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Three Dimensional Two Group Finite Difference Diffusion Equation Solver for CANDU-PHWR Analysis, FDM3D

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ABSTRACT

FDM3D is a three-dimensional(3-D) two group finite difference method diffusion equation solver adopting accelerated iterative schemes such as successive overrelaxation(SOR) or bi-conjugate gradient stabilization method(BICG-STAB) method as inner iteration schemes and Chebyshev two-parameter method or Wielant method as outer iteration schemes. It is designed to achieve an improved efficiency of the CANDU-PHWR analysis by the current RFSP code. For the efficiency test of FDM3D code, the FDM3D with SOR/Chebyshev two-parameter schemes is incorporated into the RFSP code and the benchmark problems have been analyzed by using the physics test data [6] of Wolsong units 2 and 3 and the calculation results of CANFLEX-NU physics design. It is shown that the FDM3D can reduce the CPU time of the current RFSP by 2 to 5 times.

1. INTRODUCTION

The RFSP(Reactor Fuelling Simulation Program)[1] has been the major neutronics analysis program for the core neutronics design and simulation of operational characteristics of CANDU–PHWR. But the RFSP adopts an incomplete two neutron energy group model where the fast fission term is merged into thermal fission term. It also adopts less efficient numerical iterative schemes for solutions of two group finite difference diffusion equations. Because of these, the RFSP may have an unspecified but a certain degree of computational ineffectiveness both in accuracy and computational speed. In an attempt to overcome this weakness of the RFSP, we herein present a 3-D finite difference diffusion equation solver based on the full two group model, FDM3D code, which utilizes the accelerated iteration schemes such as SOR[2][3] or BICG-

STAB[3][4] method as inner iteration schemes and Chebyshev two parameter[2][5] method or Wielandt method[2] as outer iteration schemes.

For the efficiency test of the FDM3D, the benchmark problems have been analyzed by using the physics test data [6] of Wolsong units 2 and 3 and the calculation results of CANFLEX-NU physics design. For this analysis, efficiencies of two options of inner and outer iteration schemes, e.g., SOR/Chebyshev and BICG-STAB/Wielandt schemes are examined. We observed that the former is slightly more efficient than the latter in terms of computational time. Because of this, we incorporated the FDM3D with SOR/Chebyshev iterative schemes into RFSP and the computational efficiency of the resulting FDM3D-RFSP is then compared with that of the existing RFSP. It is demonstrated that the FDM3D can reduce the CPU time of the existing RFSP by 2 to 5 times in most of benchmark problems. Because the FDM3D with SOR/Chebyshev scheme can be readily incorporated into the RFSP with its user-interface untouched, it is concluded that the FDM3D provides a useful and efficient two-group finite difference diffusion equation solver of full two-group model for the improved RFSP.

2. 3-D TWO GROUP FINITE DIFFERENCE DIFFUSION EQUATION SOLVER (FDM3D)

The FDM3D is based on the following 3-D finite difference method diffusion equations of two group model,

$$\underline{\underline{\mathbf{A}}}_1\underline{\Phi}_1 = \frac{1}{k}\left(\underline{\underline{\mathbf{F}}}_1\underline{\Phi}_1 + \underline{\underline{\mathbf{F}}}_2\underline{\Phi}_2\right) \qquad (1)$$

$$\underline{\underline{\mathbf{A}}}_2\underline{\Phi}_2 = \underline{\underline{\mathbf{R}}}\underline{\Phi}_1$$

The notations in Eq.(1) is standard. Note that the fast fission and thermal fission terms are explicitly described in Eq.(1), unlike the current RFSP in which the fast fission term is merged into the thermal fision term.

We adopted two iterative solution schemes for the above two group finite difference equations;SOR/Chebyshev two-parameter method and BICG-STAB/Wielandt method.

As will be shown in section 4, it is found that SOR/Chebyshev two parameter method is slightly more efficient than BICG-STAB/Wielandt scheme in terms of computing speed. So, we incorporated the SOR/Chebyshev two parameter method into the existing RFSP to examine the efficiency of the FDM3D code.

3. BENCHMARK PROBLEMS AND MAIN CONTORL VALUES

The benchmark problems are partly selected in the physics tests of the Wolsong units 2[6] and 3, and partly in the physics design of CANFLEX-NU advanced fuel.

Table 1 shows brief descriptions of the problems on Wolsong units 2 and 3, while Table 2 on CANFLEX-NU advanced fuel design.

Table 3 shows the main control values necessary for the iteration in RFSP input. The variable "OCON " listed below Table 3 denotes the average of relative flux errors, which is used in RFSP output to check the convergence.

Table 1 Description Of Wolsung 2 and 3 Benchmark Problems

Problem Index	Meaning of symbol #	Objective
BC#	Boron Concentration (ppm)	Boron Coefficient Calculation
LZ#	Average Liquid Zone Level (%)	Liquid Zone Worth Calculation
ADJ#	Rod INDEX	ADJ Rod Worth Calculation
ADJBNK#	Bank INDEX	ADJ Bank Worth Calculation
MCA#	Unit INDEX	MCA Worth Calculation
MCABNK#	Bank INDEX	MCA BANK Worth Calculation
SOR#	Rod INDEX	SOR Worth Calculation
MT#	Moderator Temperature (°C)	Moderator Temperature Coefficient
FLUXM#	Case INDEX	FLUX Measurement

Table 2 Description Of CANFLEX-NU Design Benchmark Problems

Problem Index	Meaning of symbol #	Objective
LOADF#	RANDOM	SIMULATION FOR LOAD
ZCR#	RANDOM	SIMULATION FOR ZONE CONTROLLER
XENON#	RANDOM	CALCULATION FOR XENON OSCILLATION

Table 3 Main Control Values For Iteration In 'E' Card Of RFSP Input

Sub Card	Objective	Contents
ISS	Set Inner Iteration Method	0 : sequential solution of fast flux, then thermal flux.(default). 1 : simultaneous solution of fast and thermal fluxes. (most fast but unstable) 2 : simultaneous solution of fast and thermal fluxes. (fast and stable)
KNT	Stabilize SOR Iteration	number of flux iterations for which k_eff is kept fixed at its initial value. Default is 10.
EPS	Judge Flux Errors	flux-shape convergence criterion. Default is 0.001
ALFA	Weighting Factor In SOR Method	Liebmann over-relaxation acceleration parameter. Default is 1.5
IOP	Accelerate Calculation	1 : use subroutine RUSH to speed convergence 2 : don't use subroutine RUSH. (default)
LIM	Constrain Number Of Iteration	Maximum number of flux iterations. Default is 100.

$$OCON = \frac{1}{2M}\sum_{m=1}^{M}\left|\frac{\sum_{g=1}^{2}\Phi^{m,\ t+1}_{\ \ g} - \Phi^{m,\ t}_{\ \ g}}{\sum_{g=1}^{2}\Phi^{m,\ t}_{\ \ g}}\right|$$

4. Results and Discussion

Table 4 and 5 shows a comparison of efficiency of SOR/Chebyshev two parameter method over BICG-STAB/Wielandt method in terms of CPU time for the problems designated B6 and FLUXM4. It is noted that SOR/Chebyshev two parameter method turned out to be faster than BICG-STAB/Wielandt method. To compare the computation speed of two schemes further, we introduced linear fitting function for the logarithmic value of residual norm versus CPU time. Figure 1 shows that SOR/Chebyshev two parameter method is better in most range of residual norm.

Because of the better efficiency of the SOR/Chebyshev scheme and easiness of its implementation in the existing RFSP from the programming standpoint, we incorporated FDM3D based on SOR/Chebyshev scheme into the RFSP code. We noted that the CPU time and convergence of flux errors(OCON) of the resulting RFSP depend on input parameters to the RFSP such as ISS, ALFA, and flux shape convergence criteria(EPS), as displayed in Tables 6 and 7 for solutions of problems, MT45. It is noted from Table 6 and 7 that ALFA(Liebmann factor)=1.5 is the best estimate value for the existing RFSP, and 1.2 for FDM3D-RFSP. It is also noted from Table 7 that FDM3D-RFSP can converge the OCON to the value of 1.0e-11 with great improvement in computational speed.

Tables 8 to 13 and Figure 2 are the computational results by FDM3D-RFSP for benchmark problems of the Wolsong units 2 and 3, which are designed for reactivity worth estimation of control devices such as adjuster rod (ADJ) and banks, mechanical control absorber(MCA) and MCA banks, liquid zone level search and moderator temperature coefficient estimation as well.

Figure 2 shows the flux shape of vanadium detector readings for 102 positions. The result shows maximum flux error 0.05% and average flux error 0.02%.

Table 14 summarizes the efficiency of the FDM3D-RFSP in terms of the benchmark problem solutions. The FDM3D-RFSP is about 1.2 ~ 2.2 faster than RFSP with much better convergence (OCON) always. It must be noted that in all these calculations, we set the values of the control variables by ALFA=1.5 or 1.2, EPS=1.0e-5 ~ 1.0e-4. These results lead us to conclude safely that the FDM3D provides a useful and efficient two-group finite difference diffusion equation solver of full two-group model for the improved RFSP.

Table 4 Comparison of SOR/CHEBY and BICG-STAB/WIELANDT (BC6)

SOR/CHEBY					BICG-STAB/WIELANDT		
Maximum Relative flux Error(1)	OCON(2)	Residual Norm(3)	CPU Time[s]	EPS(4)	Residual Norm	CPU Time[s]	ε(5)
5.25e-4	9.25e-5	2.32e-4	8	1.0e-3	-	-	-
7.27e-5	1.89e-5	4.23e-5	14	1.0e-4	-	-	-
6.07e-6	1.67e-6	3.74e-6	24	1.0e-5	2.33e-6	28	1.0e-3
5.21e-7	1.46e-7	3.25e-7	33	1.0e-6	-	-	-
6.50e-8	1.64e-8	5.79e-8	40	1.0e-7	-	-	-
9.46e-9	1.68e-9	5.90e-9	50	1.0e-8	1.53e-8	53	1.0e-5

Table 5 Comparison of SOR/CHEBY and BICG-STAB/WIELANDT (FLUXM4)

SOR/CHEBY					BICG-STAB/WIELANDT		
Maximum Relative flux Error(1)	OCON(2)	Residual Norm(3)	CPU Time[s]	EPS(4)	Residual Norm	CPU Time[s]	ε(5)
7.26e-4	1.17e-4	2.82e-4	8	1.0e-3	-	-	-
4.24e-5	9.67e-6	2.07e-5	15	1.0e-4	3.57e-5	20	1.0e-3
5.41e-6	1.41e-6	2.98e-6	21	1.0e-5	-	-	-
7.72e-7	2.05e-7	4.31e-7	27	1.0e-6	-	-	-
6.89e-8	1.71e-8	5.66e-8	34	1.0e-7	1.08e-7	42	1.0e-5
7.72e-9	1.24e-9	4.08e-9	43	1.0e-8	-	-	-

$$(1)\quad Maximum\ \ \mathrm{Re}lative\ \ Flux\ \ Error = \max\left|\frac{\sum_{g=1}^{2}\Phi^{m,}{}_{g}{}^{t+1} - \Phi^{m,}{}_{g}{}^{t}}{\sum_{g=1}^{2}\Phi^{m,}{}_{g}{}^{t}}\right|$$

$$(2)\quad OCON = \frac{1}{2M}\sum_{m=1}^{M}\left|\frac{\sum_{g=1}^{2}\Phi^{m,}{}_{g}{}^{t+1} - \Phi^{m,}{}_{g}{}^{t}}{\sum_{g=1}^{2}\Phi^{m,}{}_{g}{}^{t}}\right|$$

where, m is nodeindex , t is iteration step index , g is group index

$$(3)\quad \mathrm{Re}sidual\ \ Norm = \frac{\sqrt{\left((\underline{\underline{A}}\,\underline{x} - \frac{1}{keff}\underline{\underline{F}}\,\underline{x}) \bullet (\underline{\underline{A}}\,\underline{x} - \frac{1}{keff}\underline{\underline{F}}\,\underline{x})\right)}}{\sqrt{\left((\frac{1}{keff}\underline{\underline{F}}\,\underline{x}) \bullet (\frac{1}{keff}\underline{\underline{F}}\,\underline{x})\right)}}$$

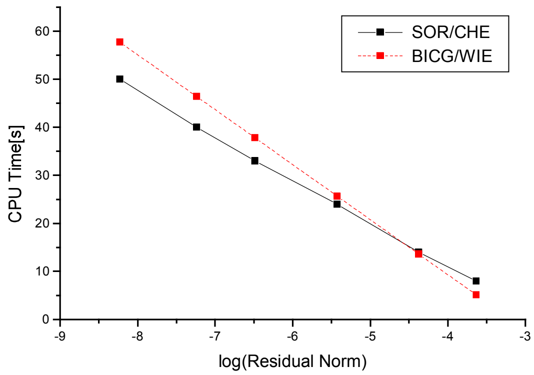
$$(4)\quad EPS\ \ :\ \ Flux - Shape\ \ Convergence\ \ Criterion$$

$$(IF)\ \ Maximum\ \ Flux\ \ Error < EPS\ \ (THEN)\ \ STOP$$

$$(5)\quad \varepsilon\ \ :\ \ \mathrm{Re}sidual\ \ Norm\ \ Convergence\ \ Criterion$$

$$(IF)\ \ \mathrm{Re}sidual\ \ Norm < \varepsilon\ \ (THEN)\ \ STOP$$

Figure 1 Residual Norm Vs CPU Time of SOR/Cheby and BICG-STAB/Wielandt



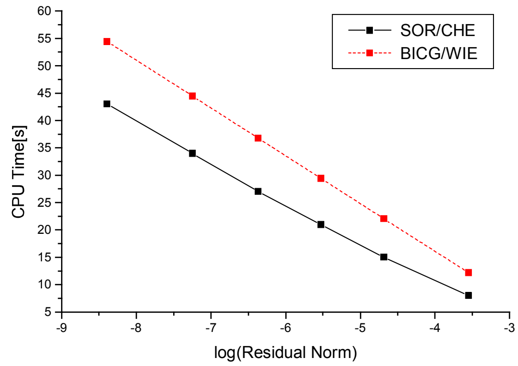


Table 6 Effects of input parameters on computational efficiency of RFSP

ISS	ALFA	RFSP				FDM3D-RFSP			
		Outer Iteration	k_eff	OCON	CPU Time (s)	Outer Iteration	k_eff	OCON	CPU Time (s)
0	1.2	512	0.999569	5.30E-06	19	74	0.999569	5.21E-06	6
	1.5	314	0.999569	4.74E-06	12	100	0.999569	8.46E-07	9
	1.8	Diverge				Diverge			
1	1.2	427	0.999569	5.04E-06	16	66	0.999569	3.41E-06	5
	1.5	258	0.999569	4.64E-06	10	Diverge			
	1.8	Diverge				Diverge			
2	1.2	507	0.999576	4.54E-06	21	73	0.999576	4.60E-06	6
	1.5	325	0.999573	5.23E-06	13	172	0.999571	3.65E-06	15
	1.8	Diverge				Diverge			

Benchmark Problem : MT45

IOP = 1, EPS = 1.0e-5, LIM=900

Table 7 Effects of input parameters on Computational efficiency

ALFA	EPS	RFSP				FDM3D-RFSP			
		Outer Iteration	k_eff	OCON	CPU Time (s)	Outer Iteration	k_eff	OCON	CPU Time (s)
1.2	1.00E-04	118	0.999567	5.16E-05	4	30	0.999564	4.78E-05	3
	1.00E-05	512	0.999569	5.30E-06	19	74	0.999569	5.21E-06	6
	1.00E-06	998	0.999569	3.57E-07	53	122	0.999569	3.15E-07	10
	1.00E-07	Out of convergence range				193	0.999569	6.59E-11	16
1.5	1.00E-04	118	0.999569	4.42E-05	5	75	0.999570	4.26E-06	6
	1.00E-05	314	0.999569	4.74E-06	12	100	0.999569	8.46E-07	9
	1.00E-06	Out of convergence range				Out of convergence range			
	1.00E-07	Out of convergence range				Out of convergence range			

Benchmark Problem : MT45

IOP = 1, ISS=0, IF (Maximum Flux Error >= 1.0e-11) STOP

Table 8 Reactivity Worth of Adjuster Rods

	RFSP					FDM3D-RFSP				
	Outer Iteration	E.R (mk)	k_eff	OCON	CPU Time (sec)	Outer Iteration	E.R (mk)	k_eff	OCON	CPU Time (sec)
Ref	252	-0.134	0.999866	9.24E-06	11	64	-0.135	0.999865	4.81E-06	5
ADJ1	281	0.095	1.000100	1.16E-05	12	52	0.090	1.000090	4.03E-06	5
ADJ2	238	0.444	1.000440	8.79E-06	10	52	0.441	1.000440	3.47E-06	4
ADJ3	231	0.601	1.000600	8.41E-06	10	40	0.604	1.000600	6.81E-06	3
ADJ4	262	0.251	1.000250	7.87E-06	11	52	0.252	1.000250	4.12E-06	4
ADJ5	234	0.594	1.000590	7.37E-06	10	52	0.600	1.000600	4.25E-06	5
ADJ6	236	0.441	1.000440	6.93E-06	10	52	0.445	1.000450	5.33E-06	5
ADJ7	215	0.088	1.000090	7.92E-06	9	52	0.088	1.000090	3.26E-06	5
ADJ8	268	0.123	1.000120	8.55E-06	11	63	0.124	1.000120	3.11E-06	5
ADJ9	266	0.582	1.000580	8.58E-06	11	52	0.573	1.000570	4.11E-06	5
ADJ10	197	0.800	1.000800	7.72E-06	8	39	0.794	1.000800	6.36E-06	4
ADJ11	268	0.378	1.000380	6.49E-06	11	52	0.378	1.000380	3.47E-06	5
ADJ12	238	0.788	1.000790	8.61E-06	10	52	0.794	1.000790	3.93E-06	4
ADJ13	246	0.576	1.000580	6.90E-06	10	52	0.573	1.000570	2.32E-06	4
ADJ14	249	0.126	1.000130	8.60E-06	11	52	0.124	1.000120	4.64E-06	4
ADJ15	281	0.090	1.000090	8.12E-06	11	74	0.090	1.000090	2.04E-06	6
ADJ16	245	0.445	1.000440	8.30E-06	10	62	0.450	1.000450	7.70E-06	5
ADJ17	214	0.598	1.000600	6.24E-06	9	40	0.599	1.000600	5.95E-06	3
ADJ18	249	0.245	1.000250	6.21E-06	10	52	0.251	1.000250	4.21E-06	5
ADJ19	253	0.595	1.000590	5.68E-06	10	52	0.603	1.000600	6.32E-06	5
ADJ20	213	0.437	1.000440	7.58E-06	9	52	0.436	1.000440	3.14E-06	5
ADJ21	218	0.087	1.000090	7.71E-06	9	52	0.095	1.000090	6.12E-06	4
Average	243	-	-	7.88E-06	10.14	53	-	-	4.52E-06	4.55

ISS=2, KNT=4, EPS=0.00002, ALFA=1.5, IOP=1, LIM=500

Table 9 Reactivity Worth of Adjuster Banks

	RFSP					FDM3D-RFSP				
	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)
Ref	242	-0.426	0.999574	7.61E-06	10	72	-0.423	0.999577	5.07E-06	6
ADJBNK1	155	0.970	1.000970	8.11E-06	6	49	0.964	1.000970	4.01E-06	5
ADJBNK2	195	2.521	1.002530	8.29E-06	8	52	2.523	1.002530	4.87E-06	5
ADJBNK3	196	4.057	1.004070	7.36E-06	8	52	4.055	1.004070	4.95E-06	5
ADJBNK4	149	6.364	1.006410	6.83E-06	6	54	6.377	1.006420	8.02E-06	5
ADJBNK5	172	8.102	1.008170	7.84E-06	7	43	8.098	1.008160	5.84E-06	3
ADJBNK6	171	9.864	1.009960	8.14E-06	7	50	9.881	1.009980	1.07E-05	5
ADJBNK7	177	13.009	1.013180	9.14E-06	7	44	13.011	1.013180	5.75E-06	4
Average	182	-	-	7.92E-06	7.38	52	-	-	6.15E-06	5.43

ISS=2, KNT=4, EPS=0.00002, ALFA=1.5, IOP=1, LIM=500

Table 10 Reactivity Worth of MCA

	RFSP					FDM3D-RFSP				
	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)
Ref	242	-0.426	0.999574	7.61E-06	10	72	-0.423	0.999577	5.07E-06	7
MCA1	352	-2.520	0.997486	8.75E-06	14	64	-2.524	0.997482	4.45E-06	6
MCA2	351	-2.512	0.997494	6.69E-06	15	75	-2.508	0.997498	4.10E-06	6
MCA3	363	-2.522	0.997484	6.56E-06	15	86	-2.521	0.997485	3.26E-06	8
MCA4	368	-2.508	0.997498	5.98E-06	15	87	-2.500	0.997506	6.80E-06	7
Average	335	-	-	7.12E-06	13.80	77	-	-	4.74E-06	4.86

ISS=2, KNT=4, EPS=0.00002, ALFA=1.5, IOP=1, LIM=500

Table 11 Reactivity worth of MCA Bank

	RFSP					FDM3D-RFSP				
	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)
Ref	242	-0.426	0.999574	7.61E-06	10	72	-0.423	0.999577	5.07E-06	6
MCABNK1	222	-6.040	0.993996	6.72E-06	9	52	-6.039	0.993997	4.56E-06	4
MCABNK2	268	-6.039	0.993997	7.41E-06	11	52	-6.040	0.993996	3.19E-06	5
Average	244	-		7.25E-06	10.00	52	-		4.27E-06	5.00

ISS=2, KNT=4, EPS=0.00002, ALFA=1.5, IOP=1, LIM=500

Table 12 Liquid Zone Level Search

	RFSP					FDM3D-RFSP				
	Outer Iteration	AVZL	k_eff	OCON	CPU Time (sec)	Outer Iteration	AVZL	k_eff	OCON	CPU Time (sec)
LZ74	377	0.74024	1.000010	4.96E-06	18	75	0.74015	1.000010	4.22E-06	8
LZ54	262	0.54115	0.999997	3.94E-06	13	94	0.54044	1.000000	2.92E-06	9
Average	320	-		4.45E-06	15.50	85	-		3.57E-06	8.50

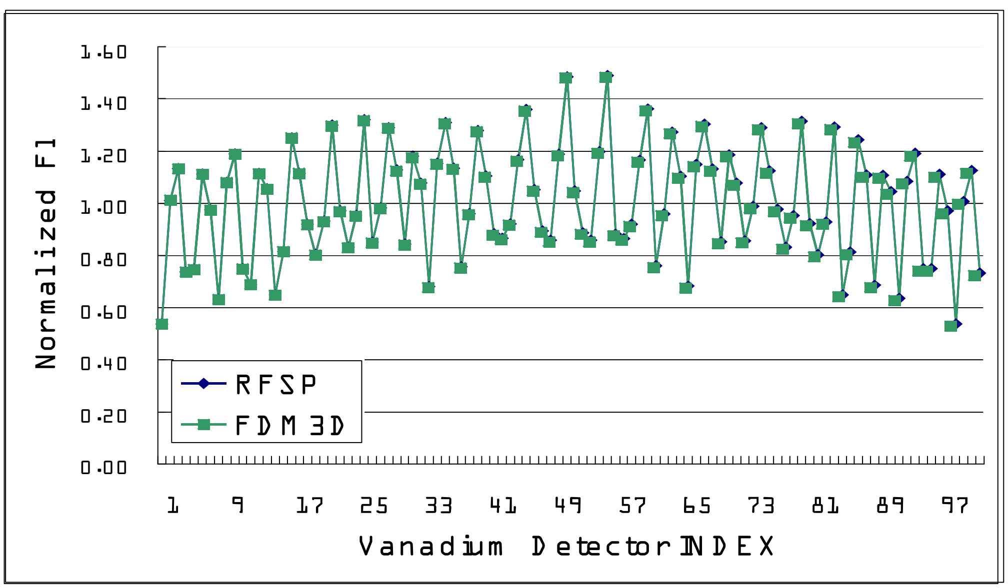
ISS=0, KNT=10, EPS=0.00001, ALFA=1.2, IOP=2, LIM=700

Table 13 Estimation of MTC

	RFSP					FDM3D-RFSP				
	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)	Outer Iteration	E.R.(mk)	k_eff	OCON	CPU Time (sec)
MT40	315	-5.973	0.994062	3.97E-06	13	74	-5.980	0.994056	1.19E-06	7
MT50	327	-5.737	0.994296	4.17E-06	14	87	-5.735	0.994298	3.68E-06	8
Average	321	-		4.07E-06	13.50	81	-		2.43E-06	7.50

ISS=0, KNT=10, EPS=0.00001, ALFA=1.5, IOP=2, LIM=700

Figure 2 Comparison of Flux Shape (Vanadium Detector Readings)



Maximum Flux Error = 0.05 % (Reference : RFSP)

Average Flux Error = 0.02 %

Benchmark Problem : FLUXM2 (ADJS IN, MCA#4 50% IN)

Table 14 SUMMARY of RFSP and FDM3D Analysis

Problems	Number of Cases	RFSP		FDM3D/RFSP		OCON RATIO (RFSP / FDM3D-RFSP)	CPU TIME RATIO (RFSP/ FDM3D-RFSP)
		OCON	CPU TIME (sec)	OCON	CPU TIME (sec)		
ADJ (See Table8)	22	7.88E-06	10.14	4.52E-06	4.55	1.74	2.23
ADJBNK (See Table9)	8	7.92E-06	7.38	6.15E-06	4.75	1.29	1.55
MCA (See Table10)	5	7.12E-06	13.8	4.74E-06	6.8	1.5	2.03
MCABNK (See Table11)	3	7.25E-06	10	4.27E-06	5	1.7	2
SOR	29	7.85E-06	13.48	5.20E-06	6.14	1.51	2.2
LZ (See Table12)	2	4.45E-06	15.5	3.57E-06	8.5	1.25	1.82
MT (See Table13)	2	4.07E-06	13.5	2.43E-06	7.5	1.67	1.8
LOADF	15	3.28E-06	44.73	2.52E-06	24.73	1.3	1.81
ZCR	5	3.69E-06	7.2	2.58E-06	5	1.43	1.44
XENON	16	4.59E-06	6.31	2.63E-06	5.19	1.74	1.22

ACKNOWLEDGEMENT

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