induced fission cross sections of \(^{242m}\text{Am}\) and \(^{243}\text{Cm}\) have very large impact. The neutron induced fission cross sections of \(^{235}\text{U},^{238-239-241}\text{Pu},^{245-247}\text{Cm},^{250-251}\text{Cf}\) are less relevant.
3. Performance of current nuclear data libraries

In order to design a nuclear plant, reactor physicists or reactor designers consider many variants and do extensive calculations to estimate their relative performance. For reliable estimates, these studies should incorporate as much as possible the available body of knowledge and the quality of the codes should be supported by extensive testing against relevant benchmark experiments. Nuclear data evaluators provide files that incorporate the best knowledge available for nuclear reactions. As nuclear data are a critical ingredient in modelling, the performance of these nuclear data files should be tested and evaluated for the intended applications. The present chapter summarizes how well the available nuclear data files can be expected to perform for advanced reactor model calculations. Two main sources of information are considered: 1) sensitivity analyses and 2) comparisons of calculated results with experimental results for benchmark experiments.

Key to both sources of information are nuclear data uncertainties and uncertainty correlations (covariances). If the evaluators provide nuclear data and the associated covariances, then in principle it is possible to derive, with appropriate software, the contributions of nuclear data to the uncertainties of core and fuel cycle characteristics. In this case, both the experimental and the calculated system results have uncertainties, thus allowing a meaningful comparison to be made. In addition, sensitivity analyses may be made that allow expressing systems target uncertainties in terms of requirements on nuclear data uncertainties. Confronting such nuclear data uncertainty requirements with current estimates of nuclear data covariances makes it possible to identify the nuclear data for which uncertainties have to be improved. Thus, under certain provisions, one may derive a list of nuclear data target uncertainties from a list of reactor systems target uncertainties.

The work of deriving design uncertainties through sensitivity analyses has been carried out by various institutes and for different nuclear data systems. Recently, a quite consistent and comprehensive work has been carried out within an international collaboration (SG26 of WPEC) [Salvatores 2008]. This is summarised here along with an effort performed within IP-EUROTTRANS that emphasises a fuel cycle with an ADS.

The inventory of discrepancies in calculated versus experimental (C/E) reactor parameters for the latest nuclear data files (e.g., JEFF-3) with both state-of-the-art deterministic (e.g., ERANOS, APOLLO2, etc.) and Monte Carlo (e.g., MCNP) software is taken to assess the present quality of nuclear data files for advanced reactor calculations. This assessment involves also irradiated fuel composition and decay heat. One difficulty of this task lies in the fact that, except for a few cases, the integral experiments being analysed cannot be directly connected to the design characteristics of advanced reactors. A measure of representativity of a benchmark experiment for a particular application is needed to bridge the gap. To this end, representativity factors were proposed that make use of sensitivity coefficients for both the experiment and plant characteristic and of the covariance information for the nuclear data file. This exercise is limited by the lack of reliable covariance data and the fact that this data is not being reported by most of experimental analysts.

The use of integral experiments for assessing the quality of nuclear data starts with an estimation of the impact of nuclear data uncertainty on the C/E comparisons. Depending on the value of this uncertainty compared to the experimental uncertainty, it may be justified, under certain conditions, to use this information for attempting to improve nuclear data as part of a global statistical adjustment, for instance, as has
been done with JEF-2.2 in the 1990’s (see Section 4.4). This has not been repeated for JEFF-3.1. Instead, a more direct approach is being used, in which integral experiments are analyzed selectively. This leads to trends in individual nuclear data, but not to adjusted nuclear data libraries. This approach has also been used for a subset of fast core experiments in order identify the largest deficiencies of the nuclear data files.

In the end, the whole process of sequential assessments and improvements has the aim of producing nuclear data libraries that meet the requests of designers of nuclear plants. With every iteration, predictions of plant characteristics will certainly improve, but might remain short of the designers’ target uncertainties. It may then be necessary to use all the information available from both differential and integral experiments in a combined evaluation to try to overcome these difficulties. However, for economic and regulatory bodies, the final justification for a claim of adequate modelling accuracy of a nuclear installation will be state-of-the-art representative integral experiments.

3.1. JEFF-3.1 performance for criticality and other reactor parameters

In recent years, extensive partly-automated validation schemes have been set up to probe the quality of the JEFF-3.1 data file. Validation studies have included MCNP (NRG, SCK), TRIPOLI (CEA) and APOLLO (CEA) criticality calculations for an unprecedented set of benchmarks. An example is given in refs. [vanderMarck 2005, vanderMarck 2006], where more than 700 criticality benchmark cases were tested. Current-day computer power should enable revisions of libraries to be quickly tested within such schemes. Additional validation is now possible by means of a Monte Carlo approach to the calculation of the effective delayed-neutron fractions [vanderMarck 2005a]. A wider range of validation exercises has been performed [Duhamel 2008, Zwermann 2008, Pescarini 2008] using different methods and codes to study various integral quantities. In addition to reactivity predictions in UO2-fuelled systems (CEA), JEFF-3.1 has exhibited improvements in isotopic inventory predictions as inferred from post irradiation examination data. All cases show improvements over the JEFF-3.0 library. However, some deficiencies do remain: core calculations with TRIPOLI4 [Litaize 2006] revealed an overestimation of k-eff when simulating a MOX core, implying the need for an improved 239Pu evaluation [Bernard 2006]. A detailed analysis of the MINERVE oscillation experiment (OSMOSE) and PIE data for UOX fuel led to the conclusion that the calculated reactivity worth is underestimated, indicating the possible adoption of a capture value for 237Np that is too low [Bernard 2006a]. The MINERVE oscillation measurements also established the quality of some important JEFF-3.1 fission products [Courcelle 2002].

Of particular interest is to validate the new JEFF3.1 library for fast reactor calculations, and for this a reanalysis of a selected set of integral experiments has been performed. These integral experiments were taken from the MASURCA facility at CEA/CADARACHE and from the PHENIX Power Reactor. To validate JEFF-3.1, various experiments have been analysed, such as MASURCA 1A’ and 1B (1968/69), CIRANO ZONA2A and 2B [Finck 1996] Pu-burning fast reactors (CAPRA project) and Na-voiding, MUSE4 [Lebrat 2008] to study the neutronic behavior of Accelerator Driven Systems (ADS), and PROFIL and PROFIL2 [Tommasi 2006] to provide
accurate information on capture cross sections for many actinides and fission products.
The analysis of the reactivity prediction in MASURCA experiments points out, via
perturbation and sensitivity calculation, the main changes due to new nuclear data.
The synthesis of JEFF3.1 results for the PROFIL and PROFIL-2 sample irradiation
experiments in PHENIX gives straightforward results for nuclear data changes.
Pulsed sphere experiments are a lot more sensitive to cross section data and even
angular distributions when compared to integral benchmarks. This aspect alone makes
them prime candidates for validating nuclear data because even the smallest
differences will be very clear. In these benchmarks, the calculated parameter is
exactly the measured one, viz the emission spectrum and the benchmark exercise
identify for what isotope and which energy range further experiments or further
nuclear data evaluation effort should be focused.
In heavy liquid metal fast spectrum systems, the inelastic scattering interactions play
an increasing role in the neutron slowing down above 1 MeV. For $^{238}$U (the most
important isotope as regards to the Doppler effects) and many MA, the fission cross-
section is higher than the capture one above 1 MeV and vice-versa. This explains the
positive coolant temperature effect observed in Pb-cooled systems such as BREST or
ELSY.

For thermal systems, experiments are performed in “zero-power” pool-reactor such as
EOLE at CEA Cadarache. The JEFF-3.1 experimental validation is based on several
experimental programs, including UH1.2, MISTRAL1, MISTRAL2, BASALA-Cold.
Other experiments being considered are those of reactor plants such as:
- the Chooz-N4-PWR reactor start up experiments at Hot Zero Power conditions.
- ICSBEP benchmarks.
- Post-irradiated experiments consist in analyzing UOX spent fuel rod cuts (2cm
  height). The irradiation of spent fuels are performed during 5 cycles in the
  French PWR-900MWe Gravelines ($^{235}$U w/o=4.5%) and during 4 cycles in the
  German BWR-900MWe Gundremingen ($^{235}$U w/o=3.14%).

The use of integral experiments is of significant importance to bring evidence that the
available nuclear data evaluations are satisfactory or not. Whatever the method used
to demonstrate that current experiments are covering the domain of interest for current
designs or not, possible remaining biases should be tracked down to the nuclear data.
This requires the use of sensitivities relating the measurement to all the influential
nuclear data. An almost direct relation exists only with specially-designed separate-
effect experiments, such as substitution measurements or sample irradiation
experiments in well-known conditions. In most situations, however, the relationship is
not simple or straightforward; therefore, sensitivity and perturbation calculations have
to be performed. This point is further discussed under Section 4.4.

3.2. JEFF-3.1 performance for fuel inventory

JEFF-3.1 validation of spent fuel inventory, decay heat and neutron emission
calculations is reviewed in JEFF Report 22, on the basis of the available benchmarks
[in preparation]. This is based upon open publications which only include results for
current thermal reactors. These results show quite good agreement for the major
nuclides and decay heat, but to be useful in the development of advanced reactor systems and fuel cycles, which are predominately fast neutron systems, validation will be required on fast reactor fuels including those fuels containing high loading of minor actinides. Thus experimental activities on fast reactor fuel analyses and their benchmarking will be required to allow validation of calculations for advanced reactor fuel composition and subsequent fuel cycles and waste management. It is strongly recommended that any new fuel irradiated within EC programmes in fast systems be analysed (ideally, by several independent groups) for important constituents and the corresponding irradiation history recorded in sufficient detail for the fuel composition to be accurately calculated and compared to the measurements. The assay results, irradiation details and any validation should be published to support future development. In addition, existing databases such as SFCOMPO should be extended to include fast reactor spent fuel analyses from future projects and any existing historic data recorded within national programmes be retrieved and archived. In this regard, an EC project to recover, store and validate existing fast reactor fuel assays held within national programmes would be beneficial.
4. Practices and limitations in nuclear data production

Generally there are two main classes of nuclear data users: nuclear industry and large, usually government-funded, research infrastructures for the development of innovative technological designs (GEN-IV, ITER, ADS, etc.). The interface of such users with nuclear data is depicted in Fig. 1. Nuclear data needs are specified and prioritized and through a combination of differential measurements, nuclear modelling, data evaluation, library production, processing and validation with integral measurements, ready-to-use qualified nuclear data libraries are returned. Depending on the complexity, the total time of such a cycle may take several months to several years, especially if in the latter stages of nuclear data validation (the inner circle of Fig. 1) new needs for differential data improvement emerge (bringing us in the outer circle again).

In this chapter, we will review the current practices for the four main fields of nuclear data development: differential measurements, nuclear models and codes, data evaluation and library production, and validation and integral measurements.

4.1. Differential measurements

In chapter 2 it was explained that sensitivity studies of advanced reactor systems, thermal or fast, and critical or sub-critical, can be used to define a list of first priorities for improvement of nuclear data. These are key data for which current uncertainties exceed the target uncertainties derived from reactor performance criteria for more
than one system. Tight requirements emerge for cross sections in the energy range from 50 keV to 6 MeV; for fission of \( ^{238,240-242}_{\text{Pu}} \) (2-3%), \( ^{241,242}_{\text{Am}} \) (3%), \( ^{244,245}_{\text{Cm}} \) (5-7%), for inelastic scattering off \( ^{23}_{\text{Na}} \) (4%), \( ^{28}_{\text{Si}} \) (3%), \( ^{56}_{\text{Fe}} \) (3%), \( ^{206,207}_{\text{Pb}} \) (3%) \( ^{238}_{\text{U}} \) (2-3%) and for capture of \( ^{238}_{\text{U}} \) (1.5%) and \( ^{239}_{\text{Pu}} \) (4%). Current measurement practices are reviewed, for these three categories and for the higher energy range that is specific to accelerator driven systems (ADS). A more extensive description is given in [CANDIDE 2008:3] while a summary is given here.

Ionization chambers, proportional counters and various types of silicon detectors are being used to measure fission cross sections. There are considerable ongoing efforts in several laboratories using either quasi-monoenergetic neutrons or white neutron sources in combination with the time-of-flight technique. The latter allow comprehensive studies of excitation functions over a wide energy range. Measurement accuracies critically depend on 1) the quality of fission deposits, 2) the determination of the detection efficiency, 3) the determination of the flux or normalization, and 4) discrimination against background. In principle, these factors can be controlled and the target uncertainties appear achievable. However, there is considerable spread in the measurement results for the above cases of interest. Therefore, new efforts should focus on methodology and take guidance from the accurate work performed for \( ^{235}_{\text{U}} \) and \( ^{239}_{\text{Pu}} \) to identify all required corrections and properly determine uncertainties and their correlations.

For inelastic scattering the emitted neutrons \("(n,n')\)-technique" or the associated gamma-rays \("(n,n'\gamma)\)-technique" are detected to measure cross sections. For actinides the first technique yields the most complete determination of the cross section, while for structural materials the latter technique may also be used successfully. For \( ^{238}_{\text{U}} \), the best results to date state 7% uncertainty for the first excited state. However the spread in results indicates an overall uncertainty of about 10%. There is little activity in this field and there are no clear indications that improvements are possible. For structural materials recent advances with the \((n,n'\gamma)\)-technique indicate that a final uncertainty of 5% is achievable and improvement may be possible.

A number of new experimental devices to study radiative capture have recently been established at neutron time-of-flight facilities around the world. Significant advances in methodology were made primarily from improved data-handling and more sophisticated modelling. Studies of the \( ^{232}_{\text{Th}}(n,\gamma) \) reaction at IRMM and the CERN n_TOF facility have demonstrated that uncertainties at the level of 2% may be achieved for non-fissile nuclides. Thus, the required accuracy for \( ^{238}_{\text{U}} \) appears within reach. For fissile nuclides like \( ^{239}_{\text{Pu}} \), prompt gamma-ray measurements have to distinguish between gammas emitted by the capture and by the fission process. Completed works date from the seventies but the accuracies obtained are promising. The best results were obtained for \( ^{235}_{\text{U}} \) and involved fission tagging of the gamma-ray spectrum to deduce the fission response and subtract it from the total. A similar effort for \( ^{239}_{\text{Pu}} \) may be feasible but is complicated by the much higher alpha emission rate.

Nuclear data above 20 MeV have been motivated by ADS [CANDIDE 2008:4]. Below 20 MeV, a single cross section can be of paramount importance, while above 20 MeV the situation is fundamentally different. For one system there are a large number of reactions and cross sections vary slowly with energy and target nuclide. No specific reaction strongly dominates. Getting a grip on the overall picture is the natural goal and several recent experiments have been made to cater the needs. From 20 up to 200 MeV these concerned fission, elastic and inelastic scattering and reactions that emit light charged particles. At higher energies considerable efforts have been made to study proton-induced spallation reactions.
4.2. Models and codes

Nuclear reaction theory, modelling and the associated computer codes are core elements in contemporary nuclear data development. Often, the types of experimental facilities required to obtain key nuclear data may not be available or too costly to construct and operate. In addition, nuclear simulations are dependent on nuclear data tables for many materials, many reaction channels at many incident energies, angles etc. and not only on those data points that happen to be available from measurement. Therefore, nuclear model codes, particularly when based upon the latest advances in theory, can offer cost effective alternatives to measurements in some very important instances. Model calculations, however must be referenced to critical measurements to provide a basis for confidence on limits and accuracy. Thus tightly coupled, calculations and measurements can reinforce each other and have a productivity far beyond that available from either separately.

Indeed, the strong increase in computer speed and memory has led to nuclear data libraries which nowadays rely much more on nuclear model calculations. Sophisticated reaction theories have become amenable for implementation and even large-scale production of covariance data using nuclear models is now taking place. In general, two families of nuclear reaction models and associated codes are available to provide nuclear data for applications, and they will be briefly described here.

4.2.1. Nuclear models and codes for the fast and high energy range.

These codes contain an implementation of various theoretical models of a nuclear reaction, the most important being the statistical model, the optical model, level densities, pre-equilibrium model and fission model, as well as a large nuclear structure data library. Since an exact description of a nuclear reaction does not exist, each of these models necessarily contains several parameters which allow the evaluator to adjust the calculated results to available experimental data. Systematic comparisons of a nuclear model code with large databases containing experimental cross sections (EXFOR) result in trends for the adjustable parameters, so that nuclear reaction data for unmeasured or non-measurable energies, reaction channels or nuclides can be predicted with some confidence.

In the past decade a few model codes have particularly dominated the field of nuclear reaction prediction, both in the nuclear physics literature and for the evaluation of nuclear data libraries; GNASH, developed in Los Alamos, EMPIRE, developed by the Brookhaven and IAEA data centers, and TALYS, developed by NRG Petten and CEA Bruyères-le-Chatel. EMPIRE and TALYS are the only widespread all-in-one codes (meaning that all required reaction mechanisms are implemented in one software package) of which the main authors are still (officially) active in the field, although some new initiatives are being taken in the USA and Japan. Restricting ourselves to Europe, TALYS [Koning 2008a] now serves, and benefits from, a large worldwide user network and has become a standard analysis tool for important experimental facilities such as TSL, Uppsala, JRC/IRMM, Geel, and others. TALYS has been highly successful in data analysis and data library production for non-fissile nuclides, and an important statement is that this also holds if the code is used by others than the authors. For actinides, a similar high performance can be achieved, though the ability to do that is not yet as widespread as it should be. This is an important issue that can and must be solved soon, preferably on the European level. While TALYS is currently able to reliably describe or predict many nuclear reaction data with phenomenological models, which are rather versatile through parameter adjustment,
there is now a tendency to add more microscopic physics (effective nucleon-nucleon force and Hartree-Fock models) to the code, thereby putting the evaluation results on firmer ground.

The main use of TALYS is currently in the range from several keV up to a few MeV (fast reactors) and around 14 MeV (fusion), but the code is reliable up to about 200 MeV. For ADS-specific data needs, around that energy intra-nuclear cascade codes, such as BRIC or INCL4, come into play to simulate nuclear reactions for energies up to the GeV bombarding energy.

4.2.2. Codes for the analysis of the resonance region

In this energy range, the availability of measured data is essential, as the evaluation process largely relies on parameter fitting. Evaluators combine the compound nucleus theory with experimental data to derive sets of resonance energies and parameters for direct use in data libraries. The Breit-Wigner formalism has progressively been replaced by the more rigorous Reich-Moore formalism. In principle, the various open reaction channels are considered simultaneously. The evaluation usually proceeds from the thermal range to the resolved resonance range, and then to the unresolved resonance range. This data reduction process is iterative; an essential aspect being the selection of a consistent set of measurements. Existing evaluated files are used as priors. For complex nuclei (actinides), this evaluation is often a complicated and lengthy task. The most widely used resonance codes are (in this order) SAMMY and REFFIT. The main authors of these codes have retired. Many resonance evaluations in the current nuclear data libraries are based on the SAMMY code and represent the work of a handful of specialized evaluators. A specific issue in contemporary resonance evaluation is the handling of covariance data for resonance parameters. To take correlations into account between all resonances, a huge covariance matrix is required, which poses specific challenges to data evaluation and processing. A new French initiative has recently started in CEA Cadarache with the development of the CONRAD code. The most important capabilities of the aforementioned codes are taken on board of CONRAD to ensure that resonance analysis remains a European competence.

4.3. Nuclear data libraries and evaluation

Nuclear data for reactor and fuel cycle analyses by end users (e.g. industry, or other parts of nuclear science) are generally provided in the form of processed nuclear data libraries, in direct usable form for reactor software and, if necessary, post-adjusted to (often proprietary) integral reactor experiments. Before this stage is reached, the entire process of Fig. 1 has taken place.

Well-known, routinely-used processing codes are the NJOY and CALENDF systems. A nuclear data evaluator uses a combination of results generated by nuclear reaction models and experimental data (if available) to produce a nuclear data library that gives a complete description of all reaction channels, with maximum quality of the cross sections and other quantities such as resonance and fission parameters. An essential feature, which is still too often ignored, is to include covariance data in the evaluation, so that the user knows to what precision the nuclear data are assumed to be known and how they are correlated. Reactor and fuel cycle calculations may provide feedback to the evaluator, leading to an iterative process that eventually

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results in a nuclear data file that embodies the best compromise between requirements from integral experiments and microscopic data (in that order of importance).

There are several Evaluated Nuclear Data Libraries (ENDL) or Files (ENDF) in the world, but by far the largest part of nuclear science and industry makes use of one of the following three libraries: ENDF/B of the USA, JEFF of the OECD (in practice, Europe), and JENDL of Japan. The data in these libraries are stored in a format that dates back to the 1960’s: ordered punch card requirements can still be recognized. Unfortunately, since most processing and reactor software that has been developed depends on this so-called ENDF-6 format, all initiatives to modernize the format have died in the initial stages, even though both the nuclear data needs and the possibilities of nuclear model codes have gone beyond the possibilities of the present representation. It would be in line with a modern nuclear science approach for new reactors to adopt a more flexible modern nuclear data format.

In the case of Europe, the JEFF library is the result of a collection of voluntary efforts from a few European OECD member states. It consists of a general purpose neutron library, an activation library, a thermal scattering library, a fission yield library, a radioactive decay data library and a proton library. Currently, most effort is invested in the neutron general purpose file and the fission yield and radioactive decay data file, and they will be briefly described here.

### 4.3.1. Status and evaluation of neutron data library

For the neutron data library, the evaluation activities are generally divided into two classes: evaluation in the low energy (thermal + resonance) range and evaluation in the fast energy range. For high quality nuclear data evaluation, several ingredients are essential

- A modern, robust nuclear model code. In Europe, TALYS is available.
- Tools to evaluate the resonance range (SAMMY, CONRAD).
- The experimental nuclear reaction database EXFOR (maintained by the international nuclear reaction data centers) in a largely error-free and user friendly form [CANDIDE 2008:6].
- Software for error-free translation of nuclear reaction data into the ENDF format, to ensure the subsequent seamless processing into application libraries.
- Tools to combine experimental and theoretical uncertainties into complete covariance matrices.
- Evaluators who know how to combine the above items in an adequate way.

We face the situation that all current nuclear reaction data libraries in the world are not as consistent in terms of contents and quality as they could be. This has to do with the commonly adopted incremental approach of nuclear data evaluation: improvements to nuclear data libraries are usually performed on a nucleus-by-nucleus or even channel-by-channel basis, driven by a particular evaluation request. These “ad hoc” evaluation methods, sometimes assembled from contributions made by different people, lead to a collection of nuclear data files of varying quality, which are partially complete, originate from different eras, of which the quality is only known to the evaluator (who, especially in this branch of nuclear science, may be retired), and which is not always processable for more than one reactor code. A related
disadvantage is the delay of adopting data from new measurements in the data file: it often requires a whole new manual evaluation. As we will argue in the roadmap (§5), a large step forward in efficiency is within reach by adopting a more quality-assured approach; currently the evaluation process is already more consistent and more complete than described above.

In recent years, a particular effort has been devoted to the generation of covariance data, both of experimental and theoretical origin, and in both the resonance and fast neutron range. Experimental covariance matrices are hard to find (see section 5.1.2. on how to change this) while for nuclear model covariance data, uncertainties on model parameters are assumed, after which a Bayesian or Monte Carlo process of uncertainty propagation leads to covariance matrices and uncertainty bands. The first attempts to produce credible covariance data are certainly promising, but more resources need to be invested into a systematical development of covariance data, especially for actinides.

4.3.2. Status and evaluation of decay data and fission yields

The evaluation skills currently available in decay data and fission yields are extremely limited worldwide. In terms of evaluators who have produced the current US, Japanese and European files very few remain active and most have retired. It is important that these skills be maintained within Europe to support development of new reactors and their fuel cycles with their requirements for improved data.

For fission yields, it should be noted that the currently available files are mostly based on measurements from the thermal fission of $^{235}$U and $^{239}$Pu, the dominant reactions in the current commercial nuclear reactors. However, advanced systems will require more accurate data on the fission of minor actinides and fission from fast and higher energy neutrons. New experimental measurements and subsequent evaluation will be required to improve the data for advanced systems.

In decay data, a divide needs to be drawn between nuclear structure and the decay data used in applied calculations. The first is an academically driven field, and the second is driven by the needs of those applying technology such as the nuclear power industry and users of radioactive materials, for example in medical imaging and treatment. Nuclear structure research is covered by the world-wide ENDSF collaboration that compiles and summarises the current literature and publishes its compilations in the Nuclear Data Sheets journal. Very few European institutions are active in the ENDSF collaboration and most will leave soon due to staff and funding shortages.

4.4. Nuclear data validation and feedback from integral experiments

Over the past 20 years or so, considerable progress has been made in the nuclear data validation process. Much of this progress is the result of a systematic effort to assess carefully the various sources of errors and uncertainties in the integral experiments (E) and in the corresponding calculations (C). A better control of measurement and modelling errors has been achieved by the routine use of Monte Carlo codes in the various simulation steps. As a result, the level of confidence in the nuclear data trends derived from the C-over-E analyses has improved significantly.
A key to this progress has been the continuous availability of high-quality analytical experiments or benchmarks, typically performed in critical facilities, aimed at addressing physics effects individually. In particular, in the JEFF project, since JEF-2.2, the most important file revisions impacting reactor applications have been motivated by the careful analysis of high-accuracy integral experiments. This is an essential point, implying that, thanks to this validation work and the corresponding feedback on the data, the performance of the JEFF-3 file for current reactor applications has reached a better level that what would have been achieved with differential data and nuclear models alone.

The full validation process implies the interpretation of C-over-E values, which entails not only C-versus-E comparisons, but also an error analysis. The latter is essential to identify the most likely causes of discrepancies, and possible error compensations. This error analysis classically uses sensitivity and perturbation calculation techniques. In practice, however, many validation studies, especially those making use of Monte Carlo codes, still often limit themselves to the C-versus-E comparisons, sometimes without even considering error bars. Even if many benchmarks are considered simultaneously, thus providing a valuable consistency test of many data, the lack of an error analysis makes it difficult to infer unambiguous trends, all the more as the measurements considered tend to be very integral ones, sensitive to many nuclear data. It is therefore desirable that these practices evolve towards a more complete interpretation of the experiments.

Past fast reactor validation studies in Europe have considered a large number of integral experiments, performed in various facilities, the main focus being on sodium-cooled and PuO₂-UO₂ fuelled systems. These studies have been used to validate the JEF-2.2 file for this particular domain of application. The results are documented in Chapters 6 and 12 of OECD/JEF Report 17 (2000). As the analysis had been done in a consistent and systematic way for a relatively large number of experiments, it was possible to perform a neutron cross section adjustment, in a multigroup sense. This data adjustment was successful, in the sense that it helped detect inconsistent experiments and improve important cross sections, such as the $^{23}$Na inelastic scattering or the $^{240}$Pu capture cross section. Furthermore, it resulted in an application library which showed satisfactory performance when applied to the SUPERPHENIX reactor. However, some limitations and shortcomings were also identified, in particular in connection with the multigroup/unfolding approach and the $a$ priori uncertainty and correlation information that had to be estimated and supplied as input to the adjustment process. These shortcomings suggested that the overall process should not be repeated “as such” for JEFF-3, especially as it would require a large dedicated effort.

One important lesson learned from these past validation studies is that, in principle, if a sufficient number of well-defined, sufficiently-diverse, high-resolution and high-information content experiments are available, it should be possible to produce application libraries that meet (realistic) performance targets. This suggests that (i) future integral experiments will be essential in assuring that nuclear data have the required quality for innovative fast reactor design, and that (ii) the designers’ needs have to be carefully and reasonably assessed.
In terms of practices, another lesson drawn from past experience is that nuclear data evaluation and validation are most efficiently done when considered as part of an integrated approach, and involve closely-related groups of physicists.
5. Nuclear data roadmap

Any roadmap is limited by the foresight that its designers can be expected to have acquired. The present roadmap is drawn from studies that were performed for advanced reactors and waste minimization with accelerator driven systems, as well as from insights gained in the course of development projects for current reactors and fuel cycles. In the former case these are scientific and engineering studies essentially without feedback from operations experience, while in the latter case experience from more intensive interactions with the users’ community is available. The current roadmap for nuclear data improvements is explicitly guided by the Generation-IV Initiative, the Global Nuclear Energy Partnership and, more recently, the Strategic Research Agenda (SRA) of the Technology Platform for Sustainable Nuclear Energy (SNE-TP). Implicitly, it is guided by efforts aiming at improving the current nuclear energy infrastructure.

Through sensitivity studies for advanced reactor concepts and an accelerator driven minor actinides burner, a number of priority nuclear data improvement requests were established. In the first case this work was performed by a working group of the OECD Nuclear Energy Agency (Subgroup 26 or SG-26) [Salvatores 2008], while in the latter case the NUDATRA domain of the EUROTRANS Integrated Project was involved. In addition, the present collaboration has drawn extensively from experience gained through involvement in various nuclear data related studies in national institutes and international collaborations. Finally, input was gathered from recent conferences and workshops, in particular the CANDIDE-sponsored workshops, NEMEA-4 and NEMEA-5.

The present roadmap provides recommendations for nuclear data projects in the interest of advanced reactor development. It is argued that significant progress can be made by well focused initiatives (vertical recommendations) provided that an appropriate framework is elaborated that effectively incorporates high quality nuclear data developments in reactor modelling and model testing (horizontal recommendations). The latter require an appropriate emphasis on method development: automated, systematic, and efficient nuclear data evaluation with consistent inclusion of covariance information, processing of nuclear data, improved interfacing of disciplines including integral validation, a general upgrade of nuclear model codes for all relevant energy ranges, improved documentation of experiments and evaluations. A common direction for all aspects of nuclear data concerns the production of uncertainties and their correlations. Covariance data should properly reflect the quality of the nuclear data so that reliable uncertainty estimates of key parameters can be made to guide reactor developers and safety authorities.

Rather than a detailed timeline, this roadmap provides a list of recommendations which are fairly general, although certain aspects of vertical recommendations may be emphasised or de-emphasised according to the particular reactor system that is favoured. Nevertheless, it is difficult to assess what will be the situation 10 years from now and reviews of this roadmap may well be in order with a frequency of once in 5 years.

In this chapter, the required innovation for the categories that were discussed in the previous chapter will be outlined.
5.1. Differential measurements

Recent sensitivity studies for advanced reactors, although limited in number and scope, have established a large number of system-specific target uncertainties for a set of key nuclear data. Cross-cutting and well-understood results from these sensitivity studies have been identified as first priorities for experimental work in the interest of advanced reactors, along with a few system-specific results important for waste minimization and sustainability. These priorities primarily concern rather tight target uncertainties for cross sections of fission, inelastic scattering and a limited number of capture reactions. With few exceptions, these requests may be met by careful measurements pushing current experimental technology and methodologies ahead with evolutionary advances. The main exception is the inelastic scattering cross section of $^{238}$U for which neither evolutionary nor revolutionary advances are anticipated that meet the 2% target uncertainty. Obtaining accurate results for fission of certain isotopes ($^{241}$Pu, $^{244}$Cm, $^{238}$Pu, $^{242m}$Am, $^{241}$Am – ordered by half life) is problematic with regard to sample preparation, background and radiation protection due to a high specific activity but, according to the literature, not impossible.

It is important to put these statements in perspective. Currently, in many cases the database shows a spread in measurement results that is often larger than the recognized experimental uncertainties. This important problem should be dealt with if advances are to be made. Typically two situations occur: 1) the reported measurement results are incompletely corrected for experimental effects and an evaluation taking these effects into account can make good use of the data; 2) experimental conditions were incompletely accounted for and can no longer be reconstructed as a result of inadequate documentation – the data are of no use to new evaluations. The necessary advances are possible provided significant well-focused efforts are directed towards the real problems. Indeed evaluation is essential to make the most of the available and forthcoming experimental results. However, guidance from theory at the level of the target uncertainties of the priority data needs is at best qualitative, so that evaluation involves arbitration between and complementation of best experimental results. Thus, high quality measurements are asked for, employing the best experimental techniques, samples and data analysis procedures available.

Possible unidentified sources of error in earlier work should be carefully identified and avoided or corrected for in new efforts. Credible uncertainty and covariance analysis must become a standard part of the measurement process. Reporting standards should be developed that facilitate the straightforward re-evaluation of older data in combination with new results, taking account of all experimental specifications. Even then a sound approach requires several independent high quality results from different facilities. In short, experimental efforts must become an integral part of a comprehensive quality assurance program for nuclear data. The above requires an active community centered on main laboratories and institutes where expertise can be built up and maintained.

It is important to reflect on issues that are not identified as first priority or that were not covered by the sensitivity studies, since the CANDIDE roadmap addresses not only the short term but also the medium and long term. What are currently perceived to be lower priority issues may turn out to be key issues once a particular system is favored over the others. Such cases may readily be identified as a result of sensitivity studies. On the other hand, covariance data, which are supposed to reflect the current
status of nuclear data, are preliminary and extensive efforts in covariance production may well shift the focus when more reliable assessments become available. Furthermore, of recognized importance for current reactors are the fission neutron spectrum, fission yields, decay data and fission product reaction data. Clearly, if left unchanged, these are anticipated to become a concern also for advanced systems at some stage of their development. Thus, experimental expertise should be maintained to address the corresponding needs.

5.1.1. Specific recommendations

Recommendations for new nuclear data measurements in the interest of the development of advanced reactor systems have vertical and horizontal components and should indicate the instruments suitable for realization of the objectives. Horizontal are recommendations that should be common to new efforts: working methods, embedding in a European overall nuclear data quality assurance system, production of covariance information for measurements, reporting standards, interfacing with evaluations. They should be considered as important evaluation criteria for new projects. Vertical are recommendations for high quality measurements for targets and reactions that were identified as priorities, and for such measurements that are considered to be important for an overall sound approach to advanced reactor development. Obvious instruments are, on the one hand, projects in which key European players collaborate on new measurements of priority nuclear data and, on the other hand, transnational access to European infrastructures where a wider range of interested parties is encouraged to engage their expertise for new developments of nuclear data, thus allowing the possibility of breakthroughs and of covering lower priority issues. For each of the instruments, training of young researchers (PhDs and postdocs) and competence building in nuclear science are natural aspects that may be further augmented by workshops and schools.

5.1.2. Horizontal recommendations for new measurements

These recommendations should serve as evaluation criteria for specific applications to calls for projects having a nuclear data component.

1. **Emphasize quality, not quantity.** Various earlier projects emphasized scoping the landscape of nuclear reactions to cover poorly charted territory, in particular for ADS development but also for fusion. For the priority nuclear data needs of advanced systems, target uncertainties are very tight and dedicated, focused, high level efforts are required to meet each of these. Expertise and commitment are essential. Experience has shown that high quality experimental efforts for a single target nuclide and reaction require time and effort. A large list of deliverables to be realized by a small group in a short time span is therefore not credible.

2. **Develop and qualify working methods.** The quality of the final result should be demonstrated. It should be carefully examined which measured quantity is realized by the experiment and what experimental information (response functions, sample characteristics, backgrounds, …) are required to allow an experiment to contribute to a better quantitative understanding of the desired physical quantity. Proposals should identify the present status on the basis of earlier work and motivate the necessary developments of working methods. Certainly, in an early phase a larger development component is anticipated and should be viewed as positive by project evaluators.
3. Covariances. Develop methods for appropriate statements of measurement uncertainties and their correlations. Uncertainty statements of measurement are frequently optimistic, erring on the low side, or artificially enlarged, barring a meaningful interpretation. Proper and consistent uncertainty/covariance statements are essential to weigh measurements in the evaluation process. Discrepancies between measurements can only be made explicit through appropriate uncertainty/covariance statements. Identified discrepancies are a key starting point for identifying which measurements need to be better understood and improved, or discarded in the evaluation process. Correlations of uncertainties are practically never reported. This is no longer acceptable and this point must be covered by new experimental efforts.

4. Improve reporting, documentation and interfacing with evaluations. All pertinent experimental information should be stored and documented in the EXFOR database at an appropriate qualitative and quantitative level to allow seamless interfacing with evaluation codes. For this purpose a number of extensions to the current EXFOR format, database and processing tools should be elaborated. Currently the ideal is far from being reached and careful assessment and development efforts in the various measurement disciplines are required to elaborate reporting standards and systems to meet this goal. Open standard software interface(s) should be developed to allow automated interfacing with evaluation codes, and criteria should be established and used to validate that the best possible use is made of high quality measured data. The need and methods of auditing EXFOR entries of the new type should be investigated and implemented.

5.1.3. Vertical recommendations for new measurements

These recommendations relate to experimental efforts that should be part of well-defined projects with a nuclear data component. Although not mentioned explicitly, for each of these recommendations, the horizontal recommendations given above should be considered as an integral part.

1. Priority measurements.
   a. Fission. As reported above, the first priorities are cross sections for the target nuclei\(^2\) \(^{238,240,242}\)Pu (2-3%), \(^{241,242m,245}\)Am (3%), \(^{244,245}\)Cm (5-7%). A realistic 3-4 years project will deal with only few of these at once so that a further prioritization is in order. These cases vary in degree of difficulty and should be categorized according to their complexity. A first important guide is provided by listing these with increasing specific activity: \(^{242}\)Pu, \(^{240}\)Pu, \(^{245}\)Cm, \(^{241}\)Am, \(^{242m}\)Am, \(^{238}\)Pu, \(^{244}\)Cm, \(^{241}\)Pu. Another priority request concerns nu-bar of \(^{240}\)Pu (1-3%) in the fast energy range. Both direct and surrogate neutron-induced studies should be stimulated to address this problem.

   b. Inelastic scattering. The first priorities are cross sections\(^1\) for \(^{23}\)Na (4%), \(^{28}\)Si (3%), \(^{56}\)Fe (3%), \(^{206,207}\)Pb (3%) \(^{238}\)U (2-3%). Great advances with the \((n,n'\gamma)\)-technique and the neutron time-of-flight technique were recently demonstrated and it is of interest to push these to the limit for the study of non-actinide target nuclides. Similarly this

\(^2\) Target uncertainties in brackets
technique may bring valuable new information for $^{238}\text{U}$ despite the fact that this will be less complete than for non-actinides. Neutron emission studies should be encouraged to obtain complementary information on the angular distribution. Although it is unlikely that 2% will be achieved for $^{238}\text{U}$, any effort that may reduce significantly the present 10% uncertainty is worthwhile as it will have an important impact on advanced reactor modelling uncertainties.

c. Capture. A concerted effort should be applied to the study of $^{238}\text{U}$ taking advantage of the experience gained in recent work for $^{232}\text{Th}$. Such an effort is expected to fulfill the requested target uncertainty. For the fissile nucleus $^{239}\text{Pu}$ fission tagging is essential to separate the gamma-ray response due to fission from that due to the capture process. Fission tagging investigations could focus first on easier cases to develop the technique. However, the importance of improving the $^{239}\text{Pu}(n,\gamma)$ cross section uncertainty even below 4% cannot be overstated. A very high accuracy for this cross section will alleviate some of the other very tight requirements for advanced reactors, in particular also for the $^{238}\text{U}$ inelastic cross section.

2. Measurements currently lacking detailed prioritization from sensitivity analyses

   a. The energy range above 20 MeV.

      i. Below 200 MeV studies of neutron elastic, inelastic, light charged-particle and fission reactions should complement earlier work at 100 MeV and below, and thus bridge the gap towards the high energy regime. As explained in the previous chapter a sufficiently higher energy (e.g. 200 MeV) and few nuclides should be studied (C or O, Fe, Zr, Pb or Bi).

      ii. Spallation reactions could be studied further for protons on lead/bismuth at energies considered by present ADS design efforts (e.g. the Myrrha energy of 600 MeV).

   b. Fission neutron spectra. Sensitivities can be studied but no systematic results from such studies are available. Improving fission neutron spectra is nevertheless a long-standing problem of recognized importance. An additional requirement is the determination of a covariance matrix for the experimental work.

   c. Decay data. Decay heat is an important aspect of the safety and operation of advanced systems. An identified problem is the consistency of various estimates for the total gamma-ray energy that is released from fission products. Total absorption gamma-ray spectrometry experiments should be encouraged to relieve this problem.

   d. Fission products. Fission product yields and fission product cross sections are of recurrent concern to light water reactors (LWRs) studies. Yields will change with neutron energy, fission product cross sections for advanced reactors concern a different energy regime than those for LWRs. Although these issues were not prioritized it is evident that a balanced experimental effort in these domains must be developed.
For the development of ADS for incineration of minor actinides, two classes of differential data are requested that are far more important to ADS than to other reactor applications. At neutron energies below 1 MeV, improved data on fission and capture on minor actinides are needed for proper assessment of the transmutation properties and related design issues. At higher energies, data on neutron-induced nuclear reactions that cause materials damage are requested for the design of ADS research facilities, already in a relatively short time scale. Fortunately, the requests based on design criteria overlap to a large extent with the reaction studies needed to complete the picture on neutron-induced nuclear reactions at high energies, as measured in FP5-6 projects.

5.2. Models and codes

In the coming years, the largest challenge for nuclear models is to provide a consistent description of nuclear reactions for actinides. We are facing the situation that only for a few major actinides experimental data are available in large numbers. The advanced nuclear designs require a better description of minor actinides as well. Generally, only for a few channels and energy ranges, good experimental data are available and nuclear models are then indispensable to provide a reliable interpolation between those measured energies and reaction channels. Another related major challenge is the prediction of cross sections for minor actinides, for which only a very few data points exist, and which are important in high burn-up, advanced reactor or ADS scenarios. The theoretical modelling of fission is still highly phenomenological: many adjustable parameters are required to obtain a decent fit for the fission cross section. This means that it is difficult to apply parameters for a well-known nuclide such as Pu-239 to a neighboring actinide. The success of an actinide evaluation depends on a subtle interplay between the deformed optical model, level densities and fission (barrier) parameters. Attempts have been launched, for example in CEA Bruyères-le-Chatel, to attack the problem with fully microscopic physics, for the three abovementioned main ingredients. This should definitely be pursued, and the progress is already very promising. However, it is difficult to estimate the timescale on which such a robust approach will be good enough to provide credible actinide evaluations that can reliably be used in advanced reactor analyses. Therefore, in parallel to this development, a phenomenological approach should also be followed, in which we strive for a simultaneous, consistent description of as many important actinides as possible, while our finite theoretical ability is reflected in covariance matrices. This means that consistent optical model, level density and fission barrier descriptions need to be developed and tested. As argued before, the computer power and software is now available to make a large step forward.

A similar effort is required for modelling fission neutrons, both for the yield and the spectra. Various improvements have been published in recent years, but systematic production of nuclear data with these models has not yet become a routine activity for everybody. A new development is to explicitly calculate neutron emission from all excited fragments after fission, simply by looping over the entire fission yield curve and performing a Hauser-Feshbach calculation for each fragment.

A very high-priority development for the nuclear model community is the assessment of uncertainties generated by nuclear model calculations. Since the major part of nuclear data libraries is created by nuclear model codes, the same holds for covariance
data. New uncertainty approaches, such “Unified Monte Carlo”, in which theoretical model uncertainties are blended with experimental uncertainties, need to become routine. A particular challenge is to disentangle model uncertainties from parameter uncertainties, and to subsequently assess credible uncertainty ranges for all model parameters. After that, a Kalman filtering technique or Monte Carlo can be used to produce covariance data.

An ADS-specific topic is the performance of nuclear models above 20 MeV. For a precise estimate of ADS-target performance or accelerator shielding, sooner or later quantitative estimates of nuclear data uncertainties will be required by the design teams, as is now commonly accepted for critical reactors. For the part between 20 and 200 MeV, this is covered by the nuclear data library approach, and TALYS will be able to provide uncertainty data up to 200 MeV. A similar step could be made for the intra-nuclear cascade codes: the performance of these against experimental emission spectra and residual production cross sections is qualitatively known, but not yet quantitatively established. High-energy code developers should devise methods to quantify the limitations of their models and parameters by including an uncertainty treatment in their codes. This will boost future measurements, since a much better justification could then be given for them, and code development.

5.3. Nuclear data libraries and evaluation

The developments in experimental and theoretical nuclear physics described above, which are necessary to fulfill certain advanced reactor nuclear data needs, are rather challenging, and are slowly but surely moving forward. The situation is, or rather should be, different for the production of nuclear data libraries for applications. The computational power, i.e. speed and memory, has increased so tremendously in the past years that it requires no scientific breakthrough to push the current nuclear data libraries to a higher level by using a more systematic and efficient data evaluation approach.

5.3.1. Covariances and evaluation of neutron data

Many pre-requisites for producing modern quality-assured nuclear data libraries are there, or nearly there. Modern nuclear data evaluation requires a quality assured procedure that guarantees complete reproducibility of the results that fill the data files, i.e., automatic file regeneration and update on the basis of selected experimental data and working input files, with optimized parameters, for model codes. This should be pursued even if many actions are needed for individual reaction channels e.g., direct inclusion of experimental data, or ad hoc modifications to particular reaction channels. In this way, expertise from the past will always remain applicable.

A large, correct experimental database, EXFOR, and nuclear model codes will always remain at the heart of the future evaluation processes. In the coming years most emphasis will be put on the uncertainties of nuclear data and their correlations. These covariance data need to be complete and reliable. First, completeness of nuclear data and their covariances can now be guaranteed with the latest class of nuclear model codes. This is essential, since no nuclear data perturbation/sensitivity study will find
sensitivity to a class of data that is not present in the data library. Often encountered examples of such omissions are angular distributions (reflection of neutrons) and gamma ray production (proper prediction of heating). There may always be an excuse for lack of quality, due to experimental and theoretical challenges already outlined, but there should no longer be any excuse for lack of completeness. Once completeness is accomplished, precise data evaluation procedures should be followed for reaction channels for which high-precision data is required.

As mentioned in Section 4.3, Monte Carlo approaches are already being developed to produce reliable nuclear data covariance information. Uncertainties of nuclear model parameters and resonance parameters are the basis for the Monte Carlo sampling. One of the challenges is to merge this with the covariance information of the experimental data, leading to the so-called Unified Monte Carlo method.

A recommendation is to apply the above sketched method to the most important materials that are important in (almost) any GEN-IV or transmutation design, as emerged from the recent NEA SG-26 study:

\[ ^{235,238}\text{U}, ^{238-242}\text{Pu}, ^{237}\text{Np}, ^{241,243}\text{Am}, ^{243-246}\text{Cm} \]

for ADS

O, B, C, Na, Cr, Fe, Zr, Pb, Bi

and to store the results in a consistent high-quality nuclear data library for advanced reactor systems, including full covariance description. This would be a major step forward compared to the current data libraries, and would open up the possibility of systematic uncertainty propagations in reactor simulation codes. Also it would be timely: the current nuclear data libraries do not reflect the current status of experimental nuclear physics (i.e. latest measurements) and theoretical nuclear physics (applying model codes for all these materials).

A parallel development is to follow a completely innovative direction in which nuclear data evaluation, uncertainty propagation and integral validation becomes part of one and the same process [Koning 2008b], by subjecting the entire nuclear data library + processing + validation chain to a Monte Carlo procedure allowing an exact assessment of the uncertainties of macroscopic design features due to nuclear data uncertainties. For straightforward integral experiment validation, this method can already be applied. It is obvious that no manual intervention is allowed in such an approach: the entire nuclear data library production and integral validation process should be part of an automated simulation scheme.

5.3.2. Covariances and evaluation of decay data and fission yields

Of particular importance to the operation and safety of advanced systems are integral quantities such as decay heat, radiation fields and their spectra, that are dominated by fission products. These integral quantities are obtained by the summation over many
separate nuclides whose yields are highly correlated. To have a good estimate of the accuracy of such calculations, detailed information on the correlations of uncertainties on the fission yield and radioactive decay nuclear data (covariance matrices) are required to correctly propagate uncertainties for these integral quantities. This is an area that has not previously been explored as current reactors and fuel cycles have been developed slowly with experimental rather than modelling justification. However, for advanced reactors and their fuel cycles, there will be pressure to rapidly tighten safety margins and thus accurate uncertainties on the calculated integral quantities will be required to justify these efficiency improvements. No covariance matrices exist for these quantities and it will be necessary to develop the physics and evaluator skills to produce and use these covariance matrices.

The development of decay data for applications is a process that requires skilled scientists that understand both nuclear structure and the needs of applications. An important collaboration in this area is the Decay Data Evaluation Project [http://www.nucleide.org/DDEP.htm], which includes several European laboratories. The purpose of this collaborative effort is to provide recommendations for atomic data, half-lives, decay modes, branching ratios, radiation energies and emission probabilities. These recommendations will be important for future nuclear industrial development. In addition, the fission products from fast fission and minor actinides are different from thermal fission of major actinides, it is thus important that facilities and analysis skills for experimental total gamma-ray spectrometry measurements identified within the OECD/WPEC-25 report be maintained.

It is noted that Europe has strong skills in both fission yield and decay data evaluation but vested in very few people; if these skills are to be maintained in the longer term they will require support for both training of new staff and the production of new evaluations.

5.4. Validation and integral measurements

When considering nuclear data validation for Gen IV reactors, the most relevant experimental feedback comes from past and current FBR operation and related programmes. That is particularly true for SFRs with oxide fuel. As a consequence, among the various Gen-IV fast reactor concepts, innovative SFRs are often viewed as having the best chances for the shortest term development.

The current experimental data base for SFR contains a significant number of configurations using oxide fuel and sodium. However, given the criteria now assigned to the design of sodium fast reactors, a revisit of the fundamental choices, which have led in Europe to such advanced designs as the EFR (European Fast Reactor), is necessary. The EFR design was very much in line with the experience gained in building and operating the PHENIX and SUPERPHENIX sodium cooled fast reactors. The objectives assigned to 4th generation reactors call for different subassembly and core designs. The strategy adopted for identifying reactors with attractive features has led to two different categories of core concepts, for which the amount of required Research & Development efforts differs significantly:

- Cores called “innovative”, derived from known technologies as in the EFR (oxide fuel pin inserted in a hexagonal wrapper).
- Cores called “highly innovative”, which would use very innovative fuel
(carbide) and sub-assembly geometries. These innovative Gen IV SFR configurations are not covered by the available database of integral experiments. As a consequence, new validation data will be required, and this concerns in particular:

- The prediction of the critical mass as volume fractions of the different constituents are very different from the values of the previous designs and is particularly a problem with carbide fuel and steel reflectors,
- The sodium void for the core and possibly the plenum, especially at the end of life and for large burn up rates,
- The mass balance over the cycle,
- The power map distribution in the core (sensitive to the core radius and the mean free path) and at its boundary close to steel reflectors,
- The efficiency of control rods (sensitive to the core radius and the mean free path),
- The efficiency of the compact shielding,
- The reactivity of some hypothetical disturbed core configurations as envisaged in severe accident sequences.

An experimental programme in support of these SFR designs is being defined at CEA as the GENESIS experimental programme, to be performed in the MASURCA facility. New PROFIL-type experiments in the PHENIX reactor will complement this programme.

Because the Gas Cooled Fast Reactor (GCFR, Helium cooled) initial specifications ask for operation at very high coolant temperature (850°C), preliminary design work has focused on refractory materials for the fuel and cladding materials: UPuC, imbedded in a SiC matrix and SiC cladding. The technological feasibility of such a concept has yet to be established. From the core physics standpoint, there is essentially no corresponding validation experiment available. Therefore, new integral experiments will be needed. The ENIGMA physics programme proposed by CEA in MASURCA is aimed at fulfilling those needs.

For Pb and LBE cooled fast reactors, there are Russian integral experiments available from the BFS zero-power reactor. The Guin evere experiments at SCK/CEN Mol will provide some additional information, but only partially since the Uranium 30% Enriched core is not really representative of a Gen-IV FR nor an ADS. It was shown in the BFS experiment that the Pb scattering cross section (elastic and inelastic) is of great importance for the reduction of calculation uncertainties for these systems.

(V)HTR is one of the six Gen IV reactors. There is a large variety of HTRs, depending on the graphite moderation (moderation ratio) and the fuel management (enriched Uranium, Plutonium burner with very high burn-up or even Thorium fuelled HTR with high conversion ratio). For each of these types of HTR, high-quality cross-sections in the thermal and epithermal range are needed. One element of specific interest for HTRs is Erbium, which could be used as burnable poison and would improve the graphite temperature coefficient. Although there is feedback from past experimental programmes and from HTRs developed and operated in the 70’s, in general, the available information on the core configurations and measurements is incomplete or insufficiently accurate by modern standards, so that it is difficult to derive meaningful physics trends from it.
Different types of breeder MSR concepts are available today:

* $^{233}$U-$^{232}$Th fuelled MSR with fluoride salt and thermal neutron spectrum, moderated by graphite;
* $^{233}$U-$^{232}$Th fuelled MSR with fluoride salt and fast neutron spectrum;
* $^{238}$U-$^{233}$Pu fuelled MSR with chloride salt and fast neutron spectrum.

For the first two of these reactors, the improvement of Thorium chain isotopes at all energies from 0.1 eV to 10 MeV will reduce the design uncertainties. The knowledge of diffusion and capture cross-section of graphite and potential constituents of the salt is also needed: Li, F, Cl, Na, Be, K either in a fast or in thermal spectrum. Today’s precision is however certainly sufficient for the viability phase.

SCWR have some distinctive features with respect to either PWR or to BWR. However, feasibility studies have demonstrated that these do not induce specific nuclear data needs, except possibly for bounded Hydrogen scattering laws in Water. Extrapolation to the high pressure in which this water (in a single phase) is operating has been found to be sufficient for current design phase. Therefore, requirements at this stage are those of existing thermal reactors.

Advanced water-cooled reactors generally have a harder spectrum than today’s LWRs because they are under-moderated in order to favour the conversion of $^{238}$U into $^{239}$Pu. Integral experiments have been performed in the past, which provide validation data in epithermal spectra. As a complement to these past programmes, minor actinides and capturing isotopes oscillation experiments are foreseen by the CEA in the MINERVE reactor in the next years.

Basic data linked to the Thorium cycle ($^{232}$Th, $^{233}$U, $^{233}$Pa) in various spectra are also important insofar as they are of interest to a number of high conversion reactor concepts ($^{232}$Th to $^{233}$U), such as the heavy water cooled Thorium reactor foreseen in India. In these reactors, $^{232}$U ways of formation have to be particularly well described because highly energetic gamma emissions (hindering fuel fabrication and reprocessing) are associated with $^{232}$U and its decay products, especially $^{208}$Tl.

Finally, the campaign on differential measurements at neutron energies above 20 MeV in FP5-6 has resulted in a much improved situation in that there are fewer lacking data. It would now be necessary to perform validation studies using integral experiments. A proposal for an experiment, a transmission experiment at 96 and 175 MeV, has been developed as part of the CANDIDE project.

**Section 4.4- Post Irradiation examinations of spent fuel and decay heat experiments**

The properties of spent nuclear fuel are all dependent upon the composition of the irradiated fuel; the number densities of the nuclides present in the material. The safety and achievable throughputs of all reactor and fuel cycle operations will depend on the accuracy of such calculated compositions, including handling, storage, transport, chemical and physical processing, fuel fabrication from recycled components, waste management and disposal. It is thus important that the calculated compositions of fuel be validated against measurements on spent fuel.

An NEA expert group exists to maintain a spent fuel isotopic composition database (SFCOMPO) of existing measurements on the assay data of spent nuclear fuel. These
measurements are currently fairly limited and only exist for uranium and mixed oxide fuels from current reactors. These show quite good agreement for the major nuclides and decay heat, but to be useful in the development of advanced reactor systems and fuel cycles, which are mostly fast neutron systems, validation will be required on fast reactor fuels, including fuels containing high loading of minor actinides. Thus experimental activities on fast reactor fuel analyses will be required to allow validation of fuel cycle calculations for advanced fuel cycles. Also the existing SFCOMPO database will need to be extended to fast systems including any data on ADS and high temperature reactors.

5.5. Other issues

Competence management is a cause of general concern in the nuclear data field. The age structure of the field is not favourable, with retirements being more frequent than the recruitments. The CANDIDE project has made one modest attempt to remedy this situation by launching the EXTEND course (European course on Experiments, Theory and Evaluation of Nuclear Data). Making this highly successful course a recurring event requires, however, some type of sponsoring.

The situation on experimental facilities is to some extent even worse than on the human capacity side, since the start-up cost is so much higher. There are a few laboratories under threat of closure or re-direction. The cost to build a new laboratory is significantly larger than subsidizing existing laboratories so they can continue to work. In this context, countries and organizations such as CEA that still have operational facilities have a special responsibility; programmes open to international collaboration should be encouraged. An interesting option is that laboratories that are presently being re-directed to commercial activities after having lost public funding (e.g., Louvain-la-Neuve, TSL) could be made available for nuclear data research as a minor part of their time, given that the beam time costs could be covered. EC programs for such beam time cost support are already operational (e.g., EFNUDAT) and have turned out to be very important for continued research in the nuclear data field.
6. Conclusions and recommendations

To enable reliable analyses and design of nuclear energy systems, the following is required:

- Produce high-quality nuclear data libraries, and assess the impact of nuclear data uncertainties more systematically in reactor and fuel cycle calculations. In practice this means data libraries with complete covariance data files, certainly for neutron transport data, but also for thermal scattering data, activation data and radioactive decay and fission yield data.
- Decrease the nuclear data uncertainties in reactor and fuel cycle analyses by the combine use of more precise differential measurements, new theory development, and trends observed in clean integral experimental benchmarks.

This report emphasizes that different nuclear research activities are needed to accomplish this, and that the required potential is available in Europe. An important issue is that a large part of the progress required in nuclear data fields such as measurements, data evaluation and validation are independent of the nuclear reactor system that is eventually chosen for implementation. There is the obvious choice between thermal and fast spectra and the specific types of coolants, but in general the same materials, and their associated nuclear data problems, emerge. Lack of decision making with respect to the advanced reactor to be built is thus no excuse to delay progress in nuclear data.

All assets are present to work towards a nuclear data library of unprecedented quality to enable realistic design calculations for future sustainable nuclear reactors. There currently is a costly time delay between advances in nuclear physics, either experimental or theoretical, and their exploitation for nuclear technology. In addition, tighter constraints in safety-economy have led to calls for more and better nuclear data, including covariance data. Up to now, in Europe no sufficient action to answer these calls has been undertaken, as there is no European-funded project for the development and maintenance of a nuclear data library for reactor and fuel cycle development. This implies that technological innovation remains shielded from many important nuclear physics and computational developments. Europe has a few of the world-leading teams in nuclear data development, and is thus well equipped to change this situation. Therefore, it is recommended to create a special European targeted action for the production of high quality nuclear data libraries, including covariance data, for the materials needed for advanced reactor design.

The differential measurements required to meet advanced reactor target accuracies are very challenging, and require a step forward in experimental methodology. Again, Europe is in a good position to take up this challenge. More application-oriented awareness, in terms of complete documentation and covariance information, is required in the measurement process. Furthermore, the facilities that are capable of producing the required nuclear measurements that emerge from GEN-IV and ADS sensitivity studies need to be supported and high-priority measurements need to be carried out.

A world-leading nuclear model code has been developed and is maintained in Europe. A major challenge in nuclear modelling is a robust description of the fission process, so that all reaction channels for actinides can be properly described. With the
anticipated increase of computer power, nuclear model development will become even more important for the delivery of nuclear data and their covariances. The capability should be provided to implement new and improved nuclear reaction models within the qualified nuclear model software as they become available.

Although the impact of improved nuclear data can generally be clearly and easily proved, a modernization of reactor and fuel cycle software is required to make maximal use of nuclear data file updates. Since eventually all design aspects depend on nuclear data, it should be the responsibility of the nuclear data community, shared with reactor physicists, to ensure more flexible use of nuclear data libraries in reactor and fuel cycle calculations. When accomplished, the nuclear data community will benefit from the increased amount of, and arguably more crucial, feedback. In other words, instead of a hard-wired black box, nuclear data should become an integral and flexible part of any applied nuclear analysis. Hence, **flexible implementation of improved nuclear data libraries in nuclear technology and design should be ensured**, by developing error-free processing and data-reading procedures and possibly even by integrating nuclear data, their uncertainties and applied calculations into one approach. In parallel, systematic approaches to integral validation and sensitivity studies should be developed, to ensure that improved nuclear data (e.g. better covariance matrices) can directly be tested on relevant integral measurements such as those from the ICSBEP, IRPHE, and SINBAD collections, or on advanced reactor and ADS sensitivity cases as initiated by SG26.

A leading indicator for nuclear data development would be the quantitative economic impact of a certain improvement, e.g. a reduced uncertainty of a particular cross section, but such a study has, to our knowledge, not been performed. This is not impossible, but would be very time consuming. It could only be done after completing the “flexible implementation” mentioned above.

Finally, this report has made it clear that improvements are necessary for almost every aspect of nuclear data: high-precision measurements, new theoretical methods, more complete nuclear data libraries, inclusion of covariance data, processing for, and validation with, reactor and fuel cycle software and integral measurements. Assigning relative weights to all these aspects is difficult; however, this does not mean that all future international nuclear data projects should necessarily contain all of the above at the same time, which leads to dilution. Specific “targeted actions” with a limited number of clear deliverables can make significant steps forward. Regarding the European situation, such targeted actions are different from projects that only emphasize networking and lifetime extension of research fields. Two specific examples of such targeted actions (more could be given) are: (i) a complete nuclear data library for advanced reactor systems including covariance data, and (ii) a new set of relevant high-quality integral measurements. Both of these would require a large effort by a limited number of participants, the combination of which is probably at variance with the current European funding structure. It thus seems to be a challenge at least as large as the scientific one, to realize funding for nuclear data improvements in accordance with the economic relevance that such improvements may bring according to industry.
References


1. Preliminary identification of Nuclear data performances for future nuclear systems
2. Current Status of Nuclear data performances
3. Prospects for high level measurements below 20 MeV
4. Prospects for nuclear data research at high neutron energies
5. Nuclear data needs for ADS
6. The EXFOR database


Nuclear Science and Engineering


Abstract
Final report of a coordinated action on nuclear data for industrial development in Europe (CANDIDE).

The successful development of advanced nuclear systems for sustainable energy production depends on high-level modelling capabilities for the reliable and cost-effective design and safety assessment of such systems, and for the interpretation of key benchmark experiments needed for performance and safety evaluations. High-quality nuclear data, in particular complete and accurate information about the nuclear reactions taking place in advanced reactors and the fuel cycle, are an essential component of such modelling capabilities.

In the CANDIDE project, nuclear data needs for sustainable nuclear energy production and waste management have been analyzed and categorized, on the basis of preliminary design studies of innovative systems. Meeting those needs will require that the quality of nuclear data files be considerably improved. The CANDIDE project has produced a set of recommendations, or roadmap, for sustainable nuclear data development. In conclusion, a substantial long-term investment in an integrated European nuclear data development program is called for, complemented by some dedicated actions targeting specific issues.
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