The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
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BENCHMARK CALCULATIONS OF SENSITIVITIES TO SECONDARIES' ANGULAR DISTRIBUTIONS

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ABSTRACT

A novel algorithm, based on the differential operator approach, for Monte Carlo calculation of sensitivities to secondaries' angular distributions has recently been developed. It has been implemented in a local version of the MCNP Monte-Carlo code. The quantity calculated is the sensitivity of a response such as the neutron leakage flux to possible changes in Legendre moments of the angular distribution of the neutrons scattered by a given reaction.

In the current work, this method, and its implementation, has been validated through the analysis of a fusion-relevant benchmark on an iron spherical shell assembly with a 14 MeV neutron source in the centre. The sensitivities of the neutron leakage flux to the angular distribution of the elastic scattering by ^{56}Fe have been calculated with the Monte Carlo algorithm as well as with the well-known sensitivity algorithm that uses the direct and adjoint fluxes, which are calculated using the discrete ordinates method. Additional estimates of sensitivities were obtained by calculations that were performed – both with Monte-Carlo or discrete ordinates methods – using ^{56}Fe cross-sections having a selectively perturbed elastic-scattering angular distribution. The various methods yielded consistent sensitivities. Thus, the Monte-Carlo method for calculation of sensitivities to secondaries' angular distributions, and its implementation, has been validated.

***Key Words*: cross section sensitivity and uncertainty analysis, Monte Carlo, discrete ordinates, angular distribution**

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 cross-sections and energy ranges. When applied to the analysis of integral experiments, it enables to assess the calculational accuracy and to provide information for improving the cross-section data evaluations. The Monte Carlo method is the most suitable computational technique for particle transport simulations in fusion technology applications. It allows a very flexible geometry representation such that the device can be modeled in full 3D geometry very close to reality. Cross sections can be used in a continuous energy representation as given in the nuclear data file. The accuracy of the calculation is only affected by the statistical uncertainty of the calculation itself and the uncertainties of the underlying nuclear cross section data. A dedicated approach is required, however, to enable the calculation of sensitivities and uncertainties on the basis of Monte Carlo calculations.

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 had been previously developed [2] and implemented in a local version of the Los Alamos Monte Carlo code MCNP4C [3], called MCSEN, for calculating point detector sensitivities to material parameters such as cross-sections and number densities. The point detector method is best suited for analysing integral benchmark experiments when leakage spectra are measured by detectors located far from the irradiated material assembly [4]. 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 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.

The method has been recently extended to enable also the calculation of sensitivities to secondary angular distributions [5]. In particular this is important for fusion applications where the neutron transport is strongly anisotropic and thus is affected to a large extend by the angular distribution of the secondaries.

This paper deals with the testing and validation of the Monte Carlo approach for calculating sensitivities to secondaries' angular distributions. This is achieved by means of deterministic and direct comparison calculations for a fusion-relevant benchmark on an iron spherical shell assembly with a 14 MeV neutron source in the centre.

2. SENSITIVITY AND UNCERTAINTY ANALYSIS

2.1. Sensitivity to Secondaries' Angular Distributions by Monte Carlo Methods

A method to calculate by Monte Carlo techniques sensitivities to secondaries' angular distributions (SAD) is described in Ref. [5]. When a neutron enters a collision, it can be absorbed, or one or more neutrons can exit from the collision. The angular distribution of these secondary neutrons can have an influence on the response to be calculated with Monte Carlo methods ("tally" in MCNP parlance). The method to calculate sensitivities to SAD is based on the differential operator approach, and it gives the algorithm to obtain the sensitivity to the Legendre moments of the distribution. For a given isotope and reaction, the SAD, f(μ,E), is developed into a Legendre series as function of the scattering angle cosine μ and of the incident energy E:

$$f(\mu, E) = \sum_{l=0}^{\infty} \frac{(2l+1)}{2} f_l(E) P_l(\mu) \tag{1}$$

Of course, due to normalization, for all E: $f_0(E) = 1$.

The Monte Carlo sensitivity method allows the calculation of the (absolute) sensitivity of the response ϕ to the l-th Legendre moment:

$$\frac{\partial \phi}{\partial f_l(E)} = \frac{\partial \phi}{\partial f_l(E) / f_0(E)} \tag{2}$$

In a Monte-Carlo simulation of particle transport, many paths are sampled: A path refers to the entire history of a neutron, from its appearance in the source, through collisions and zone-boundary crossings, to its effective elimination, by leakage or by explicit capture. The paths are sampled, path i having probability P_i.

According to the algorithm developed in Ref. [5], s_{xi}, the sensitivity of the response ϕ_i – sampled on path i – to the secondaries' angular distribution is defined by the partial derivative with respect to the Legendre coefficients $f_{x,l}(E)$ (for isotope/reaction x at energy E):

$$s_{xi} = \frac{\partial(\varphi_i P_i)}{\partial f_{x,l}(E)} = \sum_{j=1}^{J_i} \frac{\partial}{\partial f_{x,l}(E)} \left(\ell n\phi_{ij} + \sum_{k=0}^{j-1} \ell nP_{ik} \right) \phi_{ij} \prod_{k=0}^{j-1} P_{ik} \qquad (3)$$

The summations and the multiplication are on all collisions that occur on the path i. ϕ_{ij} is the contribution of collision j (of path i) to the response, and P_{ij} is the probability that collision j occurs (at a specific point in phase space), given that collision j-1 has occurred (at its point is phase space).

The sensitivity to $f_{x,l}(E)$ in Eq. (3) is caused by the appearance of the angular/energy distribution. According to Ref. [5], the logarithmic derivatives are given by

$$\frac{\partial \ell n\phi_{ij}}{\partial f_{x,l}(E)} = \frac{(2l+1)P_l(\mu_{d,j-1})}{2f_x(\mu_{d,j-1},E)} \delta_{x,x_{j-1}} \delta(E-E_{j-1}) \qquad (4)$$

for the response term in a point-detector problem only, and by

$$\frac{\partial \ell nP_{ik}}{\partial f_{x,l}(E)} = \frac{(2l+1)P_l(\mu_{k,k-1})}{2f_x(\mu_{k,k-1},E)} \delta_{x,x_{k-1}} \delta(E-E_{k-1}) \qquad (5)$$

for all types of problems.

Substitution of Eqs. (4) and (5) in Eq. (3) completes the task of the calculation of the response's sensitivity to the SAD parameters $f_{x,l}(E)$. From a practical point of view, in parallel with collecting contributions to responses at collisions, additional similar terms have to be collected that are multiplied by simple functions.

Note that the actual values of $f_{x,l}(E)$ need not to be known in order to calculate the sensitivities to these very $f_{x,l}(E)$. This feature allows a straightforward calculation of these sensitivities, independent of the actual representation of the angular distribution.

This algorithm was implemented in MCSEN, a local version of the MCNP code [3].

The quantity calculated by MCSEN is the above mentioned absolute sensitivity. However, for the current comparison, we will quote in this work the relative sensitivity:

$$\frac{1}{\phi}\frac{\partial\phi}{\partial f_l(E)} = \frac{\partial\phi/\phi}{\partial f_l(E)/f_0(E)} \tag{6}$$

In the implementation of the Monte-Carlo sensitivity in MCSEN, the sensitivity is calculated in the same system of coordinates (center of mass or laboratory) as used on the cross section data file. In the case of the Fe^{56} elastic scattering considered in this work, the SAD is given in center-of-mass coordinates.

2.2. SUSD3D deterministic code methodology and comparison with MCSEN

The SUSD3D [6] code package allows one-, two-, and three-dimensional cross section sensitivity and uncertainty analyses based on direct and adjoint fluxes calculated by discrete ordinates (S_N) codes. The sensitivity and uncertainty of an integral quantity can be calculated with respect to the neutron and gamma multi-group cross sections as well as to the secondary energy and angular distributions (SAD/SED). The direct and adjoint fluxes, partial cross sections and covariance matrices are read from interface files which can be generated by different transport code systems. At present the DOORS (ANISN, DORT, TORT) and the DANTSYS (ONEDANT, TWODANT, THREEDANT) packages can be handled. This feature has the additional advantage that SUSD3D is independent of the transport codes developments.

In the discrete ordinates codes the angular dependence of the scattering cross section is described in terms of the cosine of the scattering angle μ_0 and expanded in Legendre polynomials series

$$\sigma_{g\rightarrow g'}(\mu_0) = \sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_{l,g\rightarrow g'}\cdot P_l(\mu_0) \tag{7}$$

where μ_0 is the cosine of the scattering angle and $\sigma_{g\rightarrow g'}(\mu_0)$ represents the cross section for the scattering from energy group g to g'. The Legendre series expansion is truncated after a finite number of terms. L represents the highest Legendre order taken into account.

Using first order perturbation theory the SAD sensitivity coefficient is calculated in the SUSD3D code from [6]:

$$P_g^{x,l} = \frac{1}{R}\sum_i \Delta V_i \rho_i^x \sum_{g'}(2l+1)\sigma_{l,g\rightarrow g'}^x \sum_{n=-l}^{l} M_{g,i}^{l,n}\cdot M_{g',i}^{*l,n} \tag{8}$$

where,

$M_{g,i}^{l,n}, M_{g,i}^{*l,n}$ are direct and adjoint flux moments, corresponding to the space interval *i* and energy group *g*. In the present version, the flux moments are calculated by S_N codes, but in principle they could be obtained by Monte Carlo calculations as well.

$\sigma_{l,g \to g'}^{x}$ is the *l*'th Legendre moment of the microscopic scattering cross section for reaction *x*

ΔV_i and ρ_i^x represent the volume of the space mesh interval *i*, and the corresponding atomic number density of a nuclide *k*.

In one- and two-dimensions the summation over *n* goes only from *0* to *l* due to symmetry conditions while in three dimensions all terms from *–l* to *l* must be considered.

Comparing the SAD sensitivity profiles calculated by the MCSEN and SUSD3D codes, there are a few differences:

- SUSD3D relative sensitivities correspond to the following quantity: $\frac{\partial \phi / \phi}{\partial f_1(E) / f_1(E)}$ which differs from the quantity defined in Eq. (3) by a factor of $f_1(E)/f_0(E)$ (see Fig. 3).
- All S_N SAD sensitivities are given in laboratory coordinates.

3. BENCHMARK TASK

A simple benchmark problem, typical for fusion neutronic integral experiments, has been considered. It consists of a spherical iron shell assembly with a 14 MeV neutron point source in the centre (Fig. 1). The iron shell assembly had a 4.5 cm inner radius and a wall thickness of 7.5 cm. The source was assumed to be isotropic with a flat energy distribution between 13.84 to 14.19 MeV. The benchmark task was to calculate the sensitivities for neutron flux integrals with energy boundaries 10^{-11}, 0.09804, 1.003, 4.966, 7.408, 10.0, 13.84, 14.19 MeV, i. e. 7 energy groups, at a detector location of 6.8 m. The nuclear cross-section data were taken from the ENDF/B-VI data file and processed with the ACER module of NJOY [7] in point-wise energy representation for use with MCNP-calculations. The GROUPR module of NJOY and the TRANSX code [8] were used to process the data in the 175 VITAMIN-J group structure for use with the discrete ordinates (S_N) calculations.

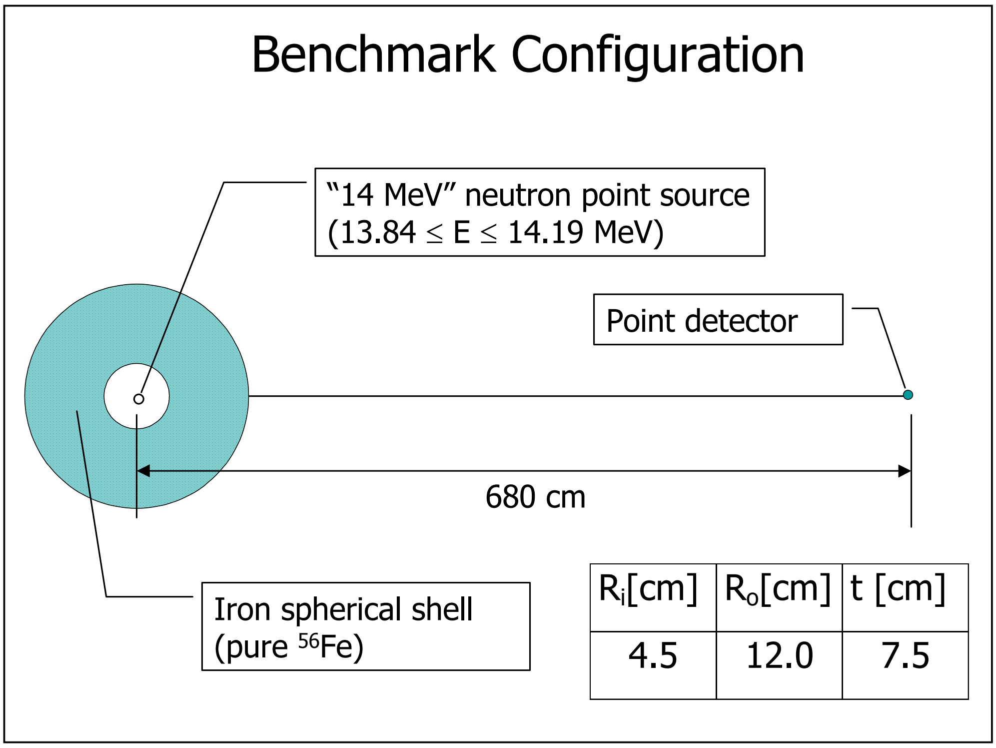

Fig. 1: Sketch of the benchmark configuration.

4. METHODOLOGICAL APPROACH

According to the benchmark task, the neutron flux spectrum at the detector location and its sensitivity to the Legendre moments of the angular scattering of neutron reactions on Fe^{56} had to be calculated with both the Monte-Carlo and the S_N method. The Monte-Carlo calculation was performed using MCNP/MCSEN with the point-detector tally (F5 in MCNP parlance). 10^6 source neutrons were sampled. The S_N-calculation was performed using the ANISN [9] code in one-dimensional spherical geometry with 71 radial intervals applying a S_{64} quadrature set for the angular segmentation (65 discrete angles) and a P_5 Legendre expansion order for the scattering kernel representation.

The fluxes were calculated in both energy group structures, the coarse 7 groups and the fine 175 VITAMIN-J group structure.

The sensitivity of the flux was calculated with both the Monte Carlo and the deterministic method making use of the specific sensitivity approaches outlined above. Profiles of the sensitivities were calculated in the fine VITAMIN-J 175 group structure for the neutron group fluxes (in the coarse group structure) to the Legendre moments. In the Monte Carlo approach, a single MCSEN run yielded all fluxes and sensitivities desired. With the S_N method, a single ANISN direct, and several adjoint calculations were performed, followed by SUSD3D runs integrating these results.

To provide further checks of the sensitivity calculations, direct transport calculations with ANISN and MCNP were performed using artificially modified cross-section data. The corresponding sensitivities were calculated from the differences of the calculated group fluxes as provided by the transport calculations using non-modified and "perturbed" cross section data that had been modified for selected reactions and energies.

5. INTERCOMPARISON OF BENCHMARK RESULTS

5.1. Flux spectra and flux energy integrals

The flux spectra calculated in the fine VITAMIN-J 175 group structure are displayed in Fig. 2. Table 1 compares the corresponding coarse group flux integrals. The different methods give very good agreement for energies above 1 MeV. Below this energy, larger differences (more than a standard deviation) may occur. These are due to the use of the same underlying cross-section data in very different ways. In particular, differences arise in the resonance region due to the use of group cross-section data in the ANISN calculation and continuous energy cross-sections in the Monte Carlo calculation. Such differences, however, do not affect the comparison of the calculated sensitivities which focuses on the energy range above 1 MeV.

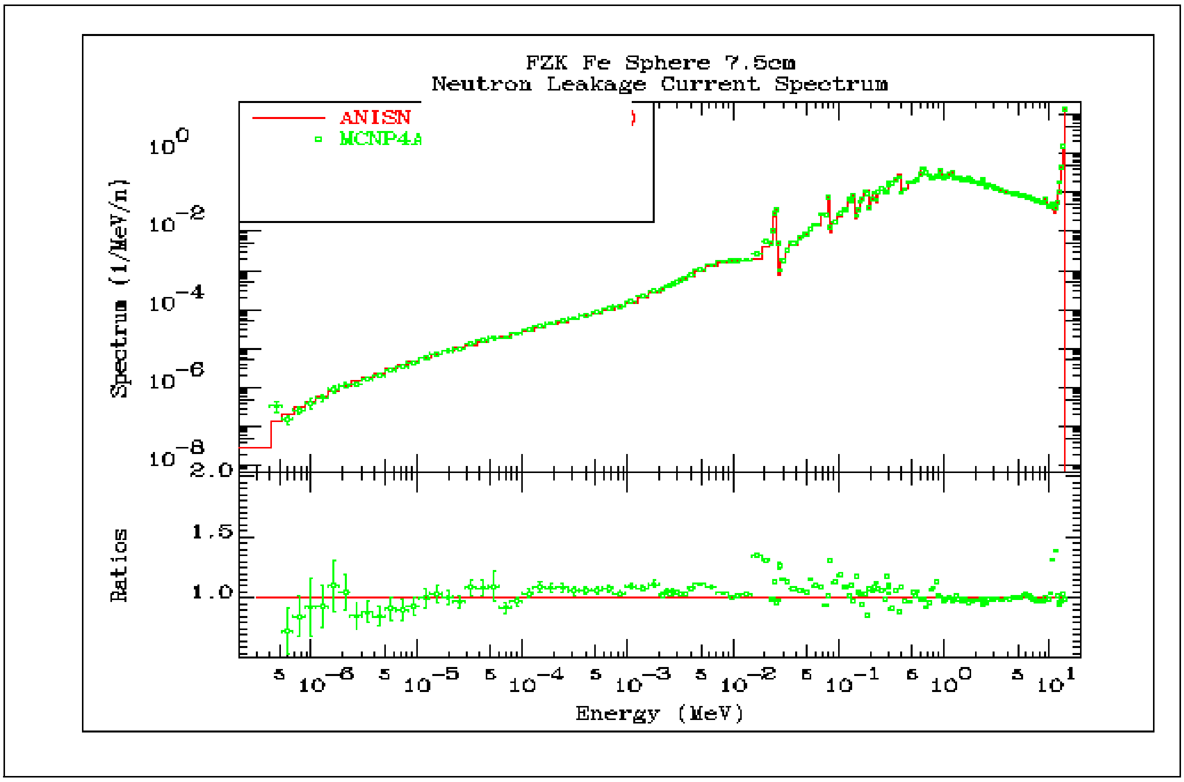

Fig. 2: The flux spectrum at the detector calculated with Monte Carlo and S_N methods

Table I: Comparison of neutron coarse group fluxes calculated directly by MCNP and ANISN

E_{high} (MeV)	MCNP[a)]	ANISN	ANISN/MCNP
0.098	$2.44 \cdot 10^{-2} \pm 0.1\%$	$2.28 \cdot 10^{-2}$	0.94
1.003	$3.64 \cdot 10^{-1} \pm 0.03\%$	$3.59 \cdot 10^{-1}$	0.99
4.966	$2.85 \cdot 10^{-1} \pm 0.02\%$	$2.88 \cdot 10^{-1}$	1.01
7.408	$3.07 \cdot 10^{-2} \pm 0.08\%$	$3.04 \cdot 10^{-2}$	0.99
10.0	$1.71 \cdot 10^{-2} \pm 0.12\%$	$1.74 \cdot 10^{-2}$	1.02
13.84	$7.63 \cdot 10^{-2} \pm 0.06\%$	$7.47 \cdot 10^{-2}$	0.98
20.0	$3.37 \cdot 10^{-1} \pm 0.02\%$	$3.42 \cdot 10^{-1}$	1.01

[a)] MCNP results include the statistical error (fractional standard deviation)

5.2. Sensitivity profiles

Profiles of the sensitivities to Legendre moments were calculated for the elastic scattering reaction. Fig. 3 displays ratios of the $f_l(E)/f_0(E)$ moments as function of the energy. Large fluctuations are observed in the energy range between about 2 and 3 MeV. Such fluctuations make the comparison between MCSEN and SUSD3D sensitivities somewhat difficult.

In the implementation of the Monte-Carlo sensitivity in MCSEN, the sensitivity is calculated in the same system of coordinates (center of mass or laboratory) as given on the cross section file. In the case of the ^{56}Fe elastic scattering considered in this work, the SAD is given in center-of-mass coordinates. The Legendre moments used by the S_N approach, on the other hand, are in laboratory coordinates. The difference between the coordinate systems, however, is small for the medium mass nucleus ^{56}Fe.

The comparison of the SAD sensitivity profiles for the neutron flux at different energy intervals calculated by the two methods is shown in Appendix A. In general there is good agreement of the sensitivity profiles calculated by the probabilistic and the deterministic approach. Minor discrepancies are due to statistical fluctuations.

The corresponding integrated sensitivities are presented in Table II. There is quite good agreement except for the energy interval between 7.41 and 10 MeV where it is difficult to get good statistics in the MCSEN calculations.

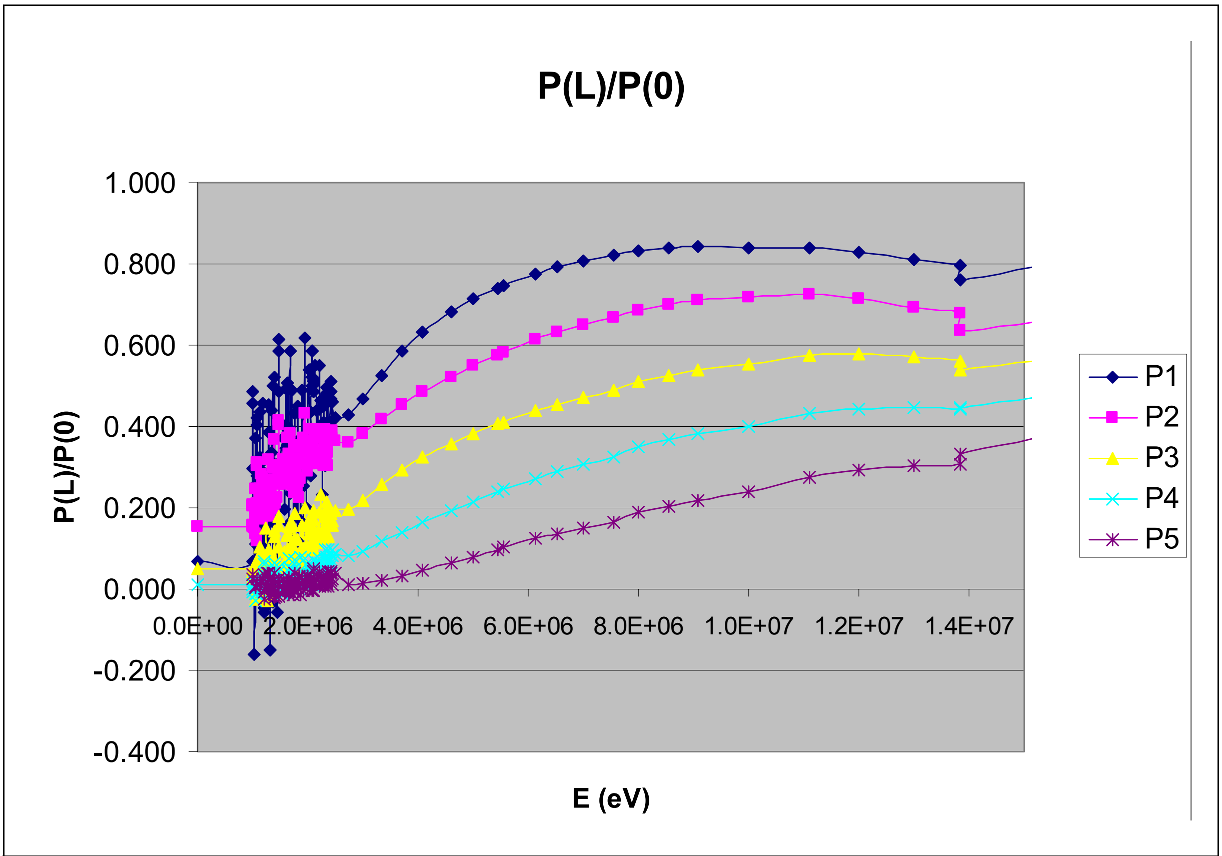

Fig. 3: Ratio of $f_l(E)/f_0(E)$ Legendre moments for elastic scattering cross sections on ^{56}Fe

Table II: Integrated SAD sensitivities, i.e. sensitivities of the neutron group fluxes to the Legendre moments of elastic scattering on ^{56}Fe (P_0 indicates the sensitivity to the elastic cross section).				
Energy	MCSEN/SUSD3D[a)]			
[MeV]	P_0	P_1	P_2	P_3
1.0 - 4.97	0.83 ±0.4%	-0.32 ±6.2%	1.09 ±2.2%	0.78 ±54.4%
4.97 - 7.41	1.00 ±1.9%	0.94 ±1.8%	0.99 ±9.1%	1.19 ±134%
7.41 - 10.0	0.85 ±6.7%	0.85 ±9.1%	1.34 ±12.5%	1.31 ±129%
10.0 - 13.8	1.00 ±0.1%	1.15 ±0.9%	0.94 ±0.4%	1.00 ±0.5%
13.8 - 19.6	1.02 ±0.1%	0.92 ±0.1%	0.95 ±0.4%	1.05 ±0.2%

[a)] MCNP results include the statistical error (fractional standard deviation)

5.3. Direct calculation with perturbed cross sections

The results of the sensitivity calculations provided by the MCSEN and SUSD3D codes were also checked with direct MCNP and ANISN transport calculations using perturbed cross-sections. The corresponding MCNP runs were performed with 10^8 source particles.

In the cross section data tables the Legendre coefficients of the elastic scattering above 13.84 MeV were modified as follows:

- f(l=1) decreased by 0.05, i. e. changed by –5% relative to f(0)).
- f(l=2) increased by 0,02, i. e. changed by +2% relative to f(0)).
- f(l=3) decreased by 0.01, i. e. changed by –1% relative to f(0)).

It is noted that these changes are nearly the maximum perturbations possible that leave f(μ) positive for all μ.

The neutron flux sensitivities were then obtained as difference between the results of the reference and the perturbed transport calculations. Figure 4 compares the calculated “direct” differences with the sensitivity results of the MCSEN and SUSD3D calculations for the first three Legendre moments. Table III displays numerical results for the case of the perturbed first Legendre moments. It is noted that that the sensitivities are expressed in terms of relative changes of the coarse group fluxes, i. e. % change per % changed Legendre moment. There is rather good agreement of the calculated sensitivity results between the applied methods for all cases. The sensitivity calculated as difference from perturbed and unperturbed MCNP calculations can show, however, rather high relative uncertainties (when calculated relative to the flux difference) although the relative uncertainties of the changes in the fluxes (uncertainties relative to fluxes) in general are acceptably small as can be seen in Fig. 4.

Table III: Comparison between sensitivity calculations and direct transport calculations with perturbed cross-sections: P-1 Legendre moment of elastic scattering decreased by 5% above 13.84 MeV energy

Upper Energy	**Δ MCNP [a)]**	**ANISN/ MCNP [b)]**	**MCSEN/ MCNP [b)]**	**MCSEN/ ANISN [b)]**	**SUSD3D/ ANISN [b)]**
[MeV]	[%]				
0.098	0.797 ± 18%	1.00	1.01±18%	1.01±1.6%	1.01
1.00	0.700 ± 5%	1.06	1.05±5%	0.99±0.5%	1.01
4.97	0.680 ± 4%	1.02	1.03±4%	1.01±0.4%	1.01
7.41	0.399 ± 28%	1.10	0.96±28%	0.88±2.6%	1.02
10.0	0.422 ± 40%	0.93	1.08±40%	1.17±3.1%	1.02
13.8	-0.618 ± 15%	0.81	1.18±15%	1.47±1.8%	0.93
19.6	-1.356 ± 2%	1.06	0.99±2%	0.93±0.1%	1.02
total	-0.015 ± 94%	1.34	0.00±138%	0.00±100.0%	1.02

[a)] Differences of neutron fluxes as calculated by MCNP with perturbed and unperturbed cross-sections.
[b)] Ratios of neutron fluxes as calculated by the mentioned codes with perturbed cross-sections.

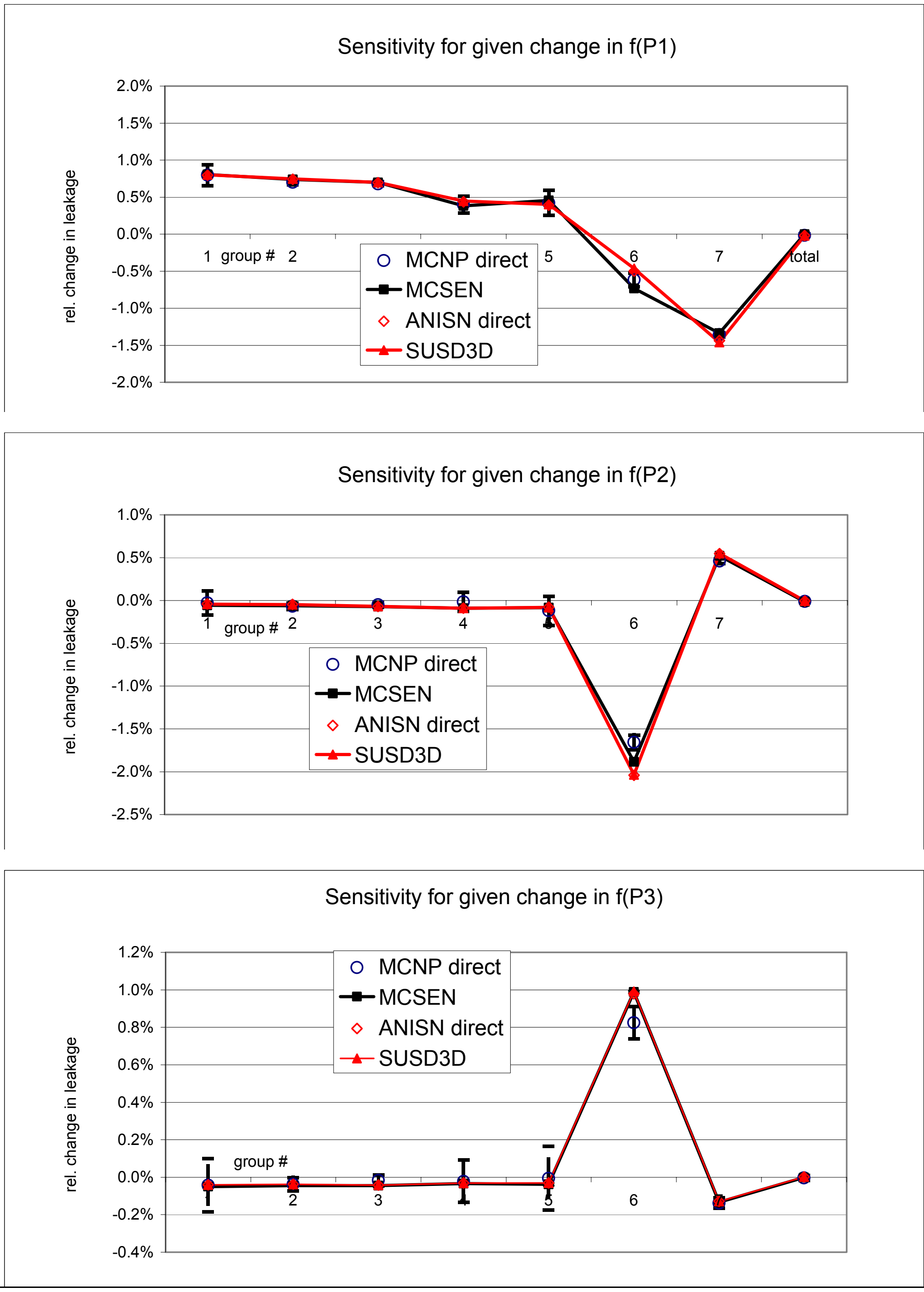

Fig. 4:Relative changes of calculated group fluxes due to modifications of the Legendre moments of the elastic scattering on ^{56}Fe: decrease of f(P1) by 5%, increase of f(P2) by 2% and decrease of f(P3) by 1% above 13.84 MeV energy.

6. CONCLUSIONS

A detailed benchmark analysis has been performed for a simple benchmark problem typical for fusion neutronic integral experiments with the objective to check and validate probabilistic and deterministic calculations of sensitivities to secondaries' angular distributions.

Good agreement has been achieved for the calculated individual sensitivity profiles, the integrated sensitivities and the neutron flux spectra. The calculated sensitivities were also shown to agree with the results of direct transport calculations using ad-hoc modified angular distributions of the elastic scattering. The Monte Carlo technique for calculating point detector sensitivities to secondaries' angular distributions is thus considered qualified for sensitivity analyses of fusion neutronics integral experiments.

7. ACKNOWLEDGMENTS

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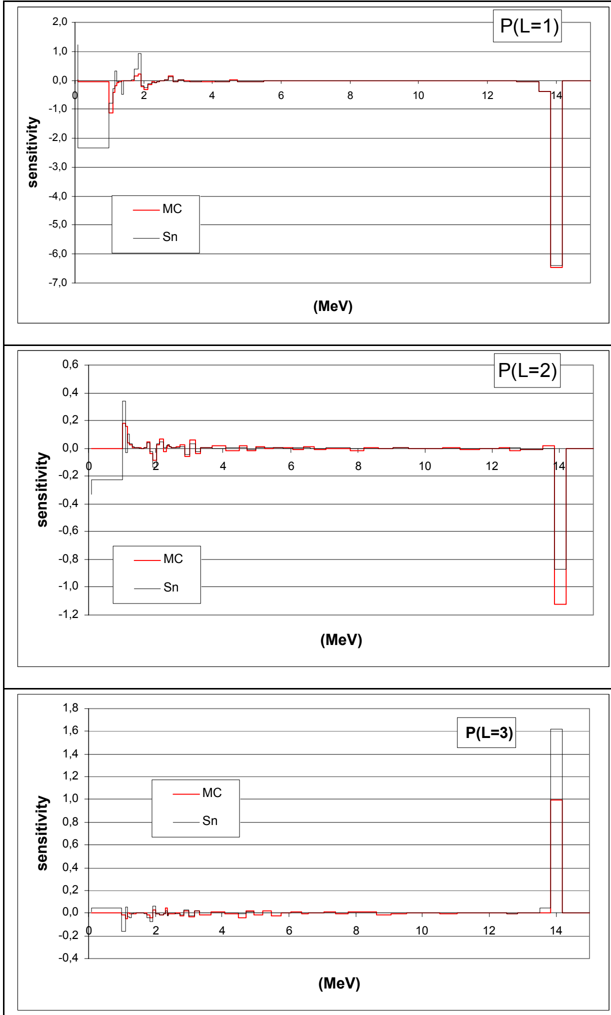
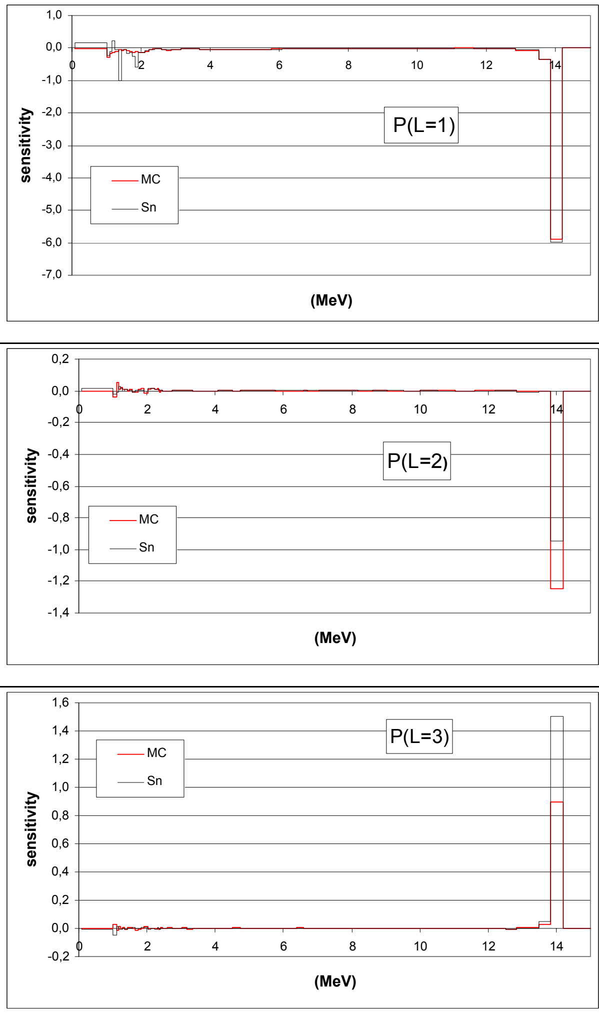
APPENDIX A

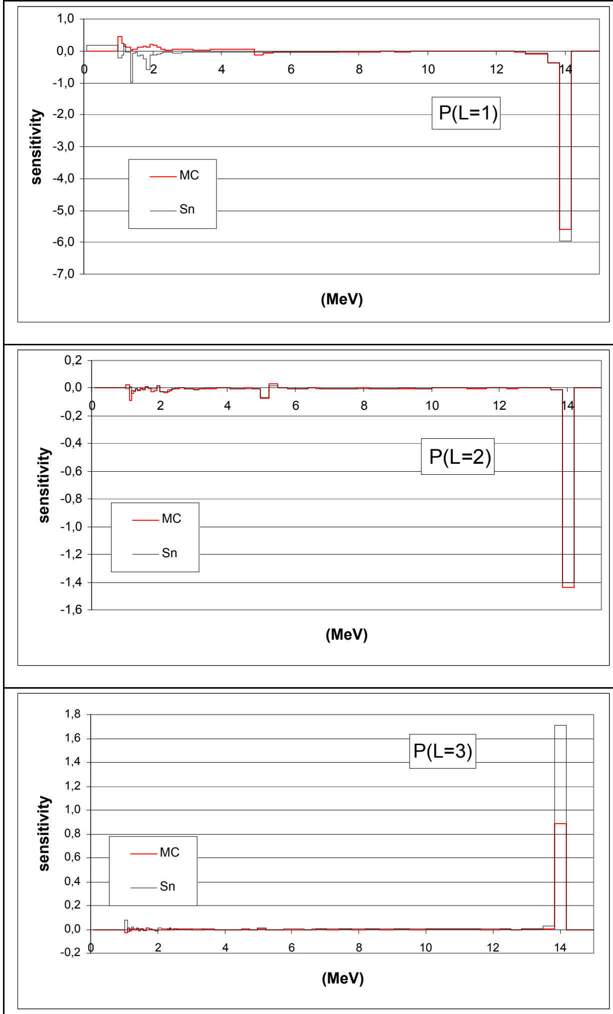
Figures A-1 to A-7 present the sensitivity profiles for the neutron leakage at indicated energies to Legendre moments of elastic scattering. The corresponding integrated sensitivities are given in Table III.



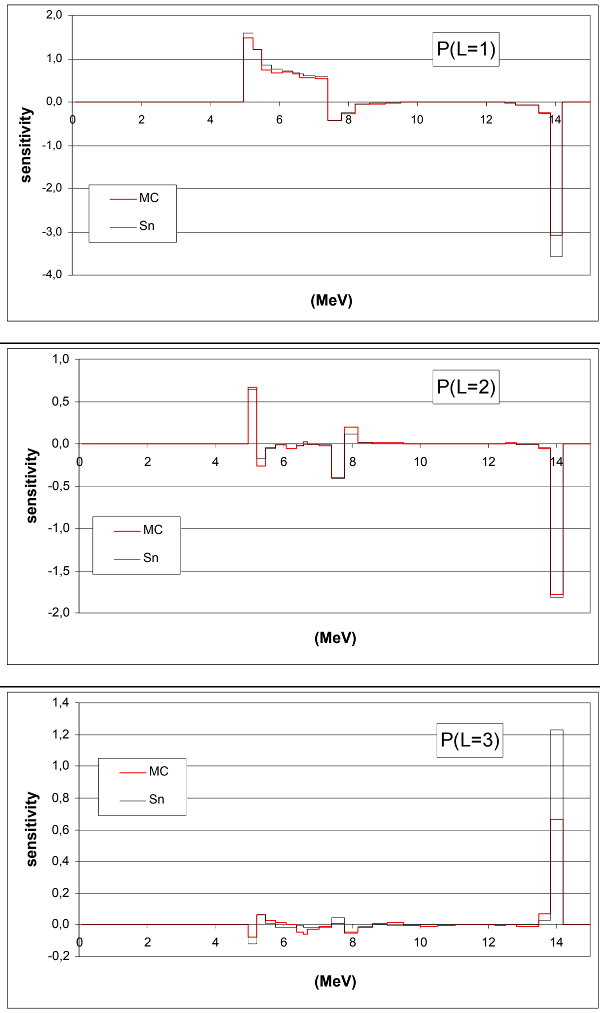
Figs. A1. Sensitivity of neutron flux below 0.1 MeV to f_l/f_0 of elastic scattering of Fe^{56}



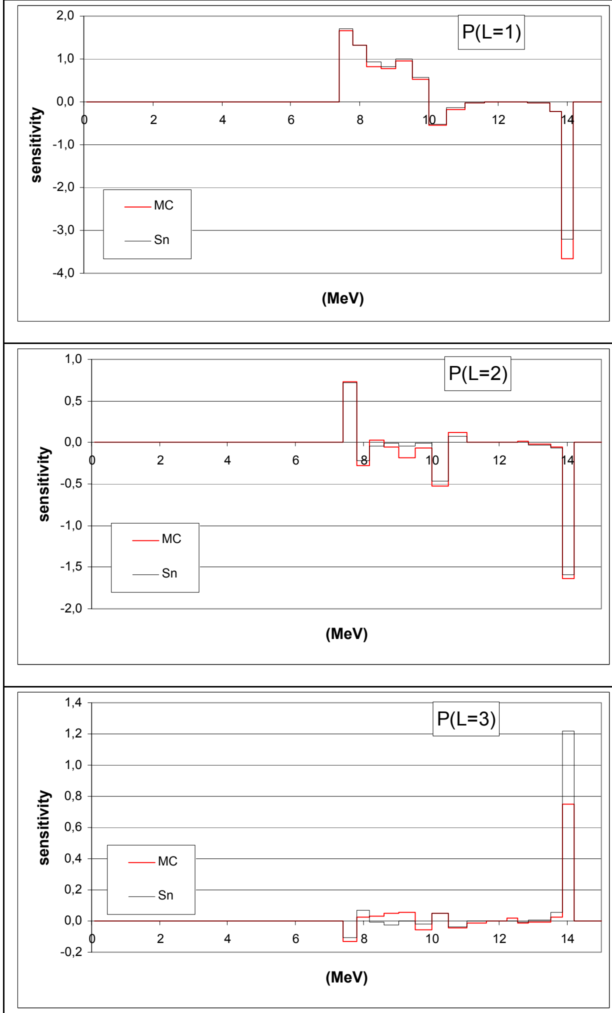
Figs. A2. Sensitivity of 0.1-1.0 MeV flux to f_l/f_0 of elastic scattering of Fe^{56}



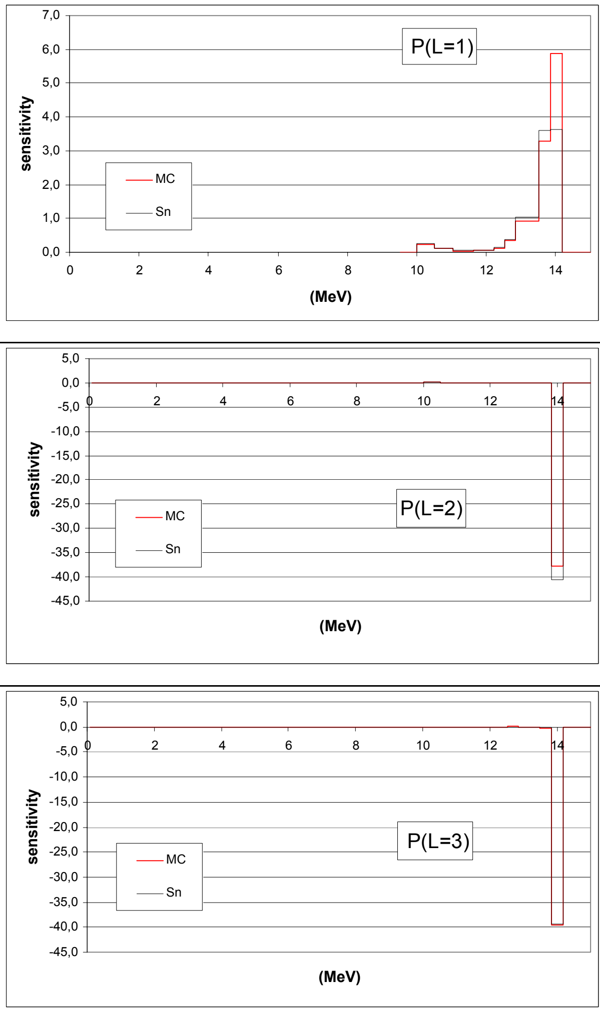
Figs. A3. Sensitivity of 1.0 - 5.0 MeV flux to f_l/f_0 of elastic scattering of Fe^{56}



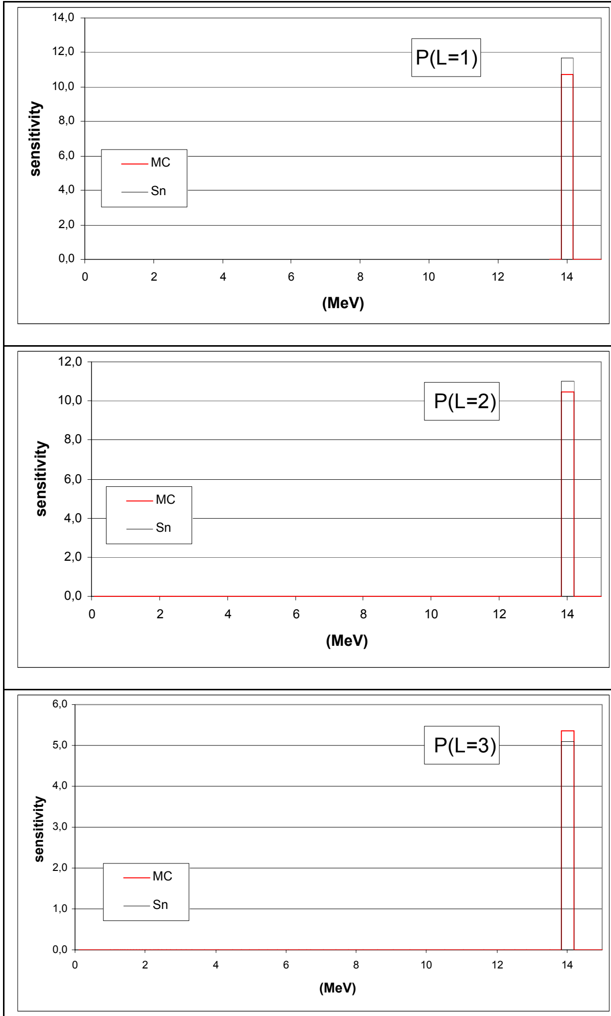
Figs. A4. Sensitivity of 5.0 - 7.4 MeV flux to f_l/f_0 of elastic scattering of Fe^{56}



Figs. A5. Sensitivity of 7.4-10 MeV flux to f_l/f_0 of elastic scattering of Fe^{56}



Figs. A6. Sensitivity of 10.0-13.84 MeV flux to f_l/f_0 of elastic scattering of Fe^{56}



Figs. A7. Sensitivity of E > 13.84 MeV flux to f_l/f_0 of elastic scattering of Fe^{56}