



Article

Nuclear Data Uncertainty Propagation in Complex Fusion Geometries

Bor Kos ^{1,*}, Henrik Sjöstrand ², Ivan A. Kodeli ^{1,†} and JET Contributors [‡]

¹ Jožef Stefan Institute, Jamova Cesta 39, SI-1000 Ljubljana, Slovenia; ivo.kodel@ijs.si

² Department of Physics and Astronomy, Applied Nuclear Physics, Uppsala University, P.O. Box 516, 751 20 Uppsala, Sweden; henrik.sjostrand@physics.uu.se

* Correspondence: bor.kos@ijs.si

† Current address: Culham Centre for Fusion Energy, Abingdon OX14 3DB, UK.

‡ See the author list of E. Joffrin et al. 2019 Nucl. Fusion 59 112021.

Received: 18 September 2020; Accepted: 30 November 2020; Published: 2 December 2020



Abstract: The ASUSD program package was designed to automate and simplify the process of deterministic nuclear data sensitivity and uncertainty quantification. The program package couples Denovo, a discrete ordinate 3D transport solver, as part of ADVANTG and SUS3D, a deterministic first order perturbation theory based Sensitivity/Uncertainty code, using several auxiliary programs used for input data preparation and post processing. Because of the automation employed in ASUSD, it is useful for Sensitivity/Uncertainty analysis of complex fusion geometries. In this paper, ASUSD was used to quantify uncertainties in the JET KN2 irradiation position. The results were compared to previously obtained probabilistic-based uncertainties determined using TALYS-based random nuclear data samples and MCNP in a Total Monte Carlo computation scheme. Results of the two approaches, deterministic and probabilistic, to nuclear data uncertainty propagation are compared and discussed. ASUSD was also used to perform preliminary Sensitivity/Uncertainty (S/U) analyses of three JET3-NEXP streaming benchmark experimental positions (A1, A4 and A7).

Keywords: nuclear data; sensitivity/uncertainty; ASUSD; TMC; JET

1. Introduction

The JET3-NEXP streaming benchmark experiment [1,2] consists of thermoluminescent and activation foil measurements in the JET torus hall up to 40 m away from the plasma source, which are computationally supported using Monte Carlo, deterministic and hybrid transport simulations. The aim of the experiment is to provide experimental results and computational models suitable for benchmarking new nuclear data (ND) and transport codes in complex, realistic fusion geometries. In order to accurately represent the measured and simulated results, all uncertainties have to be rigorously determined.

When it comes to quantification of uncertainties in neutron transport simulations, usually only uncertainties due to model simplifications (geometry and materials) and uncertainties because of the method of transport (statistical uncertainties originating from the use of Monte Carlo methods or discretization uncertainties originating from the use of deterministic methods) used are determined. Uncertainties originating from ND are often neglected in the final estimation of the total uncertainty. This is partly due to the lack of reliable covariance information and partly due to the complexity of the computations needed to propagate covariance information through the transport simulation. Different methods can be used for nuclear data uncertainty propagation including probabilistic random sampling based methods, i.e., the Total Monte Carlo (TMC) methods and Generalised Perturbation Theory (GPT)-based codes. Both approaches have advantages and disadvantages. The major

disadvantage of TMC codes is the required computational time, while the major disadvantage of GPT codes is the time and user input needed to perform such analyses using currently available codes.

In this paper, a validation and application of a new GPT-based code package ASUSD (ADVANTG + SUS3D) is presented. ASUSD (previous versions known as SUS3DwD) aims to reduce the user input needed for ND Sensitivity/Uncertainty (S/U) analyses by coupling the S/U code SUS3D [3,4] with the hybrid transport code ADVANTG [5]. ASUSD utilizes ADVANTG’s ability to automatically prepare and execute Denovo [6] deterministic calculations based on an MCNP (Monte Carlo N-Particle stochastic transport code) [7] input file and a simple additional ADVANTG input file. The programs included in the ASUSD program package are described in detail and the ASUSD computational scheme is presented in the first part of the paper. In this work, ASUSD is used for neutron ND S/U analysis but, in principle, it could also be used for gamma ND S/U analysis.

For validation purposes, ASUSD results are compared to previously obtained TMC uncertainty results [8] for KN2 irradiation position measurements at the Joint European Torus (JET) in the second part of the paper. The TMC analysis was performed using random samples created using the TALYS [9] code and MCNP transport simulations. Additionally, the ASUSD code package was used to perform a preliminary sensitivity and uncertainty analysis of three experimental positions (A1, A4 and A7) of the JET3-NEXP streaming benchmark experiment. The results of the S/U analysis of the JET3-NEXP streaming benchmark experiment are given in the third part of the paper.

2. The ASUSD Program Package

The ASUSD program package workflow is visually presented in Figure 1. In the first step, multigroup cross-sections and covariance data are prepared with GLG20 [10]. This step can only be executed sometimes as the libraries are general purpose if there is no need to include self-shielding. The MCNP input file and the ADVANTG input file are needed for the next step—execution of ADVANTG and Denovo. After the Denovo simulation has finished, the post-processing programs for SUS3D input preparation are used: Geometry.py, Materials.py and Angular_moments.py. The automatically prepared SUS3D input file using Geometry.py and Materials.py is used to run SUS3D. Angular flux moment files, forward and adjoint, needed for determining sensitivity coefficients with SUS3D are prepared by Angular_moments.py based on angular flux results from Denovo. Using multigroup cross-sections and covariance information from GLG20, the sensitivities and uncertainties due to nuclear data are calculated using SUS3D. The final sensitivity results can be visualized by ViSS.py.

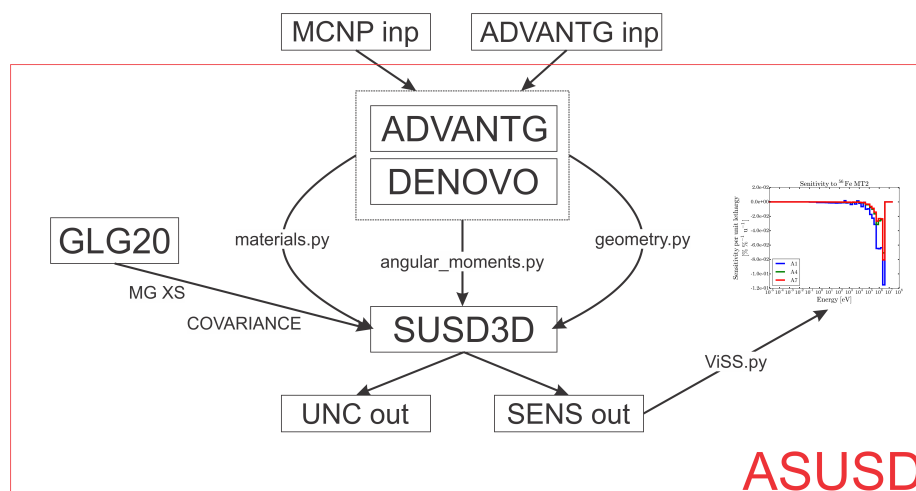


Figure 1. ASUSD program package workflow which includes Denovo as part of Automated VARIance reducTion Generator (ADVANTG), GLG20 for nuclear data (ND) processing, SUS3D for S/U analysis and several auxiliary programs.

User input is only needed in the initial step—the preparation of MCNP and ADVANTG input files. Defining an appropriate Cartesian mesh for ADVANTG is vital and can in some cases be time consuming [1]. The automated preparation of all SUSD3D input data needed for an S/U analysis allows for the analysis of complex shielding geometries such as full-scale fusion examples. i.e., KN2 irradiation position at JET and the JET3-NEXP streaming benchmark experiment. In the next few sections, individual programs from the ASUSD program package are briefly described.

2.1. SUSD3D

SUSD3D determines nuclear data sensitivity coefficients and uses them to calculate the variance in a detector response of interest by folding the sensitivity profiles with the cross-section covariance matrices [3]. The sensitivity coefficients are calculated based on the first-order perturbation theory [11]. The code execution is divided into three sequential parts which can be individually executed. In the first part—Overlay-1—SUSD3D reads and processes the forward and adjoint angular flux moments for the needs of the second step—Overlay-2—sensitivity profile calculation. In the third and final step—Overlay-3—the code folds the sensitivity profiles with the appropriate covariance information to calculate the final variance of interest.

2.2. ADVANTG

The Automated VARIance reducTION Generator (ADVANTG) [5] program was developed with the idea to automate and simplify the process of generating variance reduction parameters for continuous-energy Monte Carlo simulations of fixed-source neutron, photon, and coupled neutron–photon transport problems. ADVANTG also provides the ability to perform stand alone discrete ordinates Denovo calculations without the generation of variance reduction parameters. Denovo is a parallel (multi-core) deterministic discrete ordinates transport solver used to obtain 3-D solutions of the Boltzmann transport equation on a non-uniform Cartesian mesh.

In the initialization step, ADVANTG extracts the problem geometry, source information, tally information and material composition from a provided MCNP model. In the second step, the extracted information is used to automatically construct a Denovo compatible discretized representation of the original problem defined in the MCNP input file. In the third step, ADVANTG launches the Denovo solver to perform the forward and adjoint discrete ordinates transport calculation.

2.3. *Geometry.py, Material.py, Angular_moments.py and Viss.py*

Geometry.py, *Material.py*, *Angular_moments.py* and *ViSS.py* were developed to automate the process of preparing the input files needed by SUSD3D. They are written in Python 2.7 with dependencies on libraries included in the Anaconda 2.3.0 distribution specifically NumPy (ver. 1.14.5), H5py (ver. 2.5.0), Matplotlib (ver. 1.4.3) and SciPy (1.10). *Angular_moments.py* is used to prepare *rmflux* and *amflux* angular flux moment files needed in Overlay-1 of SUSD3D. Besides angular flux moment files, Overlay-1 requires geometry information, which is prepared by *Geometry.py*. *Material.py* reads the pure and mixed materials ray traced by ADVANTG and prepares all needed information for Overlay-2 and Overlay-3 of SUSD3D. *ViSS.py* (ViSualize SUSD3D Sensitivities) is used to prepare plots of the energy-dependent sensitivity profiles from the *fort.7* SUSD3D output file.

2.4. GLG20

The GLG20 [10] parallel nuclear data processing suite was initially developed by Charles R. Daily at ORNL and modified by the author of the paper for the needs of the ASUSD program package. Originally, the suite was used to prepare multigroup cross-sectional data for ADVANTG. Functionality to produce ACE format continuous energy data, multigroup cross-sectional data and covariance information for SUSD3D has been added. The functionality has been tested on simpler shielding benchmark experiments. The GLG20 processing suit prepares NJOY [12] input files for all nuclides included in an evaluated nuclear data library. The files are then used to process the nuclear data with

NJOY2016 on a linux machine parallel on as many cores as are available, speeding up the process of preparing multigroup ND.

3. JET KN2 S/U Analysis

Activation materials with well-known ND characteristics are routinely used to measure neutron flux or to provide information about the neutron spectrum. Such a system, KN2, is implemented in-vessel at JET in order to directly monitor the plasma without interference. Since these measurements are used for plasma power monitoring and calibration at JET, it is imperative to know all associated uncertainties. In previous work [8], a TMC approach for nuclear data uncertainty quantification was adopted. A total of 300 random ND samples were produced by TALYS for a number of key nuclides (^{52}Cr , $^{54,56}\text{Fe}$, $^{58,60}\text{Ni}$, $^{63,65}\text{Cu}$) and using MCNP transport simulations with the random samples, the uncertainty associated with nuclear data was determined from the distribution of the transport results. The TMC method was applied to several positions around KN2.

In this work, ASUSD was used to quantify the uncertainties because of the above-mentioned key nuclides (^{52}Cr , $^{54,56}\text{Fe}$, $^{58,60}\text{Ni}$, $^{63,65}\text{Cu}$) at two locations, above the activation foil stack (cell 417) and next to it, in the intermediate port (cell 395). Both locations are marked in Figure 2, which shows a cross-section of the MCNP JET model that includes a detailed KN2 model. The TENDL-2015 [9] nuclear data library was used for both uncertainty quantifications. The TENDL-2015 based ASUSD multigroup cross-sections prepared with GLG20 were non-self shielded and the ECCO-33 [13] energy group structure was used to collapse the continuous energy ND.

The results of the TALYS and ASUSD analysis are shown in Table 1. Uncertainties in the ^{115}In (n,n') $^{115\text{m}}\text{In}$ and ^{93}Nb ($n,2n$) $^{92\text{m}}\text{Nb}$ reaction rates and total neutron fluxes for the two different positions and plasma sources (Deuterium Deuterium (DD) and Deuterium Tritium (DT)) are given. Excellent agreement between the two approaches can be observed for the DD plasma source. The DT results vary significantly for some cases. This is most probably due to the coarsening of the 33 energy group structure at higher energies, whereas only five energy groups are between 19.64 MeV and 1.35 MeV (first six upper energy group boundaries of ECCO-33: 19.64 MeV, 10 MeV, 6.06 MeV, 3.68 MeV, 2.23 MeV and 1.35 MeV). In future work, a finer energy group structure needs to be used to assess the uncertainties associated with DT plasma sources. However, these results are encouraging and will be improved upon in future work.

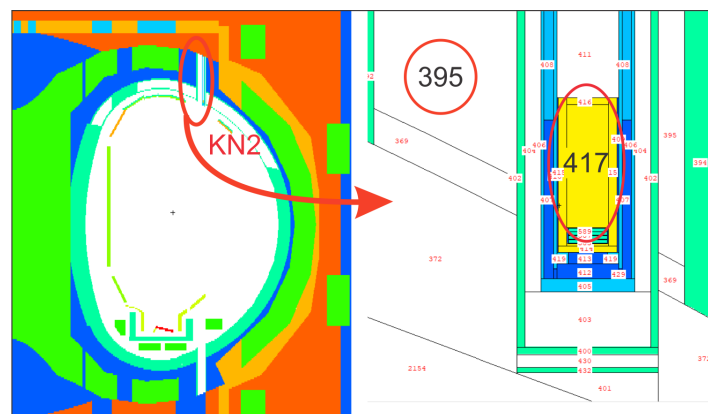


Figure 2. MCNP model of KN2 irradiation position at JET. Tokamak side view (left), close up of KN2 with the two analysed regions (right).

Table 1. Uncertainty in reaction rates and fluxes for two locations (417 and 395) in KN2 due to nuclear data uncertainty. Results from ASUSD and TALYS are compared.

		DT			DD			
		¹¹⁵ In (n,n')	^{115m} In	⁹³ Nb (n,2n) ^{92m} Nb	Flux	¹¹⁵ In (n,n')	^{115m} In	Flux
417	ASUSD	2.4%		0.6%	1.3%	0.9%		1.2%
	TALYS	3.2%		1.9%	2.8%	1.2%		0.9%
395	ASUSD	1.3%		2.1%	2.1%	1.5%		0.8%
	TALYS	4.5%		2.2%	3.3%	1.7%		1.1%

4. JET3-NEXP Streaming Benchmark Experiment S/U Analysis

All uncertainties connected to the JET3-NEXP streaming experiment [1,2] must be determined in order to assure benchmark quality data. The experimental locations in two distinct regions of the JET tokamak hall South West Labyrinth (A1–A8, B8) and South East Chimney (B1–B7) are shown in Figure 3. Since the adoption of the ADVANTG hybrid methodology in recent years, the statistical uncertainty of the simulations for all locations are negligible (<3%). The experimental part is being re-done during the current 2019 DD campaign and will be continued during the TT and DT campaigns in 2020 and 2021. The uncertainties of the experimental campaign will be re-evaluated. For the sake of completeness of the benchmark experiment, nuclear data uncertainties need to be assessed. Considering the complexity, dimensions of the model and resulting transport simulation times, TMC methods for ND uncertainty propagation are simply inadequate because of the computational time needed for such an analysis. The recent advancements in ASUSD, automated input preparation and coupling with the parallel capabilities of Denovo, are perfectly suited to analyze transport problems of this magnitude.

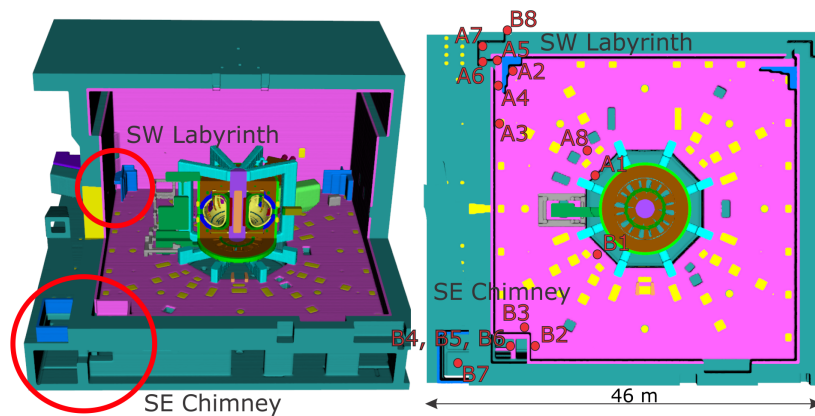


Figure 3. MCNP model of the JET3-NEXP streaming benchmark experiment with designated experimental positions.

ASUSD was used to perform preliminary sensitivity profile calculations for three measurement positions: A7 (farthest from plasma), A4 and A1 (closest to plasma). The sensitivities (percentile change of the detector response per 1% change of the cross-section), shown in Figure 4, of the total neutron fluence with regard to the elastic scattering cross-section (MT2) for ⁹Be, ¹H, ¹⁶O and ⁵⁶Fe were found to be the largest contributors to the total sensitivity. These are preliminary results which are promising but need further analysis. Namely, the geometrical mesh needs to be refined and a finer energy group structure for the multigroup cross-sections needs to be used. Since this is a streaming-dominated problem, a higher order or a specialized, e.g., forward peaking, quadrature set needs to be adopted. The corresponding total nuclear data uncertainties are in the order of 5% to 10% using both JEFF-3.3 [14] and TENDL-2015 [9] covariance information.

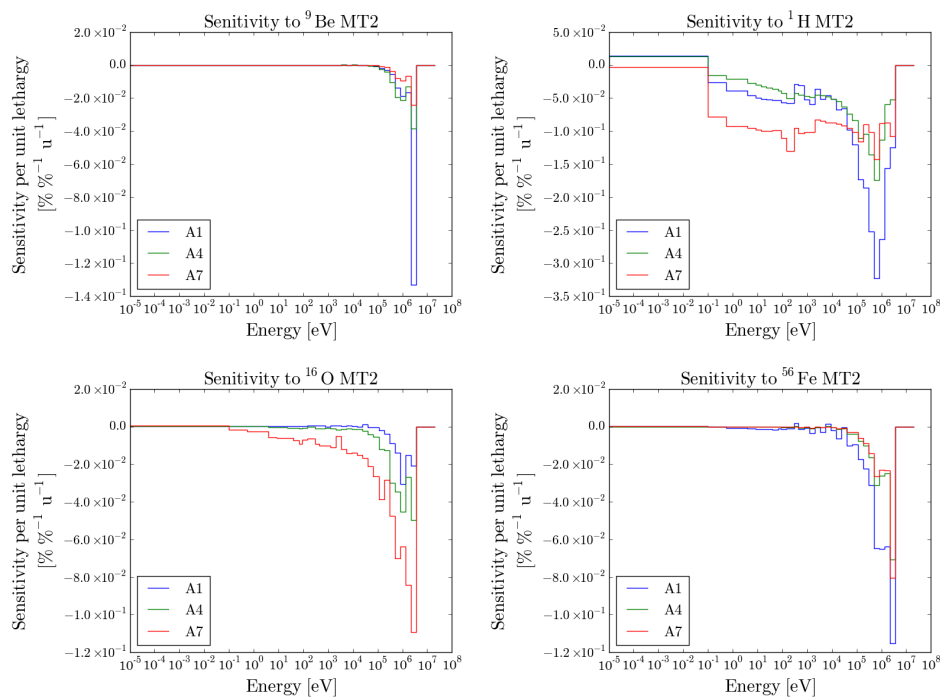


Figure 4. Sensitivities of the neutron fluence to the elastic scattering cross section (MT2) of ^9Be , ^1H , ^{16}O and ^{56}Fe at JET3-NEXP experimental locations A1, A4 and A7.

5. Conclusions

The ASUSD program package, which couples the SUSD3D first-order perturbation nuclear data sensitivity/uncertainty code with Denovo as part of ADVANTG, has been used to quantify uncertainties due to nuclear data in complex fusion geometries. The program package was developed with the idea to simplify the process of performing ND S/U analysis by automating as many steps as possible of such an analysis. This automation has opened the door for performing ND S/U analysis on complex systems, which was previously impossible with deterministic-based codes and is too computationally expensive to perform with probabilistic approaches to ND uncertainty quantification, i.e., Total Monte Carlo.

In the first part of the paper, the ASUSD computational scheme was presented alongside a detailed description of the individual components of the program package. ASUSD was used to quantify the uncertainties due to ND at two locations in the KN2 irradiation facility of JET. The results were compared to TMC results performed with TALYS random samples and MCNP. Excellent agreement between the two approaches for the DD plasma source was observed, while some discrepancies are noticeable in the case of the DT source. The most probable cause for the discrepancies is the coarsening of the energy discretization of the ASUSD deterministic calculation. The effect will be investigated in future work. ASUSD was also used to perform a preliminary ND S/U analysis of the JET3-NEXP streaming experiment. Preliminary results for the sensitivity profiles are encouraging but further work is needed to validate and evaluate the results. The resulting uncertainties are in the order of 5% to 10% using both JEFF-3.3 and TENDL-2015 covariance information.

Author Contributions: Conceptualization, I.A.K.; methodology, B.K., I.A.K.; software, B.K., I.A.K.; validation, B.K., H.S.; formal analysis, B.K.; investigation, B.K., H.S.; resources, I.A.K.; data curation, B.K.; writing—original draft preparation, B.K.; writing—review and editing, B.K., I.A.K., H.S., J.C.; visualization, B.K.; supervision, I.A.K.; project administration, B.K., J.C.; funding acquisition, I.A.K., J.C. All authors have read and agreed to the published version of the manuscript.

Funding: The authors acknowledge the financial support from the Slovenian Research Agency (research core funding No. P2-0073 and project for training young researchers No. 1000-15-0106). This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research

and training programme 2014–2018 and 2019–2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Acknowledgments: The authors would specifically like to thank Scott W. Mosher and Charles R. Daily (ORNL) for their help and insight in the process of developing ASUSD.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Kos, B.; Mosher, S.W.; Kodeli, I.A.; Grove, R.E.; Naish, J.; Obryk, B.; Villari, R.; Batistoni, P. Application of ADVANTG to the JET3-NEXP streaming benchmark experiment. *Fusion Eng. Des.* **2019**, *147*, 111252. [[CrossRef](#)]
2. Kos, B.; Vasilopoulou, T.; Mosher, S.W.; Kodeli, I.A.; Grove, R.E.; Naish, J.; Obryk, B.; Villari, R.; Batistoni, P. Analysis of DD, TT and DT Neutron Streaming Experiments with the ADVANTG Code. In Proceedings of the EPJ Web of Conferences, Portorož, Slovenia, 17–21 June 2019; EDP Sciences: Les Ulis, France, 2020; Volume 225, p. 02003.
3. Kodeli, I. Multidimensional Deterministic Nuclear Data Sensitivity and Uncertainty Code System: Method and Application. *Nucl. Sci. Eng.* **2001**, *138*, 45–66. [[CrossRef](#)]
4. Kodeli, I.; Slavic, S. SUSD3D Computer Code as Part of the XSUN-2017 Windows Interface Environment for Deterministic Radiation Transport and Cross Section Sensitivity-Uncertainty Analysis. *Sci. Technol. Nucl. Install.* **2017**. [[CrossRef](#)]
5. Mosher, S.W. *ADVANTG-An Automated Variance Reduction Parameter Generator*; ORNL/TM-2013/416 Rev. 1; Oak Ridge National laboratory: Oak Ridge, TN, USA, 2015.
6. Evans, T.M.; Stafford, A.S.; Slaybaugh, R.N.; Clarno, K.T. Denovo: A New Three-Dimensional Parallel Discrete Ordinates Code in SCALE. *Nucl. Technol.* **2010**, *171*, 171–200. [[CrossRef](#)]
7. X-5 Monte Carlo Team. *MCNP- A General Monte Carlo N. Particle Transport Code, Version 5*; LA-UR-03-1987; Los Alamos National Laboratory: Los Alamos, NM, USA, 2004.
8. Sjöstrand, H.; Conroy, S.; Helgesson, P.; Hernandez, S.A.; Koning, A.; Pomp, S.; Rochman, D. Propagation of nuclear data uncertainties for fusion power measurements. In Proceedings of the EPJ Web of Conferences, Bruges, Belgium, 11–16 September 2016; EDP Sciences: Les Ulis, France, 2017; Volume 146, p. 02034.
9. Koning, A.J.; Rochman, D. Modern Nuclear Data Evaluation with the TALYS Code System. *Nucl. Data Sheets* **2012**, *113*, 2841–2934. [[CrossRef](#)]
10. Daily, C.R. (ORNL, Oak Ridge, TN, USA); Kos, B. (JSI, Ljubljana, Slovenia). Personal email communication, 2018.
11. Williams, M.L. Perturbation theory for nuclear reactor analysis. In *CRC Handbook of Nuclear Reactors Calculations*; CRC Press: Boca Raton, FL, USA, 1986.
12. MacFarlane, R.; Muir, D.; Boicourt, R.; Kahler, A. *The NJOY Nuclear Data Processing System, Version 2012*; Tech. Rep. LA-UR-12-27079; LANL: Los Alamos, NM, USA, 2012.
13. Sartori, E. *Standard Energy Group Structures of Cross Section Libraries for Reactor Shielding, Reactor Cell and Fusion Neutronics Applications: VITAMIN-J, ECCO-33, ECCO-2000 and XMAS*; JEF/DOC-315, Revision 3; NEA Data Bank: Gif-sur-Yvette, France, 1990.
14. Plompen, A.J.; Cabellos, O.; De Saint Jean, C.; Fleming, M.; Algora, A.; Angelone, M.; Archier, P.; Bauge, E.; Bersillon, O.; Blokhin, A.; et al. The joint evaluated fission and fusion nuclear data library, JEFF-3.3. *Eur. Phys. J.* **2020**, *56*, 1–108. [[CrossRef](#)]

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



© 2020 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).