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ABOUT THE APPLICATION OF MCNP4 CODE IN NUCLEAR REACTOR CORE DESIGN CALCULATIONS

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ABSTRACT

This paper provides short review about application of MCNP code for reactor physics calculations performed in SKODA JS. Problems of criticality safety analysis of spent fuel systems for storage and transport of spent fuel are discussed and relevant applications are presented. Application of standard Monte Carlo code for accelerator driven system for LWR waste destruction is shown and conclusions are reviewed. Specific heterogeneous effects in neutron balance of VVER nuclear cores are solved for adjusting standard design codes.

1. INTRODUCTION

MCNP is a general purpose Monte Carlo code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. In SKODA calculating system this code is used mainly for criticality analysis and source driven multiplied systems calculations since it has the capability to calculate eigenvalues of critical systems or reaction rates (tallies) of source driven systems. Problem of accuracy and precision are key calculation problems in application of Monte Carlo codes. Precision is the uncertainty of mean value caused by statistical fluctuations. Accuracy is a measure of how close the expected value is to the true physical quantity being estimated. The first one is given by arrangement of calculational procedure the second one is dependent on the model and cross-section library used in Monte Carlo. Namely problem of accuracy in some cases (with the lack of experimental information) can be solved by comparison with other (including deterministic) codes.
The primary source of nuclear data in our MCNP4B [1] calculations were libraries ENDF60+KIDMAN+RMCCS+ENDF5U.

2. SPENT FUEL STORAGE CASKS CALCULATIONS

In SKODA is under development transport cask SKODA 440/84. This compact cask with internal absorbers (atabor plates) is intended for transport and storage of 84 VVER-440 fuel assemblies. The VVER-440 fuel assembly has core hexagonal pitch 14.7 cm, number of fuel rods in fuel assembly is 126 arranged in lattice pitch 12.2 mm and fuel pellet stuck height is 242 cm. The 3D calculations of cask SKODA 440/84 with axial burnup distribution were provided. The cask can be loaded by up 84 fuel assemblies VVER-440 each separated by borate steel plates in hexagonal fuel assembly pitch 17.5 cm. Criticality safety analyses is at present performed for cask filled with fresh fuel assemblies and pure water (no boron) of 20°C temperature. The problem of multiplicative factor k_{eff} uncertainty is solved statistically with three components; tolerances, bias, and calculation confidence level 95/95 uncertainty. Material and constructional tolerances are assessed by the deterministic code WIMS7 [2] on the 2D radially infinite model of cask (0.01147) and bias for VVER fuel is identical with bias used in Westinghouse project of NPP Temelin (0.0048). Calculation uncertainty are determined with a 95 percent probability/95 percent confidence level from statistically combined of the three estimators of multiplicative factor; collision, absorption, and track length. Nevertheless in some cases there are problems with precision of calculation namely in the 3D structures. Differences in convergence rate of multiplicative factor k_{eff} and tally calculations needs also focus of our attention. To demonstrate it we used simple model of radially infinite fuel assembly structure called of the benchmark CB3 [3]. This benchmark consists of multiplicative factor k_{eff} comparisons and axial distribution of normalized fission densities comparisons. The errors of k_{eff} as an integral value can be well predicted by standard deviations in 1 σ approximation as it is seen from Figure 1. We can also see that the k_{eff} will depend for the same 1 σ errors on the organization of statistical process (i.e. on the relation: number of cycles to number of neutron per each cycle).

The quality of the tally of local values of fission densities as an point detector needs special attention in statistical checks. It was found that after reaching very low relative errors (RE) some tally are not stabilized - especially in the case 14 of CB3 (see Figure 2). Formal statistical check of case 14 after 2500 cycles each with 2000 neutrons will give Table 1:

Table 1 Statistical check

distance from fuel bottom	RE	VOV	FOM
0 - 25 cm	.0044	5.61e-6	30.5
25 - 50 cm	.0037	3.94e-5	43.3
50 - 175 cm	.0010	3.14e-5	565.2
175 - 200 cm	.0013	5.14e-5	354.9
200 - 225 cm	.0011	4.02e-5	467.1
225 - 244 cm	.0015	7.22e-6	253.6

where RE is relative error, VOV is variance of variance and FOM is figure of merit. In Figure 3 are depicted basic statistical characteristics of more problematic lowest value of fission densities in case 14 of CB3 in dependence on nps. In spite of relatively stabilized FOM and small relative error RE the first statistical check - monotones behavior of mean value - is not fulfilled. The process can be characterized like slow tilting of fission densities. Presented statistical check was performed for simple calculations without adopting special reduction variance techniques.

The axial and radial leakage impacts on multiplication factor were studied on SKODA 440/84 cask filled with fresh 3.6 w/o enriched fresh fuel assemblies. It was found that that radial leakage represents -3.3% in k_{eff} and axial leakage only -0.4% in k_{eff}. It means that bias value of calculation errors is on the level of axial leakage effect.

3. DESIGN CALCULATIONS OF THE THERMAL-SPECTRUM ACCELERATOR-DRIVEN SYSTEM FOR LWR WASTE DESTRUCTION

The accelerator-driven transmutation systems waste with internal graphite moderator (ATW concept proposed by Los Alamos) has been under study [4] at SKODA JS for several years. Specific physics issues used to analysis include safety, blanket multiplication, blanket reactivity temperature coefficients. The general description of SKODA Target and Blanket (T/B) design is provided in [4]. The T/B design consists of molten lead target in iron shells of the diameter 42 cm and radial centered in the multiplying blanket. The hexagonal 100 cm diameter graphite moderates the neutrons into the thermal range before they enter the blanket. The hexagonal graphite assemblies making up the blanket with the pitch 30 cm are provided with salt channel of diameter 7 cm for soft neutron spectrum version and diameter 21 cm for hard neutron specter version. Salt of Li7+BeF2+PuF3 enters at the bottom of the blanket and is pumped through the blanket. Typical blanket dimensions are up 5 m in diameter by 5 m tall. For the first stage of our calculations were adopted two reference calculation models:
a/ Reference two dimensional (2D) supercell model for calculation of molten salt fuel cycle and reactivity coefficients.
b/ Reference three dimensional (3D) model of the T/B structure which consists of 84 hexagonal graphite assemblies with fixed pitch 30 cm and of 380 cm length for power and spectral distribution calculations and reactivity coefficients calculations.

The problems with precision of calculations was analogous as are presented in above chapter for cask. Additionally was found that convergence of subcritical systems driven by external source depends on the value of subcriticality. Burn-up process of this system was simulated on 2D supercell model and calculated by WIMS7 code. For this 2D supercell model difference between WIMS7 and MCNP4B k_{eff} calculations [4] for the same isotopic composition was less then 1%.

Second source of discrepancy between WIMS7 and MCNP4B calculations is lack of some fission products in the MCNP4B ENDF60 library which causes increasing of MCNP4B k_{eff} values by 3% (according WIMS7 assessment). The limited number of isotopes in standard MCNP4B libraries is important obstacle in MCNP application for molten salt systems. The

quality of calculation of the over-moderated accelerator driven systems is dependent on the quality of thermalization library for graphite (Thermal S(α,β) Cross - Section Tables) because this effect reaches up to 10 % in k_{eff}. In detail this effect was analyzed and presented in the paper on WG F meeting [5]. It was found that this great temperature reactivity effects are caused by spectra perturbation in thermal region.

4.ANALYSIS AND UPGRADING GAMMA MATRICES IN CORE CALCULATION

In standard VVER core macrocode calculations are more heterogenous and nondiffusional structures like control fuel assemblies or outer boundary conditions obviously modeled by gamma matrices. In this paper is presented modelling of coupler which joints the fuel follower and absorber of VVER440 control fuel assembly.

Our 3D coupler models represent simplification of model presented in paper [6] and its cross-section is shown in Figure 4. The MODEL B like in [6] consists control fuel assembly surrounded by fuel assemblies which forms symmetrical hexagonal structure of five fuel assemblies with. The second MODEL C (see Figure 4) consists control FA surrounded by 6 + 2 fuel assemblies and forms symmetrical hexagonal structure of two FA width. The third MODEL D is formed only by control fuel assembly. All three models are only 80 cm height. The MODEL B and C have reflecting radial and axial outer surfaces. The neutron field in the MODEL D is driven with the external source of neutrons on given outer radial boundary and radial outer condition are vacuum and axial are reflecting. The external source used in the MODEL D had 20 group structure:
0.022 eV, 0.1, 0.625, 2.1, 27.6, 75.6, 371, 2.2 keV, 9.1, 25, 41, 111, 183, 0.5 MeV, 0.82, 1.35, 2.23, 3.86, 6.06, 20.

The 2D calculations presented in Figure 5 for comparisons were provided on the basis of cross-section of MODEL C with axial reflective boundary conditions.

Fuel assemblies consist fresh fuel 3.82% enrich. and temperature (coolant density) corresponded to 300K.

The evaluation process.

In fine axial layers were calculated partial currents that enters control assembly (J^+) and partial currents which are returning (J^-). In one group representation for diffusion approximation can be formulated relation between flux (Φ) and current (J) by formula

$$J = gamma \cdot \Phi \qquad (1)$$

where gamma can be calculated by Monte Carlo by formula :

$$gamma1 = (J^+ - J^-)/((J^+ + J^-) \cdot 2) \qquad (2)$$

or by formula

$$gamma2 = (J^+ - J^-)/\Phi. \qquad (3)$$

Differences between gamma1 and gamma2 represents also nondiffusion effects on the boundary. Relative errors of partial currents and flux calculations were lower than 0.5 %.

In two group (epithermal = epi, thermal = t) approximation gamma coefficients forms so called gamma matrix:

$$J^{epi} = gamma\ 11\ .\ \Phi^{epi} + gamma\ 12\ .\ \Phi^{t} \qquad (4)$$

$$J^{t} = gamma\ 21\ .\ \Phi^{epi} + gamma\ 22\ .\ \Phi^{t} \qquad (5)$$

In usual praxis the *gamma 12* member of gamma matrix is nearly zero. For this reason member *gamma 11* was used for comparisons of 2D and 3D gamma calculations. In Figure 5 is presented axial distribution of *gamma 11* member in two approximations equations (2) and (3). It is seen that differences between these two approximations are negligible. The axial dependence of *gamma 11* along coupler height is important. For some layers was calculated *gamma 11* in 2D approximation. Differences between 2D and 3D approximation are seen namely in the steel posts layer in which is important impact of fuel follower and in the water layer which 2D calculation is beyond the axial scale of Figure 5.

Impact of different radial modeling in 3D approximation is seen in Figure 6 from comparisons MODEL B a and MODEL C. For thermal group comparisons is used equation (6), where *gamma 12* member is taken from standard MOBY-DICK library.

$$J^{t} = (gamma\,22 + gamma\,21 \cdot \frac{\Phi^{epi}}{\Phi^{t}}) \cdot \Phi^{t} \qquad (6)$$

On the basis of MCNP4B calculations in MODEL C was provided the first derivation of corrections of standard 2D diagonal matrix coefficients of coupler calculated by codes WIMS - HECON in standard two group library. The results for layers thickness 6.1 cm are presented in Figure 7.

On the MODEL D were calculated 3D gamma matrices in two group approximation (see Table 2) for three sublayers from the coupler layer. The gamma values in Table 2 were calculated on the presumption of *gamma 12* = 0. From calculated matrix is seen that transfer of neutrons in axial direction is important for thin layers and representation of thin axial layers by 2D model can be misleading. On the other hand from Table 2 is seen that dimensions of 3D matrices should be greater then three layers which may cause problems with their application in standard macrocodes.

Table 2 3D two group gamma matrix (for 3 layers in plenum, layer dimensions according Figure 5)

	layer 1 34.4 to 36.9 cm		layer 2 36.9 to 39.4 cm		layer 3 39.4 to 41.9 cm	
	Φ^{cpi}	Φ^{t}	Φ^{cpi}	Φ^{t}	Φ^{cpi}	Φ^{t}
J^{cpi} layer 1	+0.2828	0	-0.0738	0	-0.0261	0
J^{t} layer 1	-0.0192	+0.1751	-0.0115	-0.0591	-0.0067	-0.0110
J^{cpi} layer 2	-0.0745	0	+0.2945	0	-0.0729	0
J^{t} layer 2	-0.0115	-0.0596	-0.0179	+0.1802	-0.0117	-0.0602
J^{cpi} layer 3	-0.0257	0	-0.0724	0	+0.2879	0
J^{t} layer 3	-0.0071	-0.0111	-0.0120	-0.0600	-0.0209	+0.1728

5. CONCLUSIONS

It was shown that standard Monte Carlo code MCNP4B can be used for variety neutron transport calculations and as a support of standard diffusion calculations. Beside standard criticality calculations of fuel storage casks MCNP4B code has new application in accelerator driven systems for LWR waste destruction. In some cases MCNP4B calculations should be combined with standard burn-up spectral codes.

The comparison has shown that 2D calculated gamma matrices are not correct representation of coupler. When the 3D gamma matrices can induce more problems in their application in standard macrocodes the representation of coupler by effective diffusion constants can be more attractive.

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Fig. 1 ' CB3 benchmark - case 14. Keff dependence on sigma (e.g. 2500(2000) is 2500 cycles each 2000 neutrons)

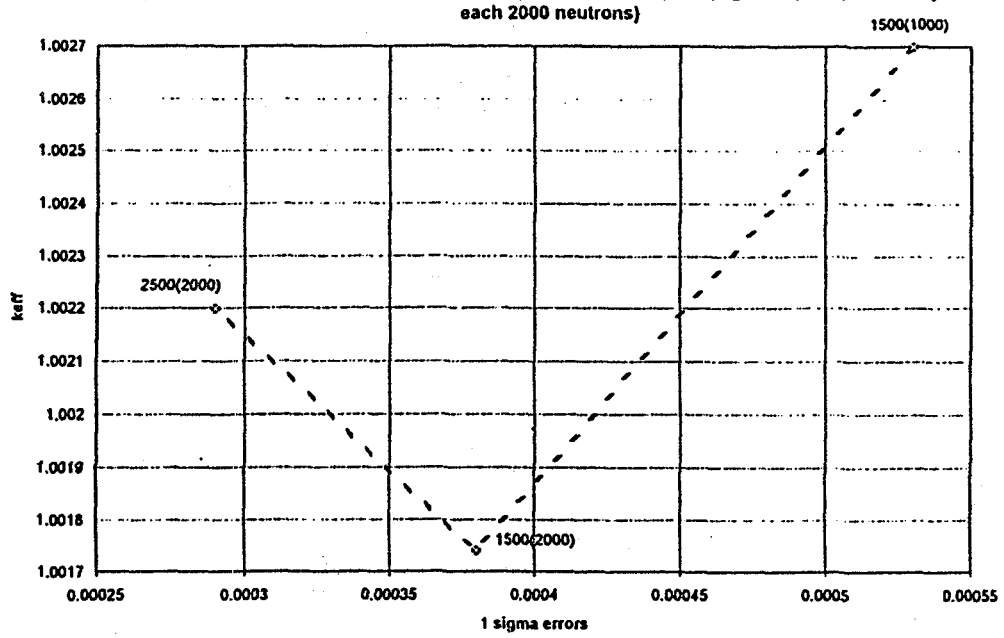
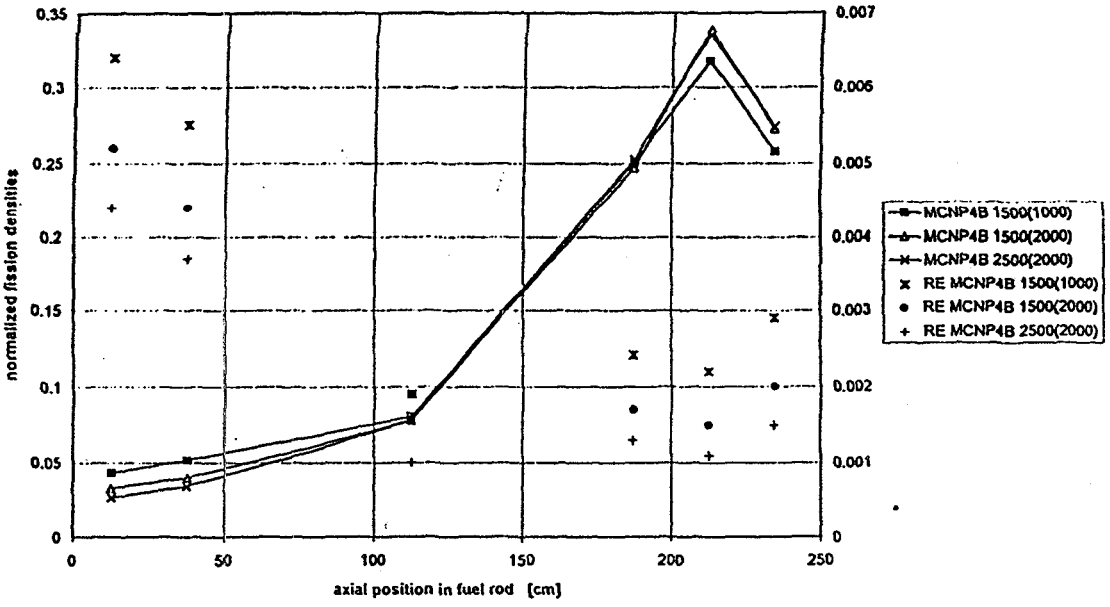


Fig. 2 CB3 benchmark - case 14. Normalized fission densities and their relative errors (RE) distributions in axial direction (cycles(neutrons in each cycle)).



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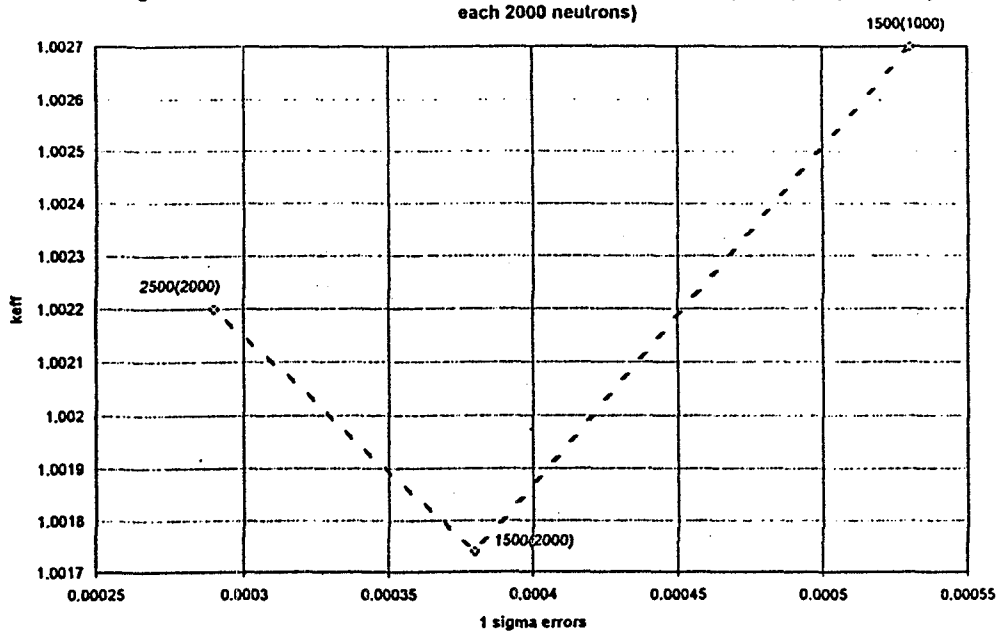

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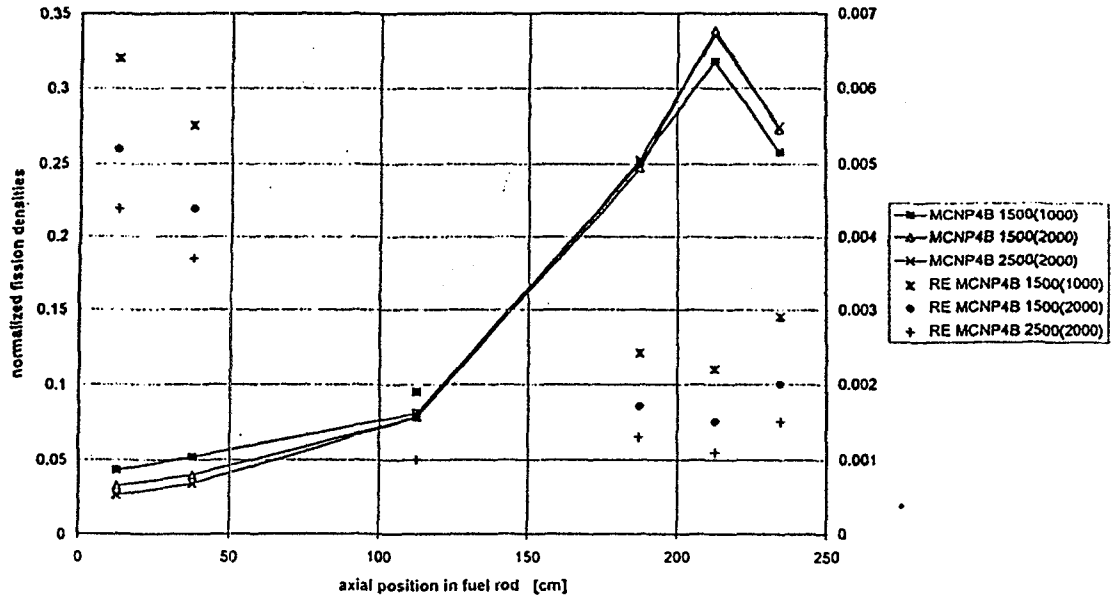
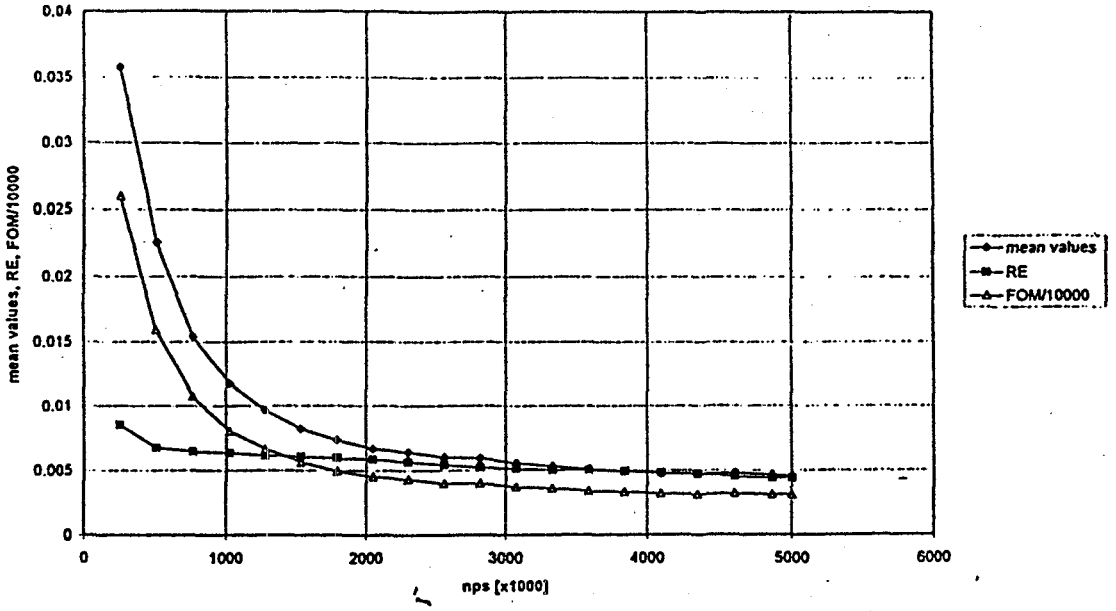
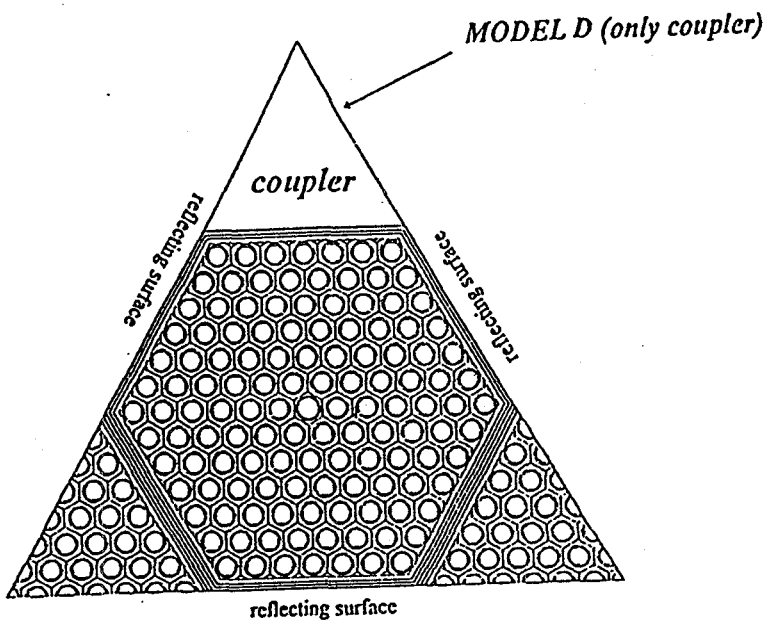


Fig. 3 CB3 benchmark - case 14. Fission densities mean values and their relative errors (RE) and FOM/10000 for position 12,5 cm dendence on nps (calculation 2500 cycles each 2000 neutrons).





MODEL C

Figure 4 Cross-section of the MODEL C and MODEL D

Fig. 5 Epithermal member (*gamma 11*) of albedo matrix axial distribution
(MCNP4B calc. 3D, 2D dashed line , model B)

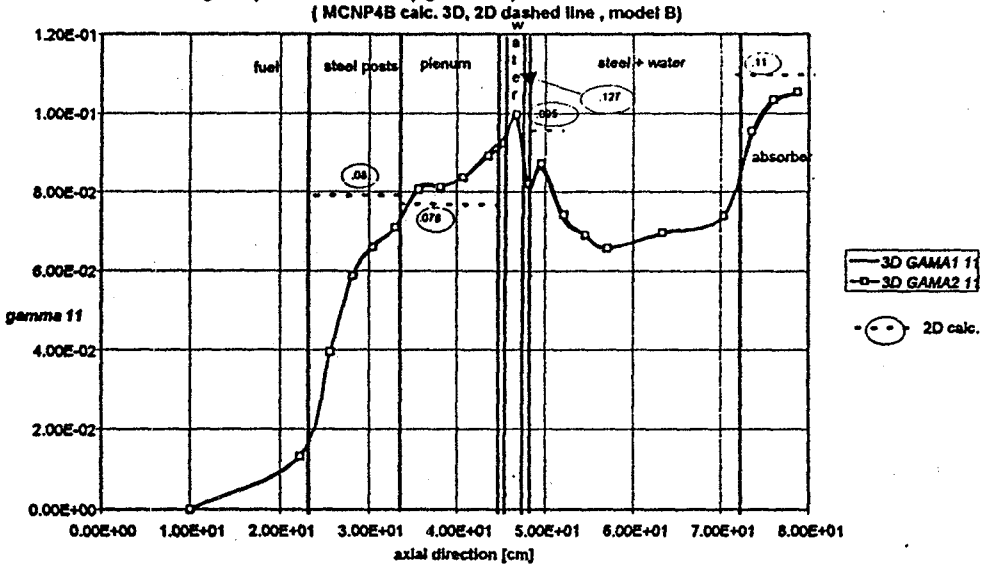


Fig. 6 Diagonal gamma matrix elements (*gamma*) for two types of calculational models of coupler
(3D MCNP4B calc., MODEL B and MODEL C) (Axial step 6.1 cm)

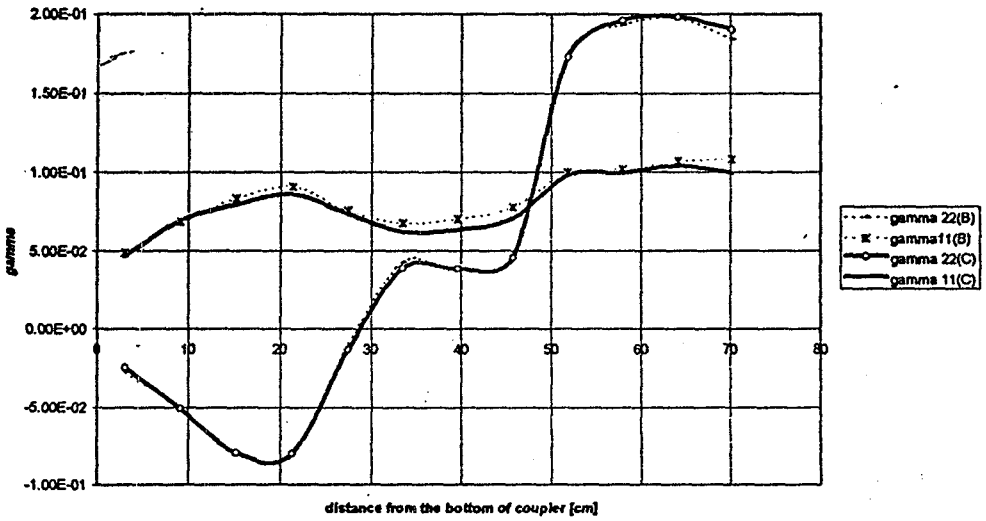


Fig. 7 Corrections factors Corr.= GAMMA(3D MCNP4B)/GAMMA(2D HECON) for diagonal elements of gamma matrix