

## HOMOGENIZATION-FREE REACTOR CORE ANALYSIS WITH GENERAL FIRST COLLISION PROBABILITIES METHOD.

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### ABSTRACT

Benchmark C5G7 MOX has been proposed as a basis to test the ability of current transport codes to treat reactor core problems without spatial homogenization. This is a seven-group form of the C5G7 MOX fuel assembly problem specified by Cavarec *et.al*. There are four fuel assemblies; two ones contain  $UO_2$  fuel elements and two ones contain MOX fuel elements. Seven group cross sections for different kinds of fuel (three enrichment of MOX and  $UO_2$ ), the guide tubes, the fission chamber and moderator are given. Thus this benchmark is just mathematical test which allows to test an accuracy of neutron transport equation analysis with different methods and codes. In this paper General First Collision Probabilities Method (GFCPM) is used to analyze the two-dimensional configuration of this benchmark. The linear flux approximation is used in the moderator. Different calculation schemes of the moderator have been used. The output results -  $K_{eff}$  and the pin powers have been analyzed. The convergence of the results has been analyzed both on dependency of subdivision way of the moderator and of the points number in the calculation scheme for general first collision probabilities. Comparison has been carried out for  $K_{eff}$  and pin powers with both the reference results (external convergence) and between the results of different approximations of GFCPM. (internal convergence).

### 1.INTRODUCTION

Expert Group on 3-D Radiation Transport Benchmarks proposed seven-group form of the C5MOX problem [1] to test the ability of current transport codes to treat reactor core problems without use the procedure of spatial homogenization. The two-dimensional and three-dimensional configurations have been described. Seven group cross sections for different kinds of fuel (three enrichment of MOX and  $UO_2$ ), the guide tubes, the fission chamber and moderator are given. The solution has been obtained by Dr. Smith (ANL,USA) with Monte-Karlo method was proposed as a reference solution.

First Collision Probabilities Method is well known method for solution of neutron transport equation. Base of this method is as following points. The system is divided into fine calculation zones (meshes). The macroscopic cross sections are supposed to be constant in every mesh and neutron flux is slowly changed in every mesh and it is approximated by its averaged value over the mesh. (So called "flat flux approximation") After this suggestion the integral kinetic equation is replaced by the linear algebraic equation system. The unknown values are just the averaged over the meshes values of the neutron flux. The coefficients of

this algebraic system are just "First Collision Probabilities". To get desirable accuracy it is necessary to divide the system into definite number of the meshes in dependence of the system dimensions. The stronger gradients neutron flux has within the system more number of the meshes is necessary to get desirable accuracy. Number of the meshes defines number of the unknown values in the algebraic system. But increasing number of the meshes is not only way of to improve the convergence of calculation method. It is possible to improve the convergence of the method if an approximation of neutron flux with some coordinates polynomial is used. Indefinite coefficients of this expansion are both the averaged neutron flux value and the moments of flux expansion over some orthogonal polynomial system. And one can get the linear algebraic system for these coefficients like the system for averaged neutron flux in FCPM. This procedure should reduce the number of unknown values to rich requisite accuracy and it should be possible to analyze not only the system like reactor's cells, but the system like reactor assemblies and even reactor core without any homogenization procedure using this method. In this paper General First Collision Probabilities Method GFCPM [2] is used to analyze C5G7 MOX benchmark. A combination of above described ways of accuracy increasing is used: there is flat flux approximation in the fuel assemblies and there is linear flux approximation in the moderator. Different ways of moderator subdivision are considered and the convergence of the method is analyzed. Beside a system subdivision there is another factor which influences on the accuracy: just number of the points in the calculation scheme for coefficients of the linear equation system of GFCPM. The convergence of the output results  $-K_{\text{eff}}$  and the pin powers distribution- is analyzed in dependence on all of these factors.

## 2. BRIEF DESCRIPTION OF GENERAL FIRST COLLISION PROBABILITIES METHOD

The General First Collision Probability is used. In this method the neutron flux is approximated with a set of the orthogonal polynomials in every calculation zones. So the set of algebraic equations are as a result of kinetic equation approximation. This algebraic system contains both the average zone neutron fluxes and the higher spatial moments of neutron flux too. The coefficients of this algebraic equation system are "general first collision probabilities".

This method is demonstrated when one-group problem with isotropic internal sources is considered:

$$\phi(\vec{r}') = \int_V d\vec{r}'' \left[ \phi(\vec{r}'') \sigma_s(\vec{r}'') + q(\vec{r}'') \right] P(\vec{r}'' \rightarrow \vec{r}') \quad (1)$$

Here the following designations are used

$\sigma_s$  - macroscopic scattering cross section

$$\tau(\vec{r}' \rightarrow \vec{r}) = \int_0^1 \sigma(\vec{r}' + s(\vec{r} - \vec{r}')) |\vec{r} - \vec{r}'| ds - \text{"optical distance" between } \vec{r} \text{ and } \vec{r}'; \quad (2)$$

$\sigma$  - total macroscopic cross section

$u(\vec{r}' \rightarrow \vec{r}) = \exp(-\tau(\vec{r}' \rightarrow \vec{r}))$  - probability for the neutron free path from  $\vec{r}'$  to  $\vec{r}$

$$P(\vec{r}' \rightarrow r) = - \frac{u(\vec{r} - \vec{r}')}{4\pi|\vec{r} - \vec{r}'|^2} \quad \text{- usual kernel of the integral kinetic equation}$$

Basic assumption of this method is that the flux is approximated by polynomial expansion in every uniform mesh:

$$\phi(\vec{r}) = \sum_t \sum_{\eta=1}^N g_t(\vec{r}) \varphi_{\eta t} f_{\eta t}(\vec{r}) \quad (3)$$

$g_t(\vec{r})$  is the characteristic function of zone "t",  $g_t(\vec{r}) = 1$  if  $\vec{r} \in t$  and  $g_t = 0$  if  $\vec{r} \notin t$

and the orthogonal relation is valid:

$$\int_{V_t} f_{\eta t}(\vec{r}) f_{\eta' t}(\vec{r}) d\vec{r} = \delta_{\eta\eta'} \quad (4)$$

The expansions (3) is substituted in the system (1); every equation is multiplied by function  $f_{\eta t}$  consequently; and the integration over "t" mesh is carried out. So, if Eq. (3) is taken into account, we deal with the set of linear algebraic equations

$$\varphi_{\eta t} V_t = \sum_{t'} (\sigma_{st'} \sum_{\eta'} \varphi_{\eta' t'} P_{\eta \leftarrow \eta'}^{t \leftarrow t'} + q_{\eta' t'}) \quad (5)$$

Here

$$P_{\eta \leftarrow \eta'}^{t \leftarrow t'} = \int_{V_t} d\vec{r} \int_{V_{t'}} d\vec{r}' f_{\eta t}(\vec{r}) f_{\eta' t'}(\vec{r}') P(\vec{r} \leftarrow \vec{r}') \quad (6)$$

$$q_{\eta' t'} = \int_{V_t} d\vec{r} \int_{V_{t'}} d\vec{r}' q(\vec{r}) f_{\eta' t'}(\vec{r}') P(\vec{r} \leftarrow \vec{r}') \quad (7)$$

The coefficients of the set of linear equations  $P_{\eta \leftarrow \eta'}^{t \leftarrow t'}$  are so called generalized first collision probabilities.

From point of view the best neutron flux approximation one would use the linear combination of some functions closed to physical behavior of flux. But just the polynomials from Cartesian coordinates have important advantage: when the integrals (6) are calculated then the calculation scheme is the best because of it is minimum of number integration parameters. The couples of points(  $\vec{r}, \vec{r}'$ ) are distributed along the trajectories of neutron flight. So it is the best way of calculation integrals (6.) is when the coordinate system is connected with the direction of neutron flight:  $\varphi, y_\varphi, x_\varphi, x'_\varphi, \lambda$

Here  $\varphi$ - the angle between neutron flight direct projection on the (x,y) plane and x-axis;

$x_\varphi, y_\varphi, z$  - coordinates of point r in the Cartesian system turned around Z-axis by  $\varphi$ -angl

$x'_\varphi, y'_\varphi, z$  - the same for point r' thus  $y'_\varphi = y_\varphi; x'_\varphi \leq x_\varphi$

After some analytical re-arrangement, equations for the general probabilities are reduced to the 2-D numerical integration:

$$P_{u'}^{\eta\eta'} = \iint \vec{P}_{i \leftarrow i'}^{\eta \leftarrow \eta'}(\varphi, y_\varphi) d\varphi dy_\varphi \quad (8)$$

The subintegral function is reduced to the combinations of trigonometric function  $\varphi$  with Bickley [6] functions of different orders from the following arguments: “optical” distances along neutron fly direction projection on the (x,y) plane from intersection of this projection with neutron birth zone boundary to the intersection of this projection with the neutron first collision zone boundary.

### 3. ALGORITHM AND CODE FOR MULTI-GROUP NEUTRON TRANSPORT CALCULATIONS.

GEFCOP-code (GEneral First COLLision Probabilities)) is multi-group neutron transport code for neutron flux distribution calculations in the different kinds of cells and assemblies of nuclear reactors. In his paper the C5G7 MOX benchmark is analyzed with this code. The universal module of combinatorial geometry SCG-5 [ 3] is used to describe the geometry of the system. The symmetrical properties of the systems are taken into account and that allows to reduce calculation zones numbers. This module provides the neutron trajectory with the optical distances between the calculation zones along this trajectory.. Boundary conditions are taken into account just on this stage so this trajectory depends on them. The coordinates of the mesh points ( and number of the trajectories) are defined using so called “uniform distributed” sequences. [4]

To use these sequences it is necessary to do the change of variables in Eq. (8):

$$\varphi = \varphi(\gamma_1, \gamma_2); \quad y_\varphi = y_\varphi(\gamma_1, \gamma_2) \quad (9)$$

These variables are coordinates of the points in the unite cube and the following relation is valid:

$$\frac{dy_\varphi d\varphi}{2\pi S_j} = d\gamma_1 d\gamma_2 \quad (10)$$

After this change of variables all integrals (8) are calculated over the unit cube with the use of the standard quadrature formula: if  $\chi(n)$  is value of the subintegral function in the mesh point number n, then the integral value is the averaged arithmetical value  $\chi(n)$  over all mesh points. The coordinates of the mesh points are defined with the use of “uniform” distributed sequences. It has been shown [4] that using of these sequences provides a high integration convergence order ( $\approx \frac{1}{N^{1-\varepsilon}}$ ) ( $\varepsilon$  is converged to zero). Thus this algorithm of numerical integration and algorithm of Monte Karlo method are similar. They differ only by

the choice of mesh points, it is possible to use the universal combinatorial geometry module SCG-5[3]. for geometry description in GFCPM codes without any essential change.

The multi-group transport eigenvalue problem is solved with the source fission method iterations.

If GFCPM is used we deal with algebraic linear equations system instead integral transport equation. In the thermalization region the internal iterations scheme is used and the spatial correction [5] is used at every iteration step to speed the iteration scheme. The corrective coefficients are got from the averaging of the linear equation system over the group index.. As a result we have got a system over only spatial (not group) dimension and the direct inversion method is used to solve it. .

A convergence of the solution (neutron flux) in the FCPM is defined by two factors:

- spatial subdivision of the system
- number of the trajectories

But the GFCPM has another possibility to increase an accuracy of the convergence of the solution: just to use polynomial flux approximation in some zones. It seems that the best convergence result would take place if optimal combination all of these factors is used in dependence of the geometrical and physical characteristic of nuclear system. .

#### **4.DESCRPTION OF CALCULATION BENCHMARK.**

Expert Group on 3-D Radiation Transport Benchmarks proposed C5G7 MOX benchmark to test the ability of current transport codes to analyze reactor core without use the procedure of spatial homogenization. The quarter of two-dimensional configuration,, shown in Figure 1 together with boundary conditions, consists of two MOX, two UO<sub>2</sub> assemblies and reflector. Overall dimension of this configuration part are 64.26\*64.26 cm while dimensions of each assembly are 21.42\*42 cm.

Each fuel assembly is made up of a 17\*17 lattice of square pin cells, as seen in Figure 1,2. All cells-fuel-pin cell with guide tube and with fission chamber-consist of two zones, in so doing, for example, the internal material of fuel -pin cell is material in which fuel, gap and cladding are homogenized and there is no fuel coolant homogenization. The side length of every cell is 1.26 cm, the radius of every internal rod cylinder is 0.54 cm. There were four types of fuel in rods, namely, one type of UO<sub>2</sub> fuel and three types of MOX fuel with enrichment 4.3% and 8.7% . A single moderator material is provided for use in all cells and external moderator. Composition layout for fuel assemblies and numbering scheme are shown in Figure 2.

Seven group cross sections were given for following seven materials: four types of fuel materials, material of fission chamber, material of guide tube and material of moderator. Scattering cross sections with transport correction were used.

## 5.PERFORMED CALCULATIOS AND RESULTS

Every fuel-pin cell has been divided into two calculation zones: the fuel zone and the moderator zone. Every guide tube has been divided into two calculation zones: the rod (mixture of clad and moderator) The flat neutron flux approximation is used in these zones. Boundary conditions are taken into account when the geometrical module SCG-5 works so the neutron trajectory contains the optical distance accordingly boundary conditions of described system There is vacuum boundary at the low and right borders of system and mirror boundary condition sat the left and upper borders of the system. When the initial data for SCG-5 are introduced the symmetrical calculation zones have the same numbers so the common number of the calculation zones is reduced to 1156 unknown values in the fuel-pin region.

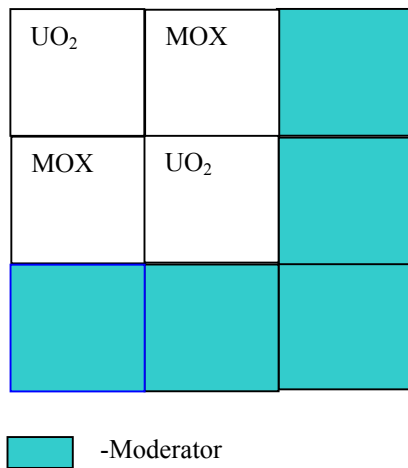


Figure 1 Calculation scheme for C5G7 benchmark number 1.

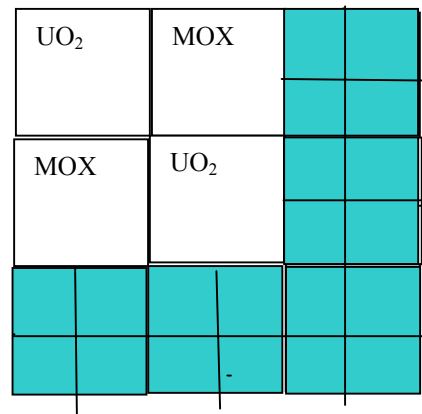


Figure 2 Calculation scheme for C5G7 benchmark number 2.

The linear flux approximation is used in the moderator. Firstly it has been divided into 5 zones (fig.1) and two linear functions are used in every zone.

$$f_{0t} = b(t); \quad f_{xt} = x + a1(t); \quad f_{yt} = y + a21(t)x + a22(t)y \quad (11)$$

The constants  $b(t)$ ,  $a1(t)$ ,  $a21(t)$ ,  $a22(t)$  are founded from orthogonality conditions of the polynomial system. So the linear equation system contains  $1156+3*5$  unknown values. The direct method of inversion is used to solve the linear algebraic system. At the next step more detail subdivision was used in the moderator. It was divided at 20 zones; the same linear function are used for the flux expansion. The output results-eigenvalue and normalized pin powers are analyzed for these two ways of system subdivisions. Also the results are analyzed in dependence on the trajectories number for every subdivisions. As it has been

mentioned the Korobov's "uniformed distributed" sequences are used in the numerical integration scheme of the GFCEP in the algorithm of this code. So the special Korobov's random generator is used to get number of trajectories. In table I different values of  $K_{eff}$  are presented for different trajectories number for subdivision number 1(fig1) and for subdivision number 2(fig2)

Table I Values of  $K_{eff}$  for 2-D C5G7 benchmark (subdivision 1)

Number of trajectories	$k_{eff}$ for subdivs. number 1	$K_{eff}$ for subdivs. Number 2
10000	1.18597	1.18598
20000	1.18597	1.18620
50000	1.18613	1.18625
100000	1.18624	1.18643
Reference	1.18655	

The first value is deviation from reference value; the second value is deviation from value  $K_{eff}$  corresponded to value for the case of 100000 trajectories subdivision 2

The results of calculation of the pin power distributions for different approximations (subdivisions and numbers of trajectories are given in the tables II,III-. Only the deviations of pin powers in separated points are given. There are the deviations of pin powers in separated points for different number of trajectories from corresponding values in reference for subdivisions 1,2 in table II. . There are the deviations of pin powers in separated points for different number of trajectories from corresponding values in the case of "100000 trajectories in subdivision 2" for subdivision 1,2 in table III. (This case corresponds the maximum accuracy for GFCEP up to day so it could be named as "GFCEP-reference") Thus one could say that the table II shows the "internal" convergence of the results for GFCEP for C5G7 MOX benchmark, and the table III shows the convergence of the GFCEP to Monte-Karlo reference solution.

Table II Percent deviations of pin power in separated points from "GFCPM reference"

N of traject, N of subdiv. Point Coordinates	10000, number 1	20000, number 1	50000, number 1	100000, number 1	10000, number 2	20000 number 2	50000 number 2
(1,1)	3.22	2.23	1.14	0.08	1.24	0.18	0.08
(1,10)	2.56	1.44	-1.25	-1.04	1.54	0.48	-0.14
(1,16)	2.98	1.68	0.88	0.10	1.87	0.877	0.04
(1,18)	-2.08	-1.86	0.45	0.32	-1.44	-0.45	0.04
(1,28)	2.68	2.33	0.97	0.45	2.08	1.24	-0.18
(1,34)	3.65	3.06	-1.22	-0.88	-2.44	-1.42	-0.06
(10,10)	-2.42	-1.12	0.98	0.82	1.88	0.56	-0.13
(10,16)	-2.54	-2.08	1.12	0.56	2.44	1.32	-0.19
(10,24)	3.08	2.56	1.06	0.88	1.24	0.08	-0.32
(10,34)	3.42	3.00	1.35	0.58	2.46	1.22	-0.16
(17,17)	-4.42	-2.88	-1.88	-0.46	-2.57	-1.78	0.16
(17,19)	2.68	2.45	0.86	0.32	1.22	0.86	-0.07
(17,25)	2.89	2.67	1.44	-0.86	-1.04	-0.12	-0.20
(17,34)	3.42	2.98	-1.32	0.22	1.22	0.12	-0.07
(19,19)	-4.03	-3.66	1.66	-0.67	-2.34	-1.84	0.22
(19,27)	2.56	2.44	0.97	0.65	1.22	0.66	-0.18
(19,34)	-3.52	-3.47	1.42	0.87	0.98	1.02	0.08
(25,27)	3.08	2.86	2.02	-0.44	-2.56	-1.86	-0.14
(25,34)	-2.89	-1.89	1.36	0.68	0.89	0.64	-0.14
(34,34)	4.87	3.68	2.00	-0.72	-2.02	-1.84	-0.12
(33,33)	4.48	3.44	-1.64	0.44	-2.06	-1.92	0.22
Max.dev. and points	5.06 (17,30)	-4.22 (23,4)	-2.02 (20,32)	-1.06 (16,34)	-2.88 (17,34)	-1.94 (34,34)	-0.8 (5,32)



Table III The deviations of pin power in separated points from M-K reference solution

N of traject, N of subdiv. Point Coordinates	10000, number 1	20000, number 1	50000, number 1	100000, number 1	10000, number 2	20000 number 2	50000 number 2	100000 number 2
(1,1)	3.85	3.08	1.24	1.02	3.45	2.34	1.18	1.02
(1,10)	4.43	3.66	1.67	1.22	3.08	2.65	1.00	0.98
(1,16)	-4.67	-3.87	-2.04	-1.46	-4.35	-2.06	-1.56	-1.42
(1,18)	4.02	3.44	1.87	1.68	4.06	2.89	1.60	1.56.
(1,28)	3.98	3.08	2.28	2.02	3.68	3.80	1.55	1.44
(1,34)	4.78	3.25	2.32	2.24	4.67	3.02	2.09	2.04
(10,10)	-5.09	-3.48	-2.57	-2.43	-4.36	-3.65	-1.45	-1.45
(10,16)	-5.33	-3.23	-2.44	-2.35	-4.08	-2.34	-2.34	-2.04
(10,24)	4.86	3.90	2.14	1.67	3.47	2.43	1.65	1.22
(10,34)	5.54	4.26	2.96	2.59	3.82	2.66	1.87	1.54
(17,17)	5.68	4.52	3.21	2.88	3.56	2.04	1.66	1.65
(17,19)	5.07	4.68	3.47	3.03	4.62	2.56	2.30	2.20
(17,25)	5.87	5.09	3.56	2.44	4.07	3.88	1.67	1.65
(17,34)	-6.08	-5.24	-3.03	-2.68	-3.86	-2.46	-1.00	-0.98
(19,19)	6.85	3.09	2.68	2.04	4.78	3.08	2.00	1.23
(19,27)	7.13	3.32	2.09	1.88	4.65	2.44	1.45	1.34
(19,34)	6.79	4.87	1.86	1.44	5.06	2.36	1.32	1.06
(25,27)	-6.65	-5.18	-3.54	-2.43	-5.48	-2.88	-1.87	-2.02
(25,34)	5.97	5.87	3.43	2.65	3.66	3.34	2.00	1.96
(34,34)	7.23	6.03	2.96	2.09	4.06	3.68	2.43	1.34
(33,33)	7.18	5.98	-3.20	-2.98	-4.87	-4.00	-2.56	-2.02
Max. dev. And Points	7.65 (16,34)	6.42 (7,34)	3.64 (16,34)	3.18 (16,33)	5.42 ((32,32)	4.68 (16,34)	2.89 (17,34)	2.44 (17,34)

These results - $K_{eff}$  and pin power distributions -are obtained on the base of neutron fluxes distributions. Group neutron fluxes distributions are obtained from fission source iteration scheme. Relative accuracy criterion of this scheme is  $10^{-6}$  for eigenvalue. The inner iteration

scheme was used in thermalisation region and relative accuracy criterion of this scheme is  $10^{-5}$  for group fluxes. All these calculations have been carried out on Pentium-4

## CONCLUSIONS.

General First Collision Probabilities Method has been used to analyze the two-dimensional configuration of C5G7 MOX benchmark. This benchmark was proposed by Expert Group on 3-D Radiation Transport Benchmarks to test the ability of current codes to analyze reactor core problem without use the procedure of spatial homogenization. Seven group cross sections for all material have been given. Expert Group GFCPM allows to use not only flat flux approximation (like the ordinary FCPM), but the polynomial flux distribution in some calculation zones accordingly the physical image of neutron flux behavior. Linear approximation was used for neutron flux in the moderator. Different ways of the moderator subdivision into the calculation zones were used. Also different number of neutron trajectories were used in the calculation scheme for General First Collision Probabilities. Output results- $K_{\text{eff}}$  and pin power distributions -have been compared both to analyze the "internal convergence" of this method and to analyze the convergence of this method to the Monte-Karlo reference solution.

Analysis of these results leads to the following conclusions

- Linear approximation of neutron flux in the moderator allows to analyze the reactor core problem without use the procedure of spatial homogenization
- The property of geometrical module SCG-5 to take into account the symmetrical relation of the system allows to reduce number of the unknown values in two times in the fuel-pin region.
- There is gradual approaching of  $K_{\text{eff}}$  both to reference solution of Monte-Karlo method and to "reference solution of GFCPM" (internal convergence).
- There is gradual approaching of pin power independence on the trajectories number both for moderator subdivision number 1 and for moderator subdivision number 2. It seems that 100000 trajectories is quite enough to get the relative accuracy for neutron flux  $\sim 10^{-4}$
- There is gradual approaching of pin power distribution obtained with GFCPM in dependence on mesh number in moderator and the trajectories number to reference solution of Monte-Karlo method
- Deviation of pin powers in the most accurate approximation of GFCPM (subdivision of the moderator number 2 and 100000 trajectories) reaches 2.4% at the point (17,34) (at the boundary MOX assembly-moderator).

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