Validation of Adjoint Sensitivity and Uncertainty Analysis Capability of McCARD

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1. Introduction

The k_{eff} uncertainties due to nuclear data uncertainties have been estimated by various sensitivity and uncertainty (S/U) analysis codes.

Recently, the Monte Carlo (MC) the adjoint-weighted perturbation (AWP) method [1,2] based on the adjoint flux estimated in the MC forward calculation was developed and implemented in *McCARD* [3]. Reference 1 noted that the uncertainties calculated by *McCARD* and *SUSD3D* [4] were quite similar except for the elastic and inelastic scattering results. In this paper, the impacts of the energy group structure of the covariance data and the applied covariance data type for inelastic scattering will be examined to address the difference of the uncertainties calculated by *SUSD3D* and *McCARD*.

2. Uncertainty Quantification

The variance of k_{eff} , $\sigma^2[k_{eff}]$, induced from the uncertainties of nuclear data can be written as

$$\sigma^{2}[k_{eff}] \cong \sum_{n,r,g} \sum_{n',r',g'} \operatorname{cov}[\mathbf{x}_{r,g}^{n}, \mathbf{x}_{r',g'}^{n'}] \left(\frac{\partial k_{eff}}{\partial \mathbf{x}_{r,g}^{n}}\right) \left(\frac{\partial k_{eff}}{\partial \mathbf{x}_{r',g'}^{n'}}\right)$$
(1)

 $\mathbf{x}_{r,g}^{n}$ is the g-th group microscopic cross-section of reaction type r of isotope n. $\partial k_{eff} / \partial \mathbf{x}_{r,g}^{n}$ is the sensitivity of \mathbf{k}_{eff} to $\mathbf{x}_{r,g}^{n}$. $\operatorname{cov}[\mathbf{x}_{r,g}^{n}, \mathbf{x}_{r',g'}^{n'}]$ denotes the covariance between $\mathbf{x}_{r,g}^{n}$ and $\mathbf{x}_{r',g'}^{n'}$.

Because $\operatorname{cov}[\mathbf{x}_{r,g}^n, \mathbf{x}_{r',g'}^n]$ in Eq. (1) is obtained by processing ENDF/B covariance data file using ERRORR/NJOY or ERRORJ [5], the uncertainty of k_{eff} can be readily calculated using $\partial k_{eff} / \partial \mathbf{x}_{r,g}^n$, which is estimated by the AWP method.

3. Numerical Results

The uncertainties of k_{eff} due to the JENDL-3.3 nuclear data uncertainties for Godiva (HEU-MET-FAST-001), Jezebel (PU-MET-FAST-001) and Bigten (IEU-MET-FAST-007) are calculated using McCARD, and compared with those from *SUSD3D*. In the *SUSD3D* calculations, SCALE [6] 44 group structure of the covariance data and detailed covariance data for the inelastic scattering according to excited states of target nucleus (MT=51-91) are used. To examine the impacts of the energy group structure of the covariance data, the *McCARD* calculations are performed using the LANL 30 group and the SCALE 44 group covariance data. To examine the impacts of covariance data type for inelastic scattering, the detailed covariance data and the merged covariance data (MT=4) for inelastic scattering are considered.

All the *McCARD* calculations are performed on 1,000 active cycles with 10,000 histories per cycle based on JENDL-3.3 nuclear data library. The ERRORR module of NJOY code is used to produce the covariance matrices from the JENDL-3.3 covariance data.



Table I and Fig 1 show the comparison of the k_{eff} uncertainties of Godiva for each reaction type due to the energy group structure and the data type of the inelastic scattering covariance. In the elastic scattering result, the difference between SUSD3D and McCARD using 30group covariance matrices is 13.1% while that between SUSD3D and McCARD using 44-group covariance matrices is 2.7%. In the inelastic scattering results, the difference of McCARD using the merged inelastic covariance data is 13.7% while that using the detailed inelastic covariance data is only 1.5%. The impact for the use of the different energy group structure is significant for the elastic scattering and the difference of the uncertainties for the inelastic scattering is mainly come from the use of the different inelastic covariance data type. Fig 2 and Fig 3 show the results of the nuclear data S/U analysis for Jezebel and Big-ten, respectively. As observed in Godiva S/U analysis, the k_{eff} uncertainties by SUSD3D are similar to those by McCARD using 44-group covariance matrices and the detailed covariance data for the inelastic scattering.

4. Conclusions

In this study, the adjoint nuclear data S/U analyses are conducted for Godiva, Jezebel and Big-ten critical assembly using McCARD. In the comparison with SUSD3D, the two codes predict similar sensitivities to the v, (n,γ) , (n,2n), fission. It is confirmed that the differences between SUSD3D and McCARD for the elastic and inelastic scattering are caused by the difference of the energy group structure of the covariance and the applied inelastic scattering covariance data type.

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section covariance for Jezebel



section covariance for Big-ten

Code		SUSD3D	McCARD			
Energy Group		44 group	Continuous Energy			
Covariance Data		44 group	30 group		44 group	
Type of inelastic scattering		Detailed	Merged	Detailed	Merged	Detailed
Unc. due to ²³⁵ U (%)	ν, ν	0.149	0.148		0.148	
	(n,γ), (n,γ)	0.171	0.159		0.159	
	(n,γ), (n,n)	0.047	0.046		0.046	
	(n,2n), (n,2n)	0.009	0.010		0.009	
	(n,fis), (n,fis)	0.168	0.168		0.168	
	(n,n), (n,n)	0.308	0.348		0.316	
	(n,n), (n,n')	-0.443	-0.512	-0.487	-0.489	-0.457
	(n,n'), (n,n')	0.694	0.790	0.730	0.776	0.707
Total		0.516	0.548	0.509	0.557	0.514

Table I: Comparison of $k_{e\!f\!f}$ uncertainties due to the covariance in ²³⁵U for Godiva