

A FISSION MATRIX APPROACH TO CALCULATE PIN-WISE 3-D FISSION DENSITY DISTRIBUTION

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ABSTRACT

This paper presents utilization of the fission matrix (FM) methodology to analyze a spent fuel pool. This FM approach utilizes a pre-calculated MCNP-generated database of fission matrix coefficients which are created at different burnups and cooling times. Certain simplifying assumptions are made based on geometric and physical considerations, greatly reducing the amount of pre-computation required. This approach is capable of quickly and accurately determine pin-wise, axial-dependent fission density distribution and subcritical multiplication (M) or criticality (k) of a spent fuel pool, in any arrangement, without recalculating FM coefficients. This paper examines the use of the FM approach for different test pool arrangements and conditions. Excellent agreements with an MCNP reference calculation have been achieved with several orders of magnitude reduction in computation time.

Key Words: fission matrix, eigenvalue, subcritical, spent fuel

1 INTRODUCTION

Neutronics calculations in a spent fuel pool are very important in terms of both safeguards and safety. For safeguards, the aim is to verify nuclear material through accurate radiation measurements. For safety, the pool must be kept sufficiently sub-critical. The work presented here can be applied to both of these problems for fast and accurate results.

This work is an extension of the fission matrix (FM) method used for the calculation of neutron sources due to sub-critical multiplication in a spent fuel pool [1–3]. Previously, the fission matrix coefficients were being obtained by using entire assemblies or fuel pins as the spatial cells. Here, we are using individual fuel pins in one-inch axial segments as the basis for the fission matrix cells. This allows not only higher accuracy, but also the ability to obtain more detailed information. This is important because in the future we plan to use this very accurate modeling to be able to estimate spent fuel composition *in situ* at the spent fuel site using various detectors. We make use of pin-wise, axially dependent pre-calculated FM coefficients to be able to quickly calculate eigenvalues and source distributions for a variety of possible scenarios in real-time.

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The FM method with Monte Carlo calculations has seen a rise in popularity in recent years [4–6], due to the problems posed by source convergence in the Monte Carlo eigenvalue problem. These methods can greatly accelerate the eigenvalue calculations, but they are still complex transport simulations. The goal of this work, using pre-calculated databases of fission matrix coefficients, is to be able to compute the eigenvalues in near real-time (seconds to minutes) rather than hours or days.

This paper will first briefly discuss the basic theory of the FM method in Section 2.1. Next, it will cover preliminary design of the reference spent fuel pool in Section 2.2. This is followed by a detailed discussion on the implementation of the algorithm for the reference pool in Section 3. Finally, the performance of the FM method will be evaluated through a set of different pool-configuration benchmark problems, shown in Section 4, followed by concluding remarks in Section 5.

2 BACKGROUND

2.1 Fission Matrix Method

The FM method can take two forms, depending on the type of problem. For a sub-critical multiplication problem, in which the fission source is driven by an independent source in the spent fuel (i.e., spontaneous fission and (α, n) reactions), the induced fission source in cell i is given by Equation (1).

$$F_i = \sum_{j=1}^N (a_{i,j}F_j + b_{i,j}S_j) \quad (1)$$

Where F_j is the induced fission source strength in fuel pin j , S_j is the intrinsic (or independent) source strength in fuel pin j , $a_{i,j}$ is the number of neutrons directly produced in fuel pin i due to a fission neutron born in fuel pin j , $b_{i,j}$ is the same as $a_{i,j}$ except for intrinsic source neutrons. These values are different because S and F should have different spatial and spectral distributions within each cell. N is the total number of computational cells (which could be a whole assembly, a single fuel pin, or a fraction thereof). This can also be written in matrix form as below.

$$\vec{F} = \mathbf{A}\vec{F} + \mathbf{B}\vec{S} \quad (2)$$

Where, \vec{F} and \vec{S} are the fission source and independent source vectors containing the N source values. \mathbf{A} and \mathbf{B} are the “fission matrices” that hold the $a_{i,j}$ and $b_{i,j}$ values.

We also consider the eigenvalue problem, as in Eq. (3).

$$F_i = \frac{1}{k} \sum_{j=1}^N a_{i,j}F_j \quad (3)$$

The fission matrix method results in a set of N linear equations, which can be solved for F and k given the $a_{i,j}$ coefficients. The chief difficulty is how to calculate the coefficients, and to decide on a computational cell size that is small enough to give detailed and accurate results, but not so large that the linear system becomes intractable. This can happen quickly as the matrix is of size $N \cdot N$.

2.2 Reference Spent Fuel Pool

Although the fission matrix method can be applied to any spent fuel pool, in this work, our reference pool is one being designed for the I²S -LWR project [7]. The I²S -LWR uses a 19×19 fuel lattice containing a total of 336 fuel rods, 24 control/guide tubes, and 1 instrument tube. The fuel used in the model is U_3Si_2 enriched to 4.95 weight-percent ^{235}U .

The spent fuel pool was developed based on the specifications of the Westinghouse AP1000 spent fuel pool [8], which was then modified to accommodate the aforementioned 19×19 I²S -LWR fuel assembly design. The segment of the spent fuel pool that we are analyzing has a capacity of 81 total fuel assemblies arranged in a 9×9 array. The neutron absorber used on storage cell walls is the material Metamic[®] [9], an alloy comprised of B_4C and Al-6061.

Figure 1a shows a unit cell of the spent fuel pool, including the assembly and cell walls. The entire 9×9 fuel pool section is shown completely filled in Figure 1b.

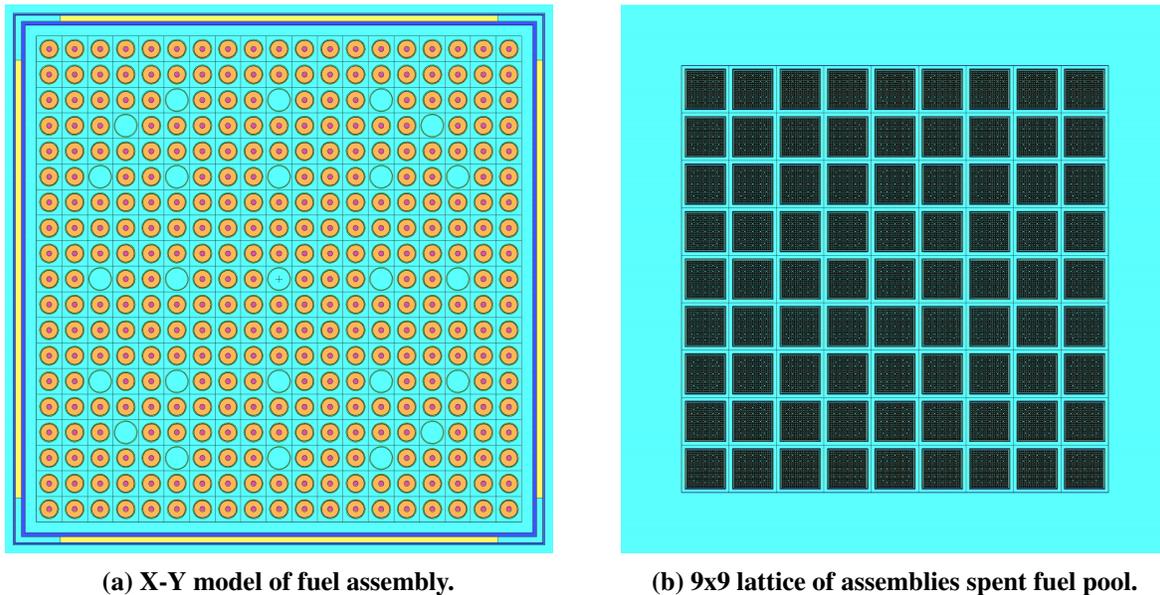


Figure 1. MCNP model used for calculating fission matrix coefficients.

3 METHODOLOGY

In theory, the fission matrix method would require N fixed source calculations in order to calculate the $N \times N$ fission matrix coefficients. If the cell size is a single pin, with 1 inch axial slices (as is done in this work), then for an entire 9×9 pool section there would be $N = 9 \cdot 9 \cdot 336 \cdot 144 = 3,919,104$ fuel segments, and thus separate fixed-source calculations. This is clearly impractical for a large problem, and defeats the purpose of “fast” calculations. However, many coefficients will be very very small (e.g., the coefficient between two distant cells), and many coefficients will be identical to each other (e.g., by observing to octal symmetry within an assembly). These will be used to greatly reduce the computational requirement of calculating the coefficients.

The first step is to decide on a computational cell size. Previously, in work with the Atucha-I reactor [1, 2], entire assemblies were used as computational cells. However, those assemblies were much smaller (37 total fuel pins per Atucha assembly vs. 336 per assembly in the I²S assembly), and there were no absorber plates between assemblies. These factors meant that for Atucha, there was little gradient in fission rate across the assembly, and so a large cell size could be used. In addition to these factors, it is also desired to have more detailed information for this project, so it was decided to use individual fuel pins with 1-inch axial segments for the computational cell. In the last version of this fission matrix work, only one cell was considered axially. This requires that the axial source distribution be known (or estimated) beforehand. This is relatively straightforward for a uniform material, but is impractical to do *a priori* for burned fuel with axial material variations.

In order to calculate the coefficients, we start with an MCNP5 [10] model of the 9×9 pool section filled with assemblies of a given fuel type (Figure 1b). Next, 49 fixed source calculations are performed, with a source located in one of each of the 49 fuel pins located in one octant of the center assembly, as shown in Figure 2. Axially, the source is located in the center one-inch segment. The total fission neutron production rate (i.e., $\int dV \phi \nu \sigma_f$) is tallied in every surrounding fuel pin for all axial levels. This tally in cell j gives $a_{i,j}$ for the source in cell i . These 49 calculations were repeated for the two different assembly types (4.95 wt% and fuel burned to 15,340GWd and cooled for approximately 2 weeks). In total, this pre-calculation of fission matrix coefficients took 47 minutes of CPU time per source location on a single processor (for a total of 4606 minutes for all source locations and for two material types). Once these have been calculated, there is no more need for detailed transport calculations.

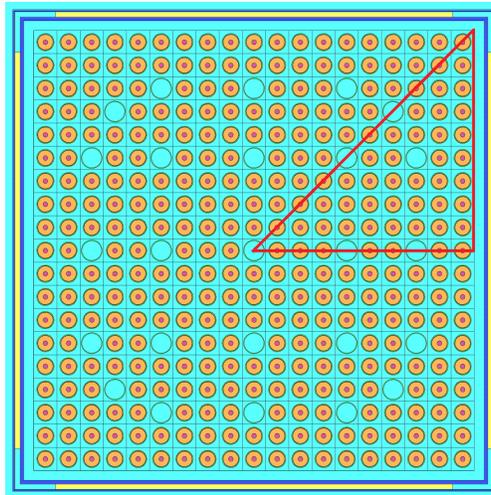


Figure 2. Pin Locations for 49 Source Calculations

Octal symmetry of the assembly is used to obtain the coefficients for the rest of the source fuel pins in this center assembly. In order to obtain the coefficients for other assemblies, it is assumed that other assemblies of the same material type have the same coefficients, except for a translation to their relative assembly position. A further simplifying assumption is that the coefficient of any pins more than 1 assembly distance away are ignored. These distant assemblies only contribute a

total of $< 10^{-4}$ of the total relative reaction rate. The translational similarity is also assumed to hold in the axial direction (e.g., the coefficient from z -level 2 to 3 is the same as from 4 to 5). These assumptions allow us to construct a fission matrix for the entire pool (for $N = 9 \cdot 9 \cdot 336 \cdot 144$ total cells) based on just 49 fixed source calculations. Additionally, we can use the same coefficients for different assembly arrangements inside the pool. The accuracy of these assumptions is investigated in Section 4.

To generate the $a_{i,j}$ FM coefficients is it necessary to assume some fission spectrum $\chi(E)$ for the fixed source calculation. It is very difficult to know this *a priori* since $\chi(E)$ for the system will depend on the fractions of fissile isotopes, their weighted ν and fission cross sections, and also the incident neutron energy. In the fixed-source MCNP calculation used to generate $a_{i,j}$ FM coefficients the Watt fission spectrum [10] is used ; Table I shows the a and b coefficients of the Watt fission spectrum used for this study. The coefficients investigated are for ^{235}U , ^{239}Pu , and a weighted average combining ^{235}U , ^{239}Pu , and ^{241}Pu ; the weighted average coefficients are calculated as in Equation (4).

$$\begin{aligned} a_{avg} &= f_{235}\nu\sigma_{f,235}a_{235} + f_{239}\nu\sigma_{f,239}a_{239} + f_{241}\nu\sigma_{f,241}a_{241} \\ b_{avg} &= f_{235}\nu\sigma_{f,235}b_{235} + f_{239}\nu\sigma_{f,239}b_{239} + f_{241}\nu\sigma_{f,241}b_{241} \end{aligned} \quad (4)$$

Where f_x is component atom fraction, $\nu\sigma_{f,x}$ is ν times the fission cross-section, and a_x and b_x are the Watt fission coefficients of component x . Note that the subscripts simply represent the mass number A of the individual component. In addition to $\chi(E)$ it is also necessary to assume a

Table I. Watt fission spectrum coefficients.

Component	a	b	$\nu\sigma_f$	f
^{235}U	0.988	2.249	512.0	0.0299
^{238}U	0.895	3.295	1.74	0.8739
^{239}Pu	0.966	2.842	1110	0.0033
Weighted	0.977	2.432	N/A	N/A

spatial source distribution. Two different spatial source distributions are considered: (i) uniformly distributed through the fuel region, and (ii) source at the outer radius of the fuel pin (which will be referred to hereafter as "Radial"). These two cases should provide coefficients which bound those of the true source distribution.

Once the coefficients have been calculated for a given pool type, the linear system in Eq. 3 is solved to determine the fission rate in each pin \vec{F} and eigenvalue k using a Jacobi iteration. First, start with a uniform, normalized source $F_i^{(0)}$ for the 0th iteration, as in Eq. 5.

$$F_i^{(0)} = \frac{1}{N} \quad (5)$$

Next, for the m 'th iteration, we have

$$F_i^{(m+1)} = \frac{1}{k^{(m)}} \sum_{j=1}^N a_{i,j} F_j^{(m)}, \quad (6)$$

where

$$k^{(m)} = \sum_{i=1}^N F_i^{(m)}. \quad (7)$$

This iteration is stopped once the k changes are below a set tolerance. A similar iterative procedure is done for the subcritical multiplication calculation, although without the normalization step.

4 RESULTS

4.1 Test Cases

To test the method, several sample problems were examined. These cases are outlined in Figure 3. All test cases use U_3Si_2 I²S fuel enriched to 4.95 wt-% ^{235}U and the fuel assembly arrangements are as follows: Case 1 is a 1×1 , Case 2 is a 6×1 , Case 3 is a 3×3 , and Case 4 is a 1×1 but using the 4.95 wt-% ^{235}U I²S fuel burned to 15,340 GWd after cooling down time of approximately 2 weeks.

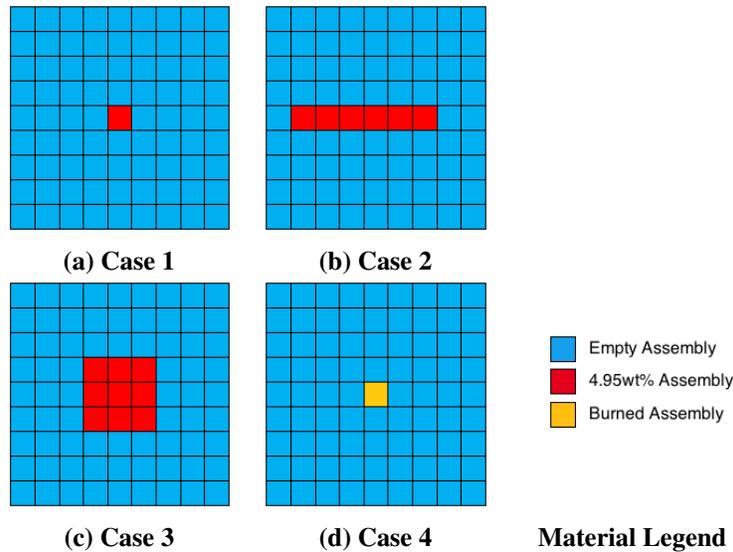


Figure 3. Pool Assembly Arrangements for Different Cases

The results of MCNP reference calculations are presented alongside the FM results in the following sections. For subcritical multiplication, the fixed-source MCNP model was run with 10^7 particles, and for the criticality problem the MCNP model was run with 40,000 histories per cycle with 500 active cycles and 400 skip cycles.

4.2 Fresh Fuel

The FM code is tested using fresh I²S fuel for the test cases outlined in Figure 3. Tables II and III present the FM k and M calculation results, respectively, for Cases 1,2, and 3 and compares

them against the MCNP reference calculation. Tables II and III also include results from a FM calculation using coefficients that are generated using both a radial source and a source uniformly distributed throughout the fuel material.

Table II. Eigenvalue calculation FM results for fresh fuel.

Case	MCNP			Uniform Source		FM Radial Source		Speedup
	k	1σ [pcm]	Time [min]	k	Rel. Err. [pcm]	k	Rel. Err. [pcm]	
1	0.79015	30	4242	0.79032	21	0.78916	-125	1547
2	0.83082	18	5200	0.83061	-26	0.82948	-161	331
3	0.86095	18	4116	0.86023	-84	0.85903	-224	167

Table III. Subcritical multiplication FM results for fresh fuel.

Case	MCNP			Uniform Source		FM Radial Source		Speedup
	M	1σ [pcm]	Time [min]	M	Rel. Err. [pcm]	M	Rel. Err. [pcm]	
1	3.33244	70	15987	3.34026	235	3.31778	-440	5769
2	4.30842	70	21356	4.32342	348	4.28620	-516	666
3	5.42369	80	27783	5.41735	-117	5.36189	-1139	537

The FM calculation results in Tables II and III show very good agreement with with the MCNP reference calculations; they also require much less computation time. In all cases k and M go down when using the radial source distribution; presumably, this is due to higher leakage rate. The lowest observed relative error is 21 pcm for the 1×1 , k calculation; a speedup of 1547 is observed for this case.

4.3 Analysis of Fission Spectrum used for Coefficient Generation

Here the effect of using different fission spectra for FM calculations using burned I²S fuel is investigated. Table IV shows the MCNP reference calculation results for Case 4 and Table V shows the FM results using the different fission sources described in Section 3.

Table IV. MCNP reference calculation results for the different test pool arrangements.

Eigenvalue Calculation			Subcritical Multiplication		
k	1σ - [pcm]	Time - [min]	M	1σ - [pcm]	Time - [min]
0.69794	18	5577	2.06625	60	10528

Table V. Fission matrix results for spent I²S fuel with different fission spectra for generation of $a_{i,j}$ FM coefficients.

Spatial Source Distribution	Spectrum	Eigenvalue Calculation			Subcritical Multiplication		
		k	Rel. Err., MCNP [pcm]	Speedup	M	Rel. Err., MCNP [pcm]	Speedup
Uniform	²³⁵ U	0.70287	706	2067	2.09951	1610	3897
	²³⁹ Pu	0.69951	225	2063	2.07787	562	3871
	Weighted	0.70244	645	2058	2.09681	1479	3906
Radial	Weighted	0.70059	379	2041	2.08469	893	3879
	²³⁹ Pu	0.69855	87	2123	2.07250	302	4002

The results in Table V indicate that, in general, the radial source lowers k and M , as does using the ²³⁹Pu spectrum. A combination of these, a radial ²³⁹Pu spectrum, produces results closest to the MCNP reference calculation. This source combination has a relative error of 87 pcm for the k calculation and 302 pcm for the subcritical multiplication calculation. A speedup of approximately 2000 for the k calculation and 4000 for the subcritical multiplication is observed.

4.4 Detailed Fission Distributions

One of the main advantages of the method over Monte Carlo is in the level of detail provided. Monte Carlo is generally good at obtaining integral results, such as k or M , but has trouble with localized results due to very poor statistical uncertainty. This is very important for example, simulation of detectors, which are generally very small compared to the system size. Here we present some detailed fission rates for Case 4 (i.e., the 1×1 case using burned fuel).

For brevity, here only the subcritical multiplication simulation is considered; the criticality simulation shows similar results. Figure 4 shows the x - y integrated (hence showing variation in z) fission distribution for MCNP and the FM method. For the FM results bounding cases with highest and lowest multiplication (uniform ²³⁵U spectrum source on the top and radial ²³⁹Pu spectrum source on the bottom). The error bars for the MCNP calculation shown are 2-sigma statistical uncertainties. The overall shape of the axial fission density distribution is in excellent agreement with the MCNP reference solution for the lowest bounding case, i.e., the radial ²³⁹Pu spectrum. Figure 5 is the same, but integrated in y - z (hence showing the variation in x); these results also match well.

Figure 6 shows the axial variation in the fission rate in a single pin (located at $x=10$, $y=11$ in the assembly). The MCNP uncertainties are approximately 5%, showing the difficulties of obtaining precise localized values. Figure 7 shows the local fission rate at z level 72 (i.e., in the axial center), at $y=10$, as a function of the pin location in x . Both of these distributions agree with the MCNP results, but without the statistical fluctuations.

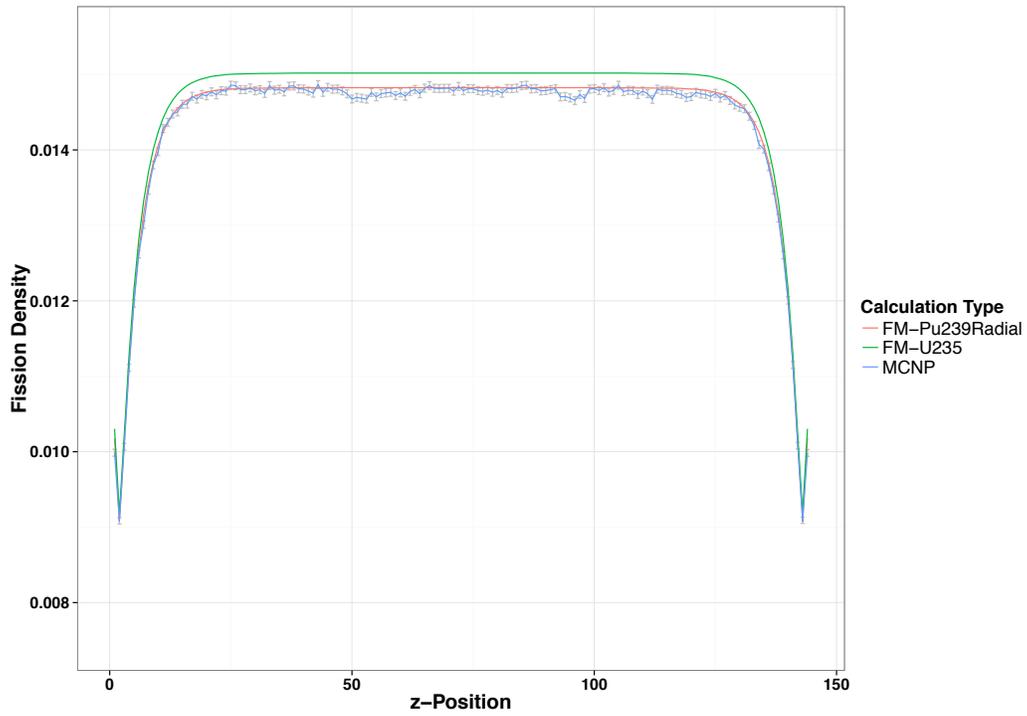


Figure 4. Axial fission density distribution of the entire fuel assembly (x - y integrated).

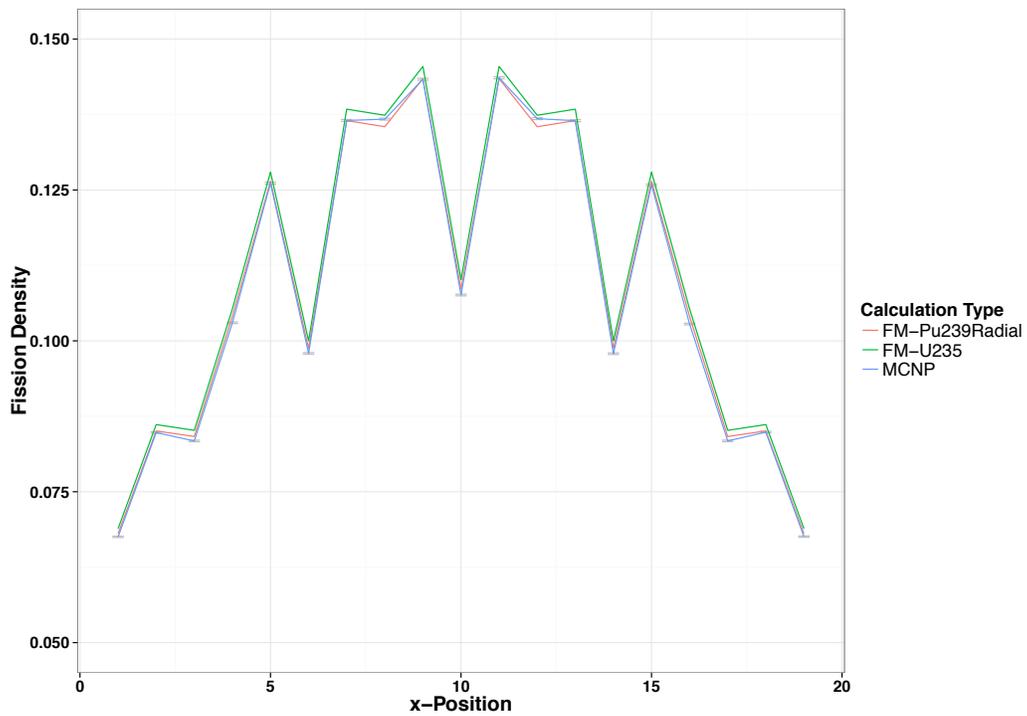


Figure 5. x fission density distribution of the entire fuel assembly (y - z integrated).

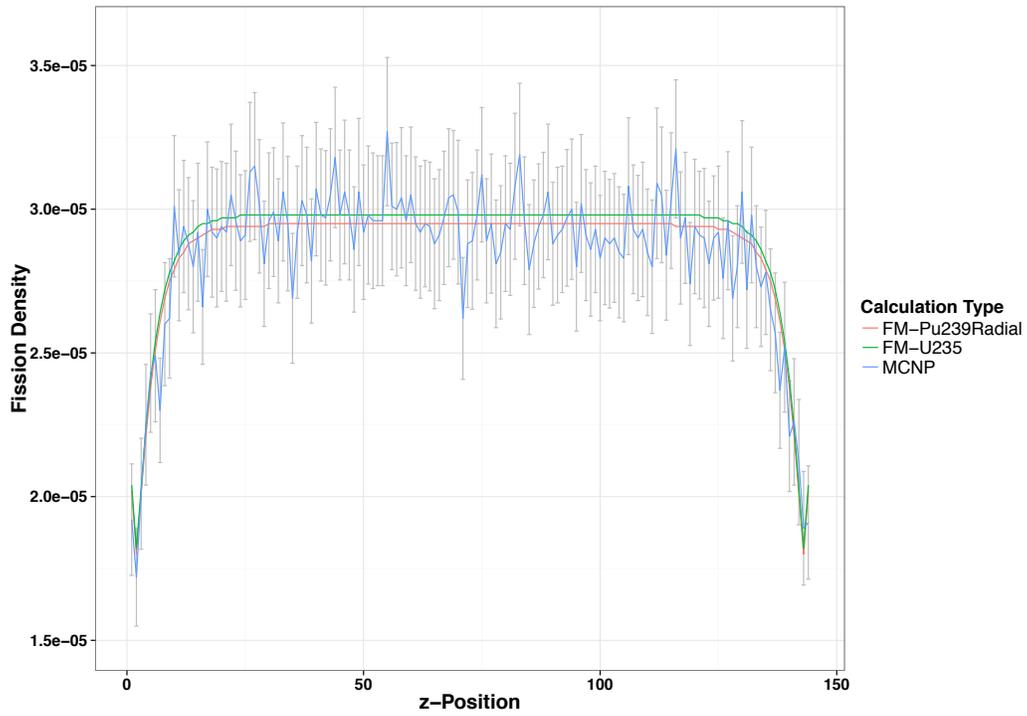


Figure 6. Axial fission density distribution of a single pin ($x=10$ and $y=11$).

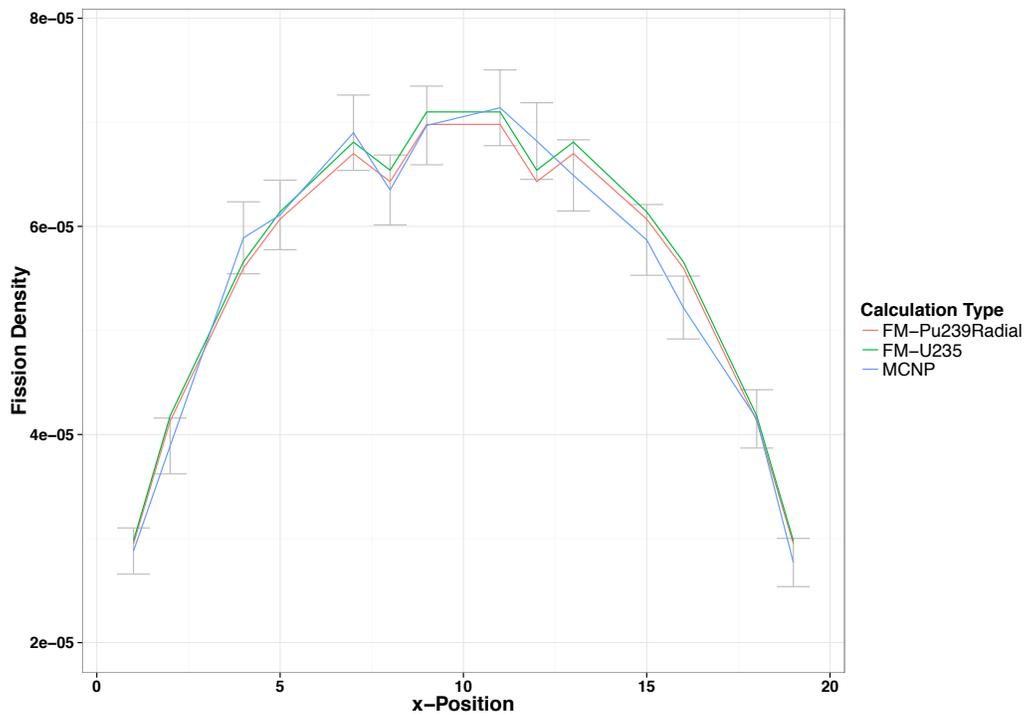


Figure 7. x fission density distribution of a single z -level (z level 72 and $y=10$).

5 CONCLUSIONS AND FUTURE WORK

In this paper, we have introduced a methodology for determination of pin-wise axial-dependent FM coefficients. This study has demonstrated that, depending on the fission spectrum or shape, the FM methodology yields k values in the range of ~ 90 to ~ 700 pcm and M values in the range of ~ 300 to ~ 1600 pcm. The methodology produces accurate axially-dependent, pin-wise fission density distribution within the statistical uncertainty of a reference MCNP calculation. Further, it is demonstrated that the FM methodology yields computational speedups of several orders of magnitude, especially if detailed fission density is needed, e.g., for determination of materials contents.

For future work, we will examine the efficacy of the methodology for a variety of fresh and burned assemblies and pool configurations.

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