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Verification of Two-Group *CERBERUS for a Loss-of-Coolant Analysis in a Simplified Reactor Model

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Abstract

A true two-energy-group three-dimensional neutron-kinetics module with history-based local-parameter lattice-cell calculations has been implemented in the *CERBERUS module of the Reactor Fuelling Simulation Program (RFSP). This project was conducted as part of the qualification of the RFSP code for analyses with lattice-cell parameters derived using the WIMS–AECL code. One component of the implementation of this calculational method is the qualification of the coding through testing and verification in computational benchmarks. In the computational benchmark problem analyzed in this paper, a simplified loss-of-coolant accident in a stylized CANDU® reactor is analyzed. The results of the benchmark problem analyses indicate proper performance of the two-energy-group version of *CERBERUS.

1 Introduction

A true two-energy-group three-dimensional neutron-kinetics module with history-based local-parameter lattice-cell calculations [1] has been implemented in the *CERBERUS module of the Reactor Fuelling Simulation Program (RFSP) [2]. History-based lattice-cell calculations is a method in which the unique history of each fuel bundle in a reactor core is simulated, and local-parameter lattice-cell calculations utilize the unique local conditions (in terms of state variables such as coolant density) of each fuel bundle. This project was conducted as one component of the qualification of the RFSP code for analyses with lattice-cell parameters derived using the WIMS–AECL [3, 4] code, which is replacing POWDERPUFS-V [5] (PPV) in this application. The true two-energy-group neutron flux solution replaces the existing one-and-a-half group (the one-and-a-half group approximation lumps non-thermal fissions into the thermal energy group and ignores up-scattering) neutron flux solution in *CERBERUS.

A necessary component of the implementation of this calculational method is the qualification of the coding through testing and verification in computational benchmarks. Although benchmarks are available for the verification of neutron kinetics calculations (such as that specified in Reference 6), the published benchmarks that have been found do not test all the features of this *CERBERUS implementation. The following are the key features that need to be tested in *CERBERUS:

1. To test the behaviour of the new two-energy-group neutron flux calculation, this calculation should be compared with the existing one-and-a-half group neutron flux calculation.
2. The implementation of the *CERBERUS interface to the history-based local-parameter lattice-cell calculation using the simple-cell method [7] (SCM) needs to be verified. The SCM is a high-speed lattice-cell calculation designed to produce results consistent with WIMS–AECL (but at speeds 100 to 200 times faster) which enables practical WIMS–AECL-based history-based local-parameter CANDU reactor analyses. The analyses in this paper do not test the history-based component of the calculations.

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3. The accuracy of the SCM calculation in this application needs to be assessed, relative to WIMS–AECL. SCM is a high-speed lattice-cell calculation designed to produce results very similar to those of WIMS–AECL.
4. The proper behaviour of the complete system of the above components under the conditions typical of a CANDU reactor during a postulated loss-of-coolant accident (LOCA) needs to be verified.

The stylized problem to be used in this verification is described as follows:

- The reactor to be analyzed is smaller than an actual CANDU reactor, having only 119 fuel channels and 1190 fuel bundles (about 25% of the number of fuel channels). This configuration is referred to as the "Baby CANDU".
- The fuel in the core is fresh natural uranium at a normal CANDU lattice spacing of 28.575 cm. Sufficient boron is added to the moderator to reduce the eigenvalue in the reference configuration to near unity.
- The only devices represented in the core are 12 shut-off rods, which are represented by an incremental thermal-absorption cross section applied over finite regions of the core.
- A simplified coolant density, coolant temperature and fuel temperature distribution are used in the initial state, representing a configuration that has coolant flowing in opposite directions in alternate channels. During the LOCA transient, the coolant densities in about half of the channels in one side of the core are linearly reduced to near zero, over the period between 0 and 1 s.
- Beginning at 0.8 s, the shutoff rods are inserted into the core at a constant speed, completing their motion at 1.8 s. The timesteps used were selected so that the ends of the shutoff-rods are aligned with mesh boundaries at the points in time that neutron flux distributions were calculated.
- The transient simulation is complete at 1.8 s.

Note that the coolant and fuel temperature distributions in the problem were uniform and not varied during the transient; this simplification will not detract from the verification of the *CERBERUS-to-lattice-cell interface as they are small effects during LOCA transients.

2 Description of Lattice-Cell Models

All the fuel bundles in the core are of a nominal 37-element natural-uranium configuration and all the lattice-cell calculations are based on a single prototype WIMS–AECL model (prepared according to the standard methodology for CANDU analysis). Two separate types of WIMS–AECL analyses and post-processing are used for this work:

1. For the SCM-based analyses, a large set of WIMS-AECL calculations was performed before the RFSP calculations, to form the fuel tables used in the SCM calculations within RFSP in both one-and-a-half and two-group neutron flux calculations. The table was generated with a full range of burnups and state-parameter perturbations, although only a small subset of the range is used in the current analyses.
2. For the "WIMS 2-group" *CERBERUS calculations, WIMS–AECL is called from within *CERBERUS to compute local-parameter lattice-cell parameters, as described in Section 4.2.

Since the SCM fuel tables were generated from the same WIMS–AECL models used in item (2) above, the SCM results should be very consistent with the results from item (2) above. All WIMS–AECL calculations were performed with version 2-5c and the ENDF/B-V library version "u2x 1.0b, 1996 Dec 13".

3 Description of the RFSP Model

The RFSP model for the "Baby CANDU" verification case has a simplified specification, and the entire transient analysis is performed from a single input file. The 119 fuel channels in the core model are organized into three "groups", according to their thermalhydraulic conditions. The three channel groups are

1. channels with a front-to-back coolant flow, not voiding during the LOCA;
2. channels with a back-to-front coolant flow, not voiding during the LOCA; and
3. channels with a back-to-front coolant flow, voiding during the LOCA.

The pre-LOCA coolant densities in g/cm^3 used in the 10 bundle positions along each channel (in the direction of coolant flow) were 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.68, 0.65, 0.62, 0.59.

The distribution of the channel groups is shown in Figure 1. Coolant temperatures at all bundle positions are held constant at 280°C during the simulations, as are the fuel temperatures at 600°C. The fuel irradiations are fixed at zero in all of these calculations. A moderator boron concentration of 7 ppm (weight) was found to make the pre-LOCA core nearly critical, and is used in all analyses. The timesteps used in the dynamic calculations are as follows: 16 steps of 50 ms between 0 and 0.8 s, and 13 steps of 76.923 ms between 0.8 and 1.8 s.

In all of the calculations, a single set of 6-group delayed-neutron plus photo-neutron data is used. The delayed neutron data are documented in Reference 8. The delayed-neutron and photo-neutron data used for ^{235}U and ^{238}U are presented in Table 1. The total reactor core thermal power is normalized to 300 MW at the beginning of the transient. Only power resulting from fissions is to be analyzed in this benchmark; all energy will be considered to be released coincident with the fissions.

The version of RFSP used in this study was an unreleased developmental version, in which the two-energy-group *CERBERUS calculations have been added to Version 2-17HP of RFSP. Version 2-17HP included the implementation of the one-and-a-half-group *CERBERUS with SCM. The new two-group *CERBERUS calculations will be included in a future officially released version of RFSP.

4 *CERBERUS Calculations

To test the behaviour of the *CERBERUS calculations, several types of neutron flux calculations are used in this verification. One calculational option varied between methods was the utilization of the fast-to-thermal flux information from the lattice-cell and core calculations, as explained in Section 4.1. The five methods of lattice-cell and core-flux coupling and calculations are shown schematically in Table 2. The methods are (in order of increasing rigor):

1. The one-and-one-half group core flux calculations using lattice-cell properties calculated using the SCM within RFSP, referred to as the "SCM 1.5-group" calculations.
2. A true two-energy-group core flux calculation using lattice-cell properties calculated using WIMS–AECL within RFSP, referred to as the "WIMS 2-group" calculations. The parameters passed to the WIMS–AECL calculations are coolant density and temperature, fuel temperature and moderator boron concentration (the last 3 were not varied during the current tests).
3. A true two-energy-group core flux calculation using lattice-cell properties calculated using SCM within RFSP, but not using fast-to-thermal flux information from the core calculations, referred to as the "SCM 2-groups(2)" calculations.

4. A true two-energy-group core-flux calculation using lattice-cell properties calculated using SCM within RFSP, but using fixed fast-to-thermal flux information from the core *SIMULATE calculations, referred to as the "SCM 2-groups(1)" calculations.

5. A true two-energy-group core flux calculation using lattice-cell properties computed using SCM within RFSP, using time-dependent fast-to-thermal flux information from the core calculations, as explained in Section 4.1, referred to as the "SCM 2-groups" calculations. This method is considered the most rigorous approach and is intended to be used in production applications.

4.1 The Fast-to-Thermal Flux Ratio in Lattice-Cell Calculations

In CANDU reactor analyses, there is normally a separation between lattice-cell and reactor-core calculations. The usual approximation made in this context in lattice-cell calculations is in the cell boundary conditions and/or leakage treatment. Several levels of approximation are used in these analyses; in order of increasing rigor they are:

- In one-and-a-half-group calculations, the approximation is made in the lattice-cell calculation that leakage is due to a single energy-independent buckling. To convert the multigroup lattice-cell parameters to one-and-a-half-group form for RFSP calculations, effective thermal fission yield and fast moderation cross sections are calculated:

$$\nu\Sigma_f = \nu\Sigma_{f,2} + \frac{\Phi_1}{\Phi_2}\nu\Sigma_{f,1}$$

and

$$\Sigma_m = \Sigma_{s,1\to 2} - \frac{\Phi_2}{\Phi_1}\Sigma_{s,2\to 1}$$

approximating that the value of $\frac{\Phi_1}{\Phi_2}$ is equal to that in the lattice-cell calculation. As the value of $\frac{\Phi_1}{\Phi_2}$ for each bundle in the core will differ from that in the lattice cell calculation, the values of $\nu\Sigma_f$ and Σ_m will be approximate.

- The two-energy-group calculations within RFSP do not require the approximations made in the one-and-a-half-group approximation, and a significant component of the core and lattice-cell coupling is simplified. The next level of approximation is in the use of bucklings to represent the energy-dependent leakage in the lattice cell calculations.

  - The approximation is made in the "WIMS 2-group" calculations that the fast and thermal bucklings are equal, because WIMS–AECL is only capable of searching for a single energy-independent buckling.
  - In the "SCM 2-groups(2)" calculations, a similar approximation to that in the "WIMS 2-group" calculations, of an energy-independent buckling, is used so that leakage treatments within the lattice-cell calculations methods are more consistent.
  - In the "SCM 2-groups(1)" calculations, a local bundle-dependent value of the cell $\frac{\Phi_1}{\Phi_2}$ from the core calculation is used, by solving for separate fast and thermal bucklings within SCM. The time-independent value of $\frac{\Phi_1}{\Phi_2}$ for each bundle is held fixed to its value from a previous *SIMULATE pre-LOCA calculation.
  - In the "SCM 2-group" calculations, local bundle-dependent values of the cell $\frac{\Phi_1}{\Phi_2}$ from the core calculation are used, by solving for separate fast and thermal bucklings. During the static reference calculations, outer iterations are used to achieve self-consistency between the core and lattice-cell values of $\frac{\Phi_1}{\Phi_2}$. These outer iterations are not currently available during dynamic *CERBERUS calculations, and the ratios from the previous timesteps are used instead.

4.2 Controlling WIMS–AECL Calculations from Within RFSP

To evaluate the consistency between SCM and WIMS–AECL lattice-cell calculations during the dynamic core analysis of a LOCA transient, a set of WIMS–AECL calculations was performed prior to each core flux calculation. In each of these lattice-cell calculations, the local value of coolant density was used, but all coolant temperatures, fuel temperatures, and fuel irradiation values were uniform.

The method used to control these WIMS–AECL calculations is quite simple and practical:

1. Within RFSP, at the point where a local-parameter lattice-cell calculation is required in *CERBERUS, the state variables for that cell are written as a single line to a specific file.
2. Within RFSP, after the loop over all local-parameter lattice-cell calculations to be performed is complete, an external procedure is used to control the execution of the required WIMS–AECL calculations. The operations performed during this external calculation are the following:
   (a) The set of required lattice-cell calculations is reduced down to the set of unique cases according to the state variables. In this benchmark problem, this reduction results in a set of only 10 or 20 cases.
   (b) For each of the unique cases, an input file is formed incorporating the state parameters.
   (c) Each WIMS–AECL case is executed, with several being executed in parallel. After each case, the summarized results are written as one line to a file.
   (d) After all cases are complete, the unique-case results are unfolded into the results for all lattices, and the lattice-cell parameter calculations are complete.
3. After the external lattice-cell calculations, the individual lattice-cell results are processed and are stored for later use within RFSP.

5 Results of Simulations

Although the initial, static eigenvalues calculated for the pre-LOCA configuration cancel out of the dynamic solutions, they do provide useful confirmation of consistency. The initial eigenvalues calculated for the configuration at the beginning of the LOCA transient were

SCM 2 Groups	1.00260
SCM 2 Groups(1)	1.00266
SCM 2 Groups(2)	1.00266
WIMS 2 Groups	1.00244
SCM 1.5 Groups	1.00359

All the two-energy-group eigenvalues are in good agreement, and the one-and-a-half-group eigenvalue differs from those by about $+1$ mk.

Because there is not yet an independent solution available outside of RFSP to this benchmark problem, the most "rigorous" solution available within RFSP has been taken as the reference solution within this document. The other solutions are all, in one or more respects, approximations to this reference solution.

The results of the reference analysis are summarized in Table 3. The variation in total core power with time during the transient in the five cases is presented in Figure 2. The results indicate a relatively small variation in total power

with method of calculation; the differential total power between the reference "SCM 2-group" results and the other 4 cases is presented in Figure 3. Between the reference case and the "SCM 2-groups(1)" case, the use of fixed local $\frac{\Phi_1}{\Phi_2}$ ratios is shown to reduce the peak power by about 40 MW. The two cases "SCM 2-groups(2)" and "WIMS 2-group" only differ in the methods of lattice-cell calculation and show an agreement within 12 MW in peak power. The one-and-a-half-group result shows a larger discrepancy of about +30 MW at the power peak.

The variation in dynamic reactivity with time during the transient in the five cases is presented in Figure 4. The results indicate a small variation in dynamic reactivity with method of calculation; the differential dynamic reactivity between the reference "SCM 2-group" results and the other 4 cases is presented in Figure 5. For times before about 1.4 s, all the two-group results agree to within approximately 0.2 mk, whereas the one-and-a-half-group result shows a larger discrepancy of approximately +0.3 mk near the time of the peak power. The cases "SCM 2-groups(2)" and "WIMS 2-group" only differ in the lattice-cell calculation method and are in good agreement. After the power pulse, the discrepancy between the two-group and one-and-a-half-group dynamic reactivity grows. After about 1.4 s, the discrepancy between the reference two-group case (SCM 2-group) and the other two-group cases grows.

Two important integral quantities related to neutron kinetics are the prompt reactivity, β^*, and the prompt-neutron lifetime, Λ^*. In all cases, the calculated β^* value was similar, equal to 7.91 mk in the SCM-based cases and 7.99 mk in the WIMS–AECL-based case. The Λ^* value was very consistent between all the two-group cases, 870 μs, and was equal to 953 μs in the one-and-a-half-group case.

6 Discussion of Results

The good agreement between the "SCM 2-groups(2)" and "WIMS 2-group" solutions is very significant, because, outside of the lattice-cell calculations themselves, the two solutions within RFSP are the same, and thus the results indicate the level of consistency between the lattice-cell calculations. The key results are as follows:

- Over the period up to 1.4 s, the dynamic reactivities in the two cases agree to within 0.04 ± 0.03 mk. This level of agreement is consistent with comparisons of coolant-density-change reactivities calculated in stand-alone SCM and WIMS–AECL analyses [7], where an agreement of about 1% was found.
- The agreement in the total core powers and peak bundle powers is consistent with the deviations in dynamic reactivity: during the period between 0.8 and 1 s the "WIMS 2-group" reactivity is lower on average by about 0.06 mk, and this is sufficient to generate a total power discrepancy of about 14 MW by 1.1 s.

The discrepancies between the one-and-a-half-group approximation and the true two-group neutron-flux solution result in a 30 MW higher peak core power in the one-and-a-half-group case, and 0.3 mk higher peak dynamic reactivity. This reactivity difference is consistent with one-and-a-half- and two-group static (*SIMULATE) calculations of the reactivity change during the same changes in the coolant density distribution, 5.63 versus 5.33 mk. The strong downward trend in the reactivity discrepancy in the one-and-a-half-group case in Figure 5 is considered to be due to the different reactivity worth of the shutoff rods in the one-and-a-half- and two-group models.

The differences between the "SCM 2-group" and the "SCM 2-groups(1)" and "SCM 2-groups(2)" cases indicate the effect of achieving self-consistency in the $\frac{\Phi_1}{\Phi_2}$ ratios between the core and lattice-cell calculations. Using a time-independent value of $\frac{\Phi_1}{\Phi_2}$ at each bundle location results in a 40-MW decrease in peak core power, and a 0.3-mk decrease in peak dynamic reactivity. Not using core values of $\frac{\Phi_1}{\Phi_2}$ at all in the lattice-cell calculations resulted in similar and opposite changes, relative to using time-independent ratios. From the slope of the "SCM 2-groups(1)" dynamic reactivity discrepancy in Figure 5, the error in the reference calculation because of the use of the $\frac{\Phi_1}{\Phi_2}$ ratios from the previous timestep can be estimated to be small, about 0.01 mk $\left(\simeq \frac{0.2 \text{ m k}}{16 \text{timesteps}}\right)$. The upward trend in the

reactivity discrepancy in the two-group cases in Figure 5 at the end of the simulations is believed to be due to the effect of the shutoff rods on $\frac{\Phi_1}{\Phi_2}$ being accounted for in the reference "SCM 2-group" calculations, but not in the other two-group SCM calculations.

The change in Λ^* of from 870 to 953 μs between the two- and one-and-a-half-group calculations is due to the changes in the time-to-fission for the non-thermal fissions. In the two-group case, the non-thermal fissions will occur at much earlier times than thermal fissions, but in the one-and-a-half-group calculations they are assumed to occur at the same times as actual thermal fissions.

7 Conclusions

The results of the analyses of this benchmark problem indicate proper performance of the two-energy-group version of *CERBERUS in RFSP in the reactor-kinetics analysis of a three-dimensional CANDU LOCA transient. The results of comparisons between different methods of solution available for this problem within RFSP indicate that:

1. The use of the one-and-a-half-group approximation, rather than using a true two-energy-group solution, is a weakness and is not recommended for CANDU LOCA analyses.
2. When consistent three-dimensional true-two-energy-group neutron-flux calculations are performed using lattice-cell data from SCM and WIMS-AECL, the dynamic reactivity calculations during the power-pulse calculation are in very good agreement.
3. Performing the two-energy-group core and lattice-cell calculations with self-consistent local values of $\frac{\Phi_1}{\Phi_2}$ affects analysis results, and is recommended.

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			1	2	1	3	1			
		1	2	1	2	1	3	1		
	1	2	1	2	1	3	1	3	1	
1	2	1	2	1	3	1	3	1	3	1
2	1	2	1	2	1	3	1	3	1	3
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2	1	2	1	2	1	3	1	3	1	3
1	2	1	2	1	3	1	3	1	3	1
	1	2	1	2	1	3	1	3	1	
		1	2	1	2	1	3	1		
			1	2	1	3	1			

Figure 1: Fuel Channel Groups in the Baby CANDU Core Model

	Nuclide				
	^{235}U		^{238}U		(γ,n)
Group	Yield	Decay (s^{-1})	Yield	Decay (s^{-1})	Yield
1	0.0380	0.0133	0.0139	0.0136	3.0172e-4
2	0.1918	0.0325	0.1128	0.0313	—
3	0.1638	0.1219	0.1310	0.1233	—
4	0.3430	0.3169	0.3852	0.3237	5.5121e-4
5	0.1744	0.9886	0.2540	0.9060	—
6	0.0890	2.9544	0.1031	3.0487	—
Total	0.0177		0.0354		

Table 1: Six-Group Delayed-Neutron and Photo-Neutron Data Used

In this table, the group-dependent values for ^{235}U and ^{238}U are the fractional yields of the total yield per fission below. The photo-neutron yields are the total to each group.

Lattice Calculation	With $\frac{\Phi_1}{\Phi_2}$ Feedback		Without $\frac{\Phi_1}{\Phi_2}$ Feedback
	Fixed local $\frac{\Phi_1}{\Phi_2}$'s	Time-Dependent $\frac{\Phi_1}{\Phi_2}$'s	
WIMS-AECL			WIMS 2-Group
SCM	SCM 2-Group(1)	**SCM 2-Group (Reference Method)**	SCM 2-Group(2) SCM 1.5-Group

Table 2: *CERBERUS Calculational Methods Used

Time (s)	Total Power (MW)	Peak Channel Power (MW)	Peak Bundle Power (kW)	Dynamic Reactivity (mk)
0.0000	300.0	4.23	636.2	0.00
0.0500	302.0	4.26	641.1	0.24
0.1000	306.6	4.32	650.8	0.52
0.1500	313.3	4.41	664.9	0.79
0.2000	321.3	4.52	681.8	1.02
0.2500	330.1	4.65	700.7	1.26
0.3000	340.6	4.79	721.4	1.49
0.3500	350.8	4.94	744.7	1.73
0.4000	362.9	5.11	769.5	1.99
0.4500	376.6	5.30	799.0	2.28
0.5000	392.4	5.53	834.0	2.59
0.5500	409.9	5.78	872.3	2.84
0.6000	428.8	6.06	913.5	3.09
0.6500	449.4	6.36	959.0	3.34
0.7000	472.0	6.69	1009.6	3.60
0.7500	497.0	7.06	1065.5	3.86
0.8000	524.9	7.47	1127.8	4.12
0.8769	577.4	8.27	1248.3	4.65
0.9538	639.6	9.21	1390.0	4.99
1.0308	684.8	9.99	1505.3	4.46
1.1077	663.4	9.91	1490.2	2.70
1.1846	552.6	8.57	1283.2	−2.40
1.2615	390.5	6.26	933.3	−4.47
1.3385	244.1	4.03	599.6	−10.50
1.4154	150.3	2.54	373.0	−19.07
1.4923	101.0	1.67	241.3	−30.85
1.5692	75.5	1.16	163.8	−45.51
1.6462	61.4	0.89	121.1	−61.12
1.7231	53.5	0.78	105.8	−74.50
1.8000	49.1	0.73	99.3	−83.17

Table 3: Results of SCM 2-Group Transient Results

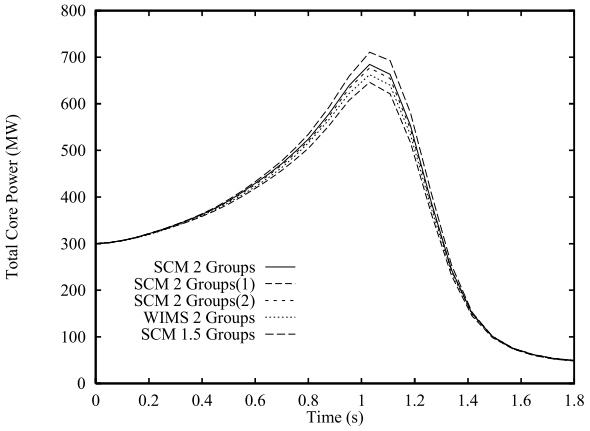

Figure 2: Calculated Total Core Power Variation

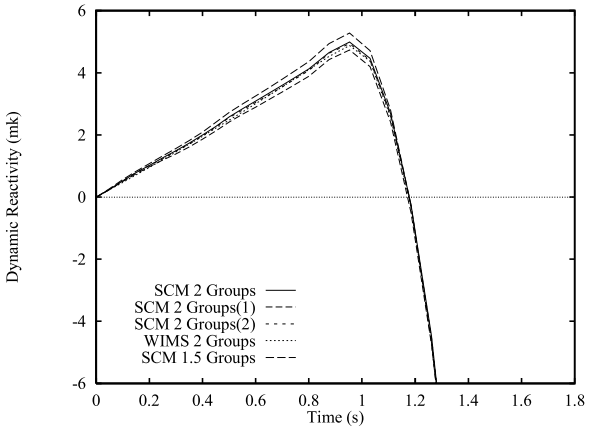

Figure 4: Calculated Dynamic Reactivity Variation

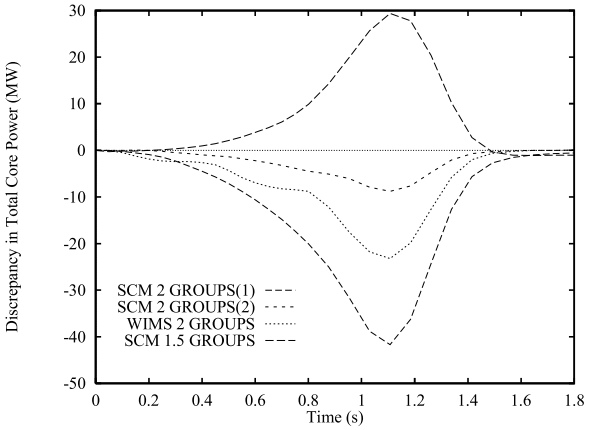

Figure 3: Difference in Total Core Power Variation

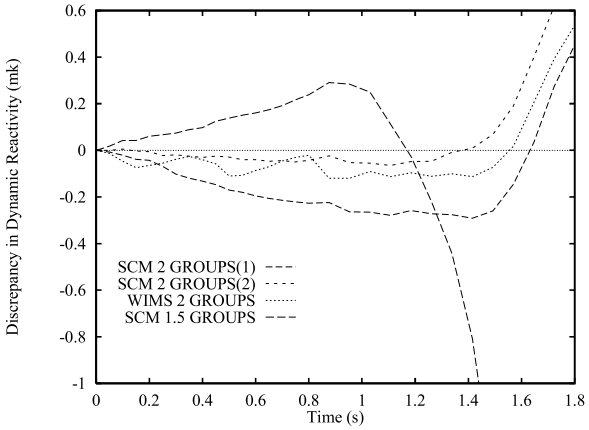

Figure 5: Difference in Dynamic Reactivity Variation