PARAGON: The New Westinghouse Assembly Lattice Code

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Abstract

This paper gives an overview of the new Westinghouse lattice code PARAGON especially its modular software structure and the theoretical physics models of the different components of the code. A brief summary of the important theoretical assumptions behind each module of the code is outlined. We have limited our discussion to the most important modules of the code which are: Self-shielding, flux solution, leakage correction, and depletion. This paper contains also some numerical benchmarks performed during the validation of the code.

1 Introduction

During early nineties, Westinghouse initiated a project to start a major renovation of its lattice code in order: to take advantage of the powerful computing environment of today, from both software as well as hardware points of view, to enhance the prediction accuracy and to have more flexibility in modeling the future and new concepts of reactor lattices that have more complicated geometry designs. Since that time, this program has been jointly carried out by Westinghouse and Mitsubishi Heavy Industries (MHI). The first phase of the program was to update the cross-section library of PHOENIX-P [Nguyen, 1988] to ENDF/B-VI based 70 groups library [Huria, 1996]. The next phase is a complete restructuring and coding. The result of this effort is the new lattice code to be called PARAGON [Ouisloumen, 1998]. PARAGON shares the same library as PHOENIX-P, but it employs more advanced numerical methods and has a completely new software architectural design. The code is written in Fortran-90 language following a well established software process [Paulk, 2001]. PARAGON is modular and uses heavily all the features of Fortran-90 like: dynamic memory management, derived type structures, data hiding, etc. The modularity of the code makes it easy to maintain and less time consuming to add any new feature.

PARAGON is designed to be a part of the Westinghouse ALPHA/PHOENIX-P/ANC (APA) design system package [Nguyen, 1988]. Consequently, the speed of the execution of

PARAGON is crucial and great care has been devoted to make PARAGON as fast as possible. For that purpose, PARAGON takes advantage of the configuration symmetries in each module to reduce the amount of calculations and data to store. A good example for that is the module of collision probability, where only necessary matrix elements are computed and others are obtained by symmetry, reciprocity relations and transformation laws [Ouisloumen, 1996].

This paper gives an overview of the different components of the code, with an emphasis on the new developments and capabilities recently added to PARAGON. Some validation tests are also included, to illustrate the good performance of PARAGON when compared to continuous energy Monte Carlo calculations of MCNP code [Breismeister, 1997].

2 Description of the Basic Modules

As in any lattice code, PARAGON has essentially four basic modules: Self-shielding, flux solution, leakage correction and depletion. Each of these modules is subdivided into sub-modules which are designed to perform a specific task. Besides these calculational modules, there are the input and output modules. We will be interested in this paper to describe only the most important basic modules.

2.1 Cross-section Library

The new standard cross-sections library of PARAGON is entirely based on ENDF/B-VI data [Huria, 1996]. It has 70 energy groups and contains data for more than 250 isotopes covering all types of fuels (including Thorium) with their explicit fission products. This library is generated by NJOY code [MacFarlane, 1994]. The only adjustment made to the basic data to better match the experimental results was in the resonance integral of Uranium-238 [Huria, 1997]. Among the data tabulated as a function of temperature and dilution are: microscopic cross-sections, shielding tables and other data required by the depletion module such as decay constants, fission product yields, gamma energies etc.

The code is designed to support an arbitrary number of energy groups. A new library with probably more energy groups is under preparation.

2.2 Self-shielding Module

For this first version of PARAGON, we are using the same resonance self-shielding model as in PHOENIX-P code. This method is based on a WIMS code [Stamm'ler, 1997] methodology where the resonances are self-shielded for an average pin cell. The non-regularity of the lattice is taken into account using space dependent Dancoff factor [Stamm'ler, 1997] corrections. This method is limited to one single region per fuel pellet. However PARAGON flux solver can divide any region of a cell into an arbitrary number of subregions. In this case, the code performs a pre-homogenization for the fuel rings before calling this module. The outcome of the module will be a set of space dependent macroscopic cross-sections with the depletion. This assumption is well justified for the fuel without a strong gradient of epithermal flux. The cases of fuel with burnable absorbers having strong thermal flux gradient, such as gadolinia, are well covered by this assumption.

A more robust method which will allow the module to generate a spatially dependent self-shielded microscopic cross-sections is under development and will be part of the next release of PARAGON.

2.3 Flux Solution Module

The flux solver module [Ouisloumen, 1996] is based on the interface current formalism using Collision Probability method within the cells. The flux at the surfaces is first discretized into a set of cones where the flux is independent of angular variables, for notations see reference [Ouisloumen, 1996]:

$$\psi^{\rho\nu}_{\pm,\alpha}(\vec{\Omega}) = \frac{1}{\sqrt{A^{\rho\nu}_{\alpha}}} H(\vec{\Omega} \in \vec{\Omega}_{\rho\nu}) \ , \tag{1}$$

where

$$A^{\rho\nu}_{\alpha} = \frac{1}{\pi} \int_{(4\pi)} (\vec{\Omega}.\vec{n}_{\pm,\alpha}) H(\vec{\Omega} \in \vec{\Omega}_{\rho\nu}) d\vec{\Omega} \ , \tag{2}$$

and $H(\vec{\Omega} \in \vec{\Omega}_{\rho\nu})$ is the Heaviside distribution defined by:

$$H(\vec{\Omega} \in \vec{\Omega}_{\rho\nu}) = \begin{cases} 1 & \text{if } \vec{\Omega} \in \vec{\Omega}_{\rho\nu} \text{ i.e. } [\varphi, \theta] \in [\varphi_{\rho}, \varphi_{\rho+1}] \times [\theta_{\nu}, \theta_{\nu+1}] \\ 0 & \text{elsewhere} \end{cases} \tag{3}$$

This leads to a coupling order parameter in the input that the user can control. The value is arbitrary. To enhance the accuracy of the solution, the user has also the ability to sub-divide the cylindrical regions into an arbitrary number of equal volumes or equal thicknesses sub-rings. The code allows also to have a diagonal sub-division of regions as described in reference [Ouisloumen, 1996]. The resulting system of equations, see reference [Ouisloumen, 1996] for the notations:

$$\begin{aligned} \phi_i &= \sum_{\alpha,\rho\nu} P^{\rho\nu}_{is_{\alpha}} J^{\rho\nu}_{-,\alpha} + \sum_{j} V_j P_{ij} \mathcal{F}_j \ , \\ J^{\rho\nu}_{+,\alpha} &= \sum_{\beta,\eta\mu} P^{\rho\nu\,\eta\mu}_{s_{\alpha}s_{\beta}} J^{\eta\mu}_{-,\beta} + \sum_{i} P^{\rho}_{s_{\alpha}i} \mathcal{F}_i \ , \\ J^{\rho\nu}_{-,\alpha} &= \sum_{\beta,\eta\mu} B^{\rho\nu\,\eta\mu}_{\alpha\beta} J^{\eta\mu}_{+,\beta} \ . \end{aligned} \tag{4}$$

is solved by iterating on flux and currents using SOR (Successive Over Relaxation) method [Thomson, 1995]. To enhance the performance of PARAGON we use the transformation laws [Villarino, 1993] to avoid repeating unnecessary computation of collision probability matrices. The code handles many assembly symmetries and boundary conditions like: reflective, infinite, albedo, etc.

2.4 Leakage Module

The leakage correction module uses the same method as in PHOENIX-P. It uses B_1 theory [Stamm'ler, 1997] to compute the diffusion coefficients and then the critical spectrum flux to be used later in the depletion module.

2.5 Depletion Module

As in PHOENIX-P, the depletion module of PARAGON is using the Laplace transform to solve the set of differential equations after linearizing the isotopic depletion chains. The module is, however more general and any new chain can be added easily without any changes in the code. We have also generalized the depletion chain to treat the cyclic chains.

The code detects automatically the regions to be depleted, but the user has the option to hold any region in the assembly as non-depletable. For boron depletion, the user has a choice on depleting it according to a letdown curve that is provided through the input or exponentially (i.e., depletion chain). For the time being, the gamma heating is modelled as follows: the total gamma energy released in the assembly is distributed equally over all electrons in the assembly, and each region will receive an amount of gamma heating proportional to the number of electrons that it contains. The gamma transport calculation will replace the above model in the future release of PARAGON.

2.6 Interface modules: input and output

2.6.1 Input description

The PARAGON input uses a free format structure. It is also modular in such a way that each module has its own input. The user can also control through the input the amount of output to be printed. We have used explicit keywords to describe different parameters required by the code, like ”coupling_order”, ”temperature”, etc. Each keyword is followed either by other keywords or by numerical values or by characters depending on what is required in that field. The key point in the design of the input is to make it easy to understand, user friendly, and as simple as possible. For that purpose we have built in this module different default options for non-mandatory parameters. The Westinghouse methodology requires that the temperature of the zones of assembly be burnup and relative power dependent. For that the user should provide a temperature table to the code for different media and associate those media to different regions of the assembly. Note also, that the user is provided with the capability to control the thermal expansion of the materials as a function of their temperature.

It is worth mentioning that the user is provided with the ability to comment the input in a flexible way.

2.6.2 Stand alone editing

Besides echoing different options that the user has chosen for his case like: geometry configuration and dimensions , temperature distribution material layout etc., PARAGON has an advantageous flexibility on printing all kinds of micro and macro physics parameters. Hence, the user can request to edit the fluxes, currents, surface fluxes, different reaction rates, isotopic distribution etc. The editing could be done for micro-regions, or as an average over a cell or as an average over a group of cells, and that for any number of energy groups (i.e., the code can collapse to any number of groups).

2.6.3 Data for core calculations

PARAGON will be a module of the APA system, the Westinghouse design tool, to provide the ANC Code (or other nodal codes) with the multi-group constants and other physics parameters necessary to analyze the nuclear power plant cores. The data is stored in Databanks that the driver of both PARAGON and ANC code can manipulate as needed. The program permitting this interface has been implemented as a module of PARAGON.

The modularity and the design structure of the code makes it easy to implement PARAGON into any other code systems with a minimum amount of work. That is mostly because of using the structures and pointers of Fortran-90. The data is structured in an ”object-oriented” way using a hierarchical structure and consequently easily accessible.

3 A word about software design

As mentioned before, PARAGON is using Fortran-90 as a programming language. The data flow in the code is designed in a hierarchical way using the derived type structures and pointers of Fortran-90. The code doesn’t contain any single ”COMMON” block containing variables nor any obsolescent features of Fortran-90 like the computed ”GOTO” statement. This has lead to a portable version of PARAGON which now is under validation in all UNIX and PC (NT and Linux) platforms. PARAGON has been developed following a well established software process used for all Westinghouse software projects. A general requirement followed by a detailed requirement for each version have been internally published. PARAGON has also a design document to make sure that all features desired by the designers are covered. The ease of maintenance of the code was one of the parameters in the design process. The development of a new code is a costly operation. For that, PARAGON has been developed using planning tools as well as a software configuration management system. The process requires also to establish a test matrix which contains problems permitting to test all the options of the code. The combination of all those facts has led us to write a high quality of software.

4 Validation Benchmarks

To test the performance of the calculational flow of PARAGON, we have chosen the following cases which represent some typical assemblies usually modelled by the designers in both Westinghouse and Mitsubishi Heavy Industries. To compare to MCNP results, the runs below are done at a constant temperature of 300 degree Kelvin for all materials (i.e. fuel, clad and moderator), but for depletion purposes, a typical operating temperature of 1031 degree Kelvin for fuel, 600 degree Kelvin for clad, and 580 degree Kelvin for moderator were used. The pin overlay of the three assemblies is given in Figure 1

4.1 A 14×14 Westinghouse fuel design assembly

This case is an example of a 14×14 fuel assembly. The pitch of the cells is about 1.414 *cm*. The assembly contains 14 guide tubes and 1 instrumentation thimble at the center. The uranium enrichment for the fuel is about 4.1 *w/o*. The assembly is surrounded by a water gap of 0.0521 *cm*.

4.2 A 17×17 MHI fuel design assembly

This second case is a MHI design of a 17×17 fuel assembly using 6 *w/o* gadolinia burnable absorber. The pitch of the cells is about 1.265 *cm*. The assembly contains 16 gadolinia rods, 24 guide tubes and 1 instrumentation thimble. The fuel enrichment is about 4.1 *w/o* for non-gadolinia cells and 2.6 *w/o* for gadolinia pins. The assembly is surrounded by a gap of 0.046 *cm*.

4.3 A 17×17 IFBA Assembly fuel type

This last test case is a Westinghouse fuel assembly design with Integral Fuel Burnable Absorbers (IFBA). The cell's pitch is about 1.262 *cm*. The fuel enrichment is about 4.8 *w/o*. The assembly contains 156 IFBA cells, 24 guide tubes and 1 instrumentation thimble. The assembly has a water gap of about 0.0716 *cm*.

4.4 Numerical Results

Table 1: Comparison of PARAGON to MCNP continuous energy.

	14×14 case	Gadolinia case	IFBA case
MCNP	1.29477 (0.00042)	1.17965 (0.00048)	1.07727 (.00056)
PARAGON	1.29329	1.17910	1.07694
delta (*pcm)*	148	55	33

To ensure a small standard deviations, MCNP runs were performed using 1.5 million particles distributed over 300 cycles. For PARAGON options, we have used a coupling order of three for all cases. The azimuthal sectors [Ouisloumen, 1996] are also used in all pin cell regions. For pins with gadolinia we have subdivided the fuel regions into six equi-volume rings. The reactivity predicted by PARAGON, for the three benchmarks, agrees very well with MCNP results, as shown in Table 1. This table is a proof that for those typical cases, the self-shielding module and the flux solution of PARAGON can predict the continuous energy Monte Carlo calculations.

The Figures 2 and 3 show the evolution of the eigenvalue as a function of the burnup. We compare PARAGON in those cases to PHOENIX-P. Our purpose here is to prove that the calculational flow of PARAGON is working properly, knowing that PHOENIX-P is well benchmarked for the typical cases that we are presenting. We are only interested in the cases of IFBA and gadolinia assemblies which are containing strong burnable absorbers. In the other case, there is no significant difference between the two codes. To generate those figures PARAGON uses a coupling order of three and azimuthal sectors (i.e. diagonal splitting) in moderator regions [Ouisloumen, 1996]. For gadolinia pins, we have used six sub-rings in the fuel regions (the sub-division of all the regions of the cells into azimuthal sectors has a negligible effect in the answers).

In Figure 2 (IFBA case), we see around 20000 MWD/MTU burnup a maximum of 100 *pcm* difference between the two codes. This difference is essentially due to the flux solution (self-shielding method is almost the same between the two codes). PHOENIX-P uses DP_0 with cylindrization and S_4 type of flux solution methods. While PARAGON uses more details in spatial representation and higher coupling order which will improve the flat-flux assumption made to compute the collision probability matrix. Throughout the depletion range the difference between the two codes in this case is acceptable and was expected.

For gadolinia case, PHOENIX-P uses a set of pre-tabulated gadolinia cross-sections which are fuel type dependent. Those cross-sections have been generated using muti-regions in the fuel, since PHOENIX-P doesn't have this capability. In Figure 3, we are also seeing the same phenomena as in the previous case, but more pronounced because of the differences in the gadolinia cross-sections. Below the burnup of 20000 MWD/MTU, the difference of about 250 *pcm* that we see in Figure 3 is due to the multi-region modeling in PARAGON and to its flux-solution. If PARAGON uses the same set of gadolinia cross-sections as PHOENIX-P and a single region in gadolinia pins, the difference will become less than 100 *pcm*. With gadolinia as a strong absorber, the multi-region permits a better Plutonium build up with the depletion (depletion is done with total flux including the thermal); that also contributes to make the difference between the two codes in this case higher than the previous IFBA case.

5 Conclusions

We have described in this paper different modules of the new lattice code PARAGON. The numerical benchmarks studied here show that PARAGON can predict the continuous energy MCNP results with high accuracy. The overall calculational flow of PARAGON was also qualified against the well established PHOENIX-P lattice code.

In the process of enhancing the physics models of PARAGON, a resonance self-shielding method which will permit generation of space dependent self-shielded cross-sections is under development. The geometrical capabilities will also be extended in the future to more geometrical configurations like hexagonal assemblies, BWR assemblies, and fuel assemblies for new generation.

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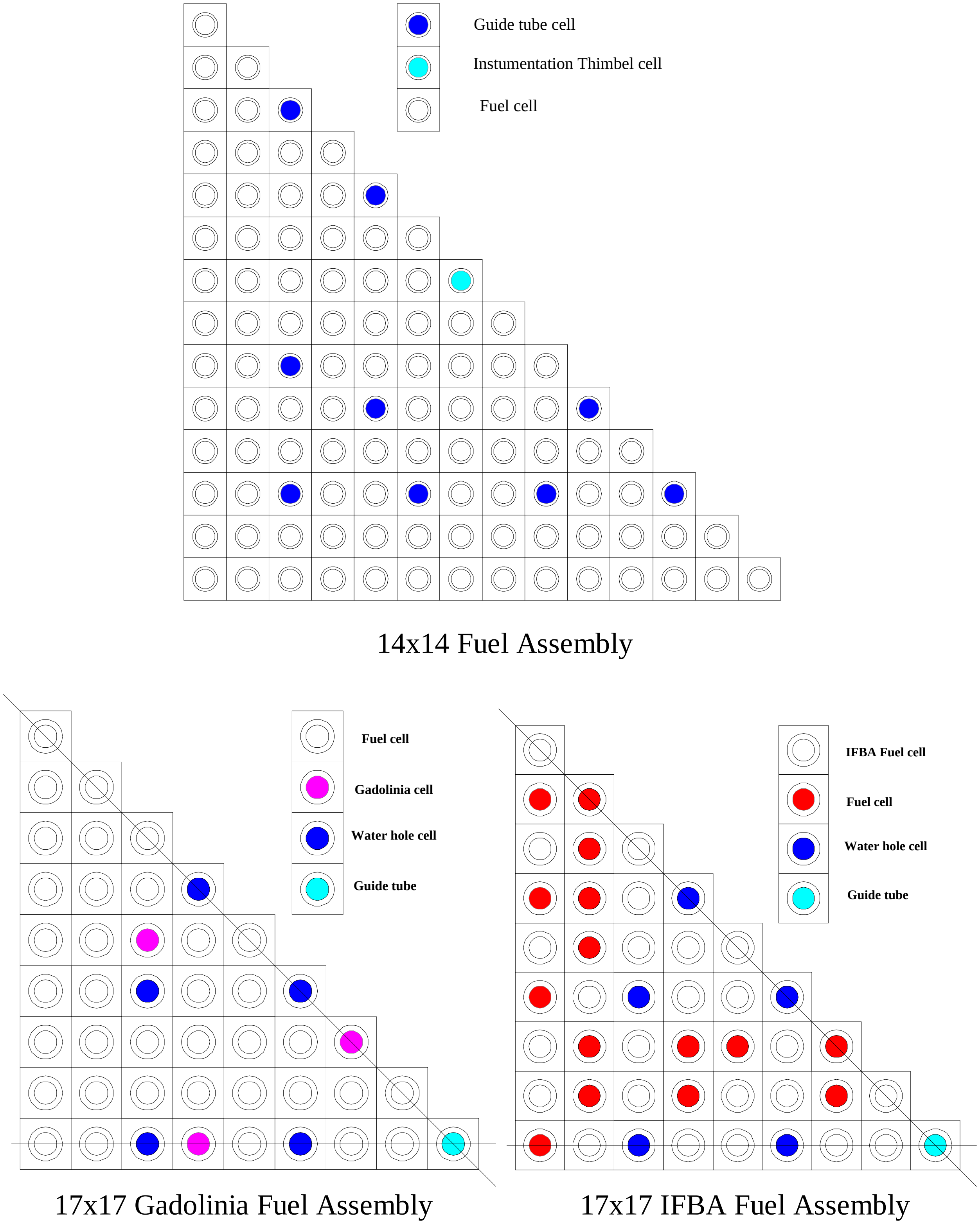

14x14 Fuel Assembly

17x17 Gadolinia Fuel Assembly

17x17 IFBA Fuel Assembly

Figure 1: Configuration of the assemblies.

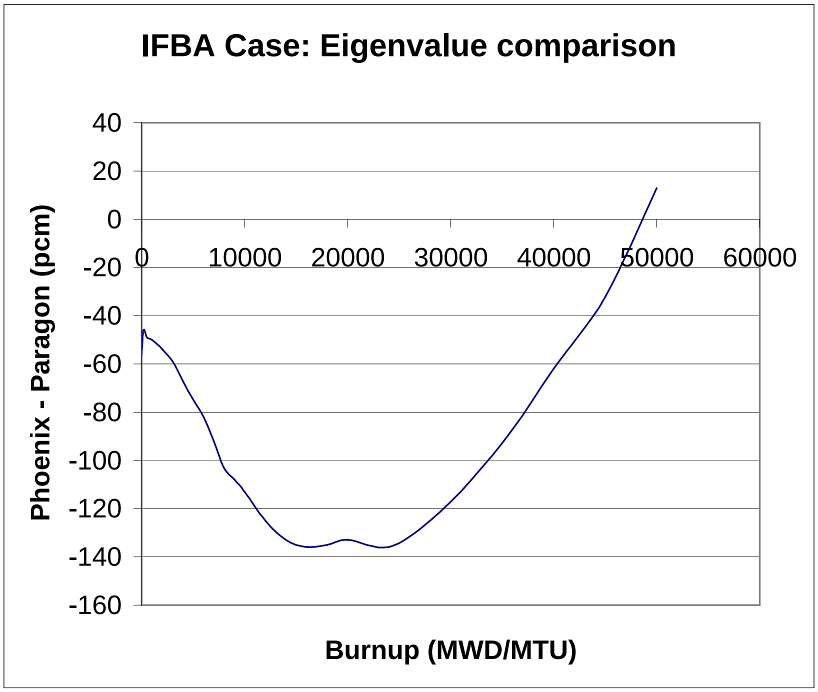

Figure 2: Eigenvalue comparison between PHOENIX-P and PARAGON for assembly with IFBA.

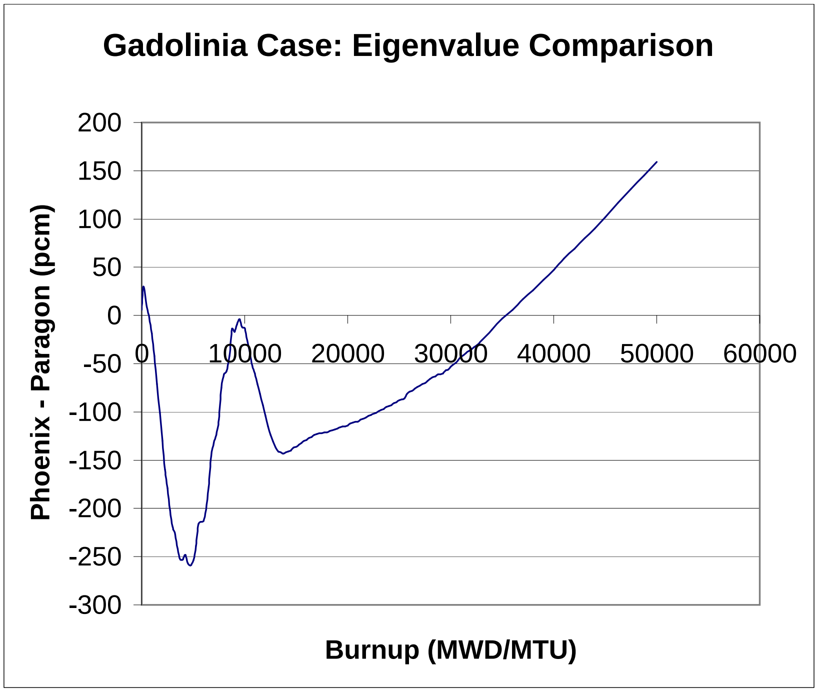

Figure 3: Eigenvalue comparison between PHOENIX-P and PARAGON for assembly with Gadolinia.