HISTORY-BASED CALCULATIONS USING WIMS-AECL IN RFSP

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ABSTRACT

The Reactor Fuelling Simulation Program (RFSP) has been modified to track core histories with local parameters based on WIMS-AECL lattice-cell properties. The lattice-cell properties are calculated with a simple-cell methodology that reproduces the WIMS-AECL lattice-cell properties of each fuel bundle using a very efficient computational scheme. The fast and thermal fluxes calculated in RFSP at each bundle location are transferred to the simple-cell model to improve the consistency between the neutron-flux spectrum in the core and lattice-cell calculations. The modified version of RFSP was used to track a one-year period of the Point Lepreau Generating Station (PLGS) operating history. The results of the simulations were compared to vanadium-detector readings from PLGS and show that the core calculations obtained with the WIMS-AECL history-based lattice-cell properties are improved, relative to non-history-based simulations.

1 Introduction

CANDU® reactor-core simulations are performed with the Reactor Fuelling Simulation Program (RFSP) [1]. An important type of simulation performed with RFSP is referred to as "history-based" calculations [2]. In history-based simulations, local parameters describing the unique state at each bundle location are used in the calculation of the lattice-cell properties. The lattice-cell properties are then used in RFSP, to calculate a new approximation to the neutron flux distribution, and lattice-cell and core-flux calculations are performed iteratively until a self-consistent solution is calculated.

Until now, lattice-cell properties used in history-based RFSP simulations were only calculated with the POWDERPUFS-V (PPV) lattice-cell code [3]. The PPV code calculates lattice-cell properties with semi-empirical methods, and the lattice-cell properties of the fuel bundles in a CANDU reactor can be calculated within a very short computation time. However, because of the semi-empirical approach used in PPV, the lattice-cell properties calculated with that code are limited to current 19-, 28- or 37-element natural-uranium fuel bundles. Current requirements for code validation, as well as the need to analyse new fuel and reactor designs, have led to the choice of the more theoretically rigorous WIMS-AECL [4] code as the lattice-cell calculation for CANDU analyses in the future.

The application of a lattice-cell code such as WIMS-AECL poses some challenges to reactor core analyses, especially in the area of history-based analyses. In principle, WIMS-AECL could be used

in conventional calculations to generate the local properties of all the bundles to be used in history-based CANDU core calculations. However, each lattice-cell calculation with WIMS-AECL requires approximately five seconds of computation on typical workstations. Therefore, the conventional approach would be unsuitable for a typical RFSP-history-based calculation that requires an average of 30,000 lattice-cell calculations, as the roughly 40 hours of computation per core burnup step is impractical.

To overcome the computation-time problem implicit in the use of a lattice-cell code such as WIMS-AECL, a simple-cell lattice-cell calculation methodology has been developed. At the specific states used to determine the parameters defining the simple-cell model, the simple-cell approach accurately reproduces WIMS-AECL results important for reactor simulations and requires a computation time of the order of 200 times less than standard WIMS-AECL lattice-cell calculations. Interfacing the simple-cell code into RFSP makes the WIMS-AECL history-based calculations practical. Sections 2 through 5 give a short description of the simple-cell model, explain how the module was linked into RFSP, and present the results of the validation simulations.

The results reported in this paper are the first demonstration of core simulations based on the WIMS-AECL history-based lattice-cell properties. Therefore, it is expected that the methodology will evolve and that the calculation scheme will improve. For that reason, the revised version of the RFSP code has not been formally released at this time.

2 Description of the Simple-Cell Model

The simple-cell model calculates the neutron-flux distributions within a lattice cell with homogenized-region one-dimensional multigroup diffusion theory, rather than two-dimensional multigroup transport theory as is applied in WIMS-AECL. Using the superhomogenization (SPH) procedure [5], the homogenized-region cross sections to be used in this calculation can be formed in such a manner that the cell-average neutron fluxes, region-averaged reactions and eigenvalues of reference WIMS-AECL solutions are preserved for the specific fuel types for which the models were prepared. These homogenized-region cross sections are stored in "simple-cell fuel tables" and are transferred to RFSP. Three homogeneous regions are used in the simple-cell CANDU lattice-cell model:

- The fuel-clad-coolant region.
- The tubes region, representing the pressure and calandria tubes and the gap between them.
- The moderator region.

In each of the three regions, the properties account for state perturbations (such as coolant and moderator temperature and composition perturbations). Within the fuel-clad-coolant region, variations due to changes in nuclide composition are treated.

A fuel region is used in the simple-cell model, but is not treated explicitly within the simple-cell neutron-flux calculations. The fuel-region neutron flux is evaluated from the calculated fuel-clad-coolant region neutron fluxes and neutron-flux disadvantage factors calculated from WIMS-AECL results. The fuel region is used to account for changes in the fuel nuclide composition and the changes in fuel-clad-coolant region cross sections that are due to those changes. For the fuel-clad-coolant region of the simple-cell model, the cross sections in each energy group include the effect of state perturbations and variations in nuclide compositions.

All the cross sections in each region and in each energy group include the effect of state perturbations. Within each of the simple-cell regions, a finite-difference mesh structure is automatically constructed, and the neutron flux solution is performed using standard finite-difference multigroup diffusion theory. In the simple-cell calculations reported in this document, 5 neutron energy groups were used. During burnup calculations in the simple-cell calculation, nuclide concentrations within the fuel are explicitly integrated as functions of time and the local conditions.

2.1 Leakage Treatment in the Simple-Cell Model

The neutron-flux calculations in the simple-cell model are normally calculated with critical bucklings, as the neutron flux at each location in a reactor core will normally be at or very near critical. As good approximations to the absolute local fast- and thermal-neutron fluxes in each lattice cell are normally available within RFSP simulations, this information is used to improve the consistency between the core and cell calculations. In the simple-cell calculation, the fast and thermal energy-group bucklings are considered to be independent, and buckling values are calculated that achieve criticality at the local reactor core ratio of fast-to-thermal flux. Only the fast and thermal neutron fluxes from RFSP are used in the leakage and absolute flux normalization calculations in the simple-cell, as current RFSP calculations are only performed in two neutron energy groups.

3 Interfacing to the Simple-Cell within RFSP

The approach taken in designing and implementing the interface between RFSP and the new lattice-cell calculations for history-based simulations was to use a simple and lattice-calculation independent approach. This approach allowed a simple specification and development of the interface, as well as allowing for the possibility of the use of other types of lattice-cell calculations in the future without requiring a significant change in methodology within RFSP. The interface between RFSP and the lattice-cell calculation is defined in terms of three tables/arrays:

1. A simple-cell fuel table calculated from WIMS–AECL results, specific to each type of fuel bundle and used for all lattice-cell calculations for that type of bundle;
2. A fuel-bundle table used within the RFSP history-based calculation, specific to each bundle and used for containing the individual local parameters for each bundle; and
3. A lattice-cell parameter table, specific to each bundle, and used for storing the results of each lattice-cell calculation.

The module in RFSP that solves the neutron-flux distribution based on the history-based lattice-cell properties has not yet been modified to solve the true-two-group neutron flux solution. The flux distribution is still solved with the one-and-a-half energy-groups approximation, in which neither non-thermal fissions nor upscattering are treated explicitly. Therefore, the true-two-group lattice-cell properties generated with the simple-cell model are transformed within RFSP into the one-and-a-half energy-group formalism using the fast-to-thermal flux ratio as calculated in the simple-cell model. When the simple-cell calculation is used to determine lattice-cell properties at a fast-to-thermal flux ratio equal to the local reactor core value, the effective thermal-fission-yield and effective fast moderation cross sections are consistent with the local flux solution and the neutron flux solution will

be much closer to a true-two-group flux solution in RFSP than in the normal one-and-a-half groups approach.

3.1 Data Manipulation in RFSP

In the WIMS-AECL history-based calculations, much of the data used in the simple-cell model is the same as that used in PPV history-based calculations. Some of the data is related to the global reactor conditions, such as the moderator temperature, the moderator purity, the boron concentration in the moderator and the coolant purity. This data could be transferred to the simple-cell code using a number of approaches; however, the decision was made to use the existing method employed in PPV history-based simulations. Therefore, the user specifies the global state conditions (moderator temperature, purity, boron concentration in the moderator and the coolant purity) in the RFSP input, and these values are stored in the record corresponding to the PPV input. These global conditions are later read from that record and transferred to the simple-cell calculation.

Several other parameters besides the global state conditions are required by the simple-cell code to calculate the lattice-cell properties: the initial and final bundle irradiations, the coolant density and the coolant temperature. With these parameters specified, plus the global conditions transferred from the PPV records, plus the fuel-type specific fuel table, all of the information required for the lattice-cell calculation is available and the lattice-cell parameters may be calculated.

No major modifications were required in RFSP to handle the data for the history-based calculations based on lattice-cell properties generated with the simple-cell code. The only data-handling modification that was introduced in the code was the creation of 2 records to save the data to be sent and returned from the simple-cell code. For each history-based simulation the 2 records were stored under the energy-clock index of the "SIMULDATA" block in the RFSP database. The length of these records varies as a function of the number of energy groups and perturbations in the simple-cell fuel table and the number of nuclides treated in the simple-cell calculation. Section 3.2 gives more information on how the data is handled in the simple-cell model.

3.2 Data Manipulation in the Simple-Cell Model

The simple-cell model is called each time the lattice-cell properties of a fuel bundle need to be calculated. To perform the calculation with the appropriate local conditions, the local parameters specific to each bundle need to be stored in, and retrieved from, the fuel-bundle table. The fuel-bundle table is structured as a simple array of keywords and numerical values, with no specific order of contents. Generally, reactor global and local state conditions are stored in the table by RFSP and retrieved within the simple-cell calculation. The nuclide concentrations stored in each fuel-bundle table are calculated and manipulated only within the simple-cell calculation itself.

The simple-cell fuel table is used within the simple-cell calculation to define all the properties of the simple-cell lattice-cell model, including the number of energy groups, the specifications of all tabulated state perturbations, the values of all multigroup cross sections, as well as the nuclide cross sections and burnup information. The set of nuclides treated in each simple-cell calculation is chosen at the time of the construction of the fuel table.

In preparation for the simple-cell neutron flux calculations, the multigroup cross sections for each of the three cell regions are formed by interpolation of the information in the simple-cell fuel table as a function of the fuel thermal-neutron irradiation and the state parameters. The neutron flux

distribution in the cell is solved using finite-difference multigroup diffusion theory. The flux solution is performed within an iterative eigenvalue calculation, and that is performed within a critical buckling search.

The values of the initial and final fuel thermal-neutron irradiations for each fuel bundle are specified by RFSP. Using the absolute fuel-flux values calculated from the simple-cell flux solution, changes in the nuclide concentrations are calculated by integration between the initial and final irradiation values. The final nuclide concentrations are stored in the fuel-bundle table.

4 RFSP Simulations Performed

To validate the WIMS-AECL simple-cell history-based calculations in RFSP, a one-year period of operation of the Point Lepreau Generating Station (PLGS) [6] was simulated. The information used from the PLGS station history consisted of the time steps, the sequence of channels refuelled, the moderator and coolant temperatures and compositions, and the liquid-zone-control compartment fills.

The first step in the WIMS-AECL based simulation was the specification of the fuel irradiation values for all the bundles in the reactor at the start of the simulation period. As the "real" irradiation values of the bundles are not measured quantities, and all previous core-follow simulations of PLGS were performed with PPV-derived lattice-cell properties, it was necessary to approximate the initial irradiation distribution from existing RFSP/PPV values. As the units of fuel thermal-neutron irradiation are not consistent between WIMS-AECL and PPV, a transformation was performed by converting each PPV-based irradiation value to the corresponding PPV burnup, and then converting that burnup value to the corresponding value of WIMS-AECL fuel irradiation.

The sequence of RFSP calculations used to start the WIMS-AECL history-based core simulations was

1. An initial static-core RFSP simulation was performed with WIMS-AECL non-history-based properties and the calculated fluxes were stored.

2. A WIMS-AECL history-based RFSP calculation was performed with a zero time step, using the neutron flux distribution calculated in Step 1 as a first approximation. It is important to perform this first zero-time-step calculation based on WIMS-AECL properties to obtain an initial flux distribution consistent with the WIMS-AECL history-based lattice-cell properties.

3. WIMS-AECL history-based RFSP simulations were performed for each time step to analyse the one-year core-follow of PLGS.

The simple-cell model uses the local flux at each bundle location to irradiate the fuel at the appropriate normalization to calculate accurate nuclide concentrations. Two sets of WIMS-AECL history-based simulations were performed with RFSP. In the first set, only the local thermal flux calculated from the core calculations were transferred to the simple-cell model, and a single buckling was taken into account to generate the lattice-cell properties. In the second set, the fast and thermal local fluxes were used to calculate separate fast and thermal bucklings in the simple-cell model. In the following Sections, the two sets are referred to as the "uniform buckling" and the "two-group buckling" solutions.

The reactivity-control devices in PLGS were represented using incremental cross sections calculated using WIMS–AECL-based SPH-corrected properties in three-dimensional diffusion-theory cell calculations.

The results of two other RFSP simulations are also included in this document for comparison purposes: a non-history-based WIMS–AECL calculation, and a history-based PPV calculation (both previously reported in Reference 6).

5 Results of the Simulations

The results of the simulations obtained with the simple-cell history-based simulations are shown in Figures 1, 2 and 3. In the following discussions, when average values of the simulation results are quoted, they were obtained by averaging over the period between full-power-day (FPD) 4000 and FPD 4150, as that period in the history had the smallest variations in PLGS operating conditions. During a few short periods of PLGS operation, the reactor was not in a normal equilibrium-operating condition, either because of operation following an extended shutdown or because of operation at reduced power; as only equilibrium operation was simulated in RFSP, these non-equilibrium points have been excluded from the reported results. These "average" values should be considered as typical for the particular period of PLGS operation, and are most useful in studying relative changes that are due to changes in the methods of analysis.

Figure 1 presents the reactivity values calculated with the 4 lattice-calculation schemes. A noticeable feature of this figure is the difference in the reactivity offset between WIMS–AECL and PPV: WIMS–AECL history-based simulations result in an average offset of −3.2 mk, whereas PPV history-based simulations result in an average offset of +3.2 mk. The results indicate that core calculations based on WIMS-AECL history-based lattice-cell properties have a higher (less negative) reactivity than the non-history-based simulations do: −3.2 mk compared to −4.2 mk. The use of two-group bucklings rather than uniform bucklings in the history-based simulations resulted in a change in the reactivity discrepancy from −2.2 mk to −3.2 mk.

Figure 2 shows the standard deviation calculated between the measured vanadium-detector readings and the simulated thermal fluxes at the vanadium-detector sites. At the beginning of the WIMS–AECL simulations, the fuel irradiation distribution is not self-consistent, as it was approximated from PPV information. This can be seen in the slope of the curves during the first 100 FPD of the simulations. The results show that using the two-group buckling in the simple-cell code gives significantly better results than when a uniform buckling is used. Toward the end of the PLGS operating history, excess refuelling and changes in moderator poison occurred, and this increased simulation challenge resulted in the positive slope at the end of the uniform-buckling curve history-based and non-history-based WIMS–AECL simulations. The average detector standard deviations with WIMS–AECL history-based simulations are not quite as good as with PPV history-based simulations: 2.5% compared to 2.2%.

Figure 3 presents the difference between the calculated average inner-core thermal-neutron flux and the average of the inner-core vanadium detector measurements (a negative value indicates a calculated value lower than the measured). The results in the figure show a significant reduction in the average discrepancy when the two-group buckling history-based method is used relative to the non-history-based method: a reduction in the discrepancy from −1.58% to −0.72%. The uniform-buckling method resulted in a larger discrepancy (−2.00%) than the non-history-based method did. Again,

the discrepancy in the WIMS–AECL history-based simulation is not quite as good as in the PPV history-based simulations: −0.72% compared to −0.27%.

6 Discussion

The level of agreement between WIMS–AECL history-based calculations and measurements in PLGS is good, and is now quite comparable to the results of equivalent simulations using PPV. Considering that PPV uses an empirical approach specifically tuned for CANDU reactor analysis and has been used in that application for over 30 years, and that WIMS–AECL is a fundamentally-based code without CANDU-specific empiricism, the current level of agreement can be considered very adequate.

Of the major contributions to the discrepancies between the PLGS core-following simulations investigated during this work, the discrepancy in the radial flux shape, as characterized by the inner core flux deviation presented in Figure 3, appears to show the greatest variation with method. Between the non-history-based WIMS–AECL and uniform-buckling history-based simulations, the effect of local reactivity feedback was included and negative fuel-temperature reactivity feedback results in a preferential reduction of the thermal flux in the inner-core where the average fuel powers are higher. This feedback flattening worsened the radial shape, because the original non-history-based simulation had an overly flat radial distribution. This change in radial shape cancels out some of the other improvements expected from the use of the history-based methodology, as is seen in the detector standard deviations in Figure 2. When the fast-to-thermal flux ratio is made consistent between the local core conditions and the simple-cell lattice-cell calculations, however, there is a significant improvement (by +1.3%) in the agreement between the inner-core simulated and measured fluxes.

The radial flux shape was also a significant component in the reactivity changes between the different simulations using WIMS–AECL, as more radial flattening increases leakage from the reactor and hence reduces reactivity.

7 Conclusions

The capability of performing WIMS-AECL history-based analyses in RFSP has been implemented, demonstrated, and successfully verified. The verification study demonstrated that the WIMS-AECL history-based lattice-cell calculations using the simple-cell method improved the accuracy of the simulations compared to the results of the simulations obtained with the WIMS-AECL non-history-based lattice-cell properties. The analysis also showed that the calculated flux values agree better with the results of the measurements when both the fast- and thermal-flux values from the core calculation are used in the simple-cell lattice-cell calculation.

8 Recommendation

The true-two-energy group neutron flux solution in RFSP should be integrated with the WIMS–AECL history-based calculations. As well, the simple-cell history-based methodology should be integrated into the *CERBERUS three-dimensional prompt kinetics module in RFSP, preferably using the true-two-energy group flux solution.

References

[1] B. Rouben, "Overview of Current RFSP-Code Capabilities for CANDU Core Analysis", AECL Report, AECL-11407, 1996 January.

[2] B. Rouben and D. Jenkins, "A Review of the History-Based Local Parameters Methodology for Simulating CANDU Reactor Cores", In the Proceedings of INC93, Toronto, 1993 October.

[3] B. Rouben, "Description of the Lattice Code POWDERPUFS-V", AECL Report, AECL-11357, 1995.

[4] J.V. Donnelly, "WIMS-CRNL: A User's Manual for the Chalk River Version of WIMS", AECL Report, AECL-8955, 1986.

[5] A. Hébert and G. Mathionnière, "Development of a Third-Generation Superhomogénéisation Method for the Homogenization of a Pressurized Water Assembly", Nuclear Science and Engineering, 115, 124-141, 1993.

[6] E.V. Carruthers and J.V. Donnelly, "Validation of WIMS-AECL Against Actual Operating History: Core Follow of Point Lepreau Nuclear Generating Station with POWDERPUFS-V and WIMS-AECL", In the Proceedings of the Fifth International Conference on Simulation Methods in Nuclear Engineering, Montréal, 1996 September.

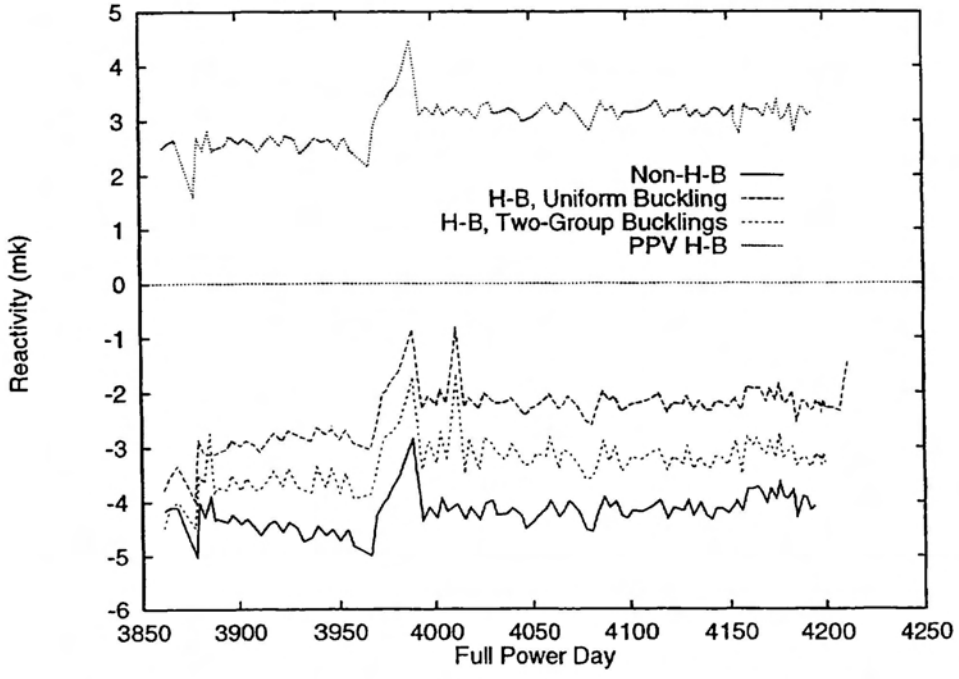

Figure 1: Reactivity Variation with Full-Power-Day in PLGS Simulations

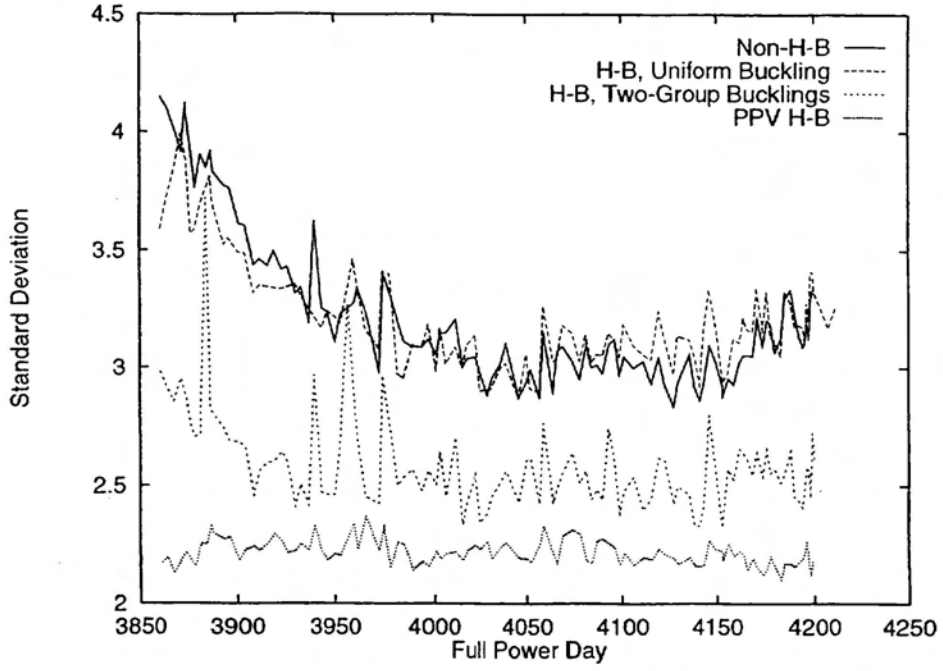

Figure 2: Standard Deviation Variation between RFSP Calculated and Measured Vanadium Detector Readings with Full-Power-Day in PLGS Simulations

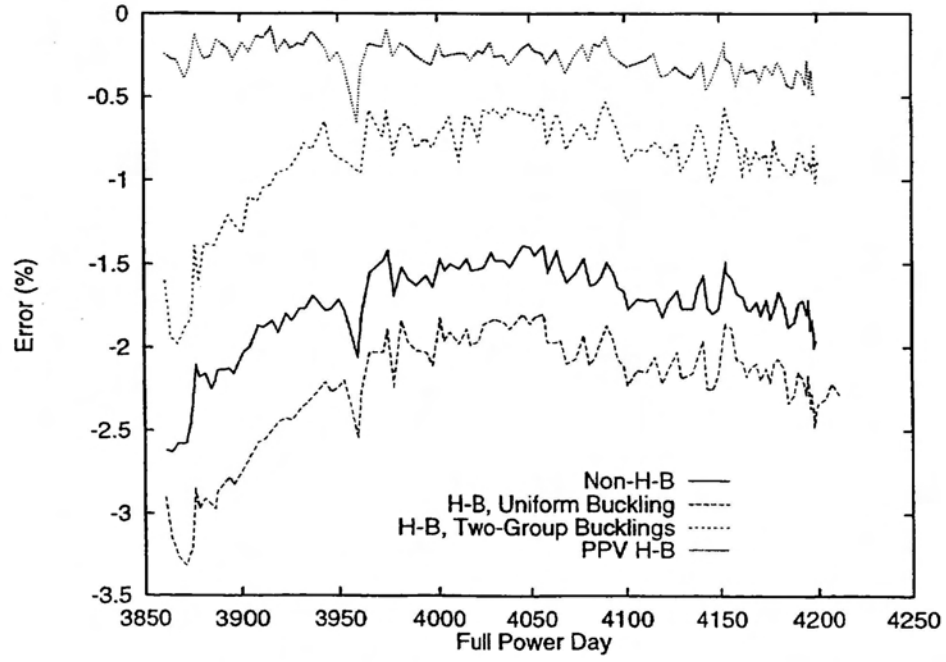

Figure 3: Inner-Core Flux Deviation Variation between RFSP Calculated and Measured Vanadium Detector Readings with Full-Power-Day in PLGS Simulations