# USE OF THE FISSION MATRIX METHOD FOR SOLUTION OF THE EIGENVALUE PROBLEM IN A SPENT FUEL POOL

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#### ABSTRACT

In this paper, we examine the use of the fission-matrix method to calculate the eigenvalue for a spent fuel pool. The fission matrix coefficients are calculated using MCNP5. In order to make the method as efficient as possible for real-time calculations, these coefficients are pre-calculated. Certain simplifying assumptions are made based on geometric considerations, greatly reducing the amount of pre-computation, and allowing the coefficients to be used on a variety of problems beyond that for which the coefficients were calculated. This methodology is applied to a reference pool that is being designed for the I2S-LWR project. Typically, the eigenvalue calculation in Monte Carlo is very difficult for loosely coupled problems such as a spent fuel pool due to source convergence issues, which are not present using the fission matrix. The fission matrix method has shown accuracy very close to that of MCNP5, while giving results in several orders of magnitude less time. Total pre-calculation time was less than a single eigenvalue calculation and can be used across many different pool configurations.

Key Words: spent fuel pool, fission matrix, real-time

### **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, 2]. Aside from being applied to a different problem, this work differs in the much higher level of detail being used. Previously, the fission matrix coefficients were being obtained by using entire assemblies as the spatial cells. Here, we are using individual fuel pins as the basis for the fission matrix cells. This allows not only higher accuracy, but also the ability 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

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*in situ* at the spent fuel site using various detectors. Furthermore, we make use of pre-calculated fission matrix coefficients to be able to quickly calculate eigenvalues and source distributions for a variety of possible scenarios in real-time.

The fission matrix method with Monte Carlo calculations has seen a rise in popularity in recent years[3–5], 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, we 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 fission matrix 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  $(\alpha, n)$  reactions), the induced fission source in cell *i* is given by Equation (1).

$$F_{i} = \sum_{j=1}^{N} (a_{i,j}F_{j} + b_{i,j}S_{j})$$
(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.

$$\vec{F} = \mathbf{A}\vec{F} + \mathbf{B}\vec{S} \tag{2}$$

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

In this work, however, only the eigenvalue problem is examined, as in Eq. (3).

$$F_{i} = \frac{1}{k} \sum_{j=1}^{N} a_{i,j} F_{j}$$
(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 now 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[6]. The I2S-LWR uses a 19x19 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 U-235. Note that for simplicity, we are examining fresh fuel, not spent fuel. Also examined in this paper, are assemblies using 4.45 w-% U-235. Table I summarizes the parameters used to develop the MCNP fuel assembly model.

Table I: I2S-LWR fuel assembly parameters.

Parameter	Value - [cm]					
Fuel Rod Pitch	1.21					
Fuel Rod Length	388.1					
Fuel Rod OD	0.914					
Fuel Rod ID	0.833					
Pellet OD	0.803					
Pellet ID	0.254					
Guide Tube OD	1.105					
Guide Tube ID	1.031					

The spent fuel pool was developed based on the specifications of the Westinghouse AP1000 spent fuel pool [7], which was then modified to accommodate the aforementioned 19x19 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 9x9 array. The neutron absorber used on storage cell walls is the material Metamic [8], an alloy comprised of B<sub>4</sub>C and Al-6061. Table II summaries the parameters used to develop the MCNP spent fuel pool model.

Figure 1a shows a unit cell of the spent fuel pool, including the assembly and cell walls. The entire 9x9 fuel pool section is shown completely filled in Figure 1b.

Parameter	Value - [cm]
Storage Cell Pitch	29.367
Storage Cell Width	24.032
Storage Cell Wall Thickness	0.191
Neutron Absorber Width	20.730
Neutron Absorber Thickness	0.269
Gap Between Absorber and Sheathing	0.031
Neutron Absorber Sheathing Thickness:	
Internal Walls	0.089
Periphery Walls	0.191

**Table II:** I2S-LWR spent fuel pool parameters.



(a) X-Y model of fuel assembly.



(**b**) 9x9 lattice of assemblies spent fuel pool.



# **3. METHODOLOGY**

In theory, the fission matrix method would require N fixed source calculations in order to calculate the NxN fission matrix coefficients. If the cell size is a single pin (as is done in this work), then for an entire 9x9 pool section there would be  $N = 9 \cdot 9 \cdot 336 = 27216$  fuel pins, 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.



(a) Pin Locations for 49 Source Calculations



(**b**) Source Location for Table III

Figure 2: Assembly Source Locations for Fission Matrix Coefficient Calculations

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 for the computational cell.

In order to calculate the coefficients, we start with an MCNP5 [9] model of the 9x9 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 2a. The total fission neutron production rate (i.e.,  $\int dV \phi \nu \sigma_f$ ) is tallied in every surrounding fuel pin. This tally in cell *j* gives  $a_{i,j}$  for the source in cell *i*. Sample results for a fission matrix calculation are shown in Table III. In this table, all values have been multiplied by 100 for readability. The source pin (i.e., cell *i*) is shown in bold and boxed, and is also shown in Figure 2b. Only the one assembly is shown. These 49 calculations were repeated for the two different assembly types (4.95 wt% and 4.45 wt% enrichment). 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.

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. An illustration of the symmetry and translation assumptions is shown in Figure 3. In this figure, all the coefficients indicated by the red arrows are assumed to be identical, as are the blue arrows. Note that there are more coefficients identical to these, but they are not shown for brevity. 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. These assumptions allow us to construct a fission matrix for the entire pool (for  $N = 9 \cdot 9 \cdot 336$  total pins) based on just 49 fixed source calculations. Additionally,

**Table III:** Fission Matrix Coefficients for a Single Source Pin (All Values Multiplied by 100)

0.02	0.04	0.02	0.05	0.00	0.10	0.11	0.1.4	0.10	0.10	0.00	0.04	0.07	0.20	0.00	0.07	0.00	0.00	0.01
0.03	0.04	0.03	0.05	0.06	0.10	0.11	0.14	0.18	0.19	0.23	0.24	0.27	0.30	0.29	0.27	0.26	0.29	0.31
0.03	0.03	0.05	0.08	0.10	0.12	0.16	0.16	0.20	0.28	0.28	0.30	0.39	0.42	0.45	0.39	0.33	0.30	0.27
0.03	0.04	0.06	0.09	0.11	0.00	0.20	0.22	0.28	0.00	0.35	0.43	0.51	0.00	0.54	0.57	0.44	0.38	0.30
0.05	0.06	0.09	0.00	0.14	0.17	0.19	0.25	0.27	0.38	0.45	0.46	0.55	0.69	0.73	0.00	0.65	0.43	0.35
0.04	0.06	0.09	0.12	0.15	0.18	0.23	0.26	0.33	0.45	0.50	0.56	0.66	0.77	0.76	0.82	0.73	0.51	0.41
0.04	0.08	0.00	0.11	0.16	0.00	0.25	0.29	0.39	0.00	0.52	0.60	0.75	0.00	1.02	0.92	0.00	0.65	0.46
0.04	0.06	0.09	0.09	0.13	0.20	0.24	0.28	0.37	0.49	0.51	0.61	0.71	0.98	2.07	0.91	0.73	0.60	0.43
0.03	0.06	0.09	0.08	0.13	0.17	0.22	0.28	0.32	0.40	0.49	0.59	0.71	0.80	0.85	0.82	0.67	0.53	0.39
0.05	0.05	0.08	0.10	0.14	0.18	0.20	0.28	0.31	0.43	0.51	0.54	0.62	0.72	0.72	0.70	0.64	0.51	0.40
0.05	0.05	0.00	0.09	0.13	0.00	0.21	0.22	0.33	0.00	0.44	0.48	0.60	0.00	0.61	0.59	0.00	0.48	0.31
0.04	0.04	0.07	0.09	0.12	0.15	0.19	0.20	0.26	0.35	0.38	0.38	0.44	0.53	0.48	0.52	0.47	0.44	0.26
0.03	0.05	0.06	0.09	0.09	0.14	0.17	0.19	0.22	0.25	0.30	0.33	0.38	0.46	0.40	0.41	0.40	0.35	0.23
0.03	0.04	0.06	0.08	0.09	0.11	0.14	0.15	0.18	0.24	0.26	0.27	0.30	0.39	0.36	0.33	0.32	0.30	0.20
0.03	0.04	0.00	0.07	0.09	0.00	0.11	0.14	0.18	0.00	0.27	0.23	0.28	0.00	0.31	0.29	0.00	0.25	0.16
0.03	0.04	0.05	0.07	0.06	0.08	0.10	0.12	0.17	0.18	0.16	0.19	0.25	0.26	0.24	0.23	0.23	0.19	0.12
0.02	0.03	0.04	0.00	0.06	0.06	0.08	0.09	0.15	0.14	0.15	0.15	0.16	0.22	0.20	0.00	0.16	0.13	0.09
0.02	0.02	0.03	0.04	0.07	0.00	0.06	0.07	0.11	0.00	0.13	0.12	0.14	0.00	0.15	0.16	0.13	0.10	0.08
0.01	0.02	0.02	0.03	0.03	0.05	0.05	0.06	0.07	0.10	0.09	0.10	0.10	0.11	0.10	0.09	0.10	0.09	0.06
0.01	0.01	0.02	0.03	0.02	0.03	0.05	0.04	0.06	0.05	0.06	0.09	0.06	0.06	0.07	0.06	0.06	0.07	0.07

we can use the same coefficients for different assembly arrangements inside the pool. The accuracy of these assumptions is investigated in Section 4.



Figure 3: Rotational and Translational Symmetry of Fission Matrix Coefficients

When a mix of fuel types is simulated in the pool, the coefficients are used from the material type in the destination pin (i.e., the *j* th cell). This approximation assumes that most of the difference in coefficients from material to material is in the value of  $\nu \sigma_f$ , not in  $\sigma_t$ . Regardless, the impact of this should be relatively small since the level of assembly-to-assembly fission is relatively weak due to the presence of the strong absorbers between assemblies.

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

Case #	Number of Assemblies	Fuel Type
1	1x1	4.95%
2	6x1	4.95%
3	3x3	4.95%
4	9x9	4.95%
5	1x1	4.45%
6	6x1	4.45%
7	3x3	4.45%
8	9x9	4.45%
9	2x1	Mixed
10	6x1	Mixed
11	3x3	Mixed

Table IV: Description of Test Cases

with a uniform, normalized source  $F_i^{(0)}$  for the 0<sup>th</sup> iteration, as in Eq. 4.

$$F_i^{(0)} = \frac{1}{N}$$
 (4)

Next, for the m th iteration, we have

$$F_i^{(m+1)} = \frac{1}{k^{(m)}} \sum_{j=1}^N a_{i,j} F_j^{(m)},$$
(5)

where

$$k^{(m)} = \sum_{i=1}^{N} F_i^{(m)}.$$
 (6)

This iteration is stopped once the k changes are below a set tolerance.

### 4. RESULTS

#### 4.1. Test Problems

To test the method, several sample problems were examined. These cases are outlined in Table IV and Figure 4. Cases 1-4 are using only the 4.95% enriched fuel, cases 5-8 are using 4.45% fuel and cases 9-11 involve a mix of assembly types.



Figure 4: Pool Assembly Arrangements for Different Cases

To obtain reference results, all of these cases were run using MCNP5. Depending on the size of the case, between 15,000 and 150,000 histories per cycle were used, with 200-300 active cycles and 100 skipped cycles. For the fission matrix method, the tolerance for the iterative solution method was set at  $10^{-6}$  for *k*-eff. Fission Matrix and MCNP5 results for k-effective, as well as timing information, are shown in Table V. These times are given for a single processor (i.e., not parallel). As mentioned earlier, the total pre-calculation time for the fission matrix coefficients for both materials was 4707 minutes. This single set of pre-calculated data is used for all of the cases, regardless of their configuration.

The fission matrix method gives results very close (within 200 pcm for all cases) to the MCNP calculations, in a fraction of time (after the first pre-calculations are finished). In addition to good keigenvalue agreement, the fission matrix also produces an accurate fission source distribution. The normalized fission sources for the 9 assemblies in cases 3 and 11 are shown in Figure 5. Figure 5b shows asymmetry due to the mix of materials, but in either case, the MCNP results line up very well with the fission matrix results.

Case	Fission	Matrix			MCNP			Com	parison
#	k-eff	time	k-eff	$1$ - $\sigma$	histories	active	time	Diff.	Speedup
		(min)		(pcm)	per cycle	cycles	(min)	(pcm)	
1	0.7905	0.04	0.7903	48	15,000	300	1555	21	35,366
2	0.8317	0.09	0.8324	28	30,000	300	4440	-56	47,037
3	0.8626	0.16	0.8636	25	30,000	300	4206	-143	26,378
4	0.8875	2.69	0.8893	15	150,000	200	11354	-192	4,222
5	0.7759	0.04	0.7751	38	15,000	300	2050	2	46,597
6	0.8162	0.10	0.8161	27	30,000	300	4381	-97	44,852
7	0.8464	0.16	0.8466	27	30,000	300	3344	-157	20,954
8	0.8709	2.50	0.8729	15	150,000	200	11397	-199	4,568
9	0.8076	0.05	0.8091	38	30,000	300	4152	26	80,745
10	0.8253	0.10	0.8260	27	30,000	300	4370	-96	42,599
11	0.8595	0.17	0.8604	27	30,000	300	4253	-135	24,331

 Table V: Test Case Results





Figure 5: Assembly-averaged Eigenfunction (i.e., Fission Source) for Cases 3 and 11

An additional benefit to the fission matrix method is that it does not suffer from the source convergence issue that is notorious in Monte Carlo simulations of loosely coupled systems[5] (as exists in the spent fuel pool with significant inter-assembly absorbers). In the full pool problems (cases 4 and 8), the materials are symmetric and so a symmetric solution is expected. However, the Monte Carlo solution (despite very high computation time) exhibits asymmetry (up to 20% in the corner assemblies), unlike the fission matrix solution. Figure 6 shows the fundamental eigenfunction for case 4, for both MCNP and the fission matrix method.



Figure 6: Principle Eigenfunction for Case 4

The fission matrix results, although fairly accurate (under 200 pcm), still sometimes lie outside the uncertainty bounds of a full Monte Carlo solution. There are several possible causes for this. The first is that the coefficients themselves have uncertainty, though this is expected to be low. Second, there is the assumption that assemblies more than one assembly distance away do not directly affect each other. This factor is small but probably not completely inconsequential. Finally, the assumption is made that the coefficients are the same for all assemblies. This is probably not true for assemblies on the edge of the pool, which might have higher coefficients due to higher reflection from the surrounding water. This item may be considered, an specific coefficients for assemblies on the edge of the array could be used in the future.

# 5. CONCLUSIONS

The fission matrix method described in this paper has given results with near to Monte Carlo accuracy (j200 pcm) in a fraction of the time. By using a pre-calculated database of fission matrix coefficients obtained with MCNP, subsequent calculations have speedups of approximately three to four orders of magnitude. This is fast enough for the subsequent calculations (even with different pool configurations) to be done in seconds of minutes as opposed to hours or days for standard Monte Carlo. The accuracy of the results will enable future work to monitor spent fuel pools for safeguards purposes and to determine material content.

### REFERENCES

- [1] William Walters *et al.* "Calculation of sub-critical multiplication using a simplified fission matrix method." *Transactions of the American Nuclear Society*, **101**: pp. 447–447 (2009).
- [2] —. "A methodology for determination of detector response for inspection of a spent fuel pool." In: *Proceedings of PHYSOR 2010, Advances in Reactor Physics to Power the Nuclear Renaissance*. Pittsburgh, Pennsylvania, USA, May 9-14, 2010 (2010).
- [3] Sean Carney *et al. Fission Matrix Capability for MCNP Monte Carlo. Technical report*, LANL. LA-UR-12-24533 (2012).
- [4] Jan Dufek and Waclaw Gudowski. "Fission matrix based Monte Carlo criticality calculations." *Annals of Nuclear Energy*, **36[8]**: pp. 1270–1275 (2009).
- [5] Michael Wenner and Alireza Haghighat. "A fission matrix based methodology for achieving an unbiased solution for eigenvalue Monte Carlo simulations." *Progress in Nuclear Science and Technology*, **2**: pp. 886–892 (2011).
- [6] Bojan Petrovic, Fausto Franceschini, and Paolo Ferroni. "Fuel cycle cost trade-off studies for I2S-LWR (Integral Inherently Safe LWR) fuel design selection." In: *Proceedings of LWR Fuel Performance Meeting*. Charlotte, NC, September 15-19, 2013 (2013).
- [7] "Spent Fuel Storage Racks Criticality Analysis". AP1000 Standard Combined License Technical Report, APP-GW-GLR-029 Rev. 0, Westinghouse Electric (2006).
- [8] "Use of METAMIC in Fuel Pool Applications". Holtec Information Report No. HI-2022871 Rev. 1, Holtec International (2002).
- [9] X-5 Monte Carlo Team. *MCNP-A General Monte Carlo N-Particle Transport Code, Version 5.* Los Alamos National Laboratory (2005).