

SENSITIVITY AND PERTURBATION THEORY IN FAST REACTOR CORE DESIGN

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This paper deals with the application of the perturbation theory in the area of fast reactor development. The basic theory and computational methods are described to point out their connection with common calculation tools. The reliability of the suggested methodology was validated by means of direct perturbations and comparison assessment. The shapes of sensitivity profiles were compared with sensitivities adopted from the International Subgroup 33 of NEA Paris. As an alternative to the used deterministic approach, sensitivity coefficients for defined sets of benchmark experiments were calculated by TSUNAMI based on a Monte Carlo flux calculation.

Key words: fast reactor design, sensitivity coefficient, perturbation theory, validation

1 INTRODUCTION

The Generation IV program has identified three fast reactor systems for further development. The most promising system in terms of the first possible deployment and actual status of development is the sodium cooled fast reactor. While for Slovakia the project ALLEGRO is of interest, for Korea it is the project KALIMER. Within the framework of sodium cooled fast reactor development in Korea a universal sensitivity analysis code APSTRACT (Analyzer of Perturbation and Sensitivity with TRANsport Calculation) has been developed [1].

Sensitivity analysis based on the Standard Perturbation Theory (SPT) offers a nuclear engineer a unique insight into the investigated system. The sensitivity processing tool in conjunction with nuclear data covariances may further serve as a powerful utility to obtain the cross section induced uncertainties in calculated quantities of interest [2]. The validation of sensitivity coefficient generation procedure is, within the frame of computational bias estimation and cross section adjustment process, a fundamental and highly requested necessity and should be carried out carefully.

The Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 33 was established to study the methods and issues of the combined use of integral experiments and covariance data, with the objective of recommending a set of the best and consistent practices in order to improve the evaluated nuclear data files [3].

2 THEORY AND TECHNIQUES

The sensitivity analysis technique has been derived from SPT which is based on steady state Boltzmann

transport equations

$$L\Phi(x) - \lambda P\Phi(x) = 0 \quad (1)$$

where x symbolically represents all independent variables, such as the neutron space, energy and direction coordinates. Operators L and P are net loss and production Boltzmann operators, respectively, and λ is the lambda mode eigenvalue, here $\lambda = 1/k_{\text{eff}}$.

After implementation of some perturbations to the transport operators and to the eigenvalue in (1), further derivation leads to the common expression of the first order sensitivity of the multiplication factor to some parameter α

$$S_{k,\alpha} = \frac{\alpha}{k} \frac{\Delta k}{\Delta \alpha} \cong \frac{\Phi^* \left(\frac{1}{k} \frac{\partial P}{\partial \alpha} \alpha - \frac{\partial L}{\partial \alpha} \alpha \right) \Phi}{\frac{1}{k} \Phi^* P \Phi} \quad (2)$$

Parameter α , appearing in (2), generally represents the nuclear data, such as the cross section (capture, fission, elastic scattering, inelastic scattering and $(n, 2n)$), fission spectrum or nuubar. Based on (2), the sensitivity coefficient can be defined as a percentage change of k_{eff} due to one percent change in parameter α , or in our case, in nuclear data.

In addition, sensitivity coefficients are often used to relate the cross section uncertainties to the uncertainty in the response, k_{eff} or reactivity [3]. The uncertainty in the response R is then given by

$$\sigma_R^2 = S_R C S_R^T, \quad (3)$$

where σ_R^2 is the variance of the response R and C_α is a covariance matrix of parameter α .

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3 CALCULATION METHODS

The computational route to determine the sensitivity coefficients by the APSTRACT code is based on 150 group MATXS and ISOTXS format data library prepared from ENDF/BVII.0 evaluated data. The KALIMER-150 equilibrium core flux was used as a weighting function in NJOY library processing [4]. The self-shielding calculation, unique for each benchmark model, was performed by TRANSX [5]. As a flux solver TWODANT, transport code included in the modular DANTSYS [6], was chosen to determine the angular forward and adjoint fluxes.

As an alternative approach, 238 group sensitivity data sets were independently generated by SCALE6.1.3 system where stochastic Monte Carlo KENO-VI module was used as a flux solver and the sensitivity coefficients were calculated by the TSUNAMI module [7]. Since the SCALE system is in general based on 238 energy group structure for multigroup calculation, the sensitivity coefficients calculated by TSUNAMI module had to be collapsed to a 33 group structure. For this case, auxiliary utility for group collapsing has been developed.

33 group ERANOS results coming from CEA (Commissariat à l'énergie atomique et aux énergies alternatives - France) and PSI (Paul Scherrer Institute - Switzerland) published on the WPEC Subgroup 33 web page were plotted in the final results comparison as a reference data [3].

In order to make an extensive validation, seven modified benchmark problems defined by Subgroup 33 were investigated, namely: Joyo, ZPPR9, ZPR6-7 (standard configuration) and ZPR6-7 (High 240Pu content) Jezebel (239Pu and 240Pu configuration) [8, 9]. The list of benchmarks with associated Handbook name can be seen in Tab. 1.

Table 1. Subgroup 33 benchmark problems

| Benchmark problem | Handbook name |
|---|--------------------|
| Jezebel ²³⁹ Pu configuration | PU-MET-FAST-001 |
| Jezebel ²⁴⁰ Pu configuration | PU-MET-FAST-002 |
| Flattop Pu configuration | PU-MET-FAST-006 |
| ZPR6-7 standard conf. | ZPR-LMFR-EXP-001 |
| ZPR6-7 high ²⁴⁰ Pu content | ZPR-LMFR-EXP-002 |
| ZPPR9 | ZPPR-LMFR-EXP-002 |
| JOYO | JOYO-LMFR-RESR-001 |

4 DISCUSSION AND RESULTS

The TWODANT deterministic flux calculation was performed with Sn-8 and P-3 Legendre order of scattering configuration. The KENO-VI stochastic calculations were run with 10,000 histories/generation for forward calculation and 100,000 histories/generation for adjoint calculation, until the computational statistic has reached sufficient accuracy. Afterwards, both fluxes were directly used

in TSUNAMI module, where the sensitivity coefficients were generated. The sensitivity coefficients provided by the SG33 participants are based on ERANOS calculations with ENDF/B-VII.0 or JEFF-3.1 evaluated data in 33 group structure.

The comparisons of sensitivities for chosen reactions and for the most important isotopes are presented below. Tab. 2 and Tab. 3 are showing the sensitivity coefficients determined by SPT technique as well as by direct perturbation calculations (DP).

Table 2. Integral sensitivity coefficients in % of k_{eff} for ²³⁹Pu calculated by direct perturbations (DP) and standard perturbation theory (SPT)

| Isotope | ²³⁹ Pu | | | |
|---------------|-------------------|---------|-------|-------|
| | ELASTIC | | NUBAR | |
| Reaction Type | DP | SPT | DP | SPT |
| Flattop | 0.02300 | 0.0233 | 0.875 | 0.879 |
| Jez_239 | 0.06500 | 0.0642 | 0.957 | 0.965 |
| Jez_240 | 0.05330 | 0.0529 | 0.813 | 0.820 |
| JOYO | 0.03220 | 0.0324 | 0.399 | 0.401 |
| ZPPR9 | 0.01730 | 0.0173 | 0.793 | 0.800 |
| ZPR6 | 0.00314 | 0.00317 | 0.801 | 0.807 |
| ZPR6_HPu | 0.00279 | 0.00280 | 0.786 | 0.792 |

The sensitivity coefficients of individual benchmark cases are in a good accordance with those achieved from direct perturbation, as is presented in Tab. 2 and Tab. 3; therefore only the graphical results from JOYO and ZPR6-7 investigation are presented.

Table 3. Integral sensitivity coefficients in % of k_{eff} for ²³⁸U calculated by direct perturbations (DP) and standard perturbation theory (SPT)

| Isotope | ²³⁸ U | | | |
|---------------|------------------|---------|---------|--------|
| | INELASTIC | | CAPTURE | |
| Reaction Type | DP | SPT | DP | SPT |
| Flattop | 0.06690 | 0.0697 | -0.039 | -0.040 |
| JOYO | 0.00613 | 0.0618 | -0.132 | -0.132 |
| ZPPR9 | -0.06040 | -0.0605 | -0.269 | -0.269 |
| ZPR6 | -0.04690 | 0.0473 | -0.244 | -0.245 |
| ZPR6_HPu | -0.04010 | -0.0403 | -0.239 | -0.239 |

In all figures, the abbreviation Aps33 denotes the results calculated by APSTARCT, SG33 represents the results calculated by the members of Subgroup 33 and SCALE represents the results calculated by TSUNAMI.

In the first three figures, the sensitivity profiles for the main fissile isotopes are shown: ²³⁹Pu in Fig. 1, ²³⁵U in Fig. 2 and ²⁴¹Pu in Fig. 3. From Fig. 1 to Fig. 3 a shift of

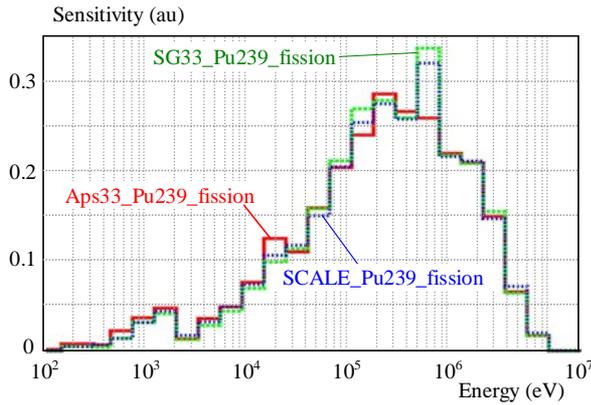


Fig. 1. Sensitivity profiles of k_{eff} for JOYO benchmark and ^{239}Pu fission

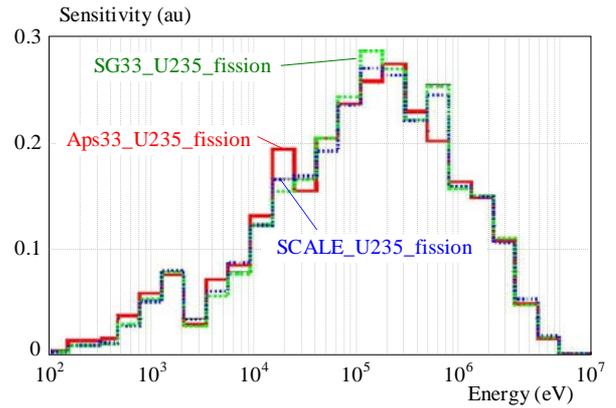


Fig. 2. Sensitivity profiles of k_{eff} for JOYO benchmark and ^{235}U fission

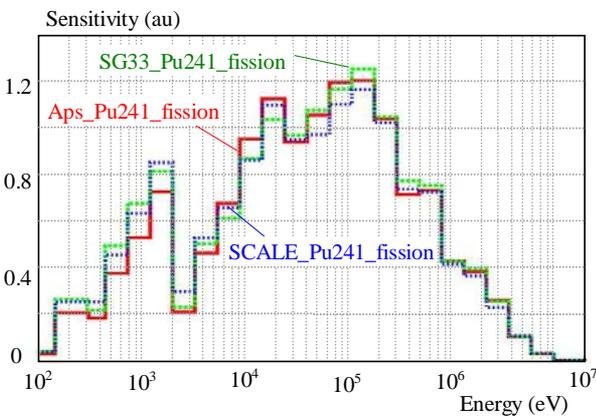


Fig. 3. Sensitivity profiles of k_{eff} for ZPR6-7 benchmark and ^{241}Pu fission

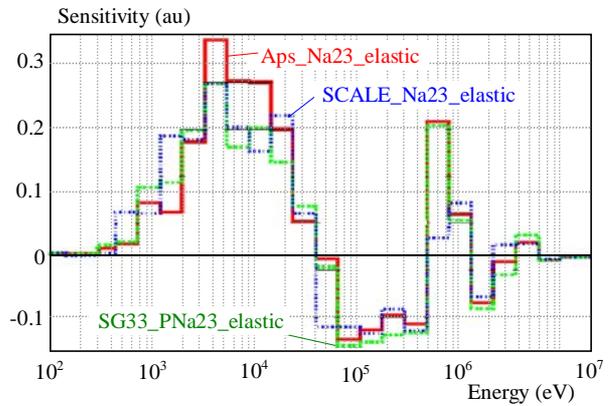


Fig. 4. Sensitivity profiles of k_{eff} for ZPR6-7 benchmark and ^{23}Na elastic scattering

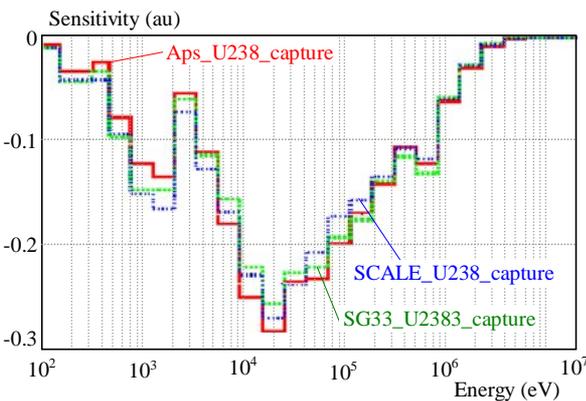


Fig. 5. Sensitivity profiles of k_{eff} for ZPR6-7 benchmark and ^{238}U capture

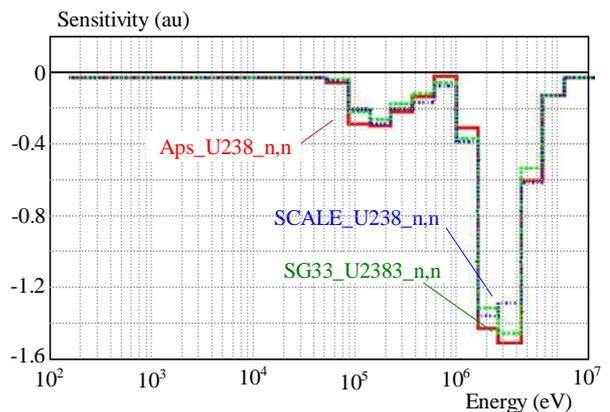


Fig. 6. Sensitivity profiles of k_{eff} for ZPR6-7 benchmark and ^{238}U inelastic scattering

the effective area of fission to lower energies can be seen. Combination of these three isotopes in the fast reactor fuel is able to cover a wide range of neutron spectrum (10 keV to 10 MeV) by fission.

This effect is probably stronger in sodium cooled fast reactors (SFR), due to sodium moderation capability, but for gas cooled fast reactor (GFR) where silicon carbide is

considered as one of the structural material, it could be also interesting.

For fission reaction, Fig. 1 to 3 demonstrate a very good consistency of individual sensitivity profiles. On the other hand, Fig. 4 presents the sensitivity profiles of sodium elastic scattering in ZPR6-7 benchmark, where the agreement is questionable. Within some groups, small

differences can be seen but all are in tolerance. An important finding of this reaction is that the overall shape is in agreement for all three cases. The variable effect of scattering reaction through energy spectrum is directly connected to capture on ^{238}U , demonstrated by positive sensitivity in lower energies, and fission on fissile isotopes, demonstrated by negative sensitivity in higher energies.

The sensitivity profiles for capture reaction of ^{238}U are presented in Fig. 5. All profiles are in very good agreement and represent the physical behavior of the system. A strong negative effect can be seen in the area of ^{238}U resonances, which plays a significant role in temperature transient analysis driven by the Doppler effect.

The last figure (Fig. 6) confirms almost perfect consistency between sensitivity profiles. The influence of ^{238}U inelastic scattering is located in the highest energy area but its effect is very strong. The integral sensitivity is several times higher than the elastic scattering of ^{23}Na in this benchmark. For specific designs like GFR, the sensitivity of k_{eff} on inelastic scattering of ^{238}U could be one of the most important issues.

The application of sensitivity coefficients to evaluate k_{eff} uncertainty is simple, which is demonstrated by (3), but the correct interpretation of these uncertainties is quiet difficult because they are strongly dependent on the quality of covariance matrices. In Tab. 4 the total uncertainties of k_{eff} for each of the investigated benchmarks are presented. The calculations were based on two different covariance data files. For the APSTRACT case, the covariance data were prepared by standard NJOY99 procedure for fast reactor application, but only for a limited number of isotopes, while in SCALE case the 44 group SCALE covariance library was used.

Table 4. Total uncertainty in % of k_{eff} coming from cross section data for investigated benchmarks

| Code | APS | SCALE |
|-----------------------|--------|--------|
| Ftattop | 0.7104 | 1.2206 |
| Jez_Pu ²³⁹ | 0.5977 | 1.3712 |
| Jez_Pu ²⁴⁰ | 0.5029 | 1.2099 |
| Joyo | 0.6071 | 1.2870 |
| ZPPR9 | 1.1698 | 1.4574 |
| ZPR6-7HPu | 1.0178 | 1.2829 |
| ZPR6-7 STD | 1.0717 | 1.2920 |

5 CONCLUSION

A proper application of the SPT has been validated by means of direct perturbation analysis on a set of seven benchmarks. Each experiment was chosen as a representative of fast reactor technology. The profile assessment has confirmed the consistency with the results calculated by the participants of NEA Paris Subgroup 33 and by Monte

Carlo flux based the TSUNAMI calculation. This paper demonstrates the ability to provide comparable sensitivity coefficient profiles with well-known codes used worldwide. Afterwards, these results can be reliably used in uncertainty analyses, cross section adjustments or determination of sensitivity to reactivity response. Finally, all sensitivity profiles are suitable for the evaluation of corresponding response uncertainties induced by cross section data. However, the final uncertainties depend mainly on the covariance data, since the sensitivities in this process serve as a weighting function.

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