WIMS-AECL CALCULATIONS FOR THE DOPPLER COEFFICIENT OF REACTIVITY

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INTRODUCTION

The Doppler coefficient of reactivity is an important parameter in the evaluation of reactor transients. The Doppler feedback, associated with changes in fuel temperature when a reactor goes from hot zero power to hot full power, is a relatively small effect which is difficult to measure directly. It is usually derived from other measured parameters. In two recent papers[1,2], Mosteller et al. calculated the Doppler coefficients for an infinite lattice of slightly idealized pressurized-water reactor pin cells using the MCNP-3A[3] Monte Carlo code with data[4] generated from the ENDF/B-V nuclear data library. The results were used as a set of numerical benchmarks to evaluate the accuracy of the CELL-2[5] code, a module within the EPRI-PRESS package for PWR lattice analysis.

At AECL, the WIMS-AECL[6] lattice code is often used in reactor physics calculations. It is of interest to compare the Doppler coefficients predicted by WIMS-AECL to those calculated by MCNP-3A. This study also serves as a numerical benchmark validation of WIMS-AECL.

LATTICE DESCRIPTION

The MCNP-3A calculations were performed for an infinite array of infinitely long pin cells. A three-region pin cell was used in the study. It consists of a circular fuel pellet region of 0.39306 cm radius surrounded by a cladding with an outer radius of 0.45802 cm. The pin cell pitch is 1.26209 cm square. The gap between the fuel pellet and the cladding was homogenized with the natural zirconium cladding.

The fuel temperatures at hot zero power and at hot full power were assumed to be 600 K and 900 K, respectively. The same pin cell dimensions were used in the MCNP-3A calculations for the fuel at 600 K and at 900 K. This was confirmed in a private communication with R.D. Mosteller. The changes in dimensions were supposed to be accounted for by the changes in density of the fuel and the cladding.

The cladding and moderator were assumed to be at a temperature of 600 K. The number density of the natural zirconium cladding was 0.0383243 atom/b.cm when the fuel was at 600 K and 0.0389087 atom/b.cm when the fuel was at 900 K. The isotopes in the light-water moderator were H^1, B^{10} and O^{16} and their concentrations were 0.0442326, 0.0000102133 and 0.0221163 atom/b.cm, respectively.

Uranium oxide fuel of various enrichments and mixed-oxide fuel with 1 and 2 atom percent (a/o) of plutonium were used in the studies. The uranium oxide fuel represents fresh fuel, while the mixed-oxide fuel represents fuel at high exposures. The uranium in the uranium oxide fuel pellet was assumed to contain only U^{235} and U^{238}. The isotopic concentrations of the fuel are shown in Table 1.

Table 1
Isotopic Concentrations of the Fuel

Uranium Oxide Fuel

Enrich. (wt%)	Temperature (K)	Number Density (atom/b.cm) O^{16}	U^{235}	U^{238}
0.711	600	0.0461309	0.000166078	0.0228994
1.6	600	0.0461355	0.000373729	0.0226940
2.4	600	0.0461397	0.000560588	0.0225093
3.1	600	0.0461433	0.000724086	0.0223476
3.9	600	0.0461475	0.000910933	0.0221163
0.711	900	0.0457561	0.000164729	0.0227133
1.6	900	0.0457607	0.000370693	0.0225096
2.4	900	0.0457648	0.000556033	0.0223264
3.1	900	0.0457684	0.000718202	0.0221660
3.9	900	0.0457725	0.000903532	0.0219827

Mixed Oxide Fuel

	Number Density (atom/b.cm) At 600 K		At 900 k	
Pu a/o	1	2	1	2
O^{16}	0.0461309	0.0461309	0.0457561	0.0457561
U^{235}	0.000164417	0.000162756	0.000163082	0.000161435
U^{238}	0.0226704	0.0224414	0.0224862	0.0222591
Pu^{239}	0.000103795	0.000207590	0.000102951	0.000205902
Pu^{240}	0.0000691965	0.000138393	0.0000686430	0.000137286
Pu^{241}	0.0000345983	0.0000691966	0.0000343170	0.0000686340
Pu^{242}	0.0000230655	0.0000461310	0.0000228780	0.0000457560

CALCULATIONS WITH WIMS-AECL

The pin cell geometry was modelled in WIMS-AECL Version 90-04-18 (Frozen), and the infinite lattice array was simulated by applying reflective boundary conditions. The WIMS ENDF/B-V Data Library[7] Version 89-03-29 (Frozen) was used.

In WIMS-AECL, the spatial mesh for the neutron transport calculation may be specified explicitly in the input, or the "MESH # n" option may be chosen. If the "MESH # n" option is chosen, WIMS-AECL will calculate and assign a mesh with n mesh points per mean free path length in each region. If n is not specified, the default value of 2.5 mesh points per mean free path length is used. Using PERSEUS, the collision probability neutron transport method in WIMS-AECL, a mesh study was performed to see if the meshes assigned by this default option were adequate. Two infinite lattice cases, one with 0.711% enriched fuel at 600 K and the other with 3.9% enriched fuel at 900 K, were used. The number of mesh points selected by WIMS-AECL was doubled for each case and the k-infinities were calculated. The results, shown in Table 2, indicate that the meshes chosen by the default "MESH #" option were adequate for these cases. This option was used in all subsequent calculations.

Table 2
Mesh Study

Fuel		Number of mesh points in			k-infinity
Enr.(wt%)	Temp.(K)	Fuel	Clad	Moderator	
0.711	600	2	1	4	0.66502
0.711	600	4	2	8	0.66500
3.9	900	3	1	4	1.22757
3.9	900	6	2	8	1.22753

Calculations were performed using the DSN and PERSEUS neutron transport methods in WIMS-AECL with the full 89-group neutron energy structure in the WIMS ENDF/B-V Data Library. Another set of PERSEUS calculations using a condensed 32-group energy structure, frequently used in light-water reactor studies at Chalk River, was also performed. The group structures are given in Table A1 of the Appendix. The convergence criterion on the eigenvalue was set to 1.0×10^{-6}.

WIMS-AECL RESULTS

Uranium Oxide Fuel

The k-infinities computed for the cases with uranium oxide fuel are compared with those from MCNP-3A calculations in Table 3.

CELL-2 results from (1) and (2) are also included, for comparison.

Table 3
Comparison of k-infinities for Uranium Oxide Fuel

Fuel Enr. (wt%)	Fuel Temp. (K)	MCNP-3A	CELL-2	WIMS-AECL DSN 89 GROUPS	WIMS-AECL PERSEUS 89 GROUPS	WIMS-AECL PERSEUS 32 GROUPS
0.711	600	0.6638 ± 0.0006	0.6652	0.6644	0.6650	0.6649
	900	0.6567 ± 0.0008	0.6578	0.6568	0.6573	0.6572
1.6	600	0.9581 ± 0.0006	0.9605	0.9589	0.9597	0.9596
	900	0.9484 ± 0.0006	0.9507	0.9490	0.9498	0.9497
2.4	600	1.0961 ± 0.0007	1.0989	1.0967	1.0977	1.0975
	900	1.0864 ± 0.0007	1.0883	1.0862	1.0871	1.0870
3.1	600	1.1747 ± 0.0007	1.1773	1.1747	1.1757	1.1755
	900	1.1641 ± 0.0006	1.1663	1.1638	1.1649	1.1647
3.9	600	1.2379 ± 0.0006	1.2404	1.2379	1.2390	1.2388
	900	1.2271 ± 0.0006	1.2291	1.2264	1.2276	1.2273

The change in reactivity due to the Doppler effect for each fuel enrichment was calculated by:

$$\text{Reactivity change} = (1/k_{600} - 1/k_{900})1000 \quad \text{mk}$$

where k_{600} and k_{900} are the k-infinities when the fuel temperatures are 600 K and 900 K, respectively. The changes in reactivity are compared in Table 4 and the Doppler reactivity coefficients are shown in Table 5.

Table 4
Comparison of Reactivity Change (mk) from 600 K to 900 K

Fuel Enrichment (wt%)	MCNP-3A	CELL-2	WIMS-AECL DSN 89 GROUPS	WIMS-AECL PERSEUS 89 GROUPS	WIMS-AECL PERSEUS 32 GROUPS
0.711	-16.3 ± 2.3	-16.8	-17.4	-17.6	-17.6
1.6	-10.8 ± 0.9	-10.7	-10.9	-10.9	-10.9
2.4	- 8.1 ± 0.8	- 8.9	- 8.8	- 8.9	- 8.8
3.1	- 7.8 ± 0.7	- 8.0	- 8.0	- 7.9	- 7.9
3.9	- 7.1 ± 0.6	- 7.1	- 7.6	- 7.5	- 7.6

Table 5
Comparison of Doppler Coefficient of Reactivity (mk/K)

Fuel Enrichment (wt%)	MCNP-3A	CELL-2	WIMS-AECL DSN 89 GROUPS	WIMS-AECL PERSEUS 89 GROUPS	WIMS-AECL PERSEUS 32 GROUPS
0.711	-0.054 ± 0.008	-0.056	-0.058	-0.059	-0.059
1.6	-0.036 ± 0.003	-0.036	-0.036	-0.036	-0.036
2.4	-0.027 ± 0.003	-0.030	-0.029	-0.030	-0.029
3.1	-0.026 ± 0.002	-0.027	-0.027	-0.026	-0.026
3.9	-0.024 ± 0.002	-0.024	-0.025	-0.025	-0.025

Mixed Oxide Fuel

The corresponding results for the mixed oxide fuel are shown in Tables 6, 7 and 8, respectively.

Table 6
Comparison of k-infinities for Mixed-Oxide Fuel

Pu Conc. (a/o)	Fuel Temp. (K)	MCNP-3A	CELL-2	WIMS-AECL DSN 89 GROUPS	WIMS-AECL PERSEUS 89 GROUPS	WIMS-AECL PERSEUS 32 GROUPS
1.0	600	0.9445 ± 0.0007	0.9478	0.9409	0.9417	0.9413
	900	0.9347 ± 0.0007	0.9366 0.9383*	0.9314	0.9322	0.9318
2.0	600	1.0182 ± 0.0007	1.0231	1.0123	1.0133	1.0129
	900	1.0077 ± 0.0007	1.0112 1.0135*	1.0024	1.0034	1.0029

(* Values using improved CELL-2 calculations, in which the scattering temperature for O^{16} in the fuel region was at 900 K instead of 600 K as in the standard CELL-2 calculations.)

Table 7
Comparison of Reactivity Change (mk) from 600 K to 900 K

Pu Conc. (a/o)	MCNP-3A	CELL-2	WIMS-AECL DSN 89 GROUPS	WIMS-AECL PERSEUS 89 GROUPS	WIMS-AECL PERSEUS 32 GROUPS
1.0	-11.1 ± 1.1	-12.6 -10.7*	-10.8	-10.8	-10.8
2.0	-10.2 ± 1.0	-11.5 - 9.3*	- 9.8	- 9.7	- 9.8

(* Values using improved CELL-2 calculations.)

Table 8
Comparison of Doppler Coefficient of Reactivity (mk/K)

Pu Conc. (a/o)	MCNP-3A	CELL-2	WIMS-AECL DSN 89 GROUPS	WIMS-AECL PERSEUS 89 GROUPS	WIMS-AECL PERSEUS 32 GROUPS
1.0	-0.037 ± 0.004	-0.042 -0.036*	-0.036	-0.036	-0.036
2.0	-0.034 ± 0.003	-0.038 -0.031*	-0.033	-0.032	-0.033

(* Values using improved CELL-2 calculations.)

OBSERVATIONS

MCNP-3A calculations with a million neutron histories were run by Mosteller et al. for each of the fourteen cases, resulting in standard deviations of no more than 0.0007 in the k-infinities. This produced standard deviations of the order of 10 percent in the Doppler coefficient of reactivity. The MCNP-3A calculations for each case took about 10 days on a Micro VAX-II (about 8 hours on a Cray-1).

DSN Calculations

The k-infinities predicted by the DSN calculations in WIMS-AECL for the cases with uranium oxide fuel are within the single standard deviation of the MCNP-3A predictions. The Doppler coefficients are therefore in excellent agreement with the MCNP-3A results. The calculations for each case took about 11 seconds on the CDC 990 mainframe computer at Chalk River Laboratories.

For the mixed-oxide fuel, the DSN calculations produced k-infinities that are less than those computed by MCNP-3A: 4 mk less for the 1 a/o Pu fuel and about 6 mk less for the 2 a/o Pu fuel. The cancellation of these biases in calculating the reactivity differences produce Doppler coefficients that are in excellent agreement with the MCNP-3A results. The calculations took about 14 seconds for the 1 a/o Pu cases and about 16 seconds for the 2 a/o Pu cases.

PERSEUS Calculations

The PERSEUS 32-group reactivity for each case is within 0.2 mk of the corresponding reactivity calculated using 89 groups. This shows that using 32 groups would be sufficient for these cases. The 89-group PERSEUS calculations took about 2, 3 and 5 seconds for the uranium oxide, the 1 a/o Pu and the 2 a/o Pu cases, respectively, on the CDC 990, and the 32-group PERSEUS calculations took about 1, 1 and 2 seconds for the corresponding cases.

Compared to MCNP-3A, the PERSEUS calculations overpredict the k-infinities of the uranium oxide cases by about 1 mk. PERSEUS underpredicts the k-infinities by 3 mk for the 1 a/o Pu fuel, and by about 5 mk for the 2 a/o Pu fuel when compared to those predicted by MCNP-3A. Again, the cancellation of these biases in calculating the reactivity differences produces Doppler coefficients that are in excellent agreement with the MCNP-3A results.

CONCLUSIONS

WIMS-AECL calculations of the Doppler coefficient of reactivity are in excellent agreement with those predicted by MCNP-3A, and are within the single standard deviation associated with the MCNP calculations.

The k-infinities calculated by the DSN calculations for the uranium oxide cases are the same as those given by MCNP-3A. For the mixed-oxide fuel, DSN calculations give k-infinities that are 4 to 6 mk less than those computed by MCNP-3A. The PERSEUS calculations overpredict the k-infinities of the uranium oxide cases by about 1 mk, and underpredict the k-infinities of the mixed-oxide cases by 3 to 5 mk when compared to MCNP-3A results.

It was also shown that using the PERSEUS calculation method with the ENDF/B-V library, the 32-group neutron energy structure with the "MESH #" option is adequate for reactivity calculations of pin cells with fresh slightly enriched uranium oxide and light-water moderator.

This study shows that the WIMS-AECL lattice code, together with the WIMS ENDF/B-V data library, can predict the Doppler coefficient of light-water reactor fuel with good accuracy. The results could be used in SLOWPOKE or MAPLE reactor calculations, and in the validation of similar calculations for other reactors using WIMS-AECL.

References

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Appendix

Table A1
89- and 32-Group Structures
(WIMS-AECL ENDF/B-V Data Library)

Energy(eV)	89	32
1.0000E+07 - 7.7880E+06	1	
7.7880E+06 - 6.0653E+06	2	1
6.0653E+06 - 4.7237E+06	3	
4.7237E+06 - 3.6788E+06	4	
3.6788E+06 - 2.8650E+06	5	
2.8650E+06 - 2.2313E+06	6	
2.2313E+06 - 1.7377E+06	7	2
1.7377E+06 - 1.3534E+06	8	
1.3534E+06 - 1.0540E+06	9	
1.0540E+06 - 8.2085E+05	10	
8.2085E+05 - 6.3928E+05	11	3
6.3928E+05 - 4.9787E+05	12	
4.9787E+05 - 3.8774E+05	13	
3.8774E+05 - 3.0197E+05	14	
3.0197E+05 - 2.3518E+05	15	
2.3518E+05 - 1.8316E+05	16	
1.8316E+05 - 1.4264E+05	17	4
1.4264E+05 - 1.1109E+05	18	
1.1109E+05 - 8.6517E+04	19	
8.6517E+04 - 6.7379E+04	20	
6.7379E+04 - 4.0868E+04	21	
4.0868E+04 - 2.4788E+04	22	
2.4788E+04 - 1.5034E+04	23	5
1.5034E+04 - 9.1188E+03	24	
9.1188E+03 - 5.5308E+03	25	
5.5308E+03 - 3.3546E+03	26	
3.3546E+03 - 2.0347E+03	27	
2.0347E+03 - 1.2341E+03	28	6
1.2341E+03 - 7.4852E+02	29	
7.4852E+02 - 4.5400E+02	30	
4.5400E+02 - 2.7536E+02	31	
2.7536E+02 - 1.6702E+02	32	
1.6702E+02 - 1.3007E+02	33	
1.3007E+02 - 1.0130E+02	34	
1.0130E+02 - 7.8893E+01	35	7
7.8893E+01 - 6.1442E+01	36	
6.1442E+01 - 4.7851E+01	37	
4.7851E+01 - 3.7267E+01	38	
3.7267E+01 - 2.9023E+01	39	8
2.9023E+01 - 2.2603E+01	40	
2.2603E+01 - 1.7603E+01	41	
1.7603E+01 - 1.3710E+01	42	9
1.3710E+01 - 1.0677E+01	43	
1.0677E+01 - 8.3153E+00	44	
8.3153E+00 - 6.4760E+00	45	
6.4760E+00 - 5.0435E+00	46	10
5.0435E+00 - 4.0000E+00	47	
4.0000E+00 - 3.3000E+00	48	11
3.3000E+00 - 2.6000E+00	49	12
2.6000E+00 - 2.1000E+00	50	13
2.1000E+00 - 1.5000E+00	51	14
1.5000E+00 - 1.3000E+00	52	
1.3000E+00 - 1.1500E+00	53	15
1.1500E+00 - 1.1230E+00	54	16
1.1230E+00 - 1.0970E+00	55	
1.0970E+00 - 1.0710E+00	56	
1.0710E+00 - 1.0450E+00	57	17
1.0450E+00 - 1.0200E+00	58	
1.0200E+00 - 9.9600E-01	59	18
9.9600E-01 - 9.7200E-01	60	
9.7200E-01 - 9.5000E-01	61	19
9.5000E-01 - 9.1000E-01	62	20
9.1000E-01 - 8.5000E-01	63	
8.5000E-01 - 7.8000E-01	64	21
7.8000E-01 - 6.2500E-01	65	
6.2500E-01 - 5.0000E-01	66	22
5.0000E-01 - 4.0000E-01	67	
4.0000E-01 - 3.5000E-01	68	23
3.5000E-01 - 3.2000E-01	69	
3.2000E-01 - 3.0000E-01	70	
3.0000E-01 - 2.8000E-01	71	24
2.8000E-01 - 2.5000E-01	72	
2.5000E-01 - 2.2000E-01	73	25
2.2000E-01 - 1.8000E-01	74	
1.8000E-01 - 1.4000E-01	75	26
1.4000E-01 - 1.0000E-01	76	27
1.0000E-01 - 8.0000E-02	77	28
8.0000E-02 - 6.7000E-02	78	
6.7000E-02 - 5.8000E-02	79	29
5.8000E-02 - 5.0000E-02	80	
5.0000E-02 - 4.2000E-02	81	
4.2000E-02 - 3.5000E-02	82	30
3.5000E-02 - 3.0000E-02	83	
3.0000E-02 - 2.5000E-02	84	
2.5000E-02 - 2.0000E-02	85	31
2.0000E-02 - 1.5000E-02	86	
1.5000E-02 - 1.0000E-02	87	
1.0000E-02 - 5.0000E-03	88	32
5.0000E-03 - 2.0000E-04	89	