VALIDATION OF VISWAM SQUARE LATTICE MODULE WITH MOX PIN CELL BENCHMARK

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Development and validation of computational tools for the design analysis of modern light water reactors (LWR) has become important in view of the renewed interest in LWRs to Indian nuclear power programme. Development of a comprehensive code system called VISWAM has been undertaken based on the experience with the Tarapur BWR code system and its subsequent hexagonal version developed for the analysis of the Russian VVER, which has been commissioned recently at Kudankulam, Tamil Nadu. The new code system is being developed as a modular code package in Fortran-90 language. This paper presents the validation of the lattice burnup model for a square lattice pin cell problem. The pin cell problem with MOX fuel has been taken from the benchmark problem suite for the LWR next generation fuels. The VISWAM code results and their comparison with results of other research labs are presented in this paper. The problem was independently analyzed using the DRAGON code system. The results thereof are also presented in the comparison. In addition, the effect of (n,2n) cross-section on ^{237}Npnumber density prediction and the importance of considering two different capture products of ^{241}Am are also discussed.

Keywords: VISWAM Code, DRAGON Code, LWR MOX Benchmark, JEFF-3.1.2

1. Introduction

With a view to analyze the modern LWRs which are planned to be included in the Indian nuclear power programme, the computational tools already developed in the 1970-90's are being integrated in a single code system called VISWAM [1]. At present VISWAM code system has reached the level of lattice burnup computation. It can presently be used for burnup calculations of Pressurized Water Reactor (PWR) assemblies in both square and hexagonal (as

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in Russian VVER) geometries. It has provisions for modeling all the heterogeneities present in a typical PWR such as rod cluster control absorbers (RCCA), burnable absorber rods of gadolinium and boron type, water rods, instrumentation tubes, and assembly channels.

2. VISWAM Code System

The VISWAM code system is being developed to perform the physics design computations of LWR cores. The lattice burnup code has been developed and is being tested. The 1-D option in the VISWAM code is essentially same as that of SUPERB code used for square lattice [2] and EXCEL code used for hexagonal lattice [3]. The lattice model considers one dimensional multi group transport calculations and two dimensional few group diffusion calculations with transport-diffusion correction for strong absorber cells. The operation experience of Tarapur BWR has proven the overall reliability of the lattice and core computation models [4].

2. 1 Basic Nuclear Data

The basic cross section library considers 172 energy groups in WIMS/D format. Currently the library based on the JEFF-3.1 nuclear data library is being used for most of the LWR design computations. For the analysis of the benchmark problem we used the WIMS/D library based on ENDF/B6 dataset as well. The JEFF-3.1 library contains cross sections for 185 nuclides up to ^{252}Cf, and the temperature for important resonant nuclides is extended up to 2500K. Resonance integrals are available for 48 nuclides up to ^{252}Cf. The ENDF/B6 library has 173 nuclides up to ^{244}Cm and the temperature for resonance integral tabulation is up to 1100°K. Resonance treatment is done for 28 nuclides.

2.2 Brief Description of VISWAM Code Lattice Model

The resonance treatment is based on the equivalence principle and semi-empirical formulae as described in LWR-WIMS report [5]. Mutual shielding of different resonant isotopes is treated as per the procedures described by Stamm'ler and Abbate [6]. The two dimensional fuel assembly cell problem is solved in three stages. First, a series of one dimensional (1-D) transport calculations in 172 energy groups is done for every fuel pin cell type by the first flight collision probability method (P_{ij}). In the second set of computations, each heterogeneity is treated separately by appropriate 1-D supercell model. The multi-group neutron spectra obtained by the supercell calculations is appropriately chosen for condensing the 172 group cross sections to five broad energy groups. For absorber cells, a diffusion iterative technique is used to modify the few group cross sections such that the transport leakage in the

absorber cell is preserved by a diffusion treatment of the same problem. Finally the entire assembly is treated by 2-D diffusion theory in five energy groups. Assembly homogenized few group cross sections are obtained in five and two energy groups for subsequent core calculations. Isotopic density changes as a function of irradiation is carried out for several burnup zones representing each fuel pin and burnable absorber. One group microscopic cross sections are obtained for each burnup zone with neutron spectrum corrected for criticality. Multiple ring regions are considered in burnable absorber rods and fuel pins. However in fuel pins with no Gd, it is found that single region is adequate. The burnup equations are solved by using 5^{th} order Runge-Kutta method.
Some salient features of VISWAM code system are the following. The code input supplies the enrichment distribution, along with the heterogeneities present in the problem. The classification of pin cell types depending on enrichment and Dancoff factors is done internally by the code. The pin cell types are further differentiated into several burnup types according to the fuel layer count from the centre of the assembly. The same data is used to make the choice of the supercell spectra for collapsing of cross sections. Options for handling both hexagonal and square lattices are available.

All the routines in the VISWAM code are written in Fortran 90 with extensive use of features such as dynamic memory allocation, modular attributes, array operations; user defined data structures and derived types.
This paper presents the results of the validation exercise for one of the PWR pin cell benchmark problem with MOX fuel. [7]

3. Analysis of MOX Pin Cell Benchmark

Yamamoto et.al [7] have proposed a benchmark problem suite for the LWR next generation fuels. This benchmark problem suite has been formulated for progressive checking of code system from simple pin cell level to complex assembly level. In pin cell level two types of ceramic fuels are considered, viz., low enriched uranium (LEU) and Mixed Oxide (MOX). At assembly level, the problems represent a typical PWR or BWR fuel assemblies with both LEU and MOX type fuel pins. The LEU version considers some fuel pins mixed with Gd_2O_3. The VISWAM code is being developed and tested against each of these problems. In view of the massive data collected for comparison of each of these problems we present only selected results of the MOX fuel pin cell analysisin this paper. This benchmark problem has been analyzed by many other lattice codes popularly used worldwide and their results have been compiled as per the requirements of the benchmark Working Group at selected burnup steps [8]. The comparison of VISWAM results with the Benchmark Mean (BM) values of the results of sixteen codes is presented.

4.DRAGON Code System

The analysis of the benchmark problem has also been carried out using the Canadian DRAGON code system [9]. DRAGON calculations reported in this paper employed LIB, GEO, EXCELT, USS, ASM, FLU and EDI modules of DRAGON code for generation lattice level results. The LIB: module was used to read 172 group DRAGLIB library format based on the JEFF-3.1.2 nuclear data library. Functions of other modules used are: GEO to model specific geometry with material compositions, EXCELT, which creates integration lines for full cell calculations (i.e.) to generate tracking files containing regional volumes and track lengths, Universal Self-Shielding module, USS to calculate the resonance self-shielded cross sections using subgroup method, ASM to determine the multi-group complete collision probability matrices, FLU to solve the multi-group transport equation for the flux, the adjoint flux and the multiplication constant and EDI module was used to edit the output and at the same time perform Flux-Volume Weighting (FVW) or Super homogenization (SPH) method homogenization and condensation. In the present self-shielding calculations USS module employs PTSL approach, where mathematical probability tables and slowing down correlated weight matrices can be computed in selected energy groups using the Ribbon extended approach.

5. Benchmark Problem

5.1 Description

The details of the MOX pin cell problem are given in benchmark problem suite for the LWR next generation fuels [7]. The broad specifications of the fuel pin are summarized in Table 1.

Table 1

Broad Specifications of the MOX Pin cell Benchmark Problem

Description	Units	Nominal values	Fuel Composition	Units	Nominal values
Fuel pin pitch	cm	1.265	**U-235**	%	0.2
Pellet outer diameter	cm	0.824	**Pu-total**	%	17.2
Clad inner diameter	cm	0.824	**Pu Composition**		
Clad outer diameter	cm	0.952	**Pu-238**	%	2.1
Fuel density	g/cc	10.4	**Pu-239**	%	54.5
Zr-Clad density	g/cc	6.53	**Pu-240**	%	25.0
Coolant density	g/cc	0.66	**Pu-241**	%	9.3
Clad/Coolant temp.	K	600	**Pu-242**	%	6.4
Fuel temperature	K	900	**Am-241**	%	2.7
Average Linear Heat Generation Rate				W/cm	179

Table 2

Specifications for Branching Calculations

Parameter	Change	Value
40% void	Coolant density	0.549 g/cc
70% void	Coolant density	0.409 g/cc
Doppler	Fuel temperature	1800K
Cold	Coolant density All temperatures	0.996 g/cc 300K

5.2 Benchmark Results to be collected

In the VISWAM analysis, the first flight collision probability method was used to analyze the MOX pin cell benchmark problem. The 172 group cross section libraries based on JEFF-3.1 and ENDF/B6 dataset were used[10]. The nominal parameters were used to build the number densities as a function of burnup up to 70 GWd/t. Fine burnup steps were considered. Four additional branch calculations were done using these isotopic densities with any one of the changes from the nominal parameters as shown in the Table 2.

6. Results and Discussion

Figs. 1.1, 1.2, 1.3, 1.4, and 1.5 give the values of k_∞ as a function of burnup for nominal state and for branching cases of 40% and 70% void, Doppler at 1800°K and cold state. The figures give the results of VISWAM code with JEFF-3.1 and ENDF/B6 libraries (referred henceforth as VISWAM-J and VISWAM-E) and their comparison with DRAGON and the benchmark mean (BM) values. It is seen that the VISWAM k_∞ values for both JEFF-3.1 and ENDF/B6 libraries are lower than the BM values by ~1% in nominal and 40% void. They were lower by 1.1% and 0.8% in 70% voided cases for the two libraries. In the Doppler case of 1800K and in cold case, the differences in k_∞ values are smaller. DRAGON values are similar to the VISWAM-J values.

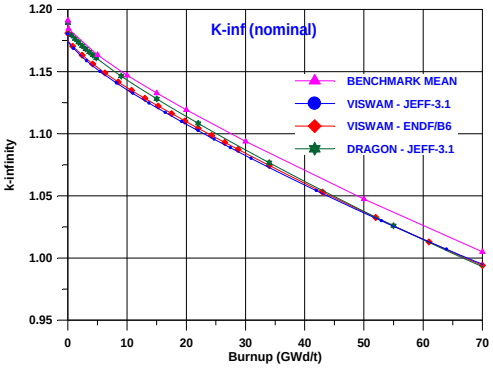

Fig.1.1 k_∞ as a function of burnup for nominal case

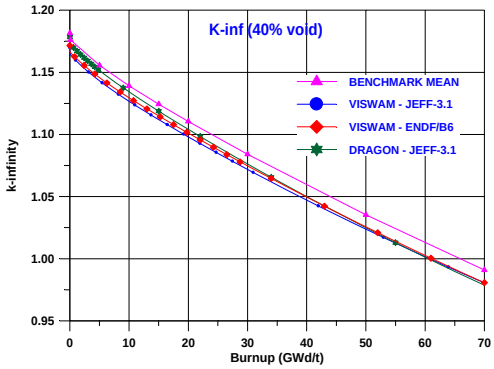

Fig.1.2k_∞ as a function of burnup for 40% voided case

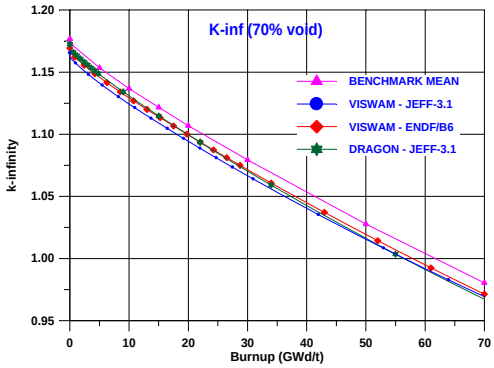

Fig.1.3k_∞ as a function of burnup for 70% voided case

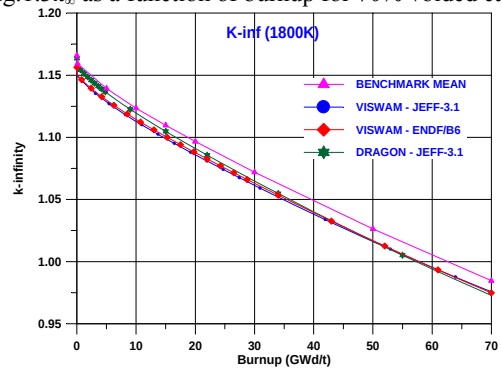

Fig.1.4k_∞ as a function of burnup for T_{fuel}=1800K case

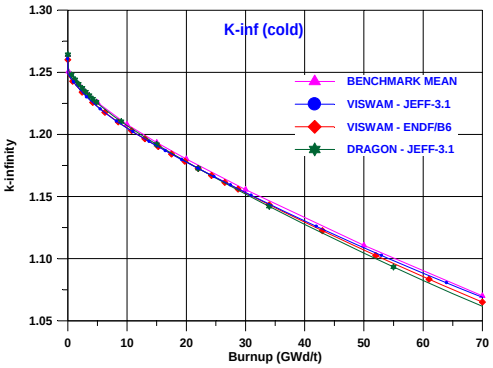

Fig.1.5k_∞ as a function of burnup for cold state (300K)

The void reactivity is over-predicted by VISWAM-J and under-predicted by VISWAM-E for 70% void. The Doppler reactivity load is under-predicted by both the libraries. The cold to hot reactivity load is over predicted by both VISWAM-J and VISWAM-E and DRAGON.

The number densities of all transuranic isotopes and fission products are in good agreement with BM values. Figs 2.1 and 2.2 show the number density comparison for U-235 and U-238 respectively. Fig. 3.1 gives the comparison of one group macroscopic absorption cross section of the fuel cell. They agree within -1.2%, -2.5% and +0.3% for VISWAM-J, VISWAM-E and DRAGON respectively. Figs.3.2 and 3.3 give the comparison of one group microscopic absorption cross section of ^{235}U and ^{239}Pu. The VISWAM and DRAGON values agree within ±5% for most of the fuel nuclides. Fig. 4.1 gives the comparison of macroscopic production cross section of the fuel cell. They agree within -0.75%, -2.2% and -0.64% for VISWAM-J, VISWAM-E and DRAGON respectively. Figs.4.2 and 4.3 give the comparison of microscopic production cross section of ^{235}U and ^{239}Pu.Here also, the VISWAM and DRAGON values agree within ±5% for most of the nuclides.

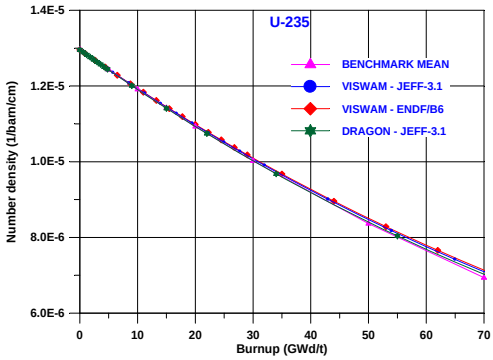

Fig.2.1 Number density of U-235

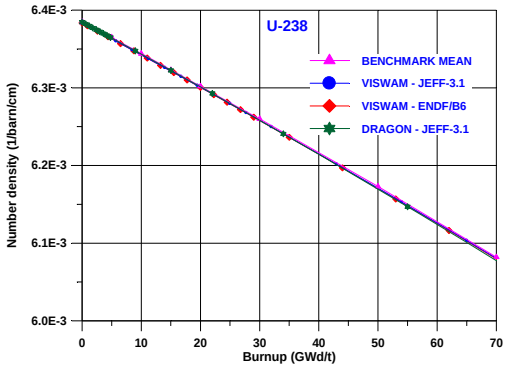

Fig.2.3 Number density of U-238

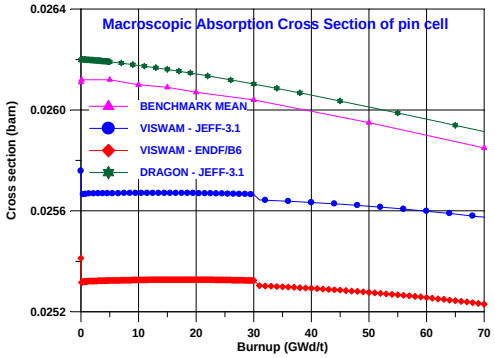

Fig.3.1 Macroscopic absorption cross section of pin cell

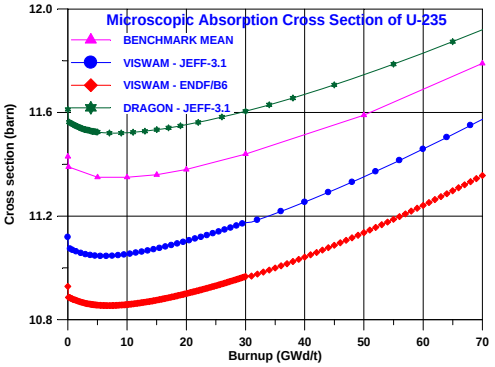

Fig.3.2 Microscopic absorption cross section of U-235

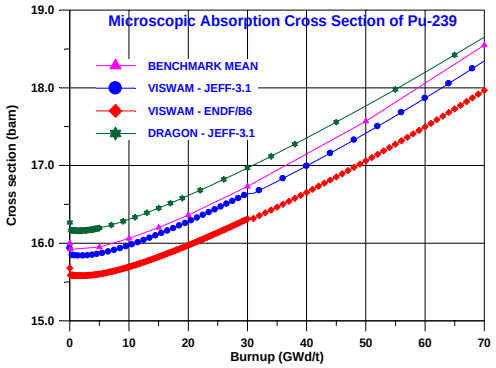

Fig.3.3 Microscopic absorption cross section of Pu-239

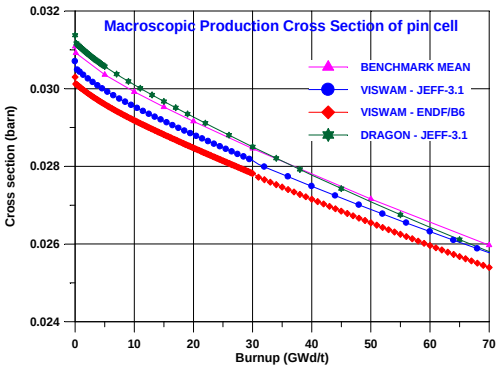

Fig.4.1 Macroscopic production cross section of pin cell

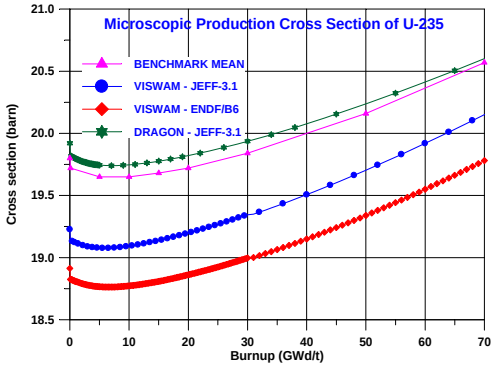

Fig.4.2 Microscopic production cross section of U-235

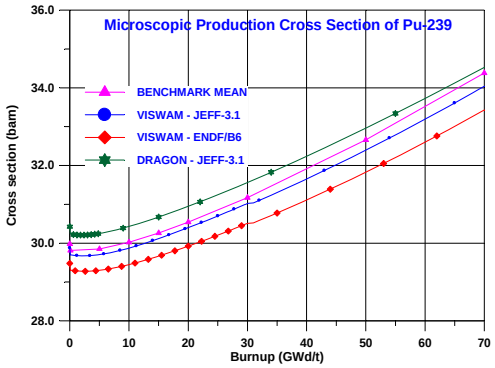

Fig.4.3 Microscopic production cross section of Pu-239

6.1 (n, 2n) cross section – Effect on ^{237}Np Number Density

In WIMS library, the (n, 2n) and other such threshold reaction cross sections are not normally available since they are subtracted from the absorption cross section in the parent library itself. When the MOX pin cell benchmark was initially analyzed without the explicit (n, 2n) chain, we noted that the ^{237}Np number density was under-predicted by a factor of 4.2 compared to BM value. Fig.5 gives the plot of ^{237}Np number density as a function of burnup. Later we introduced explicit (n, 2n) chains in VISWAM code. In the current WIMS library, the (n, 2n) cross sections are available for 8 nuclides, viz., ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu and ^{242}Pu. These cross sections are provided as absorption cross sections of some pseudo dosimetry materials. Special provisions were made to read these cross sections and collapse them to one group.The multi group (n, 2n) cross sections were added to the multi group absorption cross sections of the respective nuclides prior to obtaining the effective one group microscopic absorption cross sections. This could make the absorption cross section less negative or positive for these nuclides in high energy groups. Burnup chains were suitably modified in VISWAM code. It is seen that ^{237}Np number density is now over-predicted by 9% compared to BM value. DRAGON values are higher than VISWAM values.

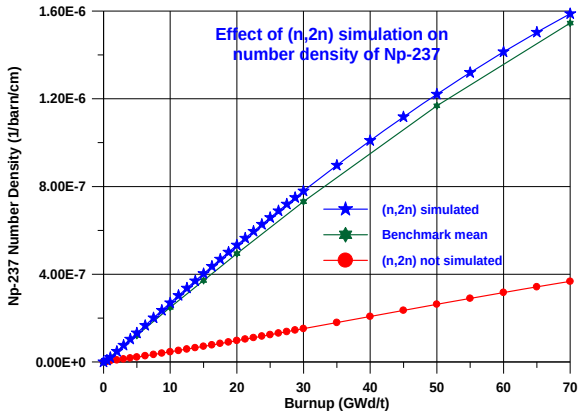

Fig.5 Effect of (n, 2n) simulation on number density of Np-237

6.2. Capture products of ^{241}Am – Effect on ^{242}Cm & ^{238}Pu Number Density

^{241}Am on neutron capture produces ^{242}Am as well as ^{242m}Am with probability of 79% and 10% respectively, rest being fission. ^{242m}Am decays to ^{242}Am with a half-life of 141 years. ^{242}Am decays to ^{242}Cm with a half life of 16 hrs. ^{242}Cm becomes ^{238}Pu by α-decay with a half-life of 163 days.

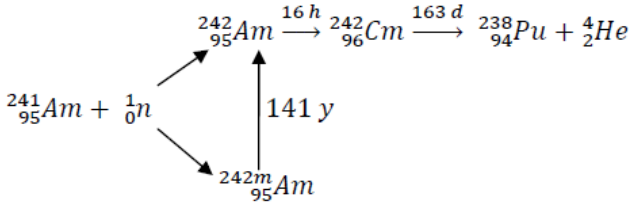

Fig.6.1. ^{241}Am neutron Capture Products

The WIMS libraries generated as part of WIMS library Update Project (WLUP) in 2001 [11], consider only one capture product for any nuclide. To enable two capture products of ^{241}Am, Trkov et al. [12] made the following provisions in the WIMS libraries of WLUP. ^{242m}Am was treated as the capture product of ^{241}Am with a branching ratio of 0.12. ^{242}Am was treated as a pseudo fission product from the fission reaction of ^{241}Am with a pseudo fission yield of '67'. To enable this second link, the fission cross section of ^{241}Amwas modified to be proportional to the capture cross section such that the capture to fission ratio (CFR) would be equal to 92. This is the CFR value assessed for typical

PWR lattice spectrum. The production cross section was also modified by preserving the value of 'ν'.

In the present study, we would like to mention that the modification of fission cross section of ^{241}Am had been done only in ENDF/B6 library and not in JEFF-3.1 library. ENDF/B 6 values are artificially decreased ones. Unfortunately, the fission product link to ^{242}Am and the pseudo fission yield was present in both the libraries. Hence when we performed the MOX benchmark calculation, the results of number density of ^{242}Cm and ^{238}Pu using ENDF/B6 library matched well with BM mean values while those of JEFF-3.1 showed large deviations. VISWAM code was modified to include ^{242}Am as second capture product of ^{241}Am with a branching ratio of 0.88. In addition to account for the β decay of ^{242}Am to ^{242}Cm a reducing factor of 0.827 was also considered for formation of ^{242}Am from capture of ^{241}Am. Formation through fission process of ^{241}Am was disabled. Unmodified fission and nu-fission cross sections of ^{241}Am were used. It was seen that these modifications could nearly reproduce the BM results for both ^{242}Cm and ^{238}Pu.

Figs. 6.2 and 6.3 show the comparison of number density of ^{242}Cm and ^{238}Pu before and after the above modifications in VISWAM code. The VISWAM-E value is seen to be closer to the benchmark mean value for both the above nuclides. The VISWAM-J values with unmodified fission cross section of ^{241}Am and single capture product is seen to be higher by 300% and 200% than BM values for ^{242}Cm and ^{238}Pu respectively. With inclusion of explicit two capture products of ^{241}Am and with non-tampered fission cross sections, it is seen that the result has substantially improved (<2%) for both the nuclides.

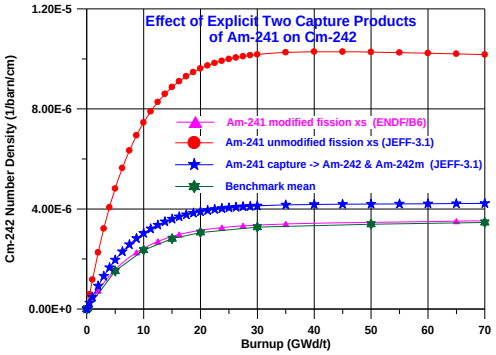

Fig.6.2 Effect of Explicit Two Capture Products of ^{241}Am on ^{242}Cm

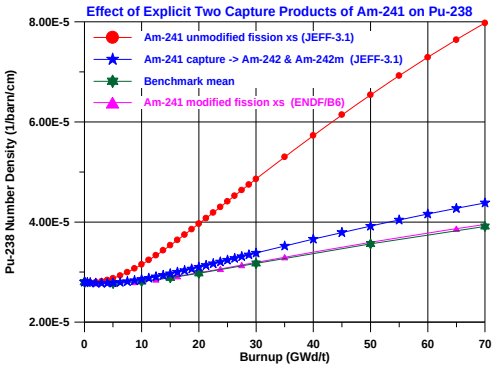

Fig.6.3 Effect of Explicit Two Capture Products of ^{241}Am on ^{238}Pu

7. Conclusions

An integrated code system VISWAM is being developed as for modern LWR design analysis. Efforts are being made to validate the newly developed code system at each successive stage of its development to enhance its predictive capability. As a part of such validation studies, the MOX pin cell problem of the LWR benchmark suite has been analyzed with two different nuclear cross section libraries viz., JEFF-3.1 and ENDF/B6 in 172 energy groups and is presented in this paper. The results of VISWAM code are compared with those of DRAGON code and the mean values of the results of sixteen labs reported in the LWR BM suite. At first, the comparisons led to theidentification of some areas which requires improvement in VISWAM calculations. To improve the same, the new calculation algorithmsare developed and are incorporated in VISWAM calculations. The main conclusions from the present study are:

- The comparisons with the results of DRAGON code and other international codesshows generally good agreement for all parameters studied and it demonstrates the capability of VISWAMcode for such calculations.
- The k_∞ values agree within 1% for nominal and other branching cases. The burnup reactivity load, void reactivity, Doppler load, cold to hot reactivity load compare reasonably well.
- Isotopic densities of actinides and fission products also agree in general within 5%. Initially, large difference by several factors was noted for ^{237}Np, ^{238}Pu and ^{242}Cm nuclide number densities. The study necessitatesthe inclusion of explicit (n, 2n) reaction to improve the ^{237}Np number density prediction. After incorporating it, the ^{237}Np number density comparison is observed to be within 9% deviation.

- The number densities of ^{242}Cm and ^{238}Pu were predicted very close to the BM value by ENDF/B6 library. On scrutiny, it was noticed that the burnup chain in this library provided a fission link between ^{241}Am and ^{242}Am instead of a branching capture link. In ENDF/B6 library, the fission cross sections had been changed to be proportional to capture cross sections. On providing the dual capture link for ^{241}Am with ^{242m}Am and ^{242}Am the results of the JEFF-3.1 library also improved for the number densities of ^{242}Cm and ^{238}Pu. This was achieved without tampering the fission cross sections of ^{241}Am.

In summary, the calculation method incorporated in VISWAM code is demonstrated to be reliable for reactor design calculations through this validation exercise.

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