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Online Kalman Filter Fission Source Convergence Diagnosis In Monte Carlo Eigenvalue Calculation

Seung-Ah Yang [a] and Ho Jin Park [b]*
[a]*Korea Atomic Energy Research Institute, 111, Daedeok-daero 989 beon-gil, Yuseong-gu, Daegeon, 34057 Korea*
[b]*Department of Nuclear Engineering, Kyung Hee University, Deogyeong-daero, Giheung-gu, Gyeonggi-do, Korea*
** Corresponding author: parkhj@khu.ac.kr*

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1. Introduction

In Monte Carlo (MC) eigenvalue transport calculations, inactive cycles are intended to provide a fully-converged fission source distribution (FSD) that is a stationary mode. There have been many studies on the FSD convergence in MC eigenvalue calculations such as Ueki's posterior method [1], Shim's stopping criterion [2], Skewness estimation method (SEM), and Kurtosis estimation method (KEM) [3]. In the previous studies, it is difficult to determine the number of inactive cycles due to large statistical fluctuations and noise occurred from FSDs.

In this study, a new methodology to diagnose the convergence of FSDs was newly introduced. Firstly, this methodology can reduce the statistical noise in the FSD by utilizing the Kalman filter [4,5], a type of mathematical algorithm that combines Gaussian distributions to reduce variance. Secondly, the number of inactive cycles can be determined from the number of the inflection points that occur during the Kalman filter calculations. The concept of inflection points is introduced as a way to determine convergence because statistical noise is shaped like inflection points. The number of inflection-points relative to the number of calculated samples must reach a certain criterion, ε, for convergence. To determine ε, which is used as the convergence criteria, the inflection point calculations with the Kalman filter on several benchmarks with various dominance ratios (DRs) are conducted. Finally, we established a formula to find the convergence criteria as a function of a DR. Using the Kalman filter and inflection points, we proposed an effective online methodology called as the Inflection-Kalman combined method (IKCM), designed to accurately diagnose convergences.

2. Methodology

2.1. Kalman Filter Algorithm

In the Kalman filter algorithm, the prediction and measurement functions are combined using Gaussian distribution. Figure 1 shows the overview of the Kalman filter algorithm. The characteristics of the Kalman filter is used to reduce the statistical noise in the FSDs. As shown in Figure 2, the Kalman filter algorithm iteratively updates the measured and predicted values to estimate the optimal value. In this study, the McCARD [6] MC code consistently measures FSD values cycle by cycle. All McCARD calculations are performed using 100,000 neutron particles per a cycle and 10,000 cycles.

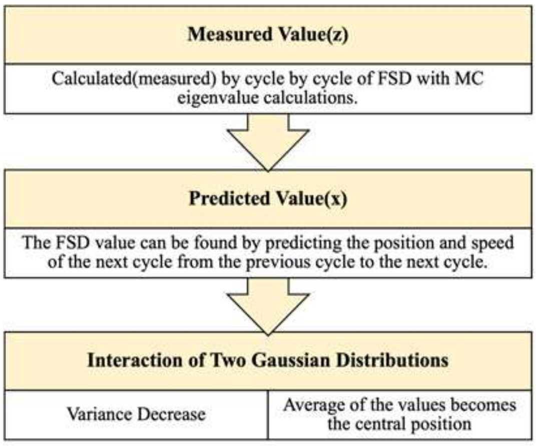


Figure 1. Overview of Kalman Filter Algorithm

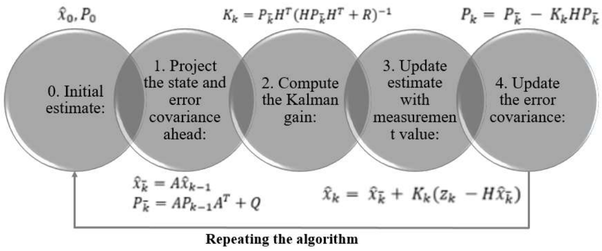


Figure 2. Structure of Kalman Filter Algorithm

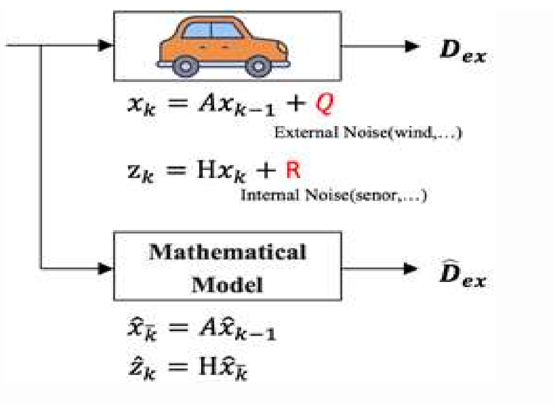


Figure 3. Example of measured and predicted model

Figure 3 demonstrates the principle of the Kalman filter using a car as an example. If the car has a rangefinder, it can measure the distance moved (measured value), that is D_{ex} as it moves over a period of time. Also, we can mathematically calculate $\widehat{D}_{ex}$ (predicted value) simply by looking at the current position of the car and how far the car moves at the end, given its speed. The values of D_{ex} and $\widehat{D}_{ex}$ may differ due to the presence of noise and uncertainty in the mathematical model. However, when corrected by the Kalman filter, it converges to the real system (i.e., $D_{ex} = \widehat{D}_{ex}$). In this simple car problem, delta T is 1 second, and in case of the eigenvalue problem, delta T is 1 cycle.

2.2. Inflection-Kalman Combined Method (IKCM)

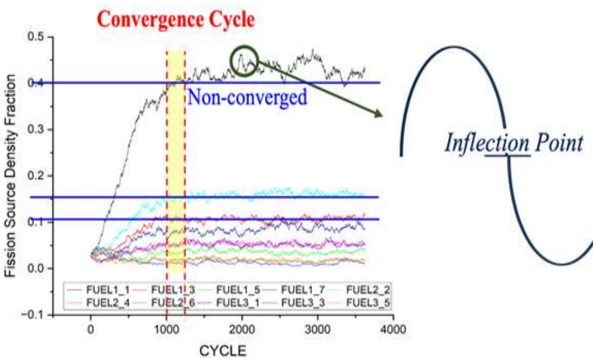


Figure 4. Example of cycle-wise cumulative FSD fraction

In a common MC eigenvalue problem, it is observed that there is a significant amount of fluctuation and noise in the FSD values, even when its convergence is achieved. It is noted that the oscillations between upward and downward movements in FSDs can be characterized as inflection points. The IKCM can be used as a convergence criterion when the number of inflection points rises above a predetermined threshold ε, as shown in Eq. (1), where ε is determined by DR.

$$\frac{N_{\infty}}{L_{\mathrm{kf}}} \geq \varepsilon\ (\mathrm{DR}), \qquad \text{…. (1)}$$

where L_{kf} is the interval or length for Kalman filter calculations and N_{∞} is the number of inflection points occurred during N cycles. The Kalman filter identifies convergence cycles by tallying the number of inflection points observed across the performed sample cycles.

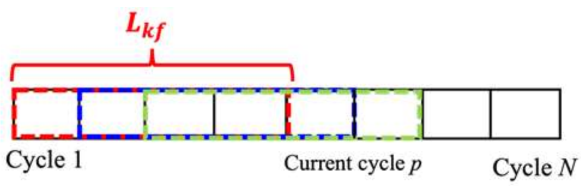


Figure 5. Convergence diagnosis with Inflection-Kalman combined Method

2.3. Determination of convergence criteria (ε)

In this section, a number of inflection points at the converged cycle was observed to determine a convergence criterion, ε, for various benchmark problem. To cover for a wide range of problems, these test problems were performed on the problems ranging from high DR to low DR.

2.3.1 1D Slab Problem with Intermediate DR

A 1D slab problem was selected for the determination of convergence criteria for problems with intermediate range DR. The 1D slab composes of the volume-equivalent 10 cells with the reflective boundary condition as shown in Figure 6. For 1D slab problem, its DR is about 0.918. It converges when the normalized FSD of each region has a ratio of 0.1, which is the 40th cycle. Firstly, after 1000 FSDs are accumulated, the Kalman filter performs online to remove noise. The next step is to count the number of inflection points occurred in the Kalman filtered 1000 samples (cycles). This study groups 1000 samples and defines them as one cycle set.

The number of inflection points occurring in a certain cycle interval was recorded by the IKCM method, and the number of inflection points increased as shown in Table I, and then stopped increasing beyond a certain number. We already know that the FSDs also converged at the 40th cycle from the other studies and the observation of FSDs. Therefore, ε becomes about 0.2.

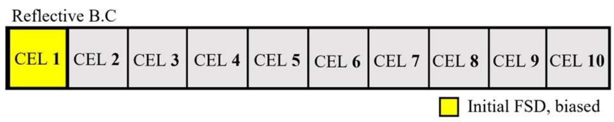


Figure 6. Vertical cross section of the 1D slab problem

Table I: Inflection points at each cycle (1D-slab)

CEL1	Inflection Point	CEL10	Inflection Point
1~1000 cycle = 1 cycle set	217	1 cycle set	136
20 cycle set	234	20 cycle set	197
30 cycle set	252	30 cycle set	197
40 cycle set	252	40 cycle set	216
50 cycle set	245	50 cycle set	219
60 cycle set	234	60 cycle set	197

2.3.2 KRITZ-2 with Low DR

The KRITZ-2 [7] reactor, operated in Sweden in the 70s, consists of a light water rectangular lattice and UO_2 and MOX fuel rods, and has a low DR problem of about 0.66. Figure 7 shows the cycle-wise cumulative FSDs before applying the Kalman filter for KRITZ-2 benchmark. In both converged and un-converged cycles, a significant number of inflection points can be observed. Thus, it is difficult for us to determine convergence solely based on the number of inflection points. Figure 8 shows the cycle-wise cumulative FSDs after applying the Kalman filter. Applying the Kalman filter to FSDs, as shown in Figure 9, the early cycles are not well predicted due to the initial slope and the number of inflection points is relatively small. However, as the cycle proceeds, the statistical noise is reduced and the predictions are well estimated, similar to the measurements.

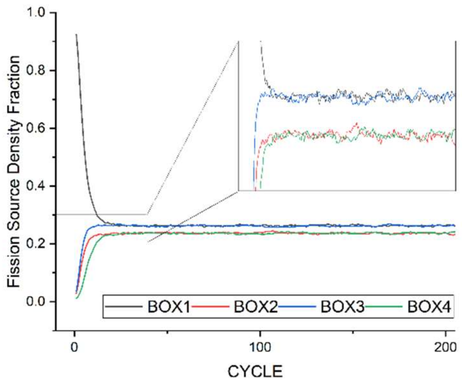


Figure 7. Cycle-wise cumulative FSD fraction before applying the Kalman filter for KRTIZ-2

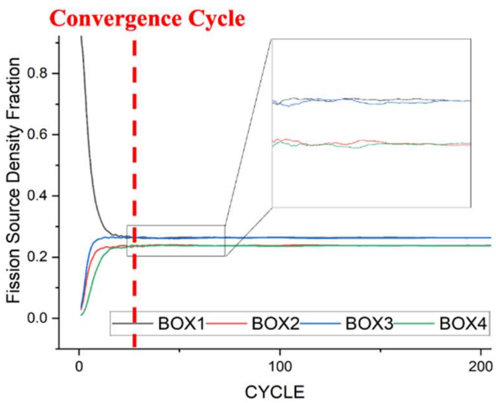


Figure 8. Cycle-wise cumulative FSD fraction after applying the Kalman filter for KRTIZ-2

In the KRITZ benchmark having low DR, we have established a criterion value of 0.26 based on the number of inflection points at the converged cycle.

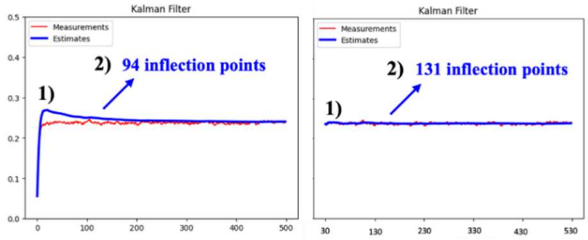


Figure 9. FSD fraction of BOX2 at 1st and 30th cycle with the Inflection-Kalman combined method (IKCM)

2.3.3 OECD/NEA Slow Convergence Benchmark Problems with High DR

In this study, two benchmark problems having high DR are considered from the OECD/NEA slow convergence benchmark. Problem 1 is a checkerboard storage of assemblies and Problem 2 is an array of pin cells with irradiated fuel. Detailed modeling and results for each benchmark problem can be found in reference [8]. The DR for Problems 1 and 2 are 0.997 and 0.976, respectively.

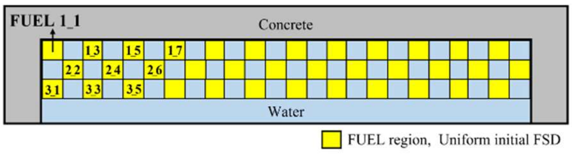


Figure 10. Checkerboard storage of assemblies (Prob.1)

In Problem 1, the FSD is biased towards the upper left corner and converges, as shown in Figure 11. Therefore, when the FUEL1_1 region converges, the other regions are already converged. After applying the Kalman filter, the first step of the IKCM, the predicted values gradually follow the measured values, as shown in Table II. The second step of the IKCM, the number of inflection points, was analyzed and ε was found to be 0.055. Figure 14 shows the configuration of the pin-cell array with irradiated fuel for Problem 2. In the same manner, in the problem 2, ε was found to be 0.05.

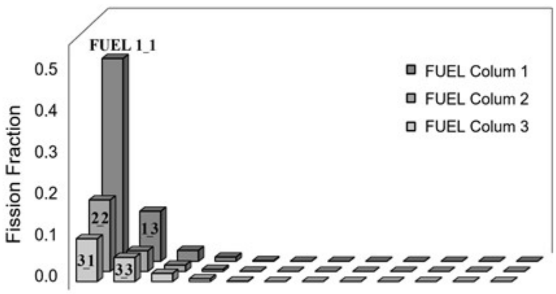


Figure 11. Fission distribution after FSD convergence

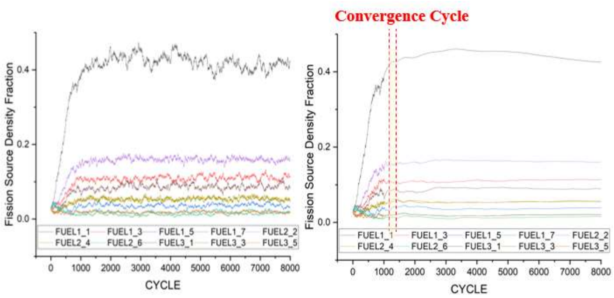
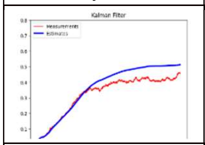
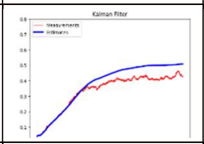
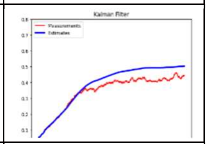
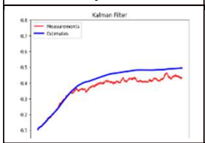
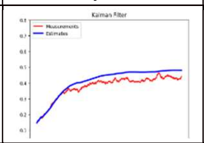
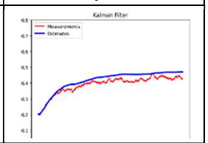
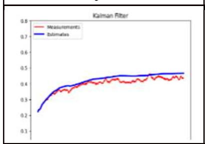
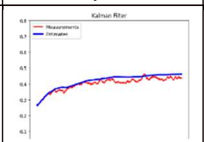
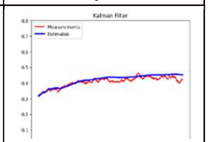
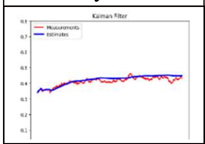
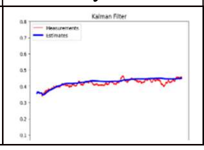
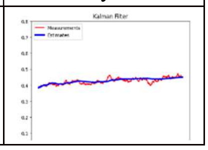


Figure 12. Cycle-wise cumulative FSD fraction before and after applying the Kalman filter of Prob.1

Table II. Calculation of Kalman filter applying for FUEL1_1

FUEL1_1		
1~1000 cycle = 1 cycle set	50 cycle set	100 cycle set
		
200 cycle set	300 cycle set	400 cycle set
		
450 cycle set	500 cycle set	600 cycle set
		
700 cycle set	800 cycle set	1000 cycle set
		

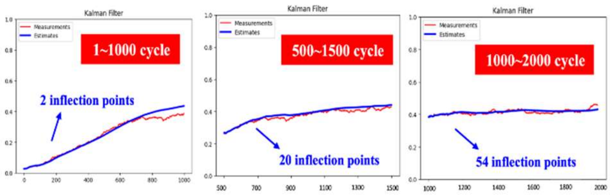


Figure 13. Using the IKCM in Prob.1

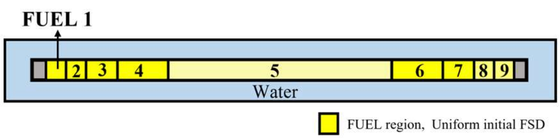


Figure 14. Pin-cell array with irradiated fuel (Prob.2)

3. Validation of the Inflection-Kalman filter Combine Method.

3.1. Results

As mentioned in the previous section, the Kalman filter was used to reduce the noise in the FSD values calculated by McCARD. In the IKCM, one can diagnose convergence when the inflection point is above a certain convergence criterion ε. In the previous section, we determined the convergence criterion ε for the problems ranged from high DR to low DR. Accordingly, the equations obtained for the approaching convergence diagnosis are Eqs. (2) ~ (4).

$$\text{High DR: } \frac{N_{\text{inflection point number}}}{L_{\text{kalman filter calculations}}} \geq 0.05 \quad \ldots (2)$$

$$\text{Intermediate DR: } \frac{N_{\text{inflection point number}}}{L_{\text{kalman filter calculations}}} \geq 0.20 \quad \ldots (3)$$

$$\text{Low DR: } \frac{N_{\text{inflection point number}}}{L_{\text{kalman filter calculations}}} \geq 0.30 \quad \ldots (4)$$

As shown in Table III, the ε as a function of DRs was determined. Based on these results, we derived Eq. (5) to cover various problems [7,8,9] by interpolation and extrapolation. This equation provides ε for determining the fission convergence cycle and can be derived for any DR and applied to benchmarks in a broad neutron energy spectrum.

$$\varepsilon = 0.0485 \ln(\text{DR}) + 0.3002 \quad \ldots (5)$$

Table III: Epsilon Derivation with DR

Benchmark	DR	Epsilon
AGN-201K	0.59	0.28
KRITZ-2:19	0.66257	0.26
1D Slab	0.9188	0.2
Prob 1.	0.976	0.055
Prob 2.	0.997	0.05

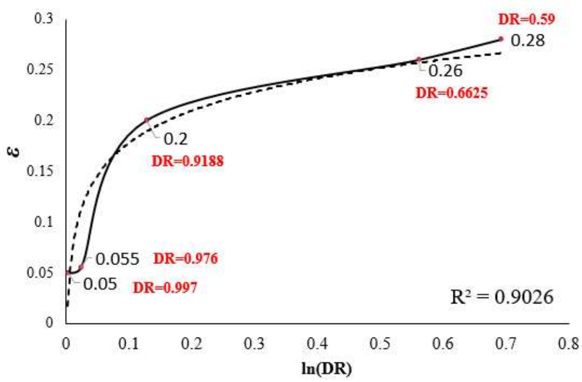


Figure 15. Convergence criterion values determined by DR and the function curve

3.2. Validation of the IKCM

To validate IKCM, we compared it to previous studied FSD convergence diagnosis methods. In the 1D slab problem, the IKCM converged at the 40^{th} cycle. The following results are similar to those diagnosed by the Ueki's posterior method, the SEM and the KEM [3,10]. In Problem 1 of the OECD/NEA slow convergence benchmark, the IKCM converged at the 1000^{th} cycle, which falls between the reference convergence cycle value and another method. In Problem 2, the IKCM showed a similar convergence cycle to the SEM and KEM methods. It was noted that the IKCM reliably and accurately diagnosed the convergence cycle of the FSDs for even high DR benchmarks.

Table IV: Convergence cycle results for the 1D Slab problem

Method	Convergence Cycle
	1D Slab
Ueki's posterior	56
Shim's Type A	97
Shim's Type B	100
SEM	31
KEM	39
IKCM	40

Table V: Convergence cycle results for OECD/NEA Slow Convergence Benchmarks

Method	Convergence Cycle	
	Prob. 1	Prob. 2
Reference [8]	700	600
Ueki's posterior	1160	1865
Shim's Type-A	163	33
Shim's Type-B	1075	39
SEM	1007	752
KEM	1127	881
IKCM	1000	800

4. Conclusion

This study introduces the inflection-Kalman combined method (IKCM). The IKCM can remove the severe noise of FSDs using the Kalman filter. The number of inflection points from the Kalman filtered FSDs can be used to diagnose the convergence cycle smoothly. The principle of the IKCM is that the number of inflection points increases as the FSDs are converged. To determine the convergence criteria, $\boldsymbol{\varepsilon}$, the equation as a function of DR was made up by performing several practical problems having various DR. Accordingly, the benchmark problems are performed: 1D slab Problem, AGN-201K, KRITZ-2:19, and OECD/NEA slow convergence benchmark. To validate the IKCM, we compared the calculated convergence cycles with those by the different methodologies. It was noted that the convergence or inactive cycles determined by the IKCM are comparable and reasonable to the other methodologies. Moreover, it was confirmed that the IKCM has the advantages in terms of the user convenience and the computation time. Therefore, the IKCM can be utilized as a practical and noble method for diagnosing the convergence of FSDs in various MC analyses.

However there is still a need for perform more calculations based on the number of neutrons per cycle to improve the DR function equation. The McCARD calculation was performed with 100,000 neutron particles per cycle, and as the number of neutrons per cycle is reduced, the statistical noise becomes more significant. The statistical noise is identified as inflection points and can impact diagnosis convergence by increases L_{kf} in Equation 1.

Acknowledgement

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