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Sensitivity analysis for a 14 MeV neutron benchmark using Monte Carlo and deterministic computational methods

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Abstract

A sensitivity analysis has been performed for a 14 MeV neutron benchmark on an iron assembly, typical for a fusion neutronic integral experiment. Probabilistic and deterministic computational methods have been used in the sensitivity calculations with the main objective to check and validate the novel Monte Carlo technique for calculating point detector sensitivities. Good agreement has been achieved between the Monte Carlo and the deterministic approaches for the individual calculated sensitivity profiles, the uncertainties and the neutron flux spectra. It is thus concluded that the Monte Carlo technique for calculating point detector sensitivities and related uncertainties as being implemented in MCSEN, a local version of the MCNP4A code with the capability to calculate point detector sensitivities, is well qualified for sensitivity and uncertainty analyses of integral experiments. © 2004 Elsevier B.V. All rights reserved.

Keywords: 14 MeV neutron benchmark; Monte Carlo technique; Computational methods

1. Introduction

Sensitivity and uncertainty analysis is a powerful means to assess uncertainties of nuclear responses in neutron transport calculations and track down these uncertainties to specific nuclides, reaction crosssections and energy ranges. When applied to the analysis of integral experiments, it enables the assessment of the calculational accuracy and provides information for improving the cross-section data evaluations.

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The differential operator method developed originally by Hall [1] is a suitable method to calculate sensitivities with the Monte Carlo technique. Based on this method, an algorithm has been developed at the Hebrew University of Jerusalem [2] for calculating point detector sensitivities which has been implemented into a local update to the Los Alamos Monte Carlo code MCNP4A [3]. The point detector method is best suited for analysing integral benchmark experiments when leakage spectra are measured by detectors that are located far from the irradiated material assembly. Experiments of this kind are in frequent use for testing and validating fusion nuclear data evaluations, as well as for assessing their uncertainty margins. In

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these experiments, material assemblies are irradiated with 14 MeV (d, t) neutrons and the neutron leakage flux spectrum is measured by means of experimental techniques such as the time-of-flight (TOF) method.

This work is devoted to the sensitivity analysis of a 14 MeV neutron benchmark on an iron assembly typical for a fusion neutronic integral experiment. Probabilistic and deterministic computational methods have been used in the sensitivity calculations with the main objective to check and validate the novel Monte Carlo technique for calculating point detector sensitivities. There follows a short description of the benchmark problem, the computational procedures for both the deterministic and the Monte Carlo calculation of point detector sensitivities as well as a detailed presentation and discussion of the sensitivity results obtained in this analysis.

2. Benchmark problem

A simple benchmark, typical for fusion neutronic integral experiments, has been defined for the sensitivity analysis. It consists of a spherical iron shell assembly with a 14 MeV neutron point source in the centre. The source is assumed to be isotropic, with a flat energy distribution between 13.84 and 14.19 MeV. The benchmark task is to calculate first the neutron flux spectra at a detector location of 6.8 m, second the sensitivity profiles for neutron flux integrals with energy boundaries 0.09804, 1.003, 4.966, 7.408, 10.0, 13.84, 14.19 MeV and, on this basis, the related uncertainties due to the uncertainties of the underlying cross-section data. Two different iron assembly configurations are considered, one with a wall thickness of 7.5 cm (4.5 cm inner and 12 cm outer radius) where single or few neutron collisions take place only, and one with a wall thickness of 28 cm (2 cm inner and 30 cm outer radius) to take into account transport phenomena involving multiple neutron collisions. The benchmark problem has been adapted from an integral 14 MeV neutron transmission experiment on spherical iron shell assemblies with measurement of the neutron leakage flux spectrum by the TOF method [4]. This enables the comparison, in an additional step, of the calculated neutron spectra with the measured ones. Nuclear data are taken from the European fusion file EFF-3.1 for ⁵⁶Fe [5] and FENDL-1 [6] for the other iron isotopes. The data were processed with the NJOY code [7] in pointwise energy representation for use with MCNP-calculations and in the 175 VITAMIN-J group structure for use with the discrete ordinates (S_N) calculations.

3. Methodological approach

The methodological approach is as follows. In the first step, neutron flux spectra are calculated and compared at the location of the detector. In the Monte Carlo calculation, the point detector estimator (MCNP tally 5) is used. In the S_N -transport calculations using spherical geometry, the neutron flux spectra are calculated at the spatial mesh of the detector location. Two different discrete ordinates codes for one-dimensional geometry, ANISN [8] and ONEDANT [9], are used in these calculations.

The second step is devoted to the calculation of the sensitivities of the specified neutron flux integrals. In the Monte Carlo approach, this requires one calculational run including the related point detector sensitivity estimator in the proper energy bin segmentation. With the deterministic approach, this step requires a direct and several adjoint ANISN or ONEDANT calculations followed by SUSD [10] calculations to provide the sensitivity profiles. Two different versions of the SUSD code are employed: SUSD-fusion neutron source (FNS) developed by Kosako et al. [11] at JAERI, and SUSD3D developed by Kodeli [12]. Another approach used in addition in this work to calculate sensitivities is based on the direct calculation of the neutron flux integrals with cross-sections modified for specific reactions and energy ranges.

The next step consists of calculating the uncertainties, using the calculated sensitivity profiles and the covariance matrices processed again with the NJOY code. The final step is devoted to a detailed comparison of the sensitivity profiles, the integrated sensitivities and uncertainties for all considered reactions.

4. Computational techniques

4.1. Monte Carlo point detector sensitivities

At the Hebrew University of Jerusalem, an algorithm has been developed for calculating point detector sensitivities based on the differential operator method. The algorithm has been implemented into MCSEN, a local update to the Los Alamos Monte Carlo code MCNP4A. With this approach, point detector sensitivities for all responses can be calculated in one single MCSEN run which is just an extension of the Monte Carlo run for calculating the responses. Sensitivity profiles can be calculated in an arbitrary group structure and subsequently used for calculating the uncertainties when folded with the covariance matrices of the underlying nuclear cross-sections. The Monte Carlo method thus provides an alternative way to determine sensitivities, avoiding some inherent drawbacks of the S_N method: complex geometries can be handled without severe constraints, there are no numerical convergence problems, and, in addition, the energy dependence of the cross-sections can be accurately described by using the pointwise energy representation. On the other hand, a larger calculational effort in terms of computer times is in general required for achieving a sufficient statistical accuracy.

4.2. Discrete ordinates sensitivity/uncertainty calculations

The deterministic approach in sensitivity and uncertainty analysis has been widely used in the past. The sensitivities of specified nuclear responses to the involved cross-section data are calculated on the basis of perturbation theory using direct and adjoint fluxes provided by discrete ordinates calculations. Several such codes were developed. Usually the direct and adjoint transport calculations are performed first using the existing discrete ordinates codes, and the fluxes are then passed to the sensitivity/uncertainty code via interface files. This makes the analysis guite flexible. On the other hand, the whole calculation requires several steps. Discrete ordinates-based methods are in general CPU time efficient although approximations are often required to describe very complex geometries and some expertise is needed for the multi-group data preparation.

Based on the direct and adjoint neutron fluxes, sensitivity and uncertainty calculations are performed with the following variants of the SUSD code.

4.2.1. SUSD3D

The SUSD3D sensitivity and uncertainty code package is suitable for one-, two-, and three-dimensional cross-section sensitivity and uncertainty analysis. The direct and adjoint fluxes generated by the transport codes of the DOORS (ANISN, DORT, TORT), or the DANTSYS (ONEDANT, TWODANT, THREE-DANT) packages can be used to construct the sensitivity profiles. To reduce the computer space requirements the method is based on the flux moments instead of the angular fluxes. The sensitivity and uncertainty of an integral quantity with respect to the neutron and gamma multi-group cross-sections, response functions, as well as the secondary energy and angular distributions (SAD/SED) can be studied. The procedure to calculate the SAD uncertainties was modified, but the SED treatment is basically the same as in the original SUSD code. The system is fully compatible with the ENDF-6 format.

4.2.2. SUSD-FNS

The SUSD-FNS sensitivity and uncertainty code package was developed from the SUSD code code independently at (FNS, JAERI). SUSD-FNS can use forward and adjoint flux interface files from the ANISN, DORT and TORT code series to calculate the sensitivity profiles. The sensitivity and uncertainty of SAD can also be evaluated. NJOY-SD, a modified NJOY-version is used for processing the nuclear data in ENDF-6 format for SUSD-FNS. NJOY-SD generates self-shielded group cross-sections with one single background cross-section s_0 for the whole energy range. A self-shielded ⁵⁶Fe group data set corresponding to $s_0 = 0.2$ was used for the iron sphere benchmark.

5. Inter-comparison of benchmark results

5.1. Neutron flux spectra

The calculated neutron leakage flux spectra are inter-compared in Figs. 1 and 2 for the iron spherical shells with 7.5 and the 28 cm wall thickness, respectively. With few exceptions the group fluxes calculated by MCNP with continuous energy crosssections and by ANISN/ONEDANT with multi-group cross-section data agree within a standard deviation.



Fig. 1. Comparison of neutron leakage spectra calculated for the 7.5 cm thick iron shell assembly.



Fig. 2. Comparison of neutron leakage spectra calculated for the 28 cm thick iron shell assembly.

Table 1						
Relative sensitivities in %/%	(percent per per	cent change) for	r neutron flux	integrals of the	e 7.5 cm thick	shell assembly

	Energy range (MeV)							
	E < 0.09804	0.09804-1.003	1.003-4.966	4.966-7.408	7.408-10.0	10.0-13.84	<i>E</i> > 13.84	Total
MT = 2								
MCSEN	0.247	0.099	-0.071	-0.051	-0.027	0.467	-0.125	0.003
SUSD-FNS	0.270	0.109	-0.094	-0.054	-0.035	0.439	-0.121	0.0
SUSD3D	0.303	0.113	-0.096	-0.051	-0.034	0.464	-0.124	0.002
MT = 16								
MCSEN	0.631	0.526	0.208	-0.128	-0.126	-0.232	-0.233	0.139
SUSD-FNS	0.625	0.524	0.215	-0.127	-0.123	-0.240	-0.237	0.141
SUSD3D	0.624	0.522	0.211	-0.127	-0.126	-0.233	-0.236	0.142
MT = 28								
MCSEN	0.032	0.027	0.006	-0.016	-0.016	-0.027	-0.030	-0.001
SUSD-FNS	0.033	0.028	0.006	-0.016	-0.016	-0.028	-0.030	-0.001
SUSD3D	0.033	0.028	0.005	-0.016	-0.016	-0.027	-0.030	-0.001
MT = 51								
MCSEN	0.237	0.196	-0.236	-0.040	-0.021	0.160	-0.042	0.001
SUSD-FNS	0.273	0.205	-0.254	-0.041	-0.019	0.170	-0.042	0.0
SUSD3D	0.271	0.205	-0.256	-0.040	-0.019	0.170	-0.042	0.001
MT = 52 - 82								
MCSEN	0.035	0.063	-0.039	-0.348	0.169	0.034	-0.027	0
SUSD-FNS	0.038	0.065	-0.039	-0.356	0.168	0.036	-0.027	0
SUSD3D	0.039	0.065	-0.040	-0.349	0.161	0.035	-0.027	0.000
MT = 91								
MCSEN	0.008	0.114	0.385	0.377	-0.075	-0.547	-0.388	-0.013
SUSD-FNS	0.013	0.112	0.377	0.391	-0.054	-0.546	-0.395	-0.015
SUSD3D	0.016	0.114	0.377	0.377	-0.071	-0.550	-0.394	-0.014
MT = 103								
MCSEN	-0.029	-0.029	-0.033	-0.045	-0.060	-0.079	-0.065	-0.045
SUSD-FNS	-0.029	-0.029	-0.033	-0.045	-0.060	-0.080	-0.066	-0.046
SUSD3D	-0.029	-0.029	-0.033	-0.045	-0.060	-0.080	-0.066	-0.045
MT = 107								
MCSEN	-0.010	-0.010	-0.011	-0.015	-0.020	-0.027	-0.023	-0.016
SUSD-FNS	-0.010	-0.010	-0.011	-0.015	-0.020	-0.028	-0.024	-0.016
SUSD3D	-0.010	-0.010	-0.011	-0.015	-0.020	-0.027	-0.023	-0.016
Total								
MCSEN	1.143	0.982	0.206	-0.269	-0.179	-0.256	-0.937	0.063
SUSD-FNS	1.205	0.999	0.163	-0.265	-0.163	-0.282	-0.947	0.058
SUSD3D	1.238	1.004	0.153	-0.268	-0.187	-0.253	-0.947	0.065

 $\overline{SUSD-FNS} = ANISN/SUSD-FNS$, SUSD3D = ONEDANT/SUSD3D; MT = 2: elastic scattering, MT = 16: (n, 2n) reaction, MT = 28 (n, np) reaction; MT = 51-91: inelastic scattering to discrete excitation levels and to the continuum; MT = 103: (n, p). MT = 107: (n, a).

Table 2						
Relative sensitivities in %/%	(percent per percent)	change for neutron	flux integrals o	of the 28 cm	thick shell	assembly

	Energy range (MeV)							
	E < 0.09804	0.09804-1.003	1.003-4.966	4.966-7.408	7.408-10.0	10.0-13.84	<i>E</i> > 13.84	Total
MT = 2								
MCSEN	0.739	0.001	-0.643	-0.356	-0.346	0.308	-0.556	-0.012
SUSD-FNS	0.731	0.003	-0.785	-0.383	-0.304	0.226	-0.497	-0.0225
SUSD-3D	0.862	-0.003	-0.794	-0.382	-0.303	0.253	-0.513	-0.011
ANISN	-	_	-0.671	-0.385	-0.309	0.230	-0.521	-0.005
MT = 16								
MCSEN	0.345	0.259	-0.046	-0.455	-0.440	-0.788	-0.878	0.196
SUSD-FNS	0.332	0.253	-0.053	-0.475	-0.456	-0.813	-0.891	0.194
SUSD3D	0.333	0.257	-0.056	-0.472	-0.454	-0.797	-0.893	0.198
MT = 28								
MCSEN	0.008	0.002	-0.024	-0.056	-0.055	-0.090	-0.113	-0.004
SUSD-FNS	0.007	0.002	-0.025	-0.059	-0.057	-0.069	-0.111	-0.004
SUSD3D	0.008	0.002	-0.025	-0.059	-0.057	-0.091	-0.115	-0.003
MT = 51								
MCSEN	0.284	0.102	-0.918	-0.157	-0.095	0.077	-0.157	-0.003
SUSD-FNS	0.325	0.100	-1.026	-0.157	-0.098	0.102	-0.159	-0.004
SUSD3D	0.320	0.101	-1.040	-0.158	-0.098	0.102	-0.160	-0.001
MT = 52 - 82								
MCSEN	0.034	0.025	-0.161	-0.971	-0.009	-0.047	-0.1	-0.003
SUSD-FNS	0.024	0.024	-0.167	-0.969	-0.024	-0.041	-0.103	-0.002
SUSD3D	0.026	0.024	-0.170	-0.975	-0.026	-0.041	-0.102	-0.002
MT = 91								
MCSEN	-0.028	0.009	0.005	-0.735	-1.615	-1.849	-1.466	-0.049
SUSD-FNS	-0.028	0.002	-0.018	-0.750	-1.615	-1.628	-1.859	-0.053
SUSD3D	-0.023	0.006	-0.017	-0.760	-1.648	-1.888	-1.491	-0.049
ANISN	-0.020	0.007	-0.020	-0.769	-1.659	-1.896	-1.500	-0.050
MT = 103								
MCSEN	-0.063	-0.068	-0.097	-0.162	-0.204	-0.269	-0.246	-0.077
SUSD-FNS	-0.064	-0.068	-0.100	-0.166	-0.208	-0.272	-0.257	-0.077
SUSD3D	-0.064	-0.068	-0.100	-0.166	-0.209	-0.274	-0.250	-0.077
MT = 107								
MCSEN	-0.022	-0.024	-0.034	-0.054	-0.067	-0.092	-0.087	-0.027
SUSD-FNS	-0.023	-0.024	-0.035	-0.055	-0.068	-0.091	-0.090	-0.027
SUSD3D	-0.022	-0.024	-0.035	-0.056	-0.069	-0.094	-0.089	-0.027
Total								
MCSEN	1.248	0.290	-1.929	-2.955	-2.841	-2.764	-3.620	0.003
SUSD-FNS	1.255	0.277	-2.220	-3.025	-2.854	-2.864	-3.605	-0.013
SUSD3D	1.389	0.280	-2.251	-3.037	-2.869	-2.848	-3.630	0.007

SUSD-FNS = ANISN/SUSD-FNS, SUSD3D = ONEDANT/SUSD3D, ANISN = direct calculation with modified cross-sections; MT = 2: elastic scattering, MT = 16: (n, 2n) reaction, MT = 28: (n, np) reaction, MT = 51-91: inelastic scattering to discrete excitation levels and the continuum, MT = 103: (n, p). MT = 107: (n, a). Thus, it is concluded that both the deterministic and the probabilistic approaches are well suited to properly describe neutron problems of the considered kind. Note, that the same underlying cross-section when com

the probabilistic approaches are well suited to properly describe neutron problems of the considered kind. Note, that the same underlying cross-section data have been used here in a very different way. In general, differences may arise through the processing of the data (which happens very frequently) and the computational procedure (due to inherent numerical approximations) for describing neutron transport.

5.2. Neutron flux sensitivities

Sensitivities to cross-section changes of ⁵⁶Fe have been calculated for the neutron flux integrals at the detector location with energy boundaries as given above. Tables 1 and 2 show the relative sensitivities when integrated over the specified energy range in terms of percentage change in the leakage flux at the indicated energy range per percentage change of the cross-section data in the whole energy range as calculated by MCSEN, ANISN/SUSD-FNS and ONEDANT/SUSD3D.

When comparing the results for the calculated sensitivities, it is revealed that there is a very good agreement between the Monte Carlo and the deterministic approaches for both the thin and the thick-spherical shells. The calculated sensitivities were also tested against a direct calculation with modified cross-section data for few specified reactions. Checks have been performed for elastic scattering and continuum-inelastic scattering reactions by changing the related cross-sections by 1%. These are displayed in Table 2. The resulting sensitivities, based on ANISN-calculations with the modified cross-section data, agree again with the sensitivities calculated by MCSEN, ANISN/SUSD-FNS and ONEDANT/SUSD3D. It is thus concluded that the Monte Carlo technique for calculating point detector sensitivities implemented in MCSEN, our local



Fig. 3. Sensitivity profiles of the leakage flux above 13.84 MeV from the 28 cm thick spherical shell.

version of MCNP4A, is well qualified for sensitivity and uncertainty analyses of integral experiments.

As for the sensitivities of the neutron flux themselves, it is revealed that for both the thin and the thick iron spherical shell the total flux is rather insensitive to changes of the cross-section data. This is due to the fact that the elastic and inelastic scattering sensitivities of the leakage above and below several mega electron volts neutron energy are negatively correlated. Neutrons with higher energies are down scattered by elastic and inelastic scattering collisions and thereby removed from the high energy part of the spectrum (negative sensitivity with a maximum in the source energy range). These neutrons appear directly or through multiple collisions, dependent on the penetration depth, in the low energy part of the spectrum (positive sensitivity with a maximum below 0.01 MeV neutron energy). Naturally, this effect is more pronounced for the 28 cm thick shell than it is for the 7.5 cm thick one. Similar behaviour is observed for the (n, 2n) reaction, except that the overall sensitivity is of course positive. Major contributors to the negative sensitivities in the source energy range (E > 13.84 MeV) are the (n, 2n) and the inelastic scattering (MT = 51 to 91) reactions. Likewise, these reactions form the main contribution to the positive sensitivity in the lower part of the spectrum. Elastic scattering removes neutrons from the source energy range; the related sensitivity is rather low for the small shell thickness but significant for the thick one. In the energy range below the source peak, the in-scattering dominates the out-scattering resulting in a positive sensitivity for elastic scattering in the interval 10-13.84 MeV. The sensitivities to the reactions like (n, γ) , (n, p), (n, d),(n, a) are of course negative at all energies. As shown in Tables 1 and 2, the total flux is most sensitive to the (n, 2n)and (n, p) reactions, and in some extent to the (n, α) reaction and continuum inelastic scattering. More insight is provided by investigating the sensitivity



Fig. 4. Sensitivity profiles of the leakage flux between 10.0 and 13.84 MeV from the 28 cm thick spherical shell.

profiles which give the energy dependent sensitivity of a specified response to a given nuclear reaction as function of the cross-section energy. Sensitivity profiles, which are also required for calculating the uncertainties, have been calculated in the VITAMIN-J 175-group structure. Figs. 3–7 show the profiles as provided by MCSEN and ANISN/SUSD-FNS for the 28 cm thick spherical shell. As for the integrated sensitivities, there is an overall good agreement for the sensitivity profiles calculated by MCSEN and ANISN/SUSD-FNS except for minor deviations in the source energy group (E > 13.84 MeV) in the case of elastic scattering.

5.3. Uncertainties

Uncertainties of the calculated neutron flux integrals due to uncertainties of the cross-section data have been assessed on the basis of the EFF-3.1 ⁵⁶Fe covariance data processed with NJOY by making use of the sensitivity profiles provided in the VITAMIN-J 175 neutron group structure. The agreement of the sensitivities as calculated by the different computational procedures provides a sound basis for a reliable assessment of the uncertainties. Differences in the calculated uncertainties, if any, may be easily traced down to differences in the calculated sensitivity profiles.



Fig. 5. Sensitivity profiles of the leakage flux between 7.408 and 10.0 MeV from the 28 cm thick spherical shell.



Fig. 6. Sensitivity profiles of the leakage flux between 4.966 and 7.408 MeV from the 28 cm thick spherical shell.

Table 3	
Uncertainties (%) of neutron flux integrals as calculated with ⁵⁶ Fe EFF-3.1 covariance data for the 7.5 cm thick iron shell	assembly

Flux energy E (MeV)	E<0.09804	0.09804-1.003	1.003-4.966	4.966-7.408	7.408–10.0	10.0-13.84	<i>E</i> > 13.84	Total
MCSEN SUSD3D	2.47 2.46	1.90 1.90	1.18 1.18	4.64 4.76	4.77 4.64	2.63 2.67	1.20 1.22	0.48 0.49
SUSD-FNS	2.41	1.90	1.17	4.00	3.15	2.62	1.22	0.49

The calculated uncertainties are displayed in Tables 3 and 4 for the 7.5 and 28 cm thick iron spherical shells. Again there is a good agreement between the Monte Carlo and the discrete ordinates-based calculations. As for the magnitude of the calculated uncertainties, the EFF-3.1 evaluation provide a largely improved uncertainty data as compared to previous evaluations. It has to be recalled; however, that in this approach we only take account of uncertainties of the excitation function. Uncertainties of secondary

Table 4

Uncertainties (%) of neutron flux integrals as calculated with ⁵⁶Fe EFF-3.1 covariance data for the 28 cm thick iron shell assembly

Flux energy E (MeV)	E < 0.09804	0.09804-1.003	1.003-4.966	4.966-7.408	7.408–10.0	10.0-13.84	<i>E</i> > 13.84	Total
MCSEN	3.64	1.00	1.43	12.11	7.46	5.73	4.35	0.72
SUSD3D SUSD-FNS	4.10 3.60	1.04 0.99	1.59 1.54	12.38 9.94	7.45 5.76	5.74 5.68	4.54 4.53	0.72 0.74



Fig. 7. Sensitivity profiles of the leakage flux between 1.003 and 4.966 MeV from the 28 cm thick spherical shell.

angular and energy distributions are not taken into account, although they may dominate the calculated uncertainties in the case of a multiple collision problem (e.g. the 28 cm spherical assembly). It remains an outstanding task to add to MCSEN the capability for describing the uncertainties of the secondary distributions.

6. Conclusions

A detailed sensitivity analysis has been performed for a 14 MeV neutron benchmark on an iron assembly, typical for a fusion neutronic integral experiment. Probabilistic and deterministic computational methods have been used in the sensitivity calculations with the main objective to check and validate the novel Monte Carlo technique for calculating point detector sensitivities. Good agreement has been achieved between the Monte Carlo and the deterministic approaches. This applies for the individual sensitivity profiles and uncertainties and the neutron flux spectra as well. In addition, the calculated sensitivities were shown to be consistent with the results of direct transport calculations using cross-sections that were changed by a specified percentage for selected reactions in selected energy ranges. It is thus concluded that the Monte Carlo technique for calculating point detector sensitivities and related uncertainties as implemented in MCSEN, our local version of MCNP4A, is well qualified for sensitivity and uncertainty analyses of integral experiments. In addition to the well established deterministic approaches, an independent and complementary method is thus available.

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