ABOUT COMPUTATION TOOL FOR A ESTIMATION OF NEUTRON-PHYSICAL CALCULATION UNCERTAINTY

N.I. Laletin, A.A.Kovalishin
Russian Research Center "Kurchatov Institute "
123182 Kurchatov sq. 1, Moscow, Russia
laletin@adis.vver.kiae.ru, kaa@adis.vver.kiae.ru

ABSTRACT

Neutron-physics calculations of nuclear reactors have always been important and are constantly improved nowadays. But independently from how precise they are, there is still plenty of sources of uncertainty for computation characteristics and one clearly needs to know their impact. For that matter, various experiments on test benches and operating reactors' measuring have been carried out. But this approach, which is rather expensive indeed, fails to fit all the needs of researchers during reactor's operating and gives little information for estimating uncertainty bands for emergency situations. In this respect, development of a computation tool for obtaining those bands is highly demanded. We can point out three main sources of uncertainty for characteristics of neutron-physics calculations. The first one - let us call it a method error - is related to inaccuracy of the mathematical model applied. The second one - a constant error - is related to uncertainty of knowledge about nuclear micro constants. The third one - technological error - is stipulated by incomplete information about nuclide structure of reactor's active zone. This incompleteness comes into existence from the very beginning of reactor's building due to technological errors and is continuously changing during reactors operating as a result of burnout, temperature changes, etc.

Estimation of every error above-mentioned requires different approaches. In presented paper are discussed of last two from these ones.

1. INTRODUCTION AND OVERVIEW

The problems of sufficiency of energy production have always been central the mankind. In the past years, nuclear energy made significant contribution to energy production, at least as electricity production is concerned.
All decisions regarding nuclear energy development, including establishment of new nuclear power plants and operating of existing ones, require a number of factors to be taken into consideration. The proper use and continuous improvement of computation tools for predicting emergency situations within the nuclear reactor play the role of no small significance in that respect. Such tools are especially important for nuclear energy since, unlike other energy-producing technologies, losses associated with emergency situations in a nuclear reactor can have really disastrous effects. Those effects should be taken into consideration even despite the low probability of a corresponding event.
In contrast, the main losses associated with other energy-producing technologies are related to more frequent but less disastrous incidents. As a result, forecasting of possible damage in the latter case is based primarily on historical analysis of operational practice. However this way is obviously inappropriate for nuclear energy and thus there is a great need in a

computation tool for predicting reactor's performance in emergency regimes [1].
The role of neutron-physics part of that tool can hardly be overestimated. Application and modernization of computation tools for predicting emergency situations, or their progress if precautionary measures failed, are of great importance for nuclear energy. This is so, since in nuclear energy, unlike other energy technologies, the probability of a failure is small but its consequences are disastrous.
Neutron-physics calculations of nuclear reactors have always been important and constantly improved. But despite improving precision of computation methods, there is always a great deal of uncertainty about characteristics being calculated. In this respect, one needs to know how large that uncertainty is. There are three main sources of uncertainty in neutron-physics calculations: (i) the first one is associated with inaccuracy of mathematical model applied - let us call it a methodological error; (ii) the second one is related to the lack of knowledge about micro constants - let it be a constant component; (iii) the third one is stipulated by imprecise knowledge about nuclide structure of reactor active zone. The latter error exists since the very first stage of reactor building due to technological errors; it also changes during the operational cycle as a result of burn-ups, temperature changes, etc. We will call this kind of error a technological one.

Estimation of every error mentioned above requires its own special approach.

A large number of papers on various aspects of radiation transport within stochastic environment can be divided into three groups.

1. Researches that account for random nature of the processes.

2. Works on determination of effective characteristics of stochastic environment.

3. Papers that use the perturbation theory of (sensibility coefficients) for estimating the impact of some factors, mainly errors in micro constants, on reactor characteristics.

4. Interesting papers of L. Pal [2] and his followers should be noted in respect to the first group of researches. By the thorough study of the history of neutron paths, L. Pal obtained the equation for reproducing function of neutron probability distribution that yields both the transport equation for average neutron density and equations for higher moments including variance. However for systems with large neutron density that probability component becomes usually insignificant and Pal equations appear to be of no help in solving problems of neutron transportation within stochastic environment. Different approach for analogues problems was presented in work [3].

2.The second group of papers, that studied the problems of neutron transportation within stochastic environment for deriving various efficiency characteristics of the environment, is also very big. Examples older works of this type were in [4,5]. General study of the problem of deriving efficiency characteristics within stochastic environment has been carried out in works of A.V. Stepanov, J.B. Keller, M.M.R.Williams [6,7,8]. These papers determine average and fluctuation parts within neutron transport In conclusion one can emphasis that this problem is raised as for as we want to develop a new stage of neutron physical calculations where one can have results for reactor values with variance at the same time.

equation, among its coefficients, and distribution function. After some transformations and approximations, one could get some deterministic equations that yield a number of important results. Unfortunately, this approach is very hard to apply for practically interesting problems due to complexity of computation of the Green function or inverse operators.
In recent years, there appeared a large number of papers on various aspects of radiation transport within stochastic environment. One can find a detailed survey of those papers in the book of G.S.Pomraning [9]. Despite great scientific importance of above-mentioned works on various transportation problems, there is no way for applying their results directly for solving the problem underlined here - creation of a computation tool for estimating uncertainty associated uses sensibility coefficients approach. with the functionals that reactor physics are

interested in.
The third group of researches actually applies some form of the perturbation theory, namely, it uses sensibility coefficients approach [for example, in 10]. Let us assume that any reactor functional can be represented in the following form with acceptable accuracy:

$$K(\vec{\gamma}) = K(\vec{\gamma}_0) + \sum_i \frac{\partial K}{\partial \gamma_i} d\gamma_i ,$$

$\vec{\gamma}$ - is vector with its components being micro cross sections, nuclide density, temperature, etc.; $\partial K/\partial\gamma_I$ – functional derivatives and $\partial\gamma_I$ – small increments of parameters. By computing numerically $\partial K/\partial\gamma_i$, i.e. carrying out a series of paired calculations where one calculation gives $K(\vec{\gamma})$, and another gives $K(\vec{\gamma}, \gamma_i+\partial\gamma_i)$, (where $\partial\gamma_i$ should be sufficiently small but large enough for not to lose accuracy when calculating difference between two similar values), one could estimate various uncertainties associated with multiplication coefficient due to inaccuracy of main microconstants (fission and absorption of fuel, dispersion of moderator, etc.).

One can see that the number of parameters should not be large since enumeration of calculation pairs is costly. This approach becomes even more difficult when trying to account for correlations between different parameters, i.e. include functional derivatives like $\partial^2 K/\partial\gamma_i\partial\gamma_j$ into the computation process.

All papers surveyed above are surely interesting and fruitful but not for the aim set here, namely, for building finite-difference equations for neutron field description similar to those recently in use that would additionally provide us with detailed information about uncertainty associated with reactor characteristics.

2. THEORY

Equations are supposed in this paper to be based upon Surface Harmonics Method (SHM) equations [see. for example,11]. SHM equations are built on two systems of initial equations. The first one links characteristics of subsections (nods) while the second one ties different characteristics of one node, i.e. actually determines response matrices. Assuming that those matrices are somehow determined (or that their probability distribution may be obtained), we are going to get equations of node links.

Note that these equations are derived from continuity of neutron distribution. That is why they all look similar either when this distribution is a deterministic function, or when it is some probabilistic function. Thus at this stage we are not losing the probabilistic component of variance related, for example, to probabilistic nature of micro-processes; although we are mainly interested in the "stochastic" component related to uncertainty about node characteristics that arises due to incorrect knowledge of nuclide composition of micro cross sections. The loss of probabilistic component becomes clear when one studies the problem with transport equation that determines mathematical expectations of the field at every point.
Let us write initial equation in the symbolic form

$$(\mathbf{L}+\mathbf{l})(\Phi+\varphi) = S + s \qquad (1)$$

Here deterministic components L,Φ,S and stochastically fluctuating components l,φ,s are marked out within operators and unknown variables. It is also assumed that $\langle\varphi\rangle=0$, $\langle s\rangle=0$ hold for average values. As will be shown later when building iteration process, these relations imply $\langle l\rangle=0$. The meaning of notation used is the following:
Φ - vector of amplitudes of group surface harmonics (in approximate cases - averaged group

cell fluxes), with components denoted as Φg,n and g – being the index of the group; n – is a number of surface harmonics; L - finite-difference operator that links neighboring nodes.

$$\mathbf{L} = \mathbf{A_{ii}}\delta_{ii} + \sum_{j \in i+\vec{k}} \mathbf{B_{ij}}\delta_{ij} \tag{2}$$

Here Aii and Bij - are matrices with deterministic components, k– is a 3-dimention discrete unity vector; φ - fluctuating component of the solution. l - finite-difference operator with fluctuating components

$$\mathbf{l} = \mathbf{a_{ii}}\delta_{ii} + \sum_{j \in i+\vec{k}} \mathbf{b_{ij}}\delta_{ij} \tag{3}$$

S and s- are average and fluctuating components of the source within the node under consideration.
Let us divide the equation into two parts. The first one links relatively sluggish variables.

$$\mathbf{L}\Phi+\mathbf{l}\varphi=S$$

The second one describes rapidly oscillating variable.

$$\mathbf{l}\Phi+\mathbf{L}\varphi=s$$

This procedure is the same as that used in papers of A.V. Stepanov and actually coincides with "smoothing" term applied by J.B. Keller, M.M.R. Williams. Unlike those papers, we will not write inverse operators and Green function, which are too complex to compute. Instead, we will write the following iteration procedure combined with averaging. This yields

$$\begin{aligned} &\mathbf{L}\,\Phi^{k} + <\mathbf{l}\varphi>^{k-1} = S \\ &<\mathbf{l}^2>\Phi^{k-1} + \mathbf{L}<\mathbf{l}\varphi>^{k} + \mathbf{Z}^{k} = <\mathbf{l}s> \end{aligned} \tag{4}$$

$$\mathbf{Z}^{k} = -<\mathbf{l}^2>\Phi^{k-1} - \mathbf{L}<\mathbf{l}\varphi>^{k-2} + <\mathbf{l}s>$$

No serious difficulties arise when solving the problems on eigenvalues. One just needs one more round of iterations, iterations on source.
Let us write the system of equations for this case

$$\begin{aligned} &\mathbf{L}\,\Phi^{n,k} + <\mathbf{l}\varphi>^{n,k-1} = S^{n-1} \\ &<\mathbf{l}^2>\Phi^{n,k-1} + \mathbf{L}<\mathbf{l}\varphi>^{n,k} + \mathbf{Z}^{n,k} = <\mathbf{l}s>^{n-1,k} \end{aligned} \tag{5}$$

$$\mathbf{Z}^{n,k} = -<\mathbf{l}^2>\Phi^{n,k-1} - \mathbf{L}<\mathbf{l}\varphi>^{n,k-2} + <\mathbf{l}s>$$

$$\mathbf{Z} = <\mathbf{l}\mathbf{L}\varphi> - \mathbf{L}<\mathbf{l}\varphi>$$

The meaning of indices is clear. The system is easy to solve; it yields average fluxes and eigenvalue. The second equation we take in such form as long as averaging of the second from the initial set bring forward to trivial result. Above-mentioned equations have an opportunity to estimate a displacement of mathematical waits of calculation results..

For building equations for variances and covariances we will use the same initial equations as presented in previous section. For example, let us take the equations

$$\begin{aligned} \mathbf{L}\Phi+\mathbf{l}\varphi-S=0 \\ \mathbf{l}\Phi+\mathbf{L}\varphi-s=0 \end{aligned} \tag{6}$$

We will obtain finite-difference equation with variances $<\varphi_i^2>$, correlations $<\varphi_i\varphi_j>$ and values of the form $<a_i\varphi_i>$, $<a_i\varphi_j>$, $<b_i\varphi_i>$, $<b_i\varphi_k>$, with j index corresponding to nodes nearest to the node i and K index corresponding to nodes of the next ring, as unknowns. The problem is that the number of unknowns exceeds the number of equations. Missing equations may be easily added but there arises a problem of interconnections between a large number of nodes. In order to decrease the size of the system one should use both conditions that arise naturally when solving particular problems and acceptable approximations.
Look through three different approaches for obtaining of equations for second moments (covariance functions) of neutron distributions.

In first one obtain the following relations from second equation

$$\varphi = \mathbf{L}^{-1}\mathbf{s} - \mathbf{L}^{-1}\mathbf{l}\Phi \quad \text{and } \Sigma(i)\varphi=\Sigma\mathbf{L}^{-1}\mathbf{s}-\Sigma\mathbf{L}^{-1}\mathbf{l}\Phi \tag{7}$$

one can obtain the all necessary equations multiplying these relations on component by component with following averaging. The second one can use the local worth's which is to say solutions of equations

$$\mathbf{L}^{+}\Phi^{+} = \Sigma(i).$$

From that to obtain:

$$\Sigma\varphi = \Phi^{+}s - \Phi^{+}\mathbf{l}\,\Phi \tag{8}$$

After that the procedure for obtaining of equations for second moments is analogues one to first approach. As for equations (7) both for equations (8) functions with two arguments $\mathbf{L}^{-1}(i,k)$ and $\Phi^{+}(i,k)$ are demanded. Of course these functions not so long acting as Green functions in work's [5,6] but direct calculations and following using are highly tiresome procedures.

The construction of algorithms with more short acting is preference.
Using multiplications of values $\varphi_{i,g}$ on equations $\mathbf{l}\Phi+\mathbf{L}\varphi=s$ we construct the suitable layers of iterations with counting's " the set of worth's" of different values for calculations of interesting ones.

At this way one can develop finite different equations for pin power variance, assembly powers, analogues values for multiplication factors and all other necessary values.
Code with model name SHM-VAR is developed. For test of selectable algorithm the additional code STATISTIC was developed.
The statistic integration of inverse operator is used in the algorithm of this code. This approach is reasonable.

However one can see what it is necessary to use sufficiently many of approximations for these stages even if we want to have the tool for variance calculations that will so operative as the tool for calculations of unperturbed equations. It is very more difficult to obtain equations for calculations of variances for cell calculation stage where it is necessary to take into account of smeary zone boundaries. We think that it is a long way to construct a convenient computation tool for a estimation of neutron-physical calculation uncertainties but it is necessary this way pass out.

Actually one ought to aim at the task to transfer neutron- physical calculations at new level, where as a result of the reactor characteristics are combined with its variance at same time. As a basic physical experimental result can't be without indication error limit as the neutron-physical calculation ought to achieve the analogous level. The task is not simple. The great quantity of researches is engaged in reactor characteristic calculations. The analogues works

are required to develop the tool for calculations of variance distributions.

3. PROBLEMS DEFINITION

We considerd the VVER-1000 2D core Fig.1, with vacuum boundary conditions. There are the 2-group constants for each material type in the following form:

$$\Sigma_{a,1}^{n,k}=<\Sigma_{a,1}^{n}>(1.+\sigma_c\xi_{n,1}+\sigma_t\zeta_k)$$
$$\Sigma_{a,2}^{n,k}=<\Sigma_{a,1}^{n}>(1.+\sigma_c\xi_{n,2}+\sigma_t\zeta_k)$$
$$\Sigma_{f,1}^{n,k}=<\Sigma_{f,1}^{n}>(1.+\sigma_c\xi_{n,1}+\sigma_t\zeta_k)$$
$$\Sigma_{f,2}^{n,k}=<\Sigma_{f,2}^{n}>(1.+\sigma_c\xi_{n,2}+\sigma_t\zeta_k)$$
$$\nu_f\Sigma_{f,1}^{n,k}=<\nu_f\Sigma_{f,1}^{n}>(1.+\sigma_c\xi_{n,1}+\sigma_t\zeta_k)$$
$$\nu_f\Sigma_{f,2}^{n,k}=<\nu_f\Sigma_{f,2}^{n}>(1.+\sigma_c\xi_{n,2}+\sigma_t\zeta_k)$$
$$\Sigma_{s,1\to2}^{n,k}=<\Sigma_{s,1\to2}^{n}>(1.+\sigma_c\xi_{n,3}+\sigma_t\zeta_k)$$
$$D_g^{n,k}=<D_g^{n}>$$

Here:
n-material type,
k-fuel assembly (FA) number,
$\xi_{n,1}$, $\xi_{n,2}$, $\xi_{n,3}$, n=1,2,3,4, ζ_k k=1,2,…,16, $\in$[-1,1], are the stochastic values uniformly distributed
$<\Sigma_{*,g}^{n}>$-average cross-section for energy group g, g=1,2 and material type n, n=1,2,3,4
σ_c-cross-section's variance corresponding to the uncertainty of micro cross-sections
σ_t-cross-section's variance corresponding to the technological uncertainty

Table 1. Average group constant for the VVER-1000 problem

Material	1	2	3	4
$<D_1>$	1.4	1.4	1.4	1.4
$<D_2>$	0.3	0.3	0.3	0.3
$<\Sigma_{a1}>$	0.0086	0.0092	0.0100	0.0030
$<\Sigma_{a2}>$	0.0650	0.0810	0.1000	0.0500
$<\Sigma s_{12}>$	0.0170	0.0160	0.0150	0.0300
$<\Sigma_{f1}>$	0.0017	0.0021	0.0027	0.0000
$<\Sigma_{f2}>$	0.0310	0.0450	0.0630	0.0000
$<\nu_f\Sigma_{f1}>$	0.0043	0.0054	0.0069	0.0000
$<\nu_f\Sigma_{f2}>$	0.0760	0.1100	0.1500	0.0000

Table 2. Cross-section's variance for the problems

Problem	σ_c	σ_t
1	0.01	0.01
2	0.01	0.03
3	0.01	0.05

We should find the eigenvalues variance:

$$\sigma^2\left(k_{eff}\right)=\int_{\Omega}\left(\left\langle k_{eff}\right\rangle-k_{eff}(\vec{\xi})\right)^2P(\vec{\xi})d\vec{\xi} \tag{9}$$

and power distributions variance:

$$\sigma^2\left(W_k\right)=\int_{\Omega}\left(\left\langle W_k\right\rangle-W_k(\vec{\xi})\right)^2P(\vec{\xi})d\vec{\xi} \tag{10}$$

here:

$\vec{\xi}$ -is the set of stochastic variables;

$W_k(\vec{\xi}) = \mathbf{\Sigma}_{f,1}(\vec{\xi})\mathbf{\Phi}_1(\vec{\xi}) + \mathbf{\Sigma}_{f,2}(\vec{\xi})\mathbf{\Phi}_2(\vec{\xi})$ the power distributions for k^{th} fuel assembly.

P($\vec{\xi}$)-is the probability density of $\vec{\xi}$

We got the reference solution for the problems by straightforward integration of (9) and (10) by Monte-Carlo formalism and STATISTIC-code.

4.RESULTS AND DISCUSSION

Some results see in the table 3 and the Fig.1-3.
Calculation results for the distributions of power variances are presented for 2D problem VVER-1000 with 2 groups. These calculations are only check one for SHM-VAR and STATISTIC codes, as far as initial variances and covariances for subassemblies in the core were fixed by a arbitrary manner. Three variants were considered. The part of variance that imitate technological dispersions was characterized the variance σ_t=1% for the first variant and σ_t=3% for the second one and σ_t=5% for the third one. These values were the same ones for all fuel assemblies inside each variants. There are not correlations between variance subassemblies. The part that imitate micro cross-sections uncertain was fixed with σ_c=1% and with full correlation between Σ_a and Σ_f for all subassemblies. Results of SHM-VAR code correspond approximately to formulas (3) but $\mathbf{L}^{-1}$ was evaluated by iteration procedure. STATISTIC code results are processing of calculation set with casual dispersion (M-C) of subassemblies characteristics. Except the note about concordance SHM-VAR and STATISTIC results it is premature to discuss of results because of arbitrary manner of initial date for subassemblies variances.

Table 3. The eigenvalue's variance, % for calculations with difference cross-sections fluctuations.

$\sigma_t(\Sigma)$, %	$\sigma(K_{eff})$, %, STATISTIC	$\sigma(K_{eff})$, %, SHM-VAR
1	0.10	0.10
3	0.10	0.10
5	0.12	0.12

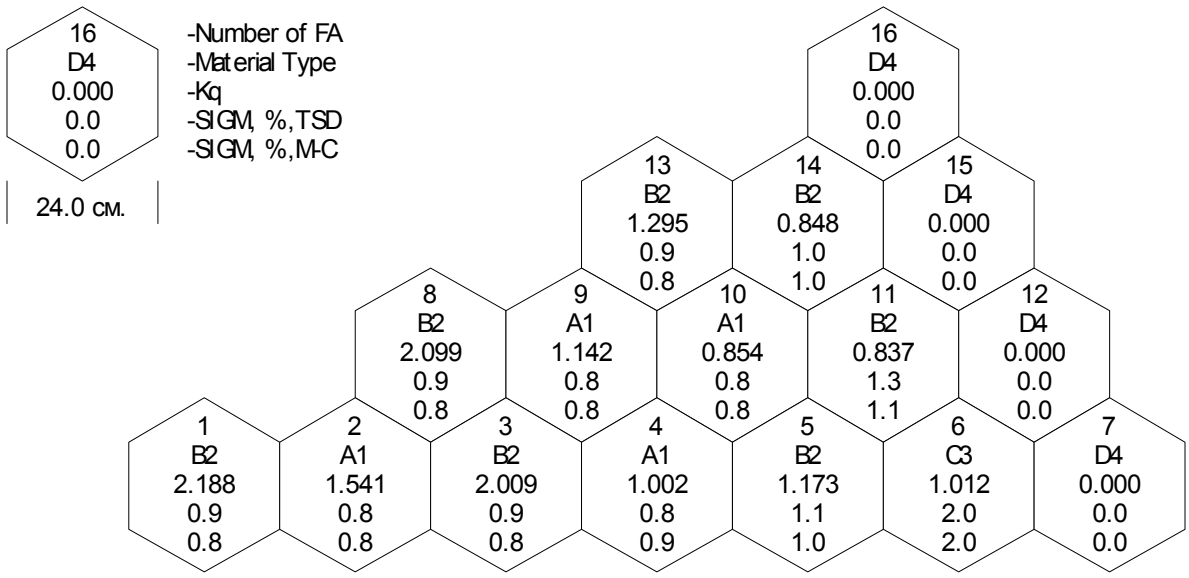

Fig.1. Power distributions variance, % for calculation with $\sigma_t(\Sigma)$=1%.

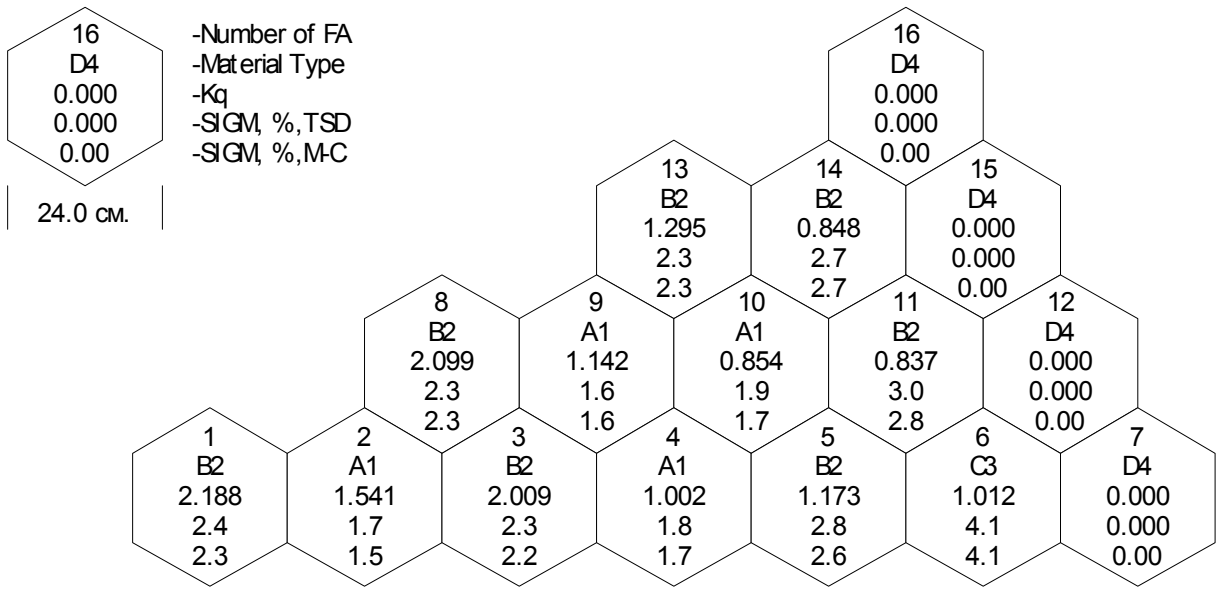

Fig.2. Power distributions variance, % for calculation with $\sigma_t(\Sigma)$=3%.

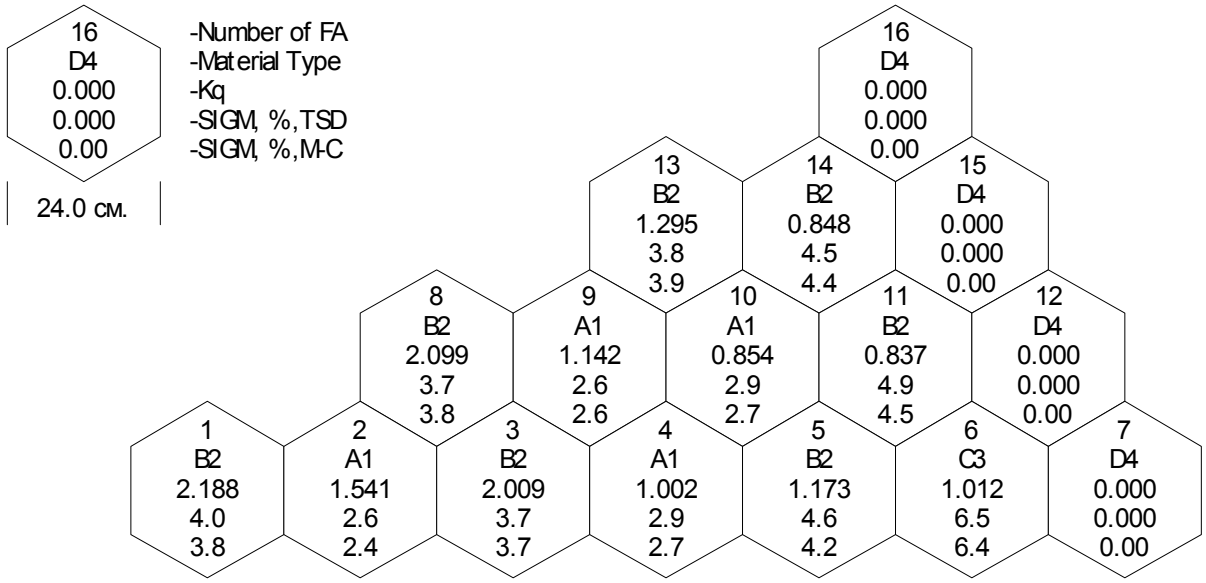

Fig.3. Power distributions variance, % for calculation with $\sigma_t(\Sigma)$=5%.

ACKNOWLEDGEMENTS

This paper had supported partly of the Russian Foundation of Basic Research, grants # 01-01-00623, and # 02-01- 00477.

REFERENCES

1. *N.I.Laletin "The Perspectives of Nuclear Energetic of Russia", J.* **Conversion in Machine Building of Russia**, *pp.6-33,v.3, 1997(in Russian)*
2. *L. Pal, Statistical fluctuation of Nutron Multiplication.* **In proc II UN Intern. Conf on the Peaceful Uses of Atomic Energy, Geneva** *1958 v.16,p.687, UN N.Y.,1959*
3. *J.L.Munoz-Cobo en al Evolution equations for two-point correlation functions in stochastic multiplicative media from a master equation theory.* **Physor-2000**, *p574 2000.*
4. *D.J.Behrens* **Proc.Phys.Soc**. *A62, p.607. 1949г.*
5. *N.I.Laletin, " The radiation loss in heterogeneous media.* **In Book Reactor shielding physics** *p.119, 1962(in Russian)*
6. *A.V.Stepanov The Macroscopic Transport Theory of Nutron in heterogeneous media. PhD work, Moscow, Russia (in Russian), 1971г.*
7. *J.B.Keller ,* **Proc.Symp.Appl.Math.** ***13,Amer.Math.Soc****.,Providence,R1.1962.*
8. *M.M.R.Williams* **Nucl.Sci.Eng**. *V.136,p34-58, 2000.*
9. *G.C.Pomraning* **Trans.Theory and St.Ph**. *V.27 #5-7 p.405-443, 1998.*

G.C.Pomraning Linear Kinetic Theory and Particle Transport in Stochastic Mixtures, **World Scientific**, *Singapore, 1991*

10.N.Usachev, U.G.Bobkov "About aggregate applications of the integral and the differential measurements in nuclear data's problem for nucl. Reactors"**, in Proc. Soviet Un. Conf. on Nutron Physics** *,part II, p.39,Kiev 24-28 May 1971. (in Russian)*
11. N.I.Laletin, N.V.Sultanov,V.F.Boyarinov.,"Surface Harmonic and Surface Pseudo-Sources Methods."-**Pro ceedings of International Conference on the Physics of Reactors***,v.2,pp.XII-39-XII-48,April 23-27, Mace ille, France, 1990.*