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Cross-section induced uncertainties in neutron source mission rate calculations

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Abstract: Analysis presented in the paper is focused on the characterization of uncertainties induced by cross-section data, which contributing to the overall uncertainty of the correction factors. Advances in computational methods and computational power shifted the calculation of correction factors among the standard steps of the manganese bath method what decrease an interest about this part of the method. Anyway, with the development of computational tools, the cross-section data were also improved, and new evaluations of nuclear data libraries include more information about the cross-section data covariances. Therefore, the propagation of uncertainties induced by neutron cross-sections can be carried out within standard transport calculation of the manganese sulphate bath model. In this paper, the super-sequence SAMPLER module that implements stochastic techniques is used to assess the uncertainty in computed results. Reaction rates on all nuclides of the solution are computed in 400 cases with uncertain parameters and the results are evaluated by an auxiliary tool. Consideration of nuclear data uncertainty in calculations is a general trend that requires the attention of nuclear researchers and should draw attention in metrology. Additional 1.5 % (one-sigma) uncertainty is introduced to the overall uncertainty through correction factor.

Keywords: *Cross-section uncertainties; neutron source; emission rate; manganese sulphate bath; SAMPLER.*

I.INTRODUCTION

The manganese sulphate bath is a globally recognized method for determination of the emission rate of radionuclide neutron sources. This method, combined with the measurement of neutron emission anisotropy, is standardly used for primary standardization of neutron dosimetry quantities. To achieve results at the metrology level it is essential to have all quantities which contribute to the overall uncertainty properly determined and contributing uncertainties minimized. In the previous analysis [1] two main contributors to the overall uncertainty of the manganese bath method were identified. Uncertainty of the activity measurement (1.41 %) and uncertainty of the detection efficiency (0.43 %) dominated in determination of the neutron source emission rate.

The manganese solution is utilized as an activation detector, where saturated activity of the ^{56}Mn corresponds to the neutron source emission rate. However, the emitted neutrons are not at all captured by ^{55}Mn. Parallel

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parasitic absorption on Oxygen, Hydrogen and Sulphur nuclei occurs accompanied by the neutrons escape from the solution tank [2]. Since the saturated ^{56}Mn activity represents just a partial neutron source strength, the neutron capture ration on manganese, as an additional correction factor, is applied on measured activity. This correction factor can be determined just based on neutron transport simulation. In a past, several parameters were calculated to properly determine manganese capture. Current computational power allows to run simple analogue Monte Carlo transport calculation and with properly defined response directly calculate the manganese correction factor. Independently to the computational power, the accuracy of neutron transport calculations is determined mainly by the accuracy of cross-section data. Improvement in the computational tools is accompanied by the improvement in cross-section data. Moreover, new evaluations of cross-section libraries include more information about cross-section covariances. Therefore, this paper is focused on the quantification of the cross-section induced uncertainties in the process of determination of neutron source emission rate through the manganese correction factor.

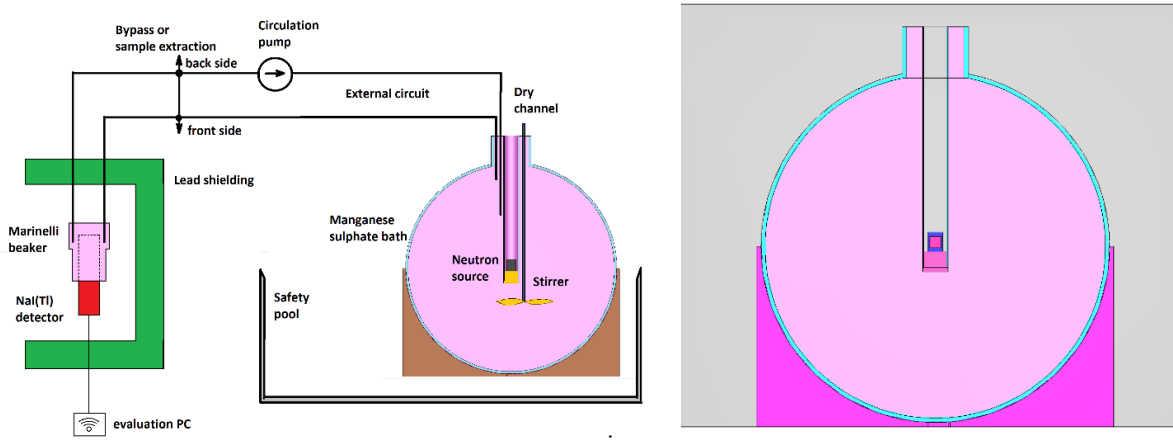
II. METHODOLOGY

The computational model for calculation of the correction factors is based on simplified representation of the bath, where just the plexiglass wall of bath with thickness 1 cm, cylindrical neck and the dry channel with real dimensions and material composition is considered. Neutron source is considered as a cylindrical shape with corresponding dimensions of real neutron sources, where just steel case and homogeneous PuBe material are considered. Whole model is placed to the void cubic volume to avoid tracking the neutrons which escape from the bath and thus speedup the calculation. The SCALE6 [3] system with MONACO code is the reference computational system for STUBA's manganese bath method. The MONACO code is based on the Monte Carlo method, which allows to model the geometry of the experiment with minimum simplifications and use nuclear data with a continuous energy structure. Principal model of the manganese bath is shown in Fig. 1-b and scheme of the experimental setup of the manganese bath is shown in Fig. 1-a.

The correction factors are calculated based on ratio of given response to neutron source strength. The response is defined as number of absorptions on ^{55}Mn nuclei in the solution. Standardly for the correction factors calculation, continuous energy library (CE) based on the ENDF/B-VII.1 [4] evaluated data is used. However, the variety of available cross-section libraries in SCALE system is relatively large, the flexibility in usage of cross-section libraries is limited to the current SCALE system release. Within the EU H2020 SANDA project, AMPX-formatted [5] version of JEFF-3.3 library [6] was prepared for direct use in SCALE6 system. Therefore, both libraries (build-in ENDF/B-VII.1 CE and JEFF3.3 CE) were used for calculations of correction factors (CF) to evaluate influence of the evaluated data. The CFs were calculated in a whole possible range of H/Mn ratio (from 1659 to 17 H/Mn). In all calculations 4 million particles were simulated within 40 batches.

To evaluate cross section data induced uncertainties the random sampling approach was applied by SAMPLER module of SCALE system. The cross sections are perturbed (sampled) based on the uncertainty and correlation information given in corresponding covariance matrices. The 400 neutron transport calculations were performed using these

perturbed input data. The SAMPLER module utilizes the previously generated perturbation factors for the 1D cross-sections on the multigroup library. The evaluation of the final uncertainty was calculated by an auxiliary tool. The calculations were performed with concentrations of $MnSO_4 \cdot H_2O$ corresponding to H/Mn ration of 962. The calculations were performed with 100000 histories per 40 batches (cycles). The standard SCALE cross-section library was used, referred as v7.1-200n47g, based on ENDF/B-VII.1 evaluated data and uses 200 neutron energy groups and 47 photon energy groups.

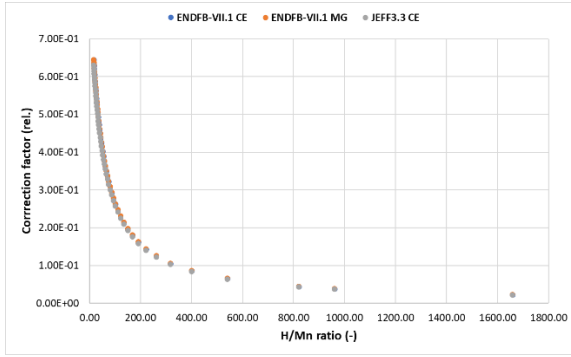


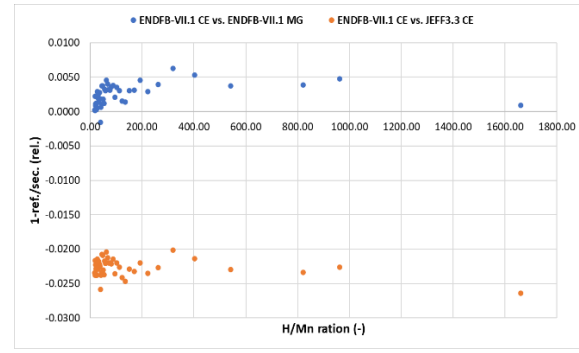
(a) (b)

Fig. 1. Manganese sulphate bath scheme and model

III.RESULTS AND DISCUSSION

Results of calculated correction factors for ENDF/B-VII.1 CE (E71_CE), ENDF/B-VII.1 200g (E71_MG) and JEFF3.3 CE (J3.3_CE) libraries are presented in Fig. 2-a. Difference between E71_CE and E71_MG is negligible, as can be seen in Fig. 2-b blue dots. Significant differences were obtained between E71_CE and J3.3_CE libraries, orange dots in Fig. 2-b. The difference varies between 2.0 and 2.5 %.





a) b)

Fig. 2. Correction factors and relative deviations between cross-section libraries

Comparison of the correction factors calculated by SCALE6 built-in libraries confirmed that both libraries provide equal results on the whole range of H/Mn ratio and

thus confirmed equivalency of utilization both libraries for determination of neutron source emission rate without any other correction. Moreover, obtained uncertainty due to cross-section data calculated by E71_MG can be then assumed for correction factors calculated by E71_CE library. Application of new JEFF3.3 library in AMPX format identified other possible source of uncertainty in the process of determination of neutron source emission rate. 2.5 % underestimation of the correction factor compared to E71_CE library exceeds currently determined uncertainties. First investigation identified that the total absorption reaction rate of ^{16}O calculated by J3.3_CE is higher than reaction rate calculated by E71_CE about 3 to 4 %. This difference is caused in the region of fast neutron which is supported by the lower total absorption rection rate of ^{1}H and lower portion of neutron which escape the solution. ^{55}Mn and ^{1}H absorb mainly thermal neutrons. If the absorption of fast neutrons is increased, it results to a decrease in the reaction rate in the thermal region and escape probability.

Results of the SAMPLER calculation for ^{55}Mn response is presented in Fig. 3. Black line represents partial results of average of calculated responses and red bars evolution of corresponding standard deviation. The convergence was reached relatively early within 250 calculated samples. The response was defined as total neutron absorption and for ^{55}Mn it is equivalent to (n, gamma) capture. All calculated responses are normalized to a neutron source strength of 5.12E5 neutrons per second to 4π and thus represent total reaction rate for the manganese solution.

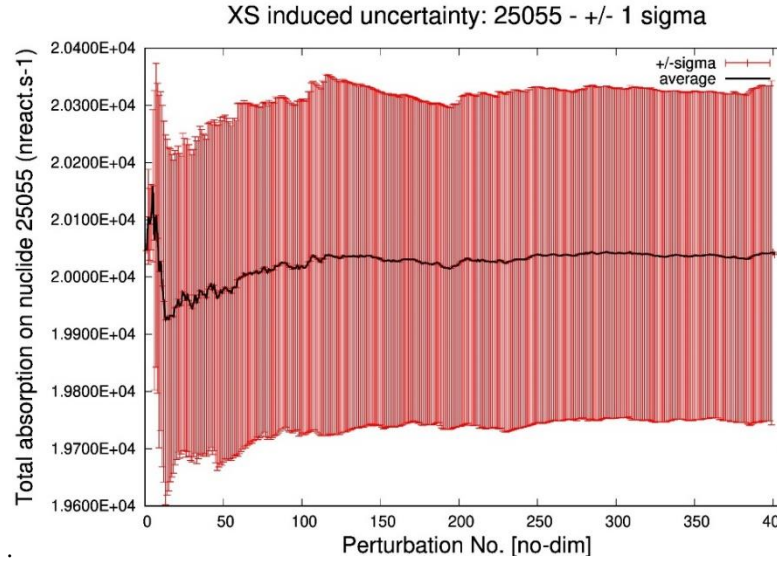
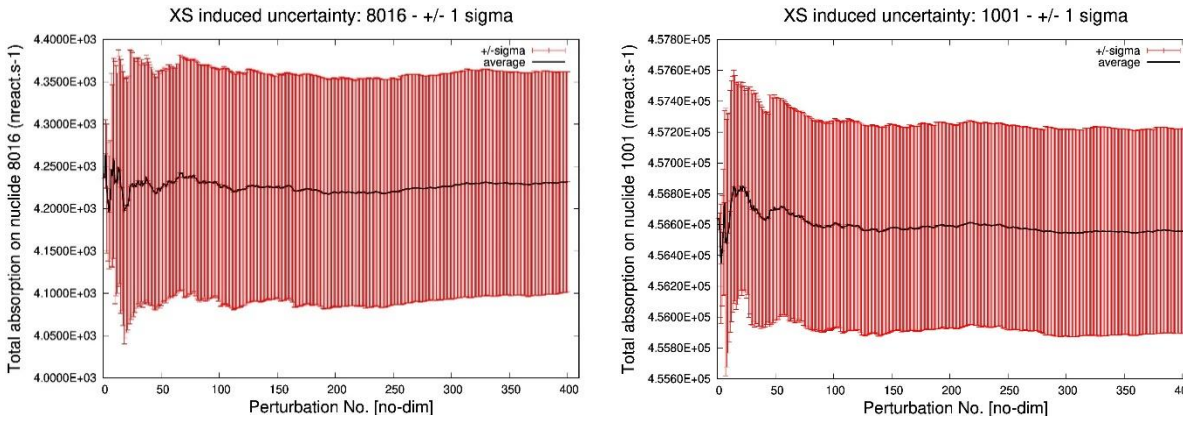


Fig. 3. Convergence of the cross-section induced uncertainty of total absorption on ^{55}Mn

The convergence of SAMPLER calculations for total absorption on ^{16}O and ^{1}H is presented in Fig. 4. Both nuclides relevantly contribute to the loss of neutrons in manganese sulphate bath and thus influencing balance between absorption on ^{55}Mn nuclei and other nuclides. The absorption on ^{1}H is driven mainly by thermal neutrons, which is direct competitive reaction to absorption on ^{55}Mn, but in the case of ^{16}O, absorption also occurs for neutrons at fast energies.



a) b)

Fig. 4. Convergence of the cross-section induced uncertainty of total absorption on ^{16}O and ^{1}H

Summary of all calculated responses are presented in Table I. Within this set of nuclides, the total neutron losses in the manganese solution are represented by the total absorption on each nuclide. The rest of neutrons are considered that escape the solution and for investigated H/Mn ration (962) it is almost 6 %. In the SAMPLER calculation, the cross-section induced uncertainties were calculated for each response and are presented in Table I in the second (absolute values) and third column (relative values). In the fourth column, the correction factors for each nuclide are calculated and represent the relative contribution to the neutron losses in the manganese solution.

Table I. Summary of the SAMPLER calculation

nuclide	response (n-react.s^{-1})	σ_R (n-react.s^{-1})	σ_R (rel.)	Corr. Factor (rel.)
1001	4.5656E+05	6.6448E+02	0.00146	8.9172E-01
1002	8.0694E-02	2.5773E-03	0.03194	1.5761E-07
8016	4.2317E+03	1.3007E+02	0.03074	8.2651E-03
16032	8.5428E+02	2.0556E+01	0.02406	1.6685E-03
16033	7.4630E+00	5.2959E-01	0.07096	1.4576E-05
16034	1.4500E+01	9.8482E-01	0.06792	2.8321E-05
16036	4.5420E-02	1.0435E-02	0.22974	8.8710E-08
25055	2.0042E+04	3.0064E+02	0.01500	3.9145E-02

Propagation of the cross-section data uncertainties using statistical sampling can determine cross-section data uncertainty of selected parameters in reasonable time and accuracy. Results presented in Table I were calculated within one set of SAMPLER run and characterized the neutrons disappearance in the manganese solution during the transport from a neutron source to shell of the bath. Currently the SAMPLER is not able to provide information about the main contributors to calculated uncertainty, but based on the results,

principal assumptions can be made. Two most competitive responses are total absorption on ^{1}H and ^{16}O. The corresponding relative uncertainties are one order of magnitude lower for ^{1}H compared to ^{55}Mn and two times higher of ^{16}O compared to ^{55}Mn. Since the total absorption on ^{16}O is just one-fifth of the total absorption on ^{55}Mn, the corresponding uncertainty of ^{55}Mn total absorption reaction rate is mainly due to uncertainties in ^{55}Mn cross-section data. For illustration, the uncertainties for ^{55}Mn (n, gamma) reaction distributed within ENDF/B-VII.1 library are presented in Fig. 5.

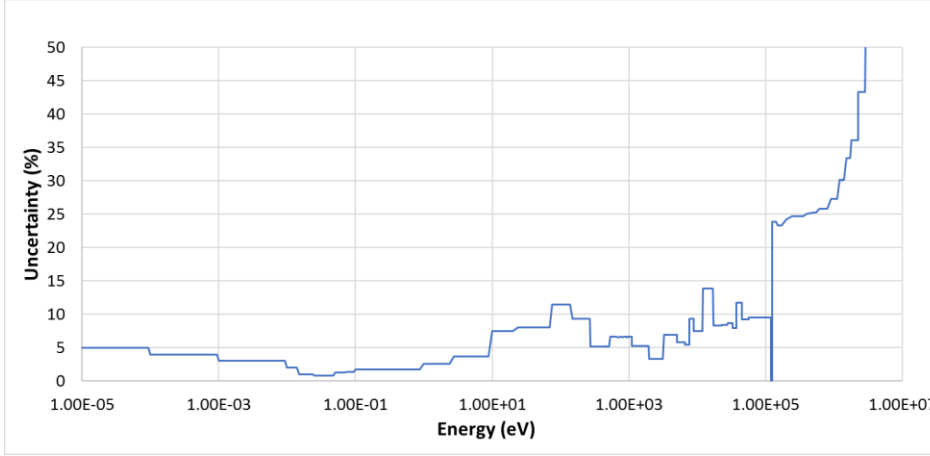


Fig. 5. Cross-section uncertainties of ^{55}Mn (n, gamma) reaction

IV.CONCLUSIONS

In the previous analyses two main contributor to the overall uncertainty of the manganese bath method were identified. Uncertainty of the activity measurement (1.41 %) and uncertainty of the manganese concentration (2.79 %) dominated in determination of the neutron source emission rate. Random sampling calculation identified additional relevant uncertainty comparable to already stated. Correction factor, which directly enter to the determination of the neutron source emission rate, is represented by 1.5 % uncertainty induced by cross-section data. Presented uncertainty analysis provides unique and first-of-kind results for the manganese sulphate bath method itself as well as for metrology community. Moreover, determination of the correction factors in the whole range of H/Mn ratio was investigated by the three cross-section data libraries. Two build-in SCALE libraries shown good agreement and thus confirm validity of the SAMPLER application with multigroup library and determination of the correction factor by CE library. New JEFF3.3 library identified a possible new source of uncertainty in determination of correction factors. More comprehensive analyses will be needed for identification of the source of this discrepancy.

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