Sensitivity Analysis and Uncertainty Propagation from Basic Nuclear Data to Reactor Physics and Safety Relevant Parameters

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Reliable knowledge of the uncertainties in important reactor parameters, like criticality, radiation load on the reactor components, neutron/gamma ray flux, nuclear heating and dose are crucial for nuclear safety concerns. Uncertainties are introduced either through the calculational algorithms or through the data uncertainties. The paper addresses the uncertainties in the reactor parameters linked to the basic nuclear data uncertainties. The method used is based on linear perturbation theory to calculate the sensitivity coefficients, and propagates these sensitivities using the basic data covariance matrices to the target reactor quantities.

The NEA Data Bank activities related to the sensitivity and uncertainty analysis are presented. This includes the collection and development of the corresponding computer codes and data libraries, the benchmark experiments studied under the projects like IRPhE, SINBAD and ICSBEP, and the Reactor Pressure Vessel surveillance project. Other areas include fusion, oil well logging, medical etc.

1. Introduction

Radiation transport codes based on Monte Carlo and deterministic methods are principally used in radiation shielding and criticality analysis. They proved to be very useful tools in many domains of application, ranging from nuclear research and power reactors, to accelerator, fusion, and medical problems. Although codes like MCNP or TORT-DORT, DANSYS etc. are widely used and extensively tested the user must still be aware that the code can never give "exact" solutions to a physical problem, as inevitably approximations are used in several steps of the calculational procedure. There are for example uncertainties, originating from the knowledge about basic nuclear reaction data and the radiation source, the geometrical description of the problem, the material compositions. The knowledge of the approximations used in the analysis and of the overall calculational uncertainties is therefore essential to gain confidence in the results obtained.

The accuracy of the transport calculations can be estimated by comparing the calculations against experiment and by uncertainty analysis. Uncertainty analysis, combined with sensitivity analysis, provides some valuable information about the radiation transport calculations. Together they give us a clear insight into the importance of different calculational parameters and tell us how much we can trust our results. The major sources of uncertainty can be identified in this way. When applied to the analysis of integral experiments, it enables to assess the calculational accuracy and provide information for improving the cross-section data evaluations.

The nuclear cross sections are among the main sources of uncertainty in the particles transport calculation, and their impact is determined by the cross-section sensitivity and uncertainty analysis.

2. NEA-DB Activity Tasks

At the NEA-DB the following ongoing or already concluded projects are related to the sensitivity and uncertainty analysis:

- Updating of the cross section sensitivity and uncertainty code SUSD3D [1], including the development of graphical tools;
- Cross section covariance matrix libraries: ZZ-VITAMIN-J/COVA [2], ZZ-COV-15GROUP-2005 (covariance matrix data review – in preparation)
- Reactor pressure vessel surveillance project focusing on the overview of the methodology for RPV surveillance [3], including uncertainty estimations. VENUS-1 and VENUS-3 benchmark analysis and interlaboratory comparison were performed [4]
- Sensitivity and uncertainty analysis of criticality benchmark experiments (KRITZ-2, VENUS-2 [5], SNEAK [6]) performed within the IRPhE project in the framework of the joint activities of the OECD/NEA Working Party on the Physics of Plutonium Fuels and Innovative Fuel Cycles (WPPR) and the Task Force on Reactor-based Plutonium Disposition (TFRPD). The aim of these exercises was to investigate the capabilities of the current production codes and nuclear data libraries for analysing UO2 and MOX systems.
- SINBAD and ICSBEP Projects [7] aiming at the preparation of the databases of internationally verified benchmarks for the validation of computational codes and nuclear data
- Fusion benchmark analysis including sensitivity/uncertainty (EFF project) [8, 9].

3. Computational tool development

One of the essential roles of the OECD NEA Data Bank is to to provide scientists in member countries with reliable computer programs and nuclear data for use in different nuclear applications. NEA DB role is to collect, develop, improve and validate these tools and make them available as requested.

For the sensitivity and uncertainty analysis both adequate computer codes and complete and reliable covariance matrix libraries are essential, and NEA actively participates in the efforts to develop such tools.

A code system SUSD3D, available from the NEA-DB, performs 1-, 2- and 3-dimensional cross section sensitivity and uncertainty analysis and is suitable to study both fission as well as fusion problems. SUSD3D uses the flux files produced by the deterministic discrete ordinates codes (DOORS and DANTSYS). The advantages of the system are the relatively low CPU time and computer space requirements. Complex 3-dimensional geometries can be treated. The SUSD3D code package was first used for PWR Pressure Vessel surveillance and fusion applications. Recently it is being used for the analysis of several critical benchmarks (KRITZ, VENUS-2, SNEAK), GEN-IV concepts (Molten Salt Reactor), fusion benchmarks, intercomparisons with stochastic methods.

Further details on SUSD3D can be found on the Web page <http://www.nea.fr/abs/html/nea-1628.html>.

Availability of reliable and complete information on the cross section covariance matrices is essential in order to be able to determine the uncertainty in the target design or safety parameters. Modern cross section evaluations usually contain the covariance matrices together with the cross section data, but unfortunately this information is too often neither complete not reliable. For many isotopes the covariance information is still not available and large differences can be found among different evaluations, although all based on the same experimental database.

In order to produce the multi-group covariance data needed for the uncertainty analysis the following codes are used today:

- NJOY99, Data Processing System of Evaluated Nuclear Data Files ENDF Format <http://www.nea.fr/abs/html/psr-0480.html>, in particular the modules ERRORR computes multigroup covariance matrices from ENDF uncertainties and COVR performs covariance plotting and output formatting operations.
- ERRORJ, Multigroup covariance matrices generation from ENDF-6 format for the JENDL 3.3 data <http://www.nea.fr/abs/html/nea-1676.html>
- Covariance data already processed into the multi-group form are also available, like:
- ZZ VITAMIN J/COVA, Covariance Matrix Data Library for Uncertainty Analysis <http://www.nea.fr/abs/html/nea-1264.html>. These data contain also auxiliary programs ANGELO2 for extrapolation/interpolation of the covariance matrices to another energy group structure and LAMBDA to verify the mathematical properties of the covariance data.
- ZZ DOSCOV, 24-Group Covariance Data Library from ENDF/B-V for Dosimetry Calculation <http://www.nea.fr/abs/html/dlc-0090.html>

More recently an overview of the available covariance data from different evaluations, including JENDL-3.2, -3.3, ENDF/B-V, -VI, EFF-3, IRDF-90, and IRDF-2002, was prepared. This evaluation of the present state provides indications on the future needs both concerning the cross section as well as the covariance matrix evaluations. Some conclusions using this work are presented in [10].

4. Pressure vessel surveillance dosimetry

The assessment of the level of metal degradation in nuclear reactor structures exposed to neutron and gamma flux during the reactor operation is one of the most important in today's reactor engineering. In particular, as many reactors throughout the world near the limits of their lives, the confident ability of judging their metal structural integrity may lead to extension of their operational licenses and hence to significant financial savings.

The radiation damage caused to the material of the pressure vessel is directly linked to the neutron field and spectrum. Damage calculation requires therefore an adequate knowledge of these quantities in particular in the surveillance capsules and at the most exposed pressure vessel location. Insufficient information about the accuracy of the neutron fluence would require large safety margins, and consequently affect the operating conditions, the life of the nuclear installations, and their cost.

The prediction of the RPV metal damage involves detailed particle transport calculations combined with experiments and modeling of basic physics phenomena of metal degradation.

The problem of accurately predicting the metal damage of the important reactor component - Reactor Pressure Vessel (RPV), has been studied by the OECD/NEA NSC Task Force on Computing Radiation Dose and Modeling of Radiation-induced Degradation of Reactor Components, which was set up in 1995. The main goals of this Task Force were to:

- Evaluate the accuracy of the calculation methods used in the NEA Member countries for predicting long-term radiation doses to reactor pressure vessels and internal structures;
- Identify points for improvements and validate the performance of improved methods for fluence calculations;
- Initiate a study on the modeling of radiation-induced damage in metals.

A critical review of the state-of-the-art computational methodologies used in the PV dosimetry programs is given in [3].

The computational system and the results applied to the French nuclear installations are described in [11]. The calculational scheme used to determine the neutron fluence and spectra in the capsules and in

the critical PV locations is based on a Monte Carlo code TRIPOLI. On the other hand the uncertainty analysis was performed by the deterministic computer codes (TWODANT, DORT, SUSD3D) and VITAMIN-J/COVA covariance matrix library. All these tools are available from the NEA-DB.

5. VENUS experimental benchmark intercomparison exercises

As a next step of the Task Force's state-of-the-art report the NSC expert group launched two intercomparison benchmark exercises to verify the claimed accuracies and to validate the calculational models used. Both benchmarks were based on the VENUS experiments performed at SCK CEN Mol, Belgium, one being a two-dimensional (VENUS-1) and the other a three-dimensional benchmark (VENUS-3). Later this was extended to VENUS-2 loaded with MOX fuel in the outer assemblies near the pressure vessel.

As part of the exercise the cross section sensitivity and uncertainty analyses were performed [12] to determine the importance of different cross sections in the transport calculation of the detector reaction rates, and assess the corresponding uncertainty. These uncertainties were finally compared with the actual spread between the measured and calculated detector reaction rates, and reasonable agreement was observed between them (Figure 1).

10 participants took part in the VENUS-1 and 8 participants in the VENUS-3 exercise. The results of the benchmark studies are discussed in [4].

6. Sensitivity & Uncertainty Analysis of Critical benchmarks (IRPhE project)

In the scope of the IRPhE (International Reactor Physics Experiment Evaluation) Project several Criticality benchmark experiments (KRITZ, VENUS-2, SNEAK) were analysed using the transport and sensitivity/uncertainty tools to determine the state of the art of the nuclear data files and suggest areas requiring further developments. This method is also used to assess the quality of the benchmark data. The results of this work are described in [13, 5, 6].

7. SINBAD integral accelerator benchmark experiments

Validation of the calculation results against integral experiments is essential in order to verify the performance of the cross section data libraries and computer codes. Integral data-bases like SINBAD (Shielding Integral Benchmark Database) [7] and ICSBEP (International Criticality Safety Benchmark Evaluation Project), established through the OECD/NEA and RSICC can be used for this purpose.

The SINBAD benchmark experiments database for shielding and dosimetry applications covers nuclear reactor shielding (including the pressure vessel surveillance), fusion neutronics and accelerator shielding. New experiments are regularly added each year. The regularly updated list of available experiments can be found in: http://www.nea.fr/html/science/shielding/sinbad/sinbadis.htm.

These projects permitted to save the information on some valuable shielding experiments. Many new experiments were added in the last years and further data is being processed. SINBAD incorporates at present 75 shielding benchmark experiments, and ICSBEP 2642 critical and sub-critical configurations.

Under specific conditions integral experiments can be used to adjust the basic data evaluations. This approach requires very reliable and consistent variance/covariance matrices for the cross sections and the measured parameters, as well as the sensitivity coefficients of the integral parameters to the basic cross

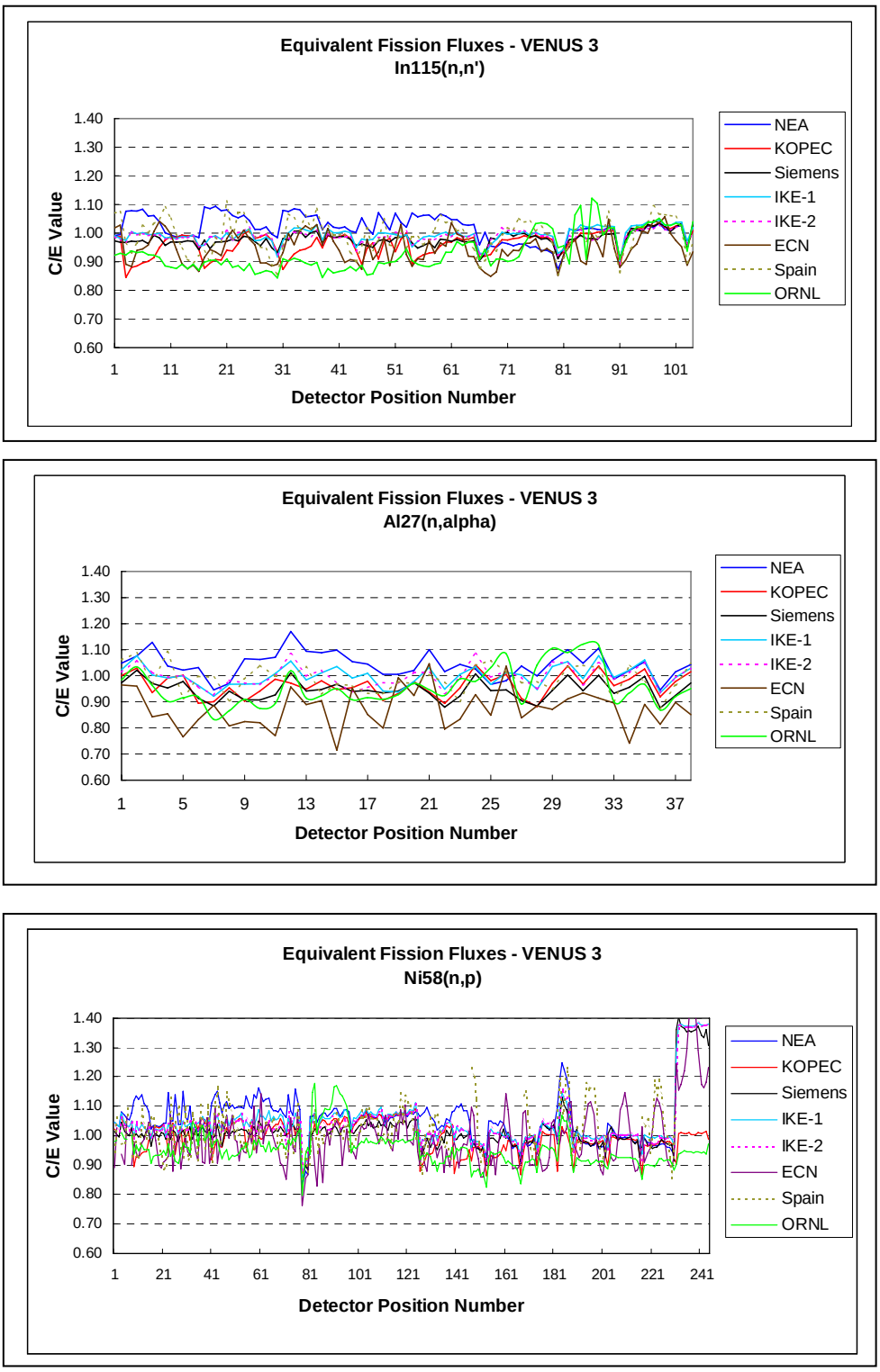

Fig. 1: The calculation to experiment (C/E) values for the indium, aluminium and nickel activation foil measurements in VENUS-3 obtained from the participants of the OECD/NEA exercise. The scatter of the C/E values was found consistent with the uncertainty in C/E estimated to 8 – 9 %.

section data. The approach is valid only if each set of experimental data is uncorrelated with the data already supplied. Even in this case it is likely that the adjustment could compensate for approximations in the processing of the data or method of calculation, therefore great caution is needed in their use.

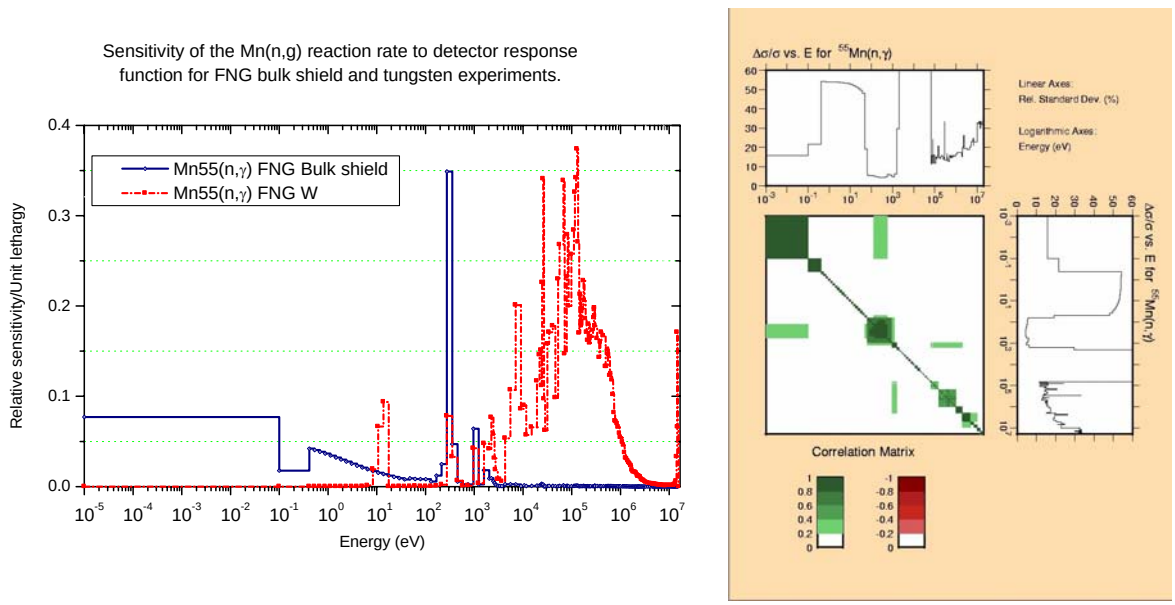

Fig. 2: Uncertainties in the cross sections can explain discrepances between the calculations and the measurements. The two examples above (steel – water array and W experimental set-ups) both using thin manganese activation foils are given. The energy dependant sensitivities are presented on the left figure, and the corresponsing Mn-55(n,gamma) covariance matrix on the right shows large uncertainties in the energy ranges between about 1 and 100 keV. In the first experiment (blue) a very good agreement between experimental and calculated reaction rates was observed, within ~10 %. In the second experiment the discrepances around 60 % were observed, due to its large sensitivity in this energy range.

8. Conclusions

Quantities of importance for reactor design and for the safe operation of reactors are biased due to uncertainties of typical parameters. These uncertainties are often substantial and in many cases exceed reactor design requirements. An improved cost efficiency of nuclear energy systems can be achieved by the reduction of uncertainties in design parameters.

Sensitivity and uncertainty analysis is a powerful means to assess uncertainties of nuclear responses in neutron transport calculations and trace down these uncertainties to specific nuclides, reaction cross-sections and energy ranges. These analyses can also identify areas of weakness in data files and thus guide further cross section evaluations. In recent years an increased interest was shown in the use of uncertainty analysis not only for dosimetry and radiation shielding but also for new reactor designs and fusion applications. Some powerful calculational tools needed for such analysis are available from the OECD/NEA Data Bank.

Examples of successful use of uncertainty analysis include the PW reactor pressure vessel surveillance, benchmark experiment analysis like shielding benchmarks ASPIS and VENUS-3, criticality benchmark analysis (KRITZ, SNEAK, VENUS-2), fusion integral experiment pre- and post-analysis. The state-of-the-art of the cross-section libraries and the corresponding covariance matrices can be evaluated from these analyses.

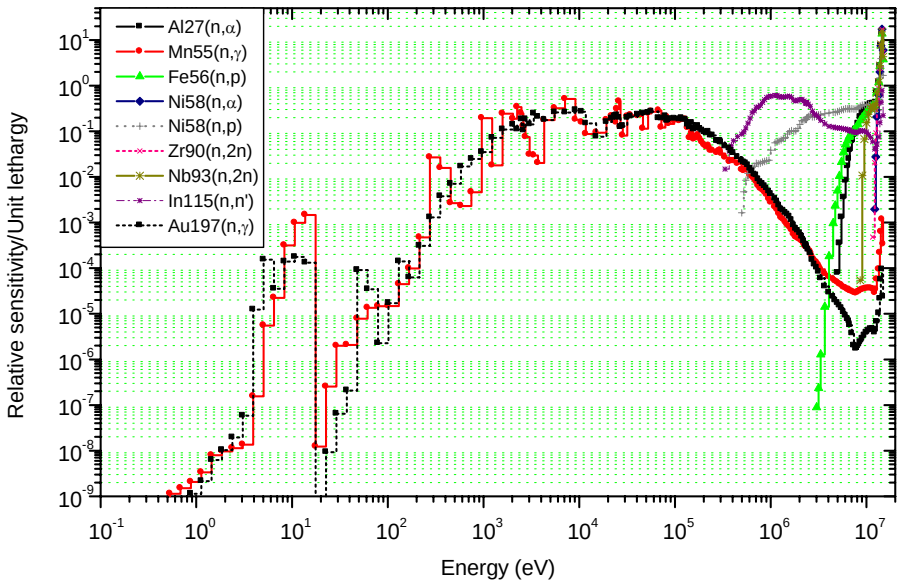

Fig. 3: Activation foils sensitive to different energies are used in experimental measurements. Sensitivity analyses provide information on the neutron energies which contribute the most to the detector response. Here an example of the energy coverage of the activation foils used for the FNG-W experiment is given.

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