NNT : 2019SACLS414

Thèse de doctorat

Uncertainty quantification of the fast flux calculation for a PWR vessel

Thèse de doctorat de l'Université Paris-Saclay
préparée à l'Université Paris-Sud

Ecole doctorale n°576 Particules, Hadrons, Énergie, Noyau, Instrumentation, Imagerie, Cosmos et Simulation (PHENIICS)
Spécialité de doctorat : Énergie nucléaire

Thèse présentée et soutenue à Saclay, le 13 Novembre 2019, par

LAURA CLOUVEL

Composition du Jury :

Pierre Désesquelles Professeur des universités, Université Paris-Sud	Président
Ivo-Alexander Kodeli Enseignant-chercheur, Institut Jožef Stefan, Slovenia	Rapporteur
Bertrand Iooss Chercheur Senior, EDF R&D /Département PRISME	Rapporteur
Claire Vaglio-Gaudard Chercheur Expert, CEA-Cadarache/DEN	Examinateur
Pietro Mosca Ingénieur-chercheur, CEA-Saclay/DEN	Superviseur
Jean-Marc Martinez Chercheur Expert, CEA-Saclay/DEN	Directeur de thèse
Stéphane Bourganel Ingénieur-Chercheur, CEA-Saclay/DEN	Invité

THESIS SUMMARY

Context

The production of electricity in Pressurized Water Reactors (PWR), consists in harnessing the heat released from the fission of atoms produced in the fuel of the reactor core, by using water as a coolant. The fission reaction results from the absorption of slow neutrons by nuclei of high atomic number. The nucleus splits into two lighter nuclei, called fission fragments and produces an average of 2.5 neutrons. In order to slow down the high-energy neutrons liberated by the fission reaction, the water also plays the role of moderator. A reflector is then installed around the reactor core to reduce neutron leakage by scattering back those which have escaped from the core. Despite the presence of the reflector, some neutrons still reach the reactor pressure vessel. The issue is that intense irradiation can alter the vessel microstructure and have an unfavourable effect on mechanical properties. This phenomenon is one of the major limiting factors to ***nuclear reactor lifetime***. The vessel, which cannot be replaced, is actually the second ***barrier against the radioactive leakage***. Surveillance programmes are therefore necessary for safety assessment and for verifying the ***vessel structural integrity*** (Steele, 1983).

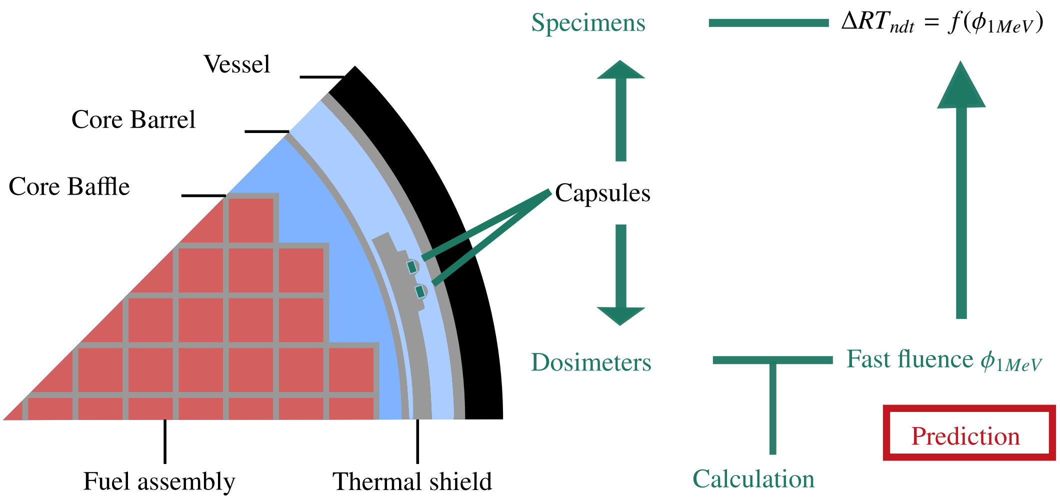

Figure 1: General Methodology in Irradiation Surveillance Programmes

Two tracks are commonly adopted to monitor the effects of neutron irradiation on the reactor vessel under actual operating conditions. They are based on the presence of surveillance capsules containing ***steel specimens*** and ***dosimeters*** and placed between the core and the vessel. During normal refuelling periods, steel specimens are removed from the reactor for performing tensile and fracture mechanics tests. Embrittlement rates by irradiation are measured as a shift of ***ductile-to-brittle transition toughness temperature*** ΔRT_{ndt} that increases with irradiation and describes the ability of material to resist fractures. On the other hand, the fracture toughness is a function of the neutron fluence. Usually, only neutrons with energies above 1 MeV are considered as the particles which produce the radiation damage on the vessel (Margolin et al., 2005). To monitor the radiation damage, it is thus also possible to use dosimeters to assess fast fluence at capsule location using activity measurements and activation codes. This assessment is notably based on tree inputs: the ***fast neutron spectrum*** ϕ_{1MeV}, the irradiation history and the cross sections drawn from activation dosimetry library (Dupré et al., 2015; Hassler et al., 1985). As capsules are placed upstream of the vessel, it is possible to predict the fast neutron flux received by the vessel and anticipate its embrittlement (OECD/NEA, 1997) following a lead factor f_{anti}. The quality of radiation damage prediction thus depends in part on the calculation of the neutron density ϕ_{1MeV}. In that sense, a lack of knowledge on the fast neutron flux will require larger safety margins on the plant lifetime affecting operating conditions and the cost of nuclear installations. To make correct decisions when designing ***plant lifetime and on safety margins*** for PWR reactors, it is therefore essential to determine the ***uncertainty in vessel flux calculations***.

State of the art and Challenges

Several publications which deal with the computational methods used in dosimetry programmes have been referenced in the OECD/NEA (1997) report. The latter document provides various methodologies used before 1996 for the fast flux computation and its associated uncertainty. It reports an average difference of 20% between measurements and the in-vessel transport calculations. The reason for this discrepancy is usually interpreted as the combination of different uncertainty and error sources in the simulation tools (Kodeli et al., 1996; Kam et al., 1990; Haghighat et al., 1996; Remec, 1996). The neutron density calculation indeed results from the implementation of successive physical models which depend on uncertain inputs, and on many assumptions involved for the calculation itself. The inaccuracy in the estimate of ϕ_{1MeV} thus arises from the combination of ***numerical errors*** (convergence criteria, computing methods, etc.), ***modelling errors*** (material, dimension and placement uncertainties, source distribution, etc.), and the propagation of ***nuclear data uncertainties*** (cross-sections, neutron spectrum, etc.). The resulting uncertainty on the calculated fast flux is finally estimated to 10 to 30 per cent (1σ) depending on the reactor type and the methodologies involved, while the uncertainty of the measurements are typically lower 5% for the dosimeters of PWR. The large number of results reported in the document shows the difficulty to analyse the calculation and measurement uncertainties according to the studied reactors and the various methodologies involving different codes, nuclear data sets and procedures. More recently, Kodeli (2001) has developed the sensitivity and uncertainty SUSD3D code package for the evaluation of sensitivity profiles and uncertainties on the cross-section data. The code allows carrying out uncertainty and sensitivity analysis and evaluating the contributions of various parameters involved in neutron flux and reaction rate calculations. It is based on a discrete ordinate sensitivity formulation of first-order perturbation theory. The code package was especially used to assess the fast flux uncertainty of the 900 MWe PWR vessel. Hence, Kodeli has shown that the uncertainty of the fast flux received in the most exposed vessel location, is in a 10% range.

However, most of past studies on the uncertainty assessment of the fast flux calculation are based on the ***methods of moments*** which assumes a ***linear output variation***. The method of moments indeed consists in approximating the statistical moments of the system response by means of a truncated Taylor series expansion y. The function of interest is expanded about the mean of input variables, and one then calculates the moments of the truncated series (mean and variance). This method was most commonly used because the calculation capabilities of computers prevented from conducting more accurate methods. In a non-linear case, the first order hypothesis appears insufficient for an accurate prediction of the output variance. Higher order expansions could be used to account for skewed distributions, but are detrimental to the rapidity in setting up this method. On the other hand, as mentioned by Smith (1994), the expansion results only return an estimate of the statistical moments and not a distribution. The method ignores the probability distribution of parameters, making it difficult to determine quantiles on the output model. In safety analysis, confidence intervals can be actually useful to quantify the level of confidence that a safety parameter lies in an interval.

An alternative method is the ***Total Monte Carlo approach*** (TMC) which consists in randomly sampling the input data and propagating the perturbations on the calculation chain. The resulting output of a computer model is therefore considered as a random variable since the inputs are uncertain. The advantage of this method is that it does not make any assumptions on the linear interactions or small input changes among data. It also allows considering the covariance data to ensure consistent perturbations. In that sense, the TMC approach provides more accurate results because it allows propagating a more precise description of input uncertainties in the output calculation while ensuring data consistency and without presupposing the linearity of interactions.

Thesis plan

It is within this context that our work was conducted. It consists in conducting a new uncertainty assessment of the fast flux calculation for the PWR vessel considering the data of recent international nuclear libraries and their associated covariances. The thesis is divided in two parts. The first part gives an overview of the background needed to carry out the uncertainty analysis. It is made in two chapters. The first chapter recalls the principle of neutron interactions and neutron transport. The second chapter is focused on methodologies of uncertainty and sensitivity analysis. The second part presents the methods and the results of the thesis. The methodology comprises three steps which are described in the different chapters of this work and illustrated in Fig.2.

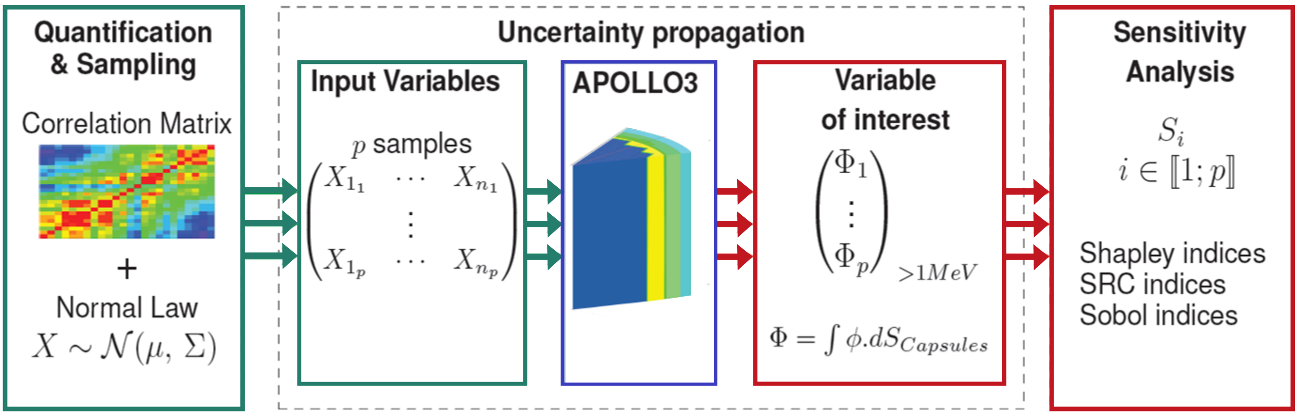

Figure 2: Uncertainty Propagation Scheme

Achievements and results

Deterministic calculation of the neutron fast flux (Part II - Chapter III)

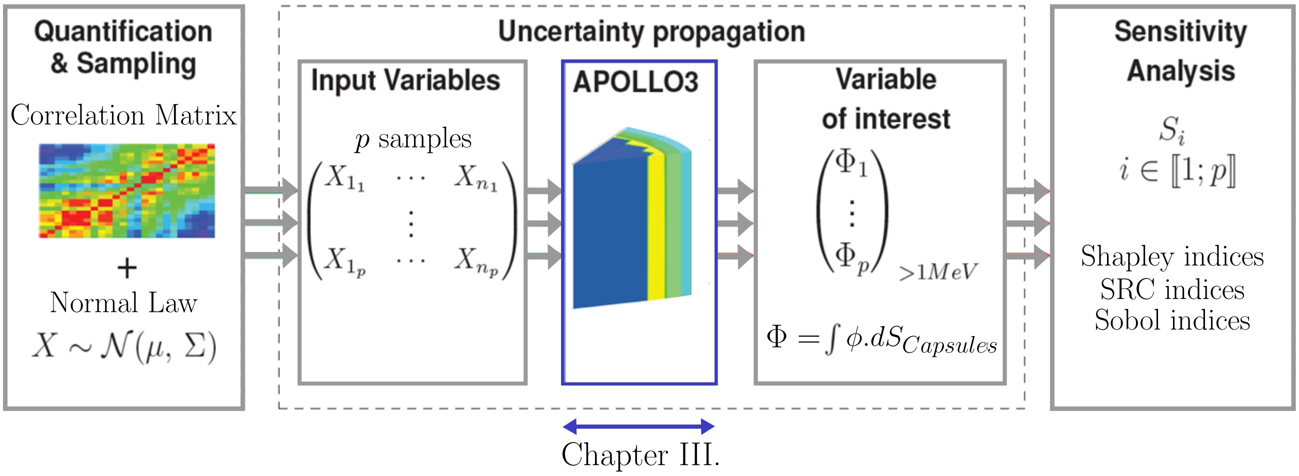

Figure 3: Uncertainty propagation scheme: in blue the specification of the deterministic calculation

The first step consists in ***defining a fast flux calculation sufficiently quick and accurate in comparison with the reference calculation***. In France, fluence calculations are usually based on a stochastic neutron transport codes like TRIPOLI-4® (Brun et al., 2014). The issue is that the TMC sampling requires many perturbations to determine the uncertainty of output accurately. The deterministic methods are computationally faster than the stochastic one and thus they are more suitable to apply the propagation of uncertainties by TMC approach. For this reason, in this chapter, a deterministic scheme for the fast flux calculation is set up. The idea is to use some approximations to reach a compromise between speed and precision which allows carrying up a sufficient number of calculations. Another advantage of deterministic methods is that they provide flux distribution in all points of a modelled system in a single calculation, allowing conducting sensitivity analysis in different locations of the reactor and for different energy groups.

The deterministic scheme which is implemented, is based on the 3D-SN solver MINARET of the APOLLO3® code which uses the Galerkin discontinuous finite elements approximation. We first determines, with the AEMC tool (Mosca et al., 2011), an optimized mesh which lies on a single group between 10^{-11}MeV and 1MeV and 18 energy groups greater than 1MeV. Self-shielded and collapsed cross-section libraries are processed from a slab calculation on the optimized energy mesh.

The final flux calculation is performed on a tridimensional PWR geometry (Mosca et al., 2018) using a P3 approximation for the scattering cross sections and a S8 angular order. ***With this scheme the total flux over 1 MeV (Φ_{1MeV}) is calculated in different locations of the reactor in less than 20 minutes with an error lower than 1% regarding to the TRIPOLI-4® reference***. At this stage of the study, we assumes that if the bias remained relatively constant regardless of the perturbations, the variability of the approached fast flux will be representative of the reference calculation variability.

Modelling uncertainties and propagation in fast flux calculations (Part II - Chapter IV)

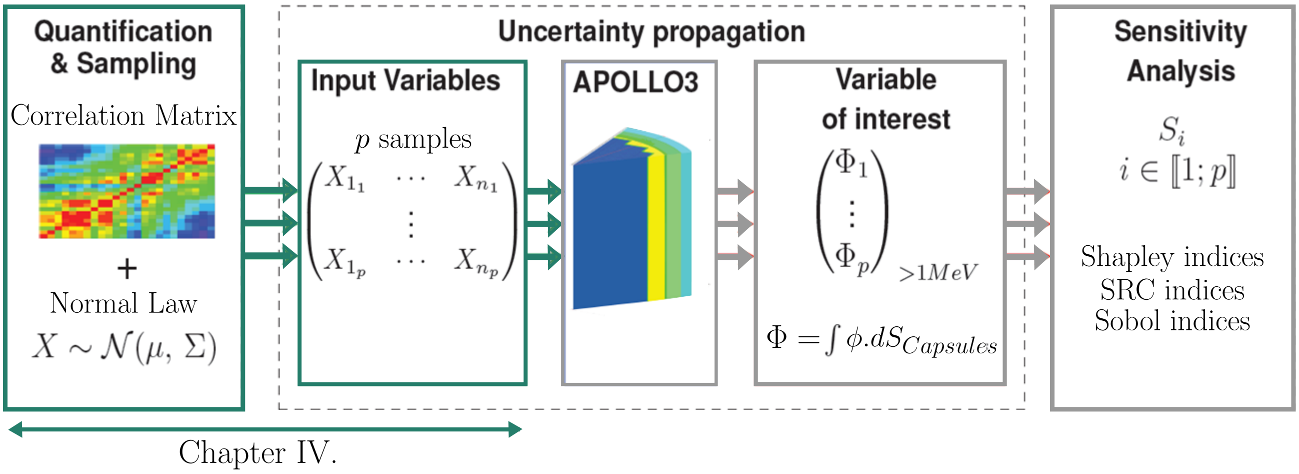

Figure 4: Uncertainty propagation scheme: in blue the specification of the deterministic calculation

The second step of our work is to ***quantify, model and propagate the input uncertainties of the deterministic flux calculation***. As the past study of Kodeli (2001), we are focussed on the sources of uncertainty which may be treated statistically, i.e. the nuclear data and the technological parameters. For each independent group of parameters, probability distributions are defined by maximum entropy principle, and the correlations, where these exist, are adapted to the deterministic calculation. To randomly sample the correlated variables, we use a Cholesky decomposition and a Maximin Latin Hypercube Sampling which ensures a good representativeness of the variation domain with a reduced number of samples.

Specifically, the ***geometry parameters*** and the ***water temperature*** are modelled by an uniform law.

By proportionality to the ***power distribution*** and the ***fission spectra***, the neutron source are perturbed. We only consider the uncertainty on the fission spectra associated with the prompt neutrons which are more likely to cause fast fission and to leak from the core, in comparison with delayed neutrons. To randomly sample the latter, we consider the covariances created by Berge et al. (2015) to describe the uncertainties on the Madland-Nix model, widely used in nuclear data libraries. The uncertainties on the source spatial distribution are defined from a covariance matrix representative of the spatial power measurements, and modelled by a standard deviation of 1% to 4% depending on the assembly position. The perturbations are finally carried out following an assembly-wise approximation, i.e. homogeneously in each pin of the same standard 17x17 UO_2 assembly.

To perturb the ***multigroup cross sections*** a calculation chain is implemented from the processing system GALILEE-1 (Coste-Delclaux et al., 2016), the NJOY code (MacFarlane, 2017) and the URANIE plateform. 343 covariance matrices (associated with the total and partial reactions of 25 isotopes) are reconstructed with the ERRORR module in coherence with the 19G-Mesh. They define the variance and the correlation of 6174 variables (343 reactions $\times$ 18 energy groups). We show that the covariance process can produce ill-conditioned matrices which make their Cholesky decomposition impossible. To deal with this issue, we propose an alternative method, based on the spectral decomposition, to simultaneously regularize these matrices and sample the random variables. We present the strategy to generate consistent perturbations between the redundant and partial cross sections. The pointwise cross sections of the

25 isotopes is then perturbed and propagated in the GROUPR procedure of NJOY. The resulting multigroup cross sections is combined in two common aggregate reactions used by APOLLO3®: the scattering and the absorption reactions.

The uncertainty related to the energy distribution of cross sections has already been propagated by many authors, but the impact of the ***angular distribution*** on the fast flux were never been evaluated (Vasiliev et al., 2018). To give a first estimation of its contribution, we assess the angular distribution uncertainty of the ^{56}Fe elastic reaction, provided by the JEFF-3.2 evaluation. The Legendre orders are then perturbed on the ENDF files directly before the NJOY multigroup processing.

Uncertainty quantification and sensitivity analysis of the fast neutron flux (Part II - Chapter V)

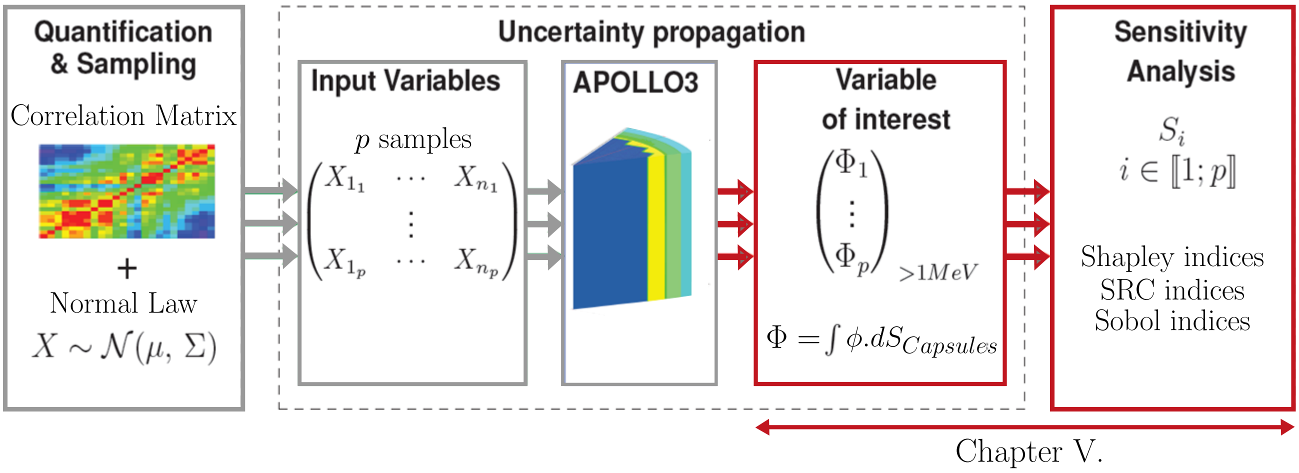

Figure 5: Uncertainty propagation scheme: in blue the specification of the deterministic calculation

Finally, the resulting perturbations are propagated in the deterministic scheme. In this context, we ***carry out a global sensitivity analysis to evaluate the impact of input uncertainties in terms of their relative contributions to the output uncertainty***. The objective of sensitivity analysis is to help to prioritise efforts for ***uncertainty reduction and data improvement***.

In order to consider the dependence among input data in the sensitivity analysis, we use the concept of the Shapley value, recently suggested by Owen et al. (2017) and Iooss et al. (2019). Especially, when a linear model describes the behaviour of the output, Shapley indices can be computed analytically (Broto et al., 2018). However, the main drawback of this method is its exponential time complexity. To avoid this issue and rank the contribution of each input, we propose to use in the case of high-dimensional input spaces an alternative method based on Johnson's indices (Johnson, 2000). The two methods are compared and give similar results. Johnson indices allow us to pursue a comprehensive sensitivity analysis and to show the importance to consider the correlation data to preserve the physical consistency of data during uncertainty propagation and sensitivity analysis.

This work is inspired by the one of Chao et al. (2008) and Bi (2012), who have provided reviews of the different methods to quantify the relative importance of variables on linear model involved respectively in public health studies and in sensory studies. The methods presented by Chao et al. (2008) and Bi (2012) are, mostly, ***not known in nuclear studies***.

In this way, we show the importance to consider the covariance matrices to propagate the input uncertainties, and analyse the contribution of each input on a physical model. We propose a global methodology to take into account the correlation data in the context of Total Monte Carlo.

Lastly, we present the results of the uncertainty propagation in the fast flux calculation and the sensitivity analysis of the relative contribution of each input on the output variance.***The final uncertainty on the fast flux Φ_{1MeV} at the vessel hot spot is in accordance with the Kodeli (2001)' work***.

Finally, the special feature of this thesis lies in the large number of uncertain parameters which are closely correlated with each other. More generally, we showed the importance to consider the covariance matrices to propagate the input uncertainties, and to analyze the contribution of each input on a physical model.

Bibliography

Berge, L. et al. (2015). Study on prompt fission neutron spectra and associated covariances for 235U(nth,f) and 239Pu(nth,f). *Physics Procedia*, 64:55–61.

Bi, J. (2012). A review od statistical methods for determination of relative importance of correlated predictors and identification of drivers of consumer liking. *Journal of Sensory Studies*, 27(2):87–101.

Broto, B. et al. (2018). Sensitivity indices for independent groups of variables. *MascotNum Annual Conference*.

Brun, E. et al. (2014). TRIPOLI-4®, CEA, EDF and areva reference monte carlo code. In *SNA+ MC 2013-Joint International Conference on Supercomputing in Nuclear Applications+ Monte Carlo*, page 06023. EDP Sciences.

Chao, Y.-C. et al. (2008). Quantifying the relative importance of predictors in multiple linear regression analyses for public health studies. *Journal of occupational and environmental hygiene*, 5(8):519–529.

Coste-Delclaux, M. et al. (2016). GALILEE-1: a validation and processing system for ENDF-6 and GND evaluations. In *EPJ Web of Conferences*, volume 111, page 06005. EDP Sciences.

Dupré, A. et al. (2015). Towards modelling and validation enhancements of the psi mcnpx fast neutron fluence computational scheme based on recent PWR experimental data. *Annals of Nuclear Energy*, 85:820–829.

Haghighat, A. et al. (1996). Uncertainties in transport theory pressure vessel neutron fluence calculations. *Transactions of the American Nuclear Society*, 74:140–142.

Hassler, L. A. et al. (1985). Babcock & wilcox reactor vessel surveillance service activities. pages 61–67.

Iooss, B. et al. (2019). Shapley effects for sensitivity analysis with correlated inputs: comparisons with sobol' indices, numerical estimation and applications. *IMT - Institut de Mathematiques de Toulouse, EDF R& D, submitted to Elsevier*.

Johnson, J. (2000). A heuristic method for estimating the relative weight of predictor variables in multiple regression. *Multivariate behavioral research*, 35(1):1–19.

Kam, F. et al. (1990). Neutron fluence calculations and uncertainty analysis. In *Proceedings*, page 179.

Kodeli, I. (2001). Multidimensional deterministic nuclear data sensitivty and uncertainty code system: Method and application. *Nuclear Science and Engineering*, 138(1):45–66.

Kodeli, I. et al. (1996). Assessment of uncertainties for PWR pressure vessel surveillance – french experience. *Transactions of the American Nuclear Society*, 74:142–144.

MacFarlane, R. E. (2017). The njoy nuclear data processing system, version 2012. Technical report, Los Alamos National Lab.(LANL), Los Alamos, NM (United States).

Margolin, B. Z. et al. (2005). Prediction of temperature dependence of fracture toughness as a function of neutron fluence for pressure-vessel steels by using the unified curve method. *Strength of materials*, 37(3):243–253.

Mosca, P. et al. (2011). An adaptative energy mesh constructor for multigroup library generation for transport codes. *Nuclear Science and Engineering*, 167(1):40–60.

Mosca, P. et al. (2018). MINARET, deterministic model of PWR fast fluence for uncertainty propagations with the code APOLLO3®. In *Reactor Dosimetry: 16th International Symposium*. ASTM International.

OECD/NEA (1997). Computing radiation dose to reactor pressure vessel and internals. Technical report, NEA/NSC/DOC (96) 5, 1997, OECD-NEA.

Owen, A. B. et al. (2017). On shapley value for measuring importance of dependent inputs. *SIAM/ASA Journal on Uncertainty Quantification*, 5(1):986–1002.

Remec, I. (1996). On the uncertainty of neutron transport calculations for reactor pressure vessel surveillance. *Transactions of the American Nuclear Society*, 74:144–145.

Smith, C. L. (1994). Uncertainty propagation using taylor series expansion and a spreadsheet. *Journal of the Idaho Academy of Science*, 30(2):93–105.

Steele, L. E. (1983). *Status of USA nuclear reactor pressure vessel surveillance for radiation effects*, volume 784. ASTM International.

Vasiliev, A. et al. (2018). On the importance of the neutron scattering angular distribution for the LWR fast neutron dosimetry. *PHYSOR*, 50.