

# XSUN-2022/SUSD3D n/ $\gamma$ sensitivity-uncertainty code package with recent JEFF-3.3 and ENDF/B-VIII.0 covariance data

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**Abstract.** A new version of the XSUN-2022 computer code package is under preparation to be released through NEA Data Bank which includes the latest updates of the SUSD3D sensitivity/uncertainty (S/U) code and the corresponding cross section and covariance matrix libraries based on the JEFF-3.3, ENDF/B-VIII.0 and FENDL-3.2 evaluations. The XSUN code package is a user-computer interface environment, written in Xbase++ ® and using Compiler 1.90.331 and Alaska 32-Bit Linker, for user-friendly pre- and post-processing of the input and output data for a complete and self-consistent set of deterministic codes. The flowchart integrates the codes TRANSX, PARTISN, and SUSD3D, all available from the OECD/NEA Data Bank and RSICC. The codes are used for the preparation of multigroup nuclear cross-section, neutron and gamma transport calculations for criticality and shielding calculations and nuclear data sensitivity and uncertainty calculations, respectively. XSUN-2022 is the 3<sup>rd</sup> released version, after XSUN-2013 and -2017.

## 1 Introduction

The development of the XSUN (Cross-section Sensitivity and Uncertainty) [1,2] Windows interface environment started in 2012 in order to facilitate the use of a suite of deterministic particle transport and nuclear data sensitivity and uncertainty codes. Deterministic codes are at present less frequently used than Monte Carlo (M/C) due to inherent approximations and complexity of their use. However, due to their fast algorithms, deterministic codes are still attractive and useful in many applications, be it for fast radiation transport providing a complete flux distribution, for the cross-section sensitivity and uncertainty analyses, deep penetration problems and validation of Monte Carlo codes and methods. XSUN package therefore integrates a complete set of deterministic tools for transport and S/U analysis, including nuclear data.

The XSUN-2013 and -2017 [1,2] code systems were released respectively in spring 2014 and in 2017 through OECD Nuclear Energy Agency Data Bank (Package-ID NEA-1882) and RSICC (Code Number CCC-825). The packages can be obtained from the two data centers, by contacting the RSICC or NEA Data Bank Computer Program Services.

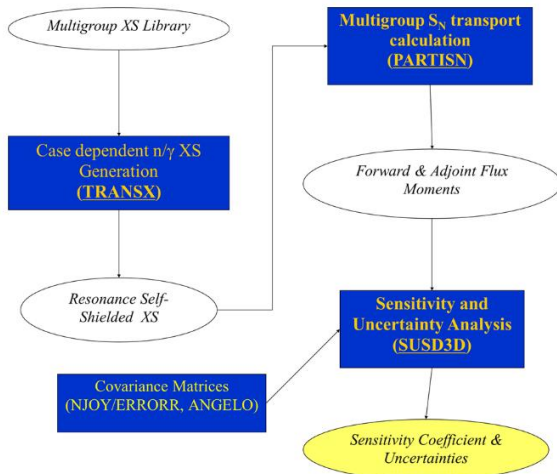
The package is a user-computer interface environment for Windows and integrating the codes TRANSX [3], PARTISN [4] and SUSD3D [5-7] (see Fig. 1), all available from the OECD/NEA Data Bank and RSICC. The system was developed to assist the users in the preparation of input cards, rapid modification and execution of this complete chain of codes for S/U analysis. XSUN-2017 package included, among others, the following nuclear data:

- Nuclear cross section data library in the ECCO 33-neutron energy group structure in MATXS format. The library includes data for 109 isotopes at different temperatures (300 K, 550 K, 600 K, 650 K, 700 K, 800 K) and for different self-shielding factors. The data were produced using the NJOY-99 code and are based mostly on the ENDF/B-VII.1 nuclear data evaluation (with a few minor data from the -VII.0 release).
- Multi-group covariance matrix libraries in the ECCO 33 energy groups based on the ENDF/B-VII.1 [8], JENDL-4.0 [9] and SCALE-6.0m [10] evaluations. The matrices were processed using the NJOY-99 [11] and the ANGELO [12] codes.

An updated version of the code system is under final testing and will be released through the NEA data Bank. Modifications and improvements were introduced in the TRANSX-2.15 code used to produce cross sections compatible with many discrete-ordinates ( $S_N$ ) transport codes (such as PARTISN), in the SUSD3D nuclear data S/U code and in the transport cross sections and covariance matrices used by the above codes. The 33-group nuclear data libraries and the material coverage were found to be insufficient for fusion applications, which therefore required extending the transport cross section and covariance matrix libraries both in terms of fine-group and material coverage. Multigroup cross-section and covariance matrix libraries for S/U analysis in 33- and 175-group structure were prepared based on JEFF-3.3 [13], ENDF/B-VIII.0 [14] and FENDL-3.2a [15] evaluations. Processing of covariance matrices included detailed verification and validation of their mathematical properties (positive definiteness, rank, etc.). The package was applied to shielding benchmark

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analysis to test the new features and cross section evaluations.



**Fig. 1.** XSUN computer code environment.

## 2 SUSD3D perturbation code

SUSD3D [5-7] is a multi-dimensional nuclear cross-section sensitivity and uncertainty code suitable for complex one-, two- and three-dimensional transport studies. Sensitivity coefficients and standard deviation in the calculated detector responses or design parameters of interest ( $k_{\text{eff}}$ ,  $\beta_{\text{eff}}$ , reaction rates) due to input cross section data and their uncertainties are calculated based on the first-order generalised perturbation theory. Several types of uncertainties can be considered, i.e. those due to: (1) neutron multi-group cross sections, (2) energy-dependent response functions, (3) secondary angular distribution (SAD) or secondary energy distribution (SED) uncertainties.

The particle transport calculations are done externally using the existing codes such as DOORS [16], DANTSYS [17], PARTISN [4], and the information on the direct and adjoint fluxes is passed to SUSD3D via the neutron flux moment files. Extensions to ADVANTG/DENOVO and DRAGON codes were also developed in the scope of PhD theses [18, 19]. At present, the XSUN package supports only the interface with the PARTISN code. Interface with the DANTSYS system can be done easily by the user, while coupling the SUSD3D/DOORS codes requires manual preparation of the DOORS and parts of the SUSD3D input cards by the user. The sensitivity profiles are folded with the cross-section covariance matrices to determine the variance in an integral response of interest. The input deck is prepared automatically by the XSUN system taking the geometry description from the PARTISN input and the isotopic cross-section composition as defined in the TRANSX input as well as the self-shielding factors calculated from the latter code. 1-, 2-, and 3-dimensional test cases are included in the package.

The development of SUSD3D started in the early 1990-ies in the scope of the French pressure vessel surveillance programme and the fusion projects of the

European Commission. Examples of the use include criticality ( $k_{\text{eff}}$ ,  $\beta_{\text{eff}}$ ) and shielding (fusion, fission, such as PV surveillance, FNG benchmark pre- and post-analyses). k-ratio derivation sensitivity method [20-21] was proposed and implemented in 2011 to calculate S/U in the effective delayed neutron fraction –  $\beta_{\text{eff}}$ . Both the unconstrained and constrained sensitivity methods [22, 23] can be used to propagate the uncertainties in fission spectra. The latter was implemented in 2008 after demonstrating the equivalence between the zero-sum correction and constrained sensitivity.

Several improvements were introduced in the SUSD3D code since the last XSUN-2017 version, such as:

- SUSD3D code and XSUN utility were updated to be able to treat of up to 440 nuclides as included in the new extended cross section libraries. Moreover, the cross section and covariance file treatment in SUSD3D was modified allowing a considerable acceleration of calculations, by up to several order of magnitudes in case of using ~200 fine energy group nuclear data libraries and many nuclides. A parameter “libx” also allows a larger flexibility of the use of nuclear data.
- Extension of the sensitivity analysis to gamma-ray quantities such as gamma flux and heating. Gamma relevant nuclear data (MF=16, MF=23, MF=26) can be processed allowing S/U for coupled n/γ problems.
- Normalisation of the sensitivities and uncertainties is done internally in the code if requested by activating the option “resp=-1”.
- Many minor corrections and modifications (e.g. printed output, plot files etc.). Top 10 reactions and isotopes causing the highest sensitivity and uncertainty are listed in the SUSD3D output. SAD S/U analysis can make use of the P<sub>1</sub> (mu-bar, MT251) data processed by NJOY-2016 or higher P<sub>N</sub> (N=1 to 5) terms processed by the ERRORR34 [24] code.

SUSD3D code now covers the sensitivity to different cross-section types: MF=3 (neutron gain term), MF=6 (neutron loss term), MF=2 (direct term-response function), MF=4 (SAD), MF=5 (SED), MF16 (gamma production), MF23, MF26 (gamma loss and gain terms).

Likewise, the TRANSX code was modified to account for the increased number of energy groups and cross section matrices.

## 3 Multi-group nuclear data in XSUN-2022

Nuclear data libraries included in the XSUN-2013 and -2017 packages were mostly based on ENDF/B-VII.1 and including a limited number of nuclear materials. The XSUN-2022 package will include data from recent cross section evaluations in both VITAMIN-J fine and broad ECCO group structures, with larger number of nuclides (up to 440):

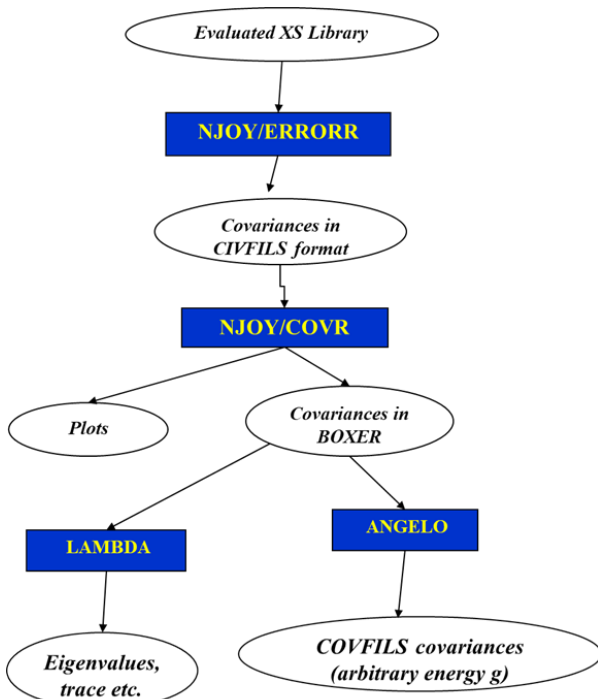
- JEFF-3.3 in ECCO 33 and VITAMIN-J 175 neutron group structures
- ENDF/B-VIII.0 (ECCO 33 and VITAMIN-J 175)

- FENDL-3.2 (211 neutron/42 gamma groups); the library is suitable for coupled neutron/gamma S/U analysis.

Older nuclear data, in particular covariances from ENDF/B-VII.1, JENDL-4.0u, COMMARA-2, SCALE-6.0 and IRDFF for a limited number of isotopes will be also included. An extension to the new JENDL-5 evaluation is planned.

### Cross section covariance data

An important factor limiting the use of S/U analysis is the availability and the quality of cross-section covariance data. The availability of covariance matrix data in several recent cross section evaluations, such as ENDF/B-VIII.0, JEFF-3.3, JENDL-4/5 etc., has been considerably improved which demonstrates an increased awareness of the importance of these data among the nuclear community.



**Fig. 2.** Covariance matrix processing and verification scheme. Covariance matrices in the Covfils format processed by NJOY and ANGELO can be used in the SUS3D code.

Although covariance matrices cannot be measured directly, and are governed by probability theory and statistics, with the inherent difficulty of estimating systematic uncertainties, they must still satisfy some basic mathematical properties such as positive semi-definiteness. The correct implementation of covariance matrix methodology in nuclear data evaluation can be therefore judged only indirectly by mathematical verification of the matrices and by the consistency, in a statistical sense, between the observed C/E values and the calculated nuclear data uncertainties.

The complete sets of recent JEFF-3.3, ENDF/B-VIII.0 and FENDL-3 covariance matrix evaluations

were processed and partly verified for mathematical properties to be included in the XSUN-2022 package.

Several computer codes were used for the processing, plotting, mathematical verification and identification of ill-defined covariance data. The computational flow-chart is shown in Figure 2 including the following codes:

- NJOY-99, -2016 and -21 codes [11], ERRORR and COVR modules,
- LAMBDA [12] code: verification of mathematical properties of covariance matrices (eigenvalues, trace, correlation coefficients exceeding  $\pm 1$ ),
- ANGELO-2 [12] code: interpolation of covariance matrices to user defined energy group structure; only file-MF33 covariance matrices can be treated using flat flux weighting.

The LAMBDA code was used to identify the matrices containing negative eigenvalues and correlation coefficients exceeding the range between -1 and +1. Verification of mathematical properties was done for the standard covariance (MF=33). Large majority of the processed matrices, in particular those relative to the important isotopes, were found to be mathematically correct, with a few exceptions listed below. Processing problems were also encountered for a few nuclides (in brackets cases with small negative eigenvalues, possibly due to numeric):

#### JEFF-3.3:

- covariance data were processed for 447 available isotopes; Processing difficulties were observed for the following nuclides:  $^{232}\text{Pa}$ ,  $^{238}\text{Np}$ ,  $^{236}\text{Np}$ ,  $^{148}\text{Nd}$ ,  $^{95}\text{Nb}$ ,  $^{92,94,96,97,98,100}\text{Mo}$ ,  $^{153}\text{Eu}$ ;
- number of nuclides with negative eigenvalues: 22 (using the present BOXER format), 18 (with an increased computational precision in BOXER code<sup>†</sup>):  $^{192}\text{Ir}$ ,  $^{103}\text{Rh}$ ,  $^{185}\text{W}$ ,  $^{88}\text{Y}$ , ( $^{190,195}\text{Pt}$ ,  $^{170}\text{Er}$ ).

#### ENDF/B-VIII.0:

- covariance data for 244 available isotopes were processed. Processing difficulties:  $^{154,159}\text{Dy}$ ,  $^{78}\text{Kr}$ ,  $^{93}\text{Nb}$ ,  $^{184,186,187,188,189,190,192}\text{Os}$ ,  $^{70}\text{Zn}$ ,  $^{192}\text{Pt}$ ,  $^{54}\text{Fe}$ ;
- number of nuclides with negative eigenvalues: 5:  $^{192}\text{Ir}$ , ( $^{190,195}\text{Pt}$ ,  $^{239}\text{Pu}$ ).

#### FENDL-3.1:

- covariance data for 58 isotopes;
- FENDL-3.1d: number of nuclides with negative eigenvalues: 2:  $^{58}\text{Ni}$ ,  $^{50}\text{Ti}$ .

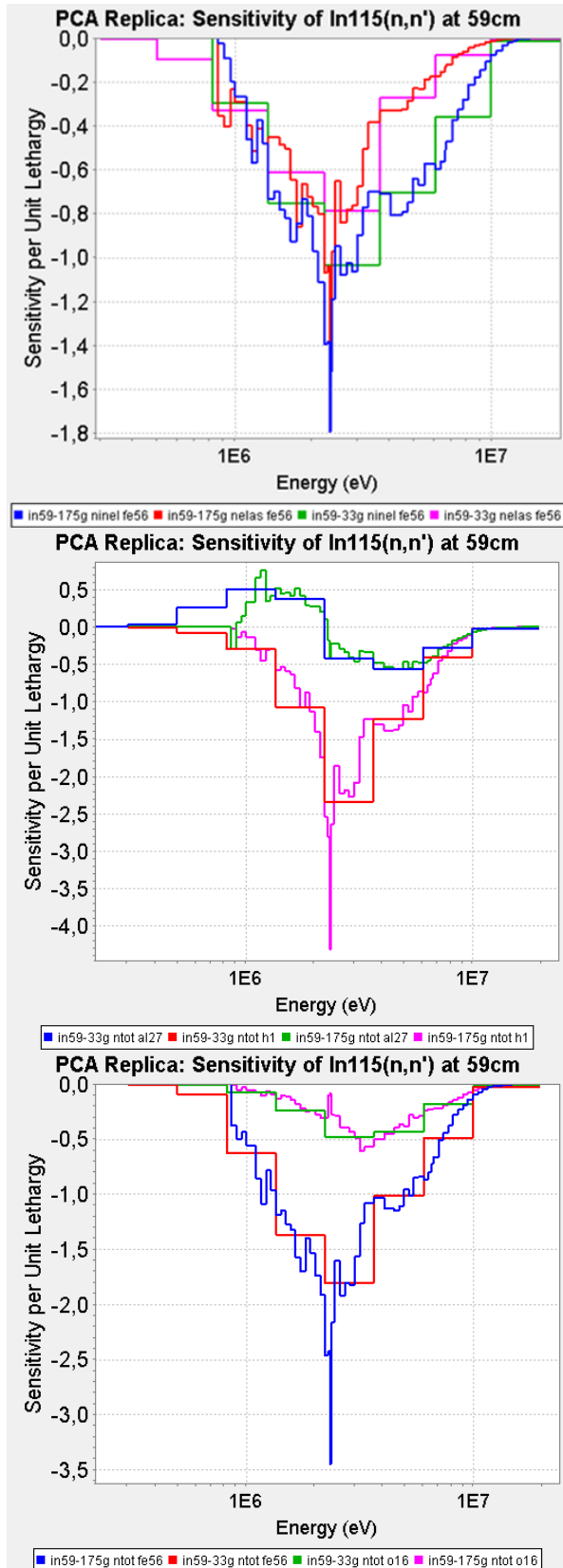
On the other hand, large correlation coefficients exceeding  $\pm 1.0$  by a factor of up to  $10^8$  were observed for threshold (but not only) reactions in large number of files processed using the NJOY code, which could be (partly) due to processing problems. A similar problem was already observed in the past, e.g. in [25] it was concluded on a "...possible problem in ERRORR in case of covariance matrix processing for threshold reactions. ERRORR seems to unphysically reduce the standard deviation in the user energy group containing the threshold when the corresponding lower energy

<sup>†</sup> In the COVR module the data precision of the BOXER format is controlled by the "nvf" parameter. It can be increased by changing the following two parameters:

- change nvf=7 to nvf=8: format '(11f7.4)' is replaced by '(10f8.5)'

- change nvf=10 to nvf=13: format '(1p8e10.3)' is replaced by '(1p6e13.6)'. The above modifications were found to resolve some (smaller) negative eigenvalues resulting from numeric problems.

group boundary extends below the threshold energy (averaging problem?).” Further studies are necessary to clarify the origin of the problems.



**Fig. 3.** Comparison of the sensitivity profiles for the reaction rates measured in the ASPIS PCA Replica benchmark. The sensitivities were obtained using the 175- and 33- energy group nuclear data.

Several integral experiments, including critical, kinetics and shielding, were studied using the SUSD3D code to verify if the matrices provide statistically credible, and quantitatively accurate nuclear data uncertainties. Shielding cases include fusion relevant (FNG) and fission reactor (ASPIS) benchmarks. Differences between various covariance matrix evaluations, both recent and older, were evaluated, which allows to judge on the progress made. An example of the analysis of the ASPIS PCA Replica benchmark experiment taken from the SINBAD database [26] - [28] is presented in Fig. 3 and Table 1 comparing the S/U analyses performed using the fine 175- and the broad 33-group nuclear data. For this fission reactor problem, a reasonable agreement is observed for most reactions. However, cases of larger differences were observed in fusion benchmark analyses, in particular for some threshold reactions such as  $(n,2n)$ ,  $(n,\alpha)$ , where the 33-group structure may be too coarse.

**Table 1.** Uncertainties in calculated  $^{115}\text{In}(n,n')$  detector reaction rates due to Fe, H, O and Al cross-section uncertainties

$^{115}\text{In}(n,n')$	Sensitivity (%/%)		Uncertainty (%)			
			33 group		175 group	
	33 group	175 group	JEFF3.3	ENDF/B-VIII	JEFF3.3	ENDF/B-VIII
$^{56}\text{Fe}(n,n')$	-1.58	-1.58	4.3	7.3	4.4	6.4
$^{56}\text{Fe}(n,n)$	-1.10	-1.03	6.0	3.1	5.8	3.0
$^1\text{H}(n,n)$	-2.74	-2.40	5.0	1.0	4.5	0.9
$^{16}\text{O}(n,n)$	-0.67	-0.58	0.8	0.8	0.7	0.7
$^{27}\text{Al}(n,n')$	-0.48	-0.46	2.1	3.6	1.9	3.4
$^{27}\text{Al}(n,n)$	0.45	0.26	3.5	1.2	3.0	0.8
<b>TOTAL</b>			9.7	9.0	9.1	8.0

In spite of the progress achieved recently, some unresolved problems and gaps persist, such as for example

- Lack of covariances relative to gamma nuclear data,
- availability and processing of covariances for the secondary angular and energy neutron distributions (SAD/SED, MF=34,35) are limited, e.g. only  $P_1$  terms in MF34 can be typically processed,
- limited information is available for some specific applications, e.g. uncertainties and correlations in delayed nu-bars (MF=31), correlations among isotopes and materials, etc.

## 4 Examples of analyses

The SUSD3D code was used since the early 1990-ies in different applications ranging from the pressure vessel surveillance, fusion and fission benchmark analysis for the nuclear data validation and guiding the design, reactor criticality ( $k_{\text{eff}}$ ) and kinetics ( $\beta_{\text{eff}}$ ) studies etc. Recent updates allow to extend the sensitivity and uncertainty analysis to gamma quantities such as gamma flux and heating. SUSD3D was recently used to determine the nuclear data uncertainty in material activation of irradiated nuclear steels.

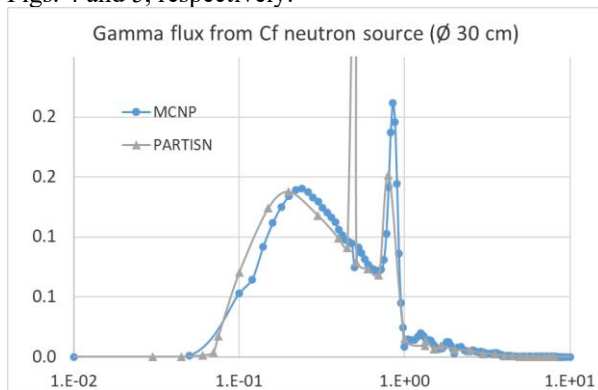


#### 4.1 Gamma-ray sensitivity of KFK $\gamma$ -ray leakage benchmark

Gamma-ray leakage spectra from a set of three iron spheres of diameters 25, 30 and 35 cm with a  $^{252}\text{Cf}$  neutron source in the centre were measured in Karlsruhe in 1977. Absolute gamma-rays in the energy range between 300 keV and 3 MeV were measured with the Si(Li) Compton spectrometer positioned on the outer surface of the iron shells. The measurement uncertainties were around 10-20%.

SINBAD evaluation of KFK-1977 measured gamma spectra from Ø25, 30 and 35 cm Fe spheres using bare  $^{252}\text{Cf}$ (s.f.) source was prepared by Stanislav Simakov within the WPEC SG47 activities, including detailed descriptions of facility, methods and final numerical results with uncertainties and MCNP model.

Comparison between the gamma spectra calculated using the PARTISN and MCNP codes and the first results of the gamma flux S/U analysis are presented in Figs. 4 and 5, respectively.



**Fig. 4.** Comparison between the gamma spectra calculated using the MCNP and PARTISN codes.

#### 4.2 Material activation analysis

Nuclear data uncertainty in material activation of irradiated nuclear steels in structural fusion reactor components were studied to estimate the safety margin to be added to the calculated mean time to reach low-level waste (LLW) disposal limit in order to account for uncertainties.

The S/U analysis on dominant radio-nuclide production rates provides uncertainty of the individual nuclide generation. The safety margin ( $\Delta t$ ) can be obtained from:

$$A_{lim} = \sum_i N_{0i} \left(1 + \frac{\Delta R}{R}\right) \lambda_i e^{-\lambda_i(t+\Delta t)}$$

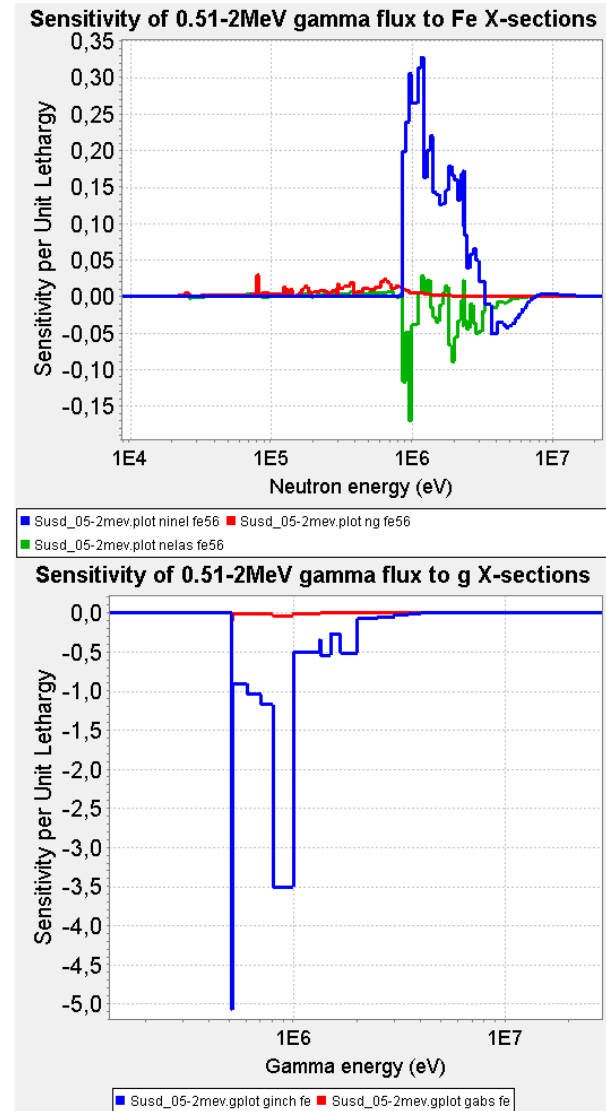
where  $A_{lim}$  refers to the specified activity level limit for LLW disposal, and  $R$  is the reaction rate for the isotope production.

In the case of a single dominant radioisotope ( $i=1$ ) the uncertainty in time to reach LLW limit can be obtained analytically from:

$$\Delta t = \frac{\ln\left(1 + \frac{\Delta R}{R}\right)}{\lambda}$$

In the general case of several dominant nuclides ( $i>1$ ) the solution is obtained by iteration.

A study simulating the neutron activation of the reduced activation ferritic/martensitic (RAFM) steels Eurofer and F82H, and two traditional steels - G91 and SS 316L(N) IG in a model of a spherical reactor geometry based on the helium-cooled pebble bed design is presented in [29].



**Fig. 5.** Sensitivity of gamma flux between 0.51 - 2 MeV at radius 16.3 - 16.8cm to neutron inelastic, elastic and capture (above) and gamma incoherent and absorption (below) cross sections (results for Ø 30 cm sphere)

#### 4.3 XSUN-2022 test cases to be provided

Test cases included in the XSUN-2022 package cover both critical and shielding applications:

- Fast critical assembly (SNEAK-7B): 1D, 2D and 3D models for the transport, sensitivity and uncertainty analysis. Nuclear data from the JEFF-3.3, ENDF/B-VIII.0 in VITAMIN-J 175- and ECCO 33-group structures are used,
- 1D shielding case: S/U of material activation in a typical fusion environment with 14 MeV neutron source involving large number of materials.

## 5 Conclusions

Deterministic codes are less frequently used today comparing to M/C due to inherent approximations and complexity of their use. However, several advantages such as lower CPU time and convenience of powerful and fast S/U analyses, still make them attractive. XSUN, an integrated environment for running a suite of deterministic codes, was developed to facilitate their use for transport and S/U analysis. The package includes the SUS3D nuclear data S/U code which was used for the analysis of fission and fusion reactor design and safety parameters since the early 1990-ies.

Several improvements and new features were introduced in the new XSUN-2022 package and the code SUS3D:

- SUS3D code was extended to S/U of gamma related quantities (gamma flux, heating, etc.)
- Nuclear data from JEFF-3.3, ENDF/B-VIII.0 in 175- and 33-groups and FENDL-3.2 for 211 neutron/42-gamma groups are included, covering large number of materials (~440).
- Considerably faster treatment of cross section and covariance data files in SUS3D to allow faster calculations for problems with large number of nuclides and energy groups.
- Many improvements and modifications in SUS3D algorithm, such as automatic normalization for fixed-source problems, extended SAD S/U analyses, printing top 10 sensitive reactions and nuclides, and several other improvements and modifications.

Mathematical verification of the JEFF-3.3, ENDF/B-VIII.0 and FENDL-3.1 covariance matrices revealed a few negative matrices (< 2-4%), but large number of inconsistent correlation coefficients. Most negative eigenvalues are small in magnitude, and it is unlikely they would have major impact on the uncertainty calculations. However, some larger negative eigenvalues may pose problems for nuclear data adjustment studies and should be corrected before their use in data assimilation studies. For several nuclides negative eigenvalues of the same magnitude were observed in several different nuclear data evaluations, suggesting a probable common origin of these covariance data. This was the case even though the corresponding nuclear cross sections differed.

On the other hand, many covariance matrices processed by the NJOY code were found to contain correlation coefficients exceeding  $\pm 1.0$ . This was in particular the case for the threshold reactions in the vicinity of the threshold, but not only.

New versions of SUS3D and XSUN-2022 are under preparation and will be available from NEA Data Bank.

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