Delayed Neutron Precursor Group Parameter and Spectra Generation in SCALE

Response to Review Comments

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Review General Response

We would like to thank the reviewers for their detailed assessment of this paper. There are now more details provided on the methods (specifically in the group structure and least-squares solver), the analysis of the results, and the potential future work. Several mistakes are corrected; your comments have resulted in changes which certainly improved the quality of the paper.

Editorial Comments

1. Page 6. The equation references are missing and show "Equations (??) through (??). Please provide the correct numbers.

   Solution: Removed sentence with the missing equation references (since the terms used in the equation are defined without an equation number).

2. Page 13 and 14. Please rewrite sentences with "forward Euler" to "...uncertainties that use the forward Euler method," and in the sentence before equation 34. Please check all places where "Euler" is used.

   Solution: Updated two sentences that used "forward Euler" instead of "the forward Euler method" (no other instance of Euler was found to have the improper phrasing).

3. Please replace "due to" phrases with "because of" on page 3 and page 17 to have proper English.

   Solution: Made suggested changes.

Reviewer 1

1. Using point kinetics simulations may not be adequate for adequately handling the uncertainty with reactor kinetics and dynamics simulations for 3-dimensional core physics needs. Modern tools exist to model 3-dimensional kinetics effects, especially in reactor core dynamics.

> **Solution:** This is a very good point. The point kinetics approach used in this work is very simple, but the main purpose was to provide the reader with a qualitative understanding of the group parameters rather than a precise quantitative assessment. A more in-depth analysis of a 3-dimensional core problem using these group parameters with uncertainties would be useful future work. Specifically, future work could use Moltres with the group parameters presented here to study 3-dimensional kinetics effects.
>
> Added to future work: "Also of interest are comparisons with kinetics benchmarks by investigating other energy spectra, fissile nuclides, and kinetics methodologies [1, 2, 3]. A tool such as Moltres can incorporate these group parameters to simulate 3-dimensional kinetics benchmark problems [4, 5, 6, 7]."

2. Please consider using a 3-dimensional benchmark from the Reactor Physics Handbook cases, to see if more dimensional detail reveals special impact of delayed neutron data. If this is not possible, please explain whether the forward Euler method used for the point kinetics evaluation would still be appropriate for 1-dimensional or 3-dimensional kinetics analyses.

> **Solution:** This would be an interesting analysis, but we believe it would be outside the scope of the current work. The forward Euler method used here can be used to solve the point kinetics equations provided the equations remain unchanged. For a multipoint kinetics method (such as a benchmark like AECL benchmark 7236, discussed by Pradhan, Obaidurrahman, and Iyer [8]), then they show that this finite differencing approach can still be used, but an implict form with the Gauss-Siedel method is used rather than the forward Euler method.
>
> The 3-D benchmark possibility is mentioned in the future work section (as mentioned in 1) by adding to the future work: "Also of interest are comparisons with kinetics benchmarks by investigating other energy spectra, fissile nuclides, and kinetics methodologies [1, 2, 3]. A tool such as Moltres can incorporate these group parameters to simulate 3-dimensional kinetics benchmark problems [4, 5, 6, 7]."

3. The fast fission U235 delayed neutron data would be significantly different from the thermal fission delayed neutron precursor data, especially considering the M fission fraction distributions by atomic number, as shown in Keepin, G. Robert, "Physics of Nuclear Kinetics," Addison Wesley, Reading Massachusetts, 1965. Also, the Argonne data book provides M distributions for fast and thermal fission.

Solution: That's right, for this work we only looked at the fast fission in U235 and not thermal fission. Because we wanted to have the direct comparison with the Keepin, Wimett, and Zeigler data, we used the fast U235 fission. Although we could have continued and investigated other neutron energy spectra and/or fissile nuclides, we determined that would be beyond the scope of this work. This raises a good point (relating to 4 as well), that this should be more explicitly indicated.

To that end, the title has been changed to "Delayed Neutron Precursor Group Parameter and Spectra Generation from Fast Fission of ^{235}U in SCALE"

4. It is good that the Godiva experiment was used for the fast fission U235 data, but a thermal reactor benchmark case should be considered. If only fast delayed neutron data is considered, please indicate this in the title.

Solution: Adjusted the title to specify fast fission of uranium-235 as: "Delayed Neutron Precursor Group Parameter and Spectra Generation from Fast Fission of ^{235}U in SCALE"

5. Please note that most fission neutrons are emitted as prompt, at fast energies, however, the delayed neutrons are also emitted as thermal neutrons. Please explain how your results with the SCALE group structure you used handles the energy emission spectrum.

Solution: The SCALE group structure used in this work was not discussed, but the main reason we didn't include it is because we made efforts to minimize self-multiplication of the sample as they did in the Keepin, Wimett, and Zeigler experiment. In their work and ours, a small sample of 3 grams is used, which leads to the spectral effect from the delayed neutrons producing fissions in the sample to be negligible. We used the v7-252 group library (ENDF/B-VII.1 252-group neutron library). This is a good point though, as the treatment of the irradiating spectra is still important to consider.

Added a sentence in the Tools and Modeling section: "Specifically, the "T6-DEPL" TRITON sequence was used with the ENDF/B-VII.1 252-group neutron library."

6. Please see the delayed neutron parameters of typical reactors used in benchmark test cases in Table 2, Ahmed Aboanber, "Generalized and Stability Rational Functions for Dynamic Systems of Reactor Kinetics," International Journal of Nuclear Energy, vol. 2013, Article ID 903904, 12 pages, here. Please see the paper for the specific reactor benchmarks used. Table 2 given below.

Solution: Comparison with this benchmark could be useful to demonstrate the differences between the results, but a slight concern is that the current work only investigates fast fission of uranium-235. This makes comparison to a "Fast reactor" complicated, as the fissions in the fast reactor are presumably not 100% from fast fission of uranium-235.

Ganapol and Picca [2, 9] are cited for the benchmark, who in turn cite Nobrega, J. A. W. da. [3] as the source of the benchmark. Nobrega states thtat the fast reactor is a representative reactor, so an analysis comparing with this benchmark might be justified in assuming a sodium fast reactor. Such an analysis would entail irradiating a sample of each fissile nuclide present in the representative reactor with the neutron energy spectra present in that reactor, after which the analysis shown in this paper could be replicated for each sample to generate a comparative set of group parameters for each fissile nuclide present in the system.

Added a sentence to the "Future Work" section noting this: "Also of interest are comparisons with kinetics benchmarks by investigating other energy spectra, fissile nuclides, and kinetics methodologies [1, 2, 3]."

7. The delayed neutron groups are usually defined by their timescales, in milliseconds to seconds put into 6 groups. Does the method you use the same group structure in terms of times?

Solution: We did notice that approach in the literature, among a few others. The approaches for putting the DNPs into groups have varied from exponential stripping (or peeling) [10, 11], defining by half-life [12], and using least-squares [13]. The exponential peeling method is less objective than the least-squares method in determining an optimal set of fits to minimize a residual. The approach of sorting by timescales is more objective, but the inability for DNPs to have an impact on multiple group parameters is a weakness. The least-squares approach is the most objective approach, though there is additional computational cost associated. A method of sorting by timescale was used to compare with the least-squares method demonstrated in this work in Figure 9 (labeled as "fractional fitting"), where each DNP could contribute some fraction to the 2 closest groups.

8. Page 10 mentions that a generic Westinghouse 17x17 PWR model was considered. Please put in a sentence on page 10 that section III.E will describe that analysis for clarity. Please provide some more details in section III.E to show your Godiva fast reactor delayed neutron data would yield similar results, and why the third precursor group has the greatest differences.

Solution: Thank you for point this out, the discussion did not previously go into sufficient detail.

In the Tools and Modeling section, added: "An additional model considered is a generic Westinghouse 17×17 pressurized water reactor (PWR), analyzed in Section III.E." In Section III.E, added: "In particular, the IAEA-ORIGEN third precursor group has a yield of 0.670, which is almost double the Pure ORIGEN third precursor group yield of 0.244. Even though fast fission of ^{235}U in the Westinghouse PWR is not the primary mode of fission, the large difference in the group yield data still leads to a difference of approximately 8% in the net group 3 yields."

9. Figure 1 uses 5,000 stochastic uncertainty simulations. Would using more simulations, such as 10,000 simulations smooth out the yield vs. frequency histogram values? Would more simulations change the mean value and narrow the 1-sigma range?

Solution:

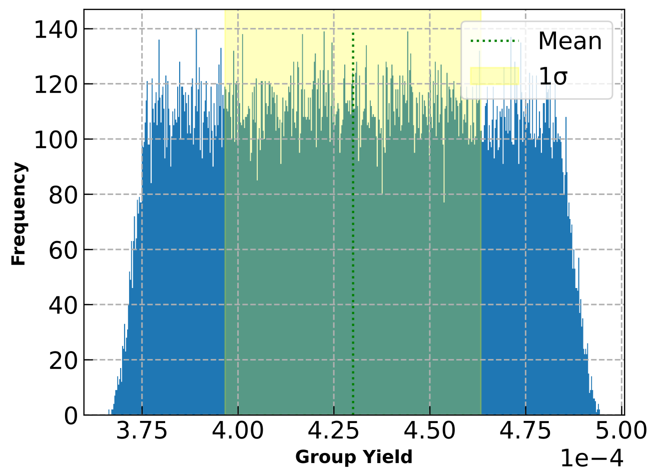

Figure 1: 50,000 stochastic uncertainty simulations of the Keepin, Wimett, and Zeigler sixth precursor group yield using a μ value of 0.5%.

Figure 1 here shows this figure with 50,000 simulations instead of 5,000. The computational cost does increase by an order of magnitude, but the result remains the same. The 1-sigma range does slightly reduce from $(4.3 \pm 0.34) \times 10^{-4}$ to $(4.3 \pm 0.33) \times 10^{-4}$.

This revealed a typo in the paper in Section II.E, where the written value read $(4.3 \pm 0.4) \times 10^{-4}$. This has been fixed.

10. Figures 2 a and b do not seem to show 2 curves on each graph. Are the results on top of each other? Please use dots or squares for one and the curve line for the other ORIGEN results so that it is clearly discernable. Please consider using dots/squares vs. lines on figure 3 as well since it is not clear.

Solution: Added squares and circles to make difference between data clearer for 2a. 2b does only have a single line, as it shows the relative percent difference between the two curves in 2a. Figures 3-5 show the absolute difference, and so are similar to Figure 2b.

Updated Figure 2a is shown below as Figure 2.

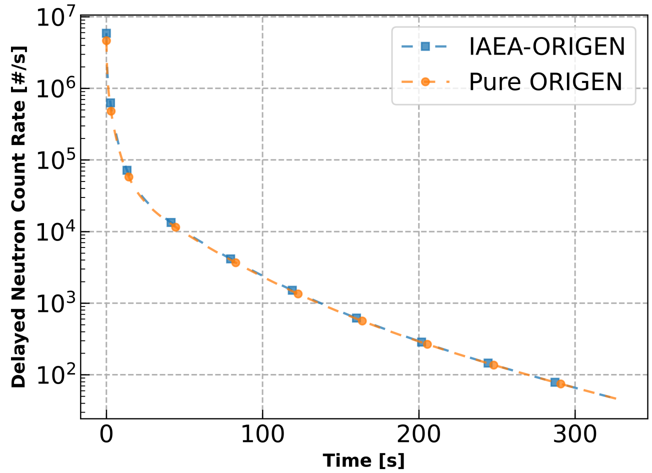

Figure 2: Pure ORIGEN and IAEA–ORIGEN count rate over time.

11. Please explain on page 18 why the emission probabilities impact of 200 pcm is considered small enough to have no significant effect on the net yield for the total number of delayed emitted.

Solution: The previous phrasing was a bit unclear, thank you for pointing this out. The change in decay constant was considered to be a non-significant impact, but the change in emission probabilities which cause a 200 pcm difference is a significant effect.

Adjusted sentence phrasing in Section III.A to: "Table II shows the net yields from various data sets, and shows that changing the decay constants does not largely impact the net yield. However, changing emission probabilities has a non-negligible impact of approximately 200 pcm."

12. On figure 6, does the blue wide band over the mean line IAEA-ORIGIN represent an error band or uncertainty level. Please clarify this in the figure caption and in the text.

Solution: The blue band is uncertainty.

This has been added in the figure caption as: "Normalized difference in emission spectra of Pure ORIGEN and IAEA–ORIGEN for ^{235}U fast-pulse irradiation at 0 s with uncertainty tracked for the IAEA-ORIGEN results." This has been added in-text as: "Figure 6 shows how the initial spectrum of the ORIGEN output compares to the IAEA–ORIGEN spectrum, with uncertainties, immediately after irradiation."

13. Figure 7 seems to show the differences between the energies. Please describe which graph or figure this is derived from or describe it in the text.

Solution: This plot takes the average energy at each time step (e.g. the average energy at time 0 from figure 6) for Pure ORIGEN and IAEA-ORIGEN and plots the difference.

Added a sentence detailing how these figures compare and what Figure 7 is showing as: "While Figure 6 shows the energy spectra at a single time step, Figure 7 shows the difference of the average of the energy spectra at each time step."

14. Tables III, IV, V, and VI may have used different evaluated cross section data sets or measurement methods, so you may need to discuss this in the text explicitly.

Solution: The Keepin, Wimett, and Zeigler results can be compared directly since their experiment was modeled explicitly in this work. The Brady and England results are calculated using a least-squares approach and preliminary data from ENDF/B-VI.

Added sentences in text to discuss this. "The results from Keepin, Wimett, and Zeigler are directly compared with this work since their experimental setup is replicated. The results from Brady and England, which use the microscopic approach, use preliminary data from ENDF/B-VI [14]. Although the methods are similar to the methods in this work, differences can be expected with the Brady and England results because of the difference in the data used."

15. On figure 8, are the color bandwidths the uncertainty ranges produced by your uncertainty analyses?

Solution: Yes, adjusted figure caption to note this as: "A comparison of the different fast fission irradiation DNP six group parameters of ^{235}U normalized to the Keepin, Wimett, and Zeigler six group count rate with uncertainties [15]."

Reviewer 2

1. Introduction, end of first paragraph ..emit multiple neutrons.. My question is. An old work by Pacilio mentions Diven numbers for multiple delayed neutrons. Can any thing be said about that or it is way outside the subject?

Solution: I believe you may be referring to the paper "TOWARD A UNIFIED THEORY OF REACTOR NEUTRON NOISE ANALYSIS TECHNIQUES" [16] where Pacilio et al. references Diven et al. [17]. A similar sort of feature can be seen in the emission probability of delayed neutrons, where there are probabilities for 1, 2 and 3 delayed neutrons to be emitted. For the vast majority of delayed neutron precursors, the average number of neutrons per decay is less than one (see The IAEA reference database for beta-delayed neutron emission data). Additionally, most of the delayed neutron precursors only have a non-zero probability to emit a single delayed neutron. I don't have much experience in neutron noise analysis, but I think such an analysis may be outside the scope of this work.

2. Equation 6 This looks like a representation of the Penrose pseudo inverse. if the matrix of the problem is well conditioned, using Eq.6 is not a problem. For an ill-conditioned matrix Using a Householder to solve the system of equation may be preferable.

> **Solution:** Thank you for pointing this out, as it allowed us to find a minor error. The matrix is fairly well conditioned, with a 2-norm condition number of approximately 200. However, the original approach used in the code was actually replaced with a Scipy Non-Negative Least Squares solve prior to generating the results (since the group yields should be positive).
>
> The pseudoinverse is no longer used in the code, and has been removed from the paper. An explanation of the method used in the current version of the code is provided. "...where the solution for the group yields with the given set of group constants is then calculated using the Scipy package's NonNegative Least Squares method [18, 19]. The 2-norm condition number of A calculated using the singular value decomposition approach in NumPy is generally approximately 200."

3. Using Keepin results raises a question Were there more recent experimental results to which the calculation may be compared?

> **Solution:** This is a very good question. There have been more recent experimental results, but the Keepin results were explicitly chosen. The Keepin data is still used for many comparisons (e.g. Loaiza and Haskin [20] where the Keepin 6-group data is compared to a proposed 7-group fit and studied using Godiva IV). Additionally, Williams [21] discusses how the Keepin data was used in ENDF until Brady's data replaced it in ENDF/B-VI. We compare our results to Keepin and Brady to provide historical background as well as to demonstrate what types of differences we could expect to see (since these changes have already been implemented into ENDF).

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