The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, Tennessee, April 17–21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

PRECISION NEUTRONICS CALCULATIONS TO RESOLVE NUCLEAR POWER SAFETY-RELATED TASKS

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ABSTRACT

Analysis of peculiarities of application of precision computing codes based on Monte Carlo statistic models to study physics of reactors and resolve nuclear safety-related tasks is considered. The procedure of precision calculations as a necessary instrument of improving computing methods to ensure reliability and accuracy of neutronics calculations is discoursed. The results of resolving criticality problems and calculations of burnup for water-cooled reactor and high-temperature reactor with helium coolant are present. Computer codes MCNP4C (MCNP5), MONTEBURNS 1.0 and ORIGEN2 were used in all calculations as base computing codes.

Key Words: neutronics calculations, burnup of fuel, reactor core, Monte-Carlo method

1 MODERN PROBLEMS AND THE REQUIRED TECHNOLOGY

The current economic situation demands the nuclear power facilities to be more efficient. Thus, the concept of excessive conservatism used for development of the first nuclear power facilities needs to be reviewed. For example, in some countries, the concept of "burnup reserve," that takes into account reduction of reactivity of the burned-up fuel, is already used for designs of spent nuclear fuel repositories with a more compact fuel assemblies (FA) storage as well as management systems for new types of fuel (uranium-gadolinium, uranium-plutonium, etc.). Reduction of excessive conservatism in development of the modern nuclear reactors (NR) and nuclear fuel cycle facilities (NFCF), search of optimum solutions to study new fuel compositions (UN, PuN, MOX), safety assessment for NR with high burnup (over 12% for operating VVER and BN reactors, up to 90% for HTGR,) may be substantiated only using the modern calculation methods, that allow full-scale simulation of NR and NFCF in a wide range of design-basis and hypothetical operation modes. Apart from application of effective calculation codes, such technique requires special methods for substantiation of the calculation results. The complex neutronics calculations and analysis of uncertainties and errors of the marked characteristics may serve as a representative basis for formulating new benchmark-tasks and required physical experiments. Such calculations will allow one speaking about a Calculation experiment by analogy with a real Physical experiment.

Nuclear Safety Institute of the Russian Academy of Sciences (IBRAE RAN) specializes in the comprehensive analysis of NR and NFCF safety using modern integral calculation codes. IBRAE experts are involved in design-theoretical analysis and development of computer modules to simulate separate NPP components, verification of developed modules in the framework of international and national programs (SURC-4/NRS, ACE, BETA /KfK, RASPLAV- OSER/RRC KI) and experiments on repeated flooding of reactor core (FZK, Germany), etc. Neutronics calculations are performed using such codes as MCNP-NJOY [1,2], MONTEBURNS [3], ORIGEN2 [4] based on the libraries of nuclear data with pointwise structure. Over last years, a number of calculations have been carried out for various NR types, including VVER, BN fast reactors with sodium coolant and HTGR high-temperature reactors with helium coolant [5]. These calculations included international benchmark-calculations for

BN-800, HTR-10, HTTR [6], GT-MHR. Nuclear safety of fresh and spent fuel transportation and storages facilities was also studied.

Analysis of the performed neutronics calculations is given in the present report for both VVER and HTGR reactors. Such analysis allows obtaining useful information to formulate requirements to advanced calculation techniques.

2 TECHNOLOGY OF PRECISION CALCULATIONS IN NEUTRON PHYSICS. CONCEPTION OF *"BURNUP RESERVE"*

Specialized reactor codes and appropriate group libraries of nuclear data, which are intended for solving neutronics problems, have been verified and tested for particular types of reactors. A definition "precision calculations" was introduced after development of universal 3D codes, libraries of nuclear data with pointwise structure, and solution of the transport equations using Monte-Carlo technique. However, precision calculations are not only the precise codes resulting in more accurate data. The precise tools require to be handled more accurately, and the calculations made regardless the specific character of the precision codes will lead to incorrect results. The precision calculations are assumed to require additional work to be carried out in order to substantiate the obtained results and to calculate the confidence intervals of the values of indicated parameters. While making such calculations, the following is to be taken into account:

- The results obtained using precision codes are considered as more significant in comparison with results of traditional calculations;
- The existing standard files of estimated nuclear data do not have any specified preferences regarding the presented data. However, the calculations made using these data frequently lead to greatly varying results. Also, the verification of the data made at the level of purely evaluated nuclear data does not ensure their correctness in neutron-physical calculations of NR and NFCF. There is also no universal set of benchmark-problems for revealing preferences and incorrectnesses. Therefore, the "problem" verification of such kind of tasks is required. If there are no direct reference values of the marked characteristics, they may be estimated by incorrect methods on the basis of solving additional benchmark-tasks.
- Stage-by-stage substantiation of the calculation correctness is required to ensure the reliability of the precision calculations. Division of the initial task into separate stages with controlled marked characteristics is an important component of performing precision calculations. Such division may be regulated for examination of standard tasks, and the solution of new tasks for NR and NFCF can require particular gains. .

Concept of the "burnup reserve" in solving the nuclear safety tasks for NR and NFCF requires accurate calculations of the isotope composition of the fuel at various stages of burnup. Thorough analysis of the fuel isotope composition behavior followed by further research of basic neutron characteristics (K_{eff}, temperature reactivity coefficients, energy distribution, etc.) is required at the stage of technical development work when designing NR and NFCF. For the existing NR, more detailed information on the isotope composition is required due to nonuniform fuel burnup and necessity of its analysis at a high burnup.

When calculating the nuclide composition of the fuel, inaccuracies may occur due to the following:

- uncertainties of the initial nuclear data and lack of the required information for separate isotopes;
- inadequacy of the mathematical model used in the calculations and the actual physical process;
- approximate character of the numerical calculations.

Lack or absence of the nuclear data for separate isotopes is a frequently occurring situation when making precision calculations. Thus, indication of the isotopes that determine the medium (BASIS) seems to be a necessary stage. Correctness of the BASIS and assessment of its incompleteness are required for carrying out the subsequent calculations and substantiation of the results. Application of the formal mathematical methods for assessment of sensitivity of the calculated values and determination of the calculation errors turns out to be unacceptable due to uncertainty of the nuclear data. For example, the perturbation method is problem-dependent and cannot be used to obtain the coefficients of sensitivity to perturbation of separate micro-constants. At the same time, the non-universal character of the correlations, even in case of using a single database of nuclear micro-data, does not allow their automatic use for various neutronics tasks even for particular NR. There is also an objective difficulty of using a large number of isotopes, for which initial errors in micro-data presentation are significantly varying or absent.

Calculation medium setup («parameters of calculation codes + libraries of nuclear data») for solution of the specific class of tasks is one of necessary stages of precision calculations. When only one calculation code is used, the medium setup is generally reduced to start of test tasks for the given code, and the main activity is connected with formation and verification of the specialized applied libraries of nuclear data. The values of the calculation parameters are set taking into account the desired accuracy of the calculated characteristics, the maximum allowed calculation time, etc. If several calculation codes are used (for example, NJOY, ORIGEN2, MCNP), each of which works with its own data and intrinsic uncertainties and the codes interaction is shuttle (not sequential), the medium setup essentially becomes complicated . The shuttle interaction, when output results of one code serve as an input for another code, requires a thorough stage-by-stage substantiation of the calculations, as the step-by-step sensitivity assessment is not possible.

The approximate character of the numerical calculations makes estimation of the calculation errors a required procedure at various stages of the calculations. Here, we speak not about the mathematical errors and indicating of confidence intervals of the values for marked characteristics. At the same time, each of the used calculation codes has its own level of accuracy and reliability of the calculated values. Special attention is paid to the tasks when solution leads to results, the adequacy of which is difficult to assess due to the lack of experimental or reference values. Therefore there is no possibility to specify any kind of substantiated error for these tasks.

3 FEATURES OF BURNUP PROBLEM SOLVING (VVER, HTGR)

Specialized libraries of nuclear data with pointwise presentation are formed for solving the transport task in order to reduce the uncertainties arising from the group libraries of nuclear data. By today, the most complete libraries of decay and yield have been assembled for solution of the burnup tasks. The libraries include yield of U234, U236, Pu240, Pu242, Np237, Np238, Am241, Am242m and Cm235, Cf252 in addition to yield of Th232, U235, U238, Pu239, Pu241. Formation of similar libraries is especially required for neutronics calculations with new fuels (regenerated fuel, uranium-plutonium fuel, etc.). The number of "transport" isotopes in the specialized nuclear data libraries is about 250. Additionally, the activation libraries contain about 450 isotopes, which include nuclear data for separate (n,γ), (n,2n) and other reactions.

The first stage of the precision calculations represents a setup of the calculation medium being adequate for the used class of tasks [7].

3.1 Choice of an effective *BASIS* of isotopes

It is in general incorrect to include all the isotopes from the cross section and fission product yield library for ORIGEN2 (around 700) in the *BASIS*. There is a considerable number of

isotopes for which the required nuclear data for calculation of neutron flux (MCNP) are not included, thus introducing uncertainty into future calculations. *BASIS* may be adjusted using the *IMP*(ortance) parameter, which is used in MONTEBURNS to set the limiting value of concentrations and macroscopic cross-sections of the isotopes included in the *BASIS*. The final *BASIS* may include additional isotopes dependent on the character of the studied tasks. Adequacy of a specific *BASIS* may be evaluated using the criteria of *« ρ density conservation »* and *«K_{eff} stability»* for the extended *BASIS* and other.

Comparative calculations were carried out for *BASIS* with IMP =1.e-2, 1.e-4, 1.e-6 and basic isotopes U, Pu, Np, Am .

Table I. K_{eff} and «ρ *density conservation*» for VVER with various *IMP*

Burnup =1.713MW*day/kg

IMP	1.e-2	1.e-4	1.e-6
Keff	1.2043±0.0004	1.1984±0.0003	1.1980±0.0005
ρ , g/cm^3	10.3009	10.3054	10.3176

Burnup = 15.42MW*day/kg

IMP	1.e-2	1.e-4	1.e-6
Keff	1.1627±0.0004	1.1137±0.0004	1.1126±0.0004
ρ , g/cm^3	10.1644	10.3023	10.3109

Burnup = 91.54MW*day/kg

IMP	1.e-2	1.e-4	1.e-6
Keff	0.7815±0.0002	0.7446±0.0002	0.7436±0.0003
ρ , g/cm^3	9.5053	10.2974	10.3043

At a *BASIS* with a fairly large list of obligatory actinides for the tasks with low burnup K_{eff} values depend on *IMP* weakly. For the case of higher burnup the difference becomes noticeable (Table I).

Table II. K_{eff} and « ρ *density conservation*» for HTGR with various *IMP*

Burnup = 1/3 Lifetime

IMP	1.e-2	1.e-3	1.e-4
Keff	1.1196±0.0027	1.1139±0.0020	1.1165±0.0004
ρ , g/cm^3	9.1639	9.4225	9.9344

Burnup = 2/3 Lifetime

IMP	1.e-2	1.e-3	1.e-4
Keff	1.1220±0.0027	1.1209±0.0020	1.1157±0.0005
ρ , g/cm^3	8.2990	8.8401	9.8888

Burnup = 3/3 Lifetime

IMP	1.e-2	1.e-3	1.e-4
Keff	1.1112±0.0027	1.1094±0.0020	11029±0.0006
ρ , g/cm^3	7.3796	8.2163	9.8431

As the *BASIS* is incomplete for IMP=1e-2 and IMP=1e-3 fuel density ρ is lower than the actual value. At the value of IMP=1e-4 the *BASIS* contains all the isotopes required for the burnup process and in this case ρ is close to the actual value of $\rho=10 g/cm^3$.

3.2 Parameter «Burnup step *Nout*»

The stability of the eventual results to *Nout* is assessed by carrying out multivariant calculations with various values of Nout. This parameter (MONTEBURNS) determines the period of time when the value of neutron flux (MCNP) is re-calculated and the corresponding libraries are updated (ORIGEN2). The available systematic data is used for determination of the optimum value of Nout. At the same time, calculations with low, medium and high burnup require specific research (Table IV-XII).

3.3 Parameter «number of internal burn steps *nint*»

Influence of the values of this parameter (ORIGEN2) on eventual results was analyzed for low and medium burnup for VVER. The value of *nint* was varied in the range of 20-10000 . The performed analysis showed that for low burnup (<0.428 MW*day/kg) there is a substantial dependency of actinides concentration on *nint*. For medium burnup the value of *nint* =400 is an acceptable one. The results of analysis of sensitivity of actinides concentration to *nint* in calculations with low and medium burnup are given in Table IV-XII. Similar calculations may be used for evaluating of calculation errors and determining the possible intervals of the values of analyzed characteristics. Also such analysis allows determining the optimum value of *nint* and verifying the value of *Nout.*

Table III. Actinide concentration for Burnup=0.0107MW*day/kg, *Nout*=1/12day with various *nint*

nint	2000	40	diff. %
Th229	0.2315E-22	0.3170E-22	-31.2
Pa230	0.2872E-24	0.3657E-24	-24.0
U231	0.2498E-25	0.1267E-24	100.0
U232	0.7538E-21	0.8163E-21	-8.0
U233	0.1607E-13	0.1961E-13	-19.8
U234	0.2349E-10	0.2422E-10	-3.1
Pu242	0.1118E-18	0.1062E-18	5.1
Pu243	0.4726E-23	0.4398E-23	7.2

Table IV. Actinide concentration for Burnup=0.0430 MW*day/kg , *Nout*=1/12day with various *nint*

nint	2000	40	diff. %
Th229	0.3972E-21	0.4596E-21	-14.6
Pa230	0.2101E-22	0.2108E-22	-0.3
U231	0.1243E-23	0.1734E-23	-33.0
U232	0.4896E-19	0.4981E-19	-1.7
U233	0.6705E-13	0.7377E-13	-9.5
U234	0.9568E-10	0.9822E-10	-2.6
Pu242	0.6865E-16	0.6766E-16	1.5
Pu243	0.9152E-20	0.8993E-20	1.7

Table V. Actinide concentration for Burnup=0.0036 MW*day/kg with various *nint, Nout*

Nout,day	1/72	1/48		1/24		1/12	
nint	10000	10000	diff ,%	10000	diff ,%	2000	diff ,%
Th229	0.1273E-23	0.2949E-23	-79.4	0.1697E-23	-28.6	0.2597E-23	-68.4
U232	0.6494E-22	0.8129E-22	-22.4	0.5816E-22	11.0	0.6888E-22	-5.9
U233	0.4863E-14	0.6255E-14	-25.0	0.4077E-14	17.6	0.5193E-14	-6.6
U234	0.7899E-11	0.7829E-11	0.9	0.7892E-11	0.1	0.7754E-11	1.9
Pu242	0.3644E-21	0.3523E-21	3.4	0.3638E-21	0.2	0.3418E-21	6.4

Table VI. Actinide concentration for Burnup=0.0430 MW*day/kg with various *nint, Nout*

Nout,day	1/24	1/12		1/4	
nint	10000	2000	diff ,%	2000	diff ,%
Th229	0.3890E-21	0.3972E-21	-2.1	0.4181E-21	-7.2
Pa230	0.1842E-22	0.2101E-22	-13.1	0.2106E-22	-13.4
U232	0.4927E-19	0.4896E-19	0.6	0.4813E-19	2.3
U233	0.6761E-13	0.6705E-13	0.8	0.6342E-13	6.4
U234	0.9594E-10	0.9568E-10	0.3	0.9651E-10	-0.6
Pu242	0.6769E-16	0.6865E-16	-1.4	0.6728E-16	0.6
Pu243	0.8996E-20	0.9152E-20	-1.7	0.8803E-20	2.2

Table VII. Actinide concentration for Burnup=0.213 MW*day/kg , *Nout*=1/4day with various *nint*

nint	2000	400	diff,%	40	diff,%
Th229	0.1000E-19	0.1049E-19	-4.8	0.1040E-19	-3.9
U231	0.3810E-23	0.4117E-23	-7.7	0.4145E-23	-8.4
U232	0.3245E-22	0.3466E-22	-6.6	0.3354E-22	-3.3
U233	0.3399E-12	0.3474E-12	-2.2	0.3436E-12	-1.1
U234	0.4850E-09	0.4932E-09	-1.7	0.4946E-09	-1.9
Pu242	0.7632E-13	0.7553E-13	1.0	0.7625E-13	0.1
Pu243	0.1976E-16	0.1960E-16	0.8	0.2001E-16	-1.3
Am240	0.1168E-21	0.1177E-21	-0.7	0.1185E-21	-1.4

Table VIII. Actinide concentration for Burnup=0.428 MW*day/kg , *Nout*=5day with various *nint*

nint	10000	4000	diff,%	400	diff,%	40	Diff,%
Th229	0.4024E-19	0.3060E-19	27.2	0.4813E-19	-17.9	0.2864E-19	33.7
Pa230	0.7212E-20	0.7232E-20	-0.3	0.7212E-20	0.0	0.7217E-20	-0.1
U230	0.4121E-22	0.4131E-22	-0.2	0.4124E-22	-0.1	0.4126E-22	-0.1
U231	0.1174E-21	0.8717E-22	29.6	0.1304E-21	-10.5	0.8541E-22	31.5
U232	0.8486E-16	0.8478E-16	0.1	0.8497E-16	-0.1	0.8448E-16	0.4
U233	0.6567E-12	0.5291E-12	21.5	0.8267E-12	-22.9	0.4494E-12	37.5
U234	0.9704E-09	0.9664E-09	0.4	0.9649E-09	0.6	0.6685E-09	36.8
Pu242	0.1581E-11	0.1487E-11	6.1	0.1599E-11	-1.1	0.1602E-11	-1.3
Pu243	0.4814E-15	0.4249E-15	12.5	0.4804E-15	0.2	0.4788E-15	0.5
Am240	0.3885E-20	0.3725E-20	4.2	0.3938E-20	-1.3	0.3776E-20	2.8

Drawing upon the Tables III-VIII, *nint*=400 is considered to be acceptable for burnup calculations. Concentrations of Th229 and U233 tend to be unstable to *nint* values, and this may be important at a choice of *nint* value at problem solving with other fuel compositions.

Table IX. Actinide concentration for Burnup=0.213 MW*day/kg , *nint*=40 with various *Nout*

Nout,day	1/12	1/4	diff,%	1.0	diff,%	5.0	diff,%
Th229	0.1052E-19	0.1040E-19	1.1	0.1039E-19	1.3	0.7636E-20	31.8
U231	0.3350E-22	0.3354E-22	-0.1	0.3344E-22	0.2	0.2626E-22	24.2
U233	0.3484E-12	0.3436E-12	1.4	0.3471E-12	0.4	0.2541E-12	31.3
U234	0.4929E-09	0.4946E-09	-0.3	0.4964E-09	-0.7	0.3363E-09	37.8
Pu242	0.7592E-13	0.7625E-13	-0.4	0.7648E-13	-0.7	0.7894E-13	-3.9
Pu243	0.1974E-16	0.2001E-16	-1.4	0.2024E-16	-2.5	0.2050E-16	-3.8
Am240	0.1164E-21	0.1185E-21	-1.7	0.1239E-21	-6.2	0.1168E-21	-0.3

Table X. Actinide concentration for Burnup=0.428 MW*day/kg , *nint*=40 with various *Nout*

Nout,day	1/4	1.0	diff,%	5.0	diff,%	10.0	diff,%
Th229	0.4186E-19	0.4260E-19	-1.8	0.2864E-19	37.5	0.2725E-19	42.3
U231	0.1161E-21	0.1186E-21	-2.1	0.8541E-22	30.5	0.8120E-22	35.4
U233	0.7078E-12	0.7370E-12	-4.2	0.4494E-12	44.6	0.4537E-12	43.7
U234	0.9780E-09	0.9916E-09	-1.4	0.6685E-09	37.6	0.6674E-09	37.8
Pu242	0.1511E-11	0.1528E-11	-1.1	0.1602E-11	-5.8	0.1696E-11	-11.5
Pu243	0.4414E-15	0.4460E-15	-1.0	0.4788E-15	-8.1	0.5108E-15	-14.6
Am240	0.3730E-20	0.3915E-20	-4.8	0.3776E-20	-1.2	0.3985E-20	-6.6

Drawing upon the Tables IX, X, *Nout*=1day is sufficient for correct calculations of actinide concentrations for low burnup.

3.4 Parameters for neutron flux calculation

The neutron flux (MCNP) is calculated on the *BASIS* with "transport" isotopes from the applied nuclear data libraries. The values of parameters should first of all ensure correct calculation (set criteria) and only then to satisfy of desired statistical accuracy. Requirements that allow estimating the correctness of the calculated values for the considered class of problems are assumed as such criteria. The number of zones throughout the FA height (*Nzon*) is important parameter for neutron flux calculation. The burnup calculations of VVER for a symmetric model of FA with *Nzon* =15 (zone height ≈25cm) and *Nzon* =40 (zone height ≈8cm) demonstrate the importance of determination of parameters for correct calculation of neutron flux. Automatic switching to calculations with large *Nzon* leads to incorrect results – first there is a considerable statistical instability of K_{eff} and second, the "zone" isotope concentrations calculated in a symmetric model are not correlated.

3.5 Parameter «*neutron source SRC*» in the burnup calculations

The significance of the *«neutron source SRC»* (both the initial one and the one formed in process of calculations) rises compared to the traditional criticality calculations in MCNP. Correct forming of *SRC* [2] is a separate task. There are two methods of *SRC* assignment in analysis of criticality in MCNP:

1. explicit determination of the coordinates (x, y, z) - *ksrc*;
2. accumulation of a special binary file (*srctp*), formed for systems with similar isotope composition and geometry.

Both types of *SRC* are characterized by three parameters: *nps* – number of neutrons per cycle, *NPS*-total statistics, *Src_Ncycle – number of* skipped cycles. Multivariant calculations

have been carried out for FA of VVER with height partitioning of fuel elements into *Nzon* =15 and 40 to examine the sensitivity of K_{eff} to *SRC*:

- SRC_K – height uniform source *ksrc* that remains constant at all stages of burnup calculation;
- SRC_0 – accumulated source *srctp* for fresh fuel that remains constant at all stages of burnup calculation;
- SRC_N – specially accumulated source *srctp* for each burnup step.

Table XI. K_{eff} of VVER cell for *Nzon*=15, *Nout*=40day, Burnup=15.38MW*day/kg with various *SRC* , *NPS*

SRC	NPS	$K_{eff}(1\sigma)$	NPS	$K_{eff}(1\sigma)$
SRC_K	300000	1.1036 ± 0.0025	3400000	1.1048 ± 0.0004
SRC_0	300000	1.1020 ± 0.0016	4600000	1.1080 ± 0.0004
SRC_N	300000	1.1039 ± 0.0017	5000000	1.1032 ± 0.0003

Table XI gives comparative results K_{eff} for a cell with various *SRC* for *Nzon*=15 and *Nout* =40day. These results demonstrate not only the strong sensitivity of K_{eff} to initial *SRC*, but in some cases (SRC_0) also demonstrate obvious statistical instability. If at a small statistics (*NPS*=300000) K_{eff} varies within statistical error (1σ), with increase of *NPS* the deviations are beyond the borders of 2σ interval of values.

The statistical instability of K_{eff} for the case when SRC_0 is used is explained by inadequacy of the neutron flux generated by SRC_0 and the real distribution of neutrons which changes dynamically with burnup.

Table XII. K_{eff} of VVER cell with various *Nzon, Nout*

Nzon	Nout, day	Burnup=15.38MW*day/kg K_{eff}	Burnup =8.55 MW*day/kg K_{eff}
1	10	1.1120±0.0003	1.1630±0.0004
15	40	1.1048±0.0003	1.1517±0.0003
15	10	1.1028±0.0002	1.1574±0.0003
40	40	1.1036±0.0002	1.1533±0.0003
40	5	1.1012±0.0003	1.1535±0.0002

Table XII contains the comparative values of K_{eff} of a macroscopic cell of VVER for various Nzon, Nout and SRC_K. Here:

- SRC_K correct source with *Src_Ncycl* =50 is used for *Nzon*=40;
- SRC_K incorrect source with *Src_Ncycl* =5 is used for *Nzon*=15;
- Correct sources SRC_K with *Src_Ncycl*=25 and *Src_Ncycl* =5 are used for *Nzon*=1 (*Nout*=10day and *Nout*=40day).

Analysis of the obtained values of K_{eff} allows an evident rule to be determined: *"for the case of medium burnup the more accurate calculations give lower values of K_{eff} in comparison to the similar values obtained using more rough calculations, while for the case of low burnup, the differences in K_{eff} are not as noticeable».*

The performed research of dynamics of SRC change with burnup allows calculation parameters to be determined for correct forming of SRC for a given class of tasks. Thus, increase of *nps* by a factor of 4 leads to a noticeable reduction of oscillations in height distribution of

SRC_0 (Fig.1). Rise of *nps* in case of a set statistics NPS leads to considerable reduction of the «*number of cycles»* and to deterioration of the accumulated SRC (Fig.2). If the «*number of cycles»* is increased simultaneously, NPS is increased by several orders of magnitude, and this may lead to deterioration of SRC. Consequently, *nps*=20000 is considered to be an optimum value.

Fig.2 gives height distribution of neutrons in SRC_0 for various NPS. For NPS=100000 (*Src_Ncycl*=5), height distribution of neutrons is close to the initial one (dotted line in Fig.2). Rise of NPS leads to redistribution of the neutrons from the central areas to the end areas and this finally leads to unlimited rise of neutron density in the end areas. The considered variant appears as a result of incorrect assignment of *NPS* and *nps*, which are used in a step-by-step calculation of the neutron flux for specified geometry. On the other hand, use of SRC_0 formed for fresh fuel in the case of a large enough *NPS* (dotted line in Fig.2), leads to results that are statistically stable, but are not fully correct in high burnup tasks, as SRC_0 remains constant at all steps of burnup calculation.

Fig.3 gives the height distribution of SRC_K dependent on *NPS* for burnup of 7,7MW*day/kg for *nps*=20000, *NPS*=100, *Src_Ncycl* =50.

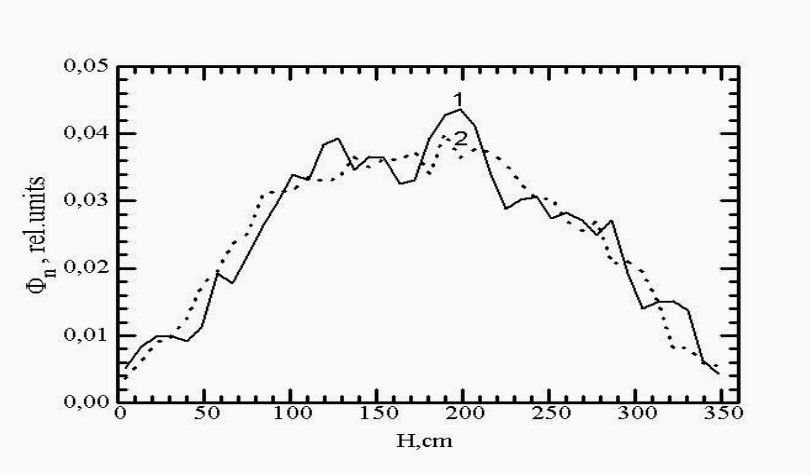

Figure 1. SRC_0 for 1 - *nps*=5000, 2 - *nps*=20000

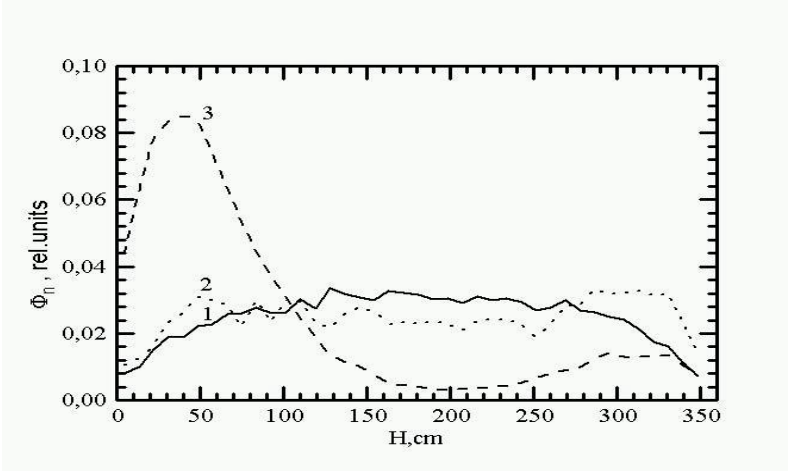

Figure 2. SRC_0 for Burnup=15,38MW*day/kg, *nps*=20000

1 -*NPS* =0.1 10^6; 2 -*NPS*=3.4 10^6; 3 -*NPS* = 7.5 10^6

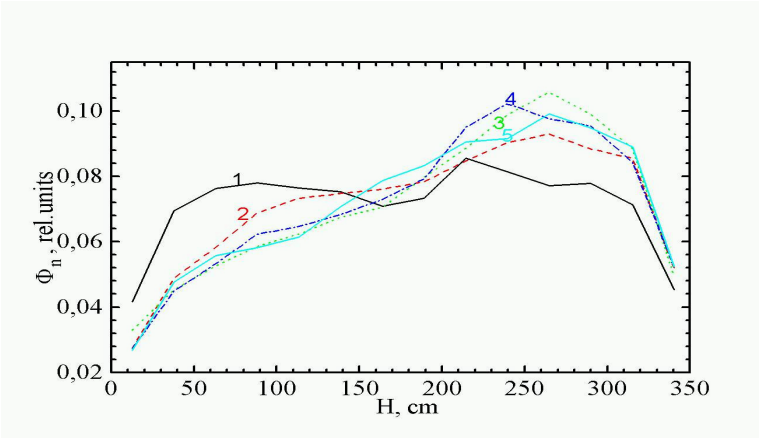

Figure 3. SRC_K for Burnup=7,7MW*day/kg, *nps*=20000 for various *NPS*

1 -*NPS*=2. 10^6, 2 -*NPS*=4.9 10^6; 3 -*NPS*=9.3 10^6; 4 -*NPS*=13. 10^6; 5 -*NPS*=27. 10^6

Fig.3 gives the dynamics of height distribution of SRC_K dependent on burnup for *nps*=20000, *NPS*=100, *Src_Ncycl* =50.

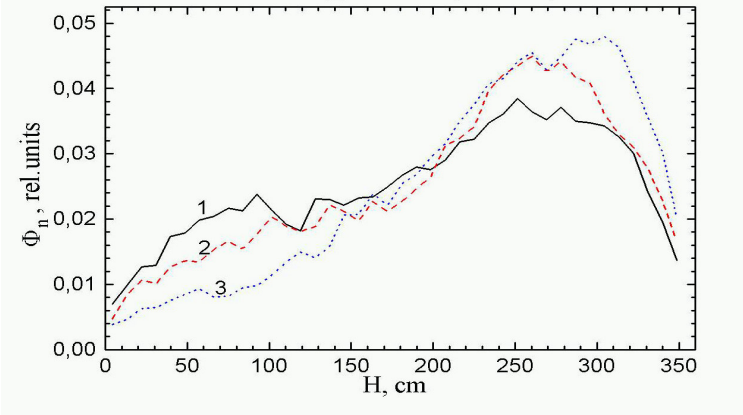

Figure 4. SRC_K for various Burnup

1 -7.70 MW*day/kg, 2 -8.55 MW*day/kg, 3 -11.96 MW*day/kg

Fig.4 gives the dynamics of height distribution of SRC_K dependent on burnup for *nps*=20000, *NPS*=150, *Src_Ncycl* =100. Here the rising dissymmetry in the symmetric areas is clearly seen. As a result *NPS*=100 and *Src_Ncycl* =50 are considered optimum for SRC_K.

4 INACCURACY OF NUCLEAR DATA & THERMALIZATION IN GRAPHITE FOR HTGR NEUTRONICS CALCULATIONS

Obviously, the correctness of the used nuclear data cannot be stated "once and for all" (for all NR and NFCF). Therefore, analysis of nuclear data of ENDF/B, JENDL, CENDL, BROND and other is required prior to carrying out neutronics calculations and forming of specialized applied libraries. Benchmark-calculations HTTR and HTR-10 initiated by IAEA demonstrate considerable dependency of the calculation results obtained using the Monte-Carlo programs (MCNP, KENO5, MCU) on the nuclear-physical constants and their compiling programs (NJOY, libraries JENDL, JEF ENDF/B6). This causes significant errors in the calculations of integral characteristics which determine the safety of NR. For example error for $K_{eff} \approx 1.5\%$, and for the temperature reactivity coefficient the error is over 20% [8]. As it turned out, the differences cannot be explained only by divergence of the reaction rate of fuel isotopes. Considerable contribution is made by graphite. Corresponding nuclear data C12 play determinative role for HTGR.

Some isotopes that are insignificant in calculations of certain types of NR and NFCF may have decisive role for neutronics calculations of other NR. Nuclear data that were formulated earlier and are currently used for these isotopes will require revision. The results of benchmark research of HTGR show considerable discrepancies in rate of reactions on C12 for various codes that use various nuclear data libraries (WIMS-D4, MCNP5 и др.). The differences in reaction of absorption on C12 reach 15% dependent on ENDF/B5, ENDF/B6, JENDL3 even when a single calculation code (MCNP4C) was used. If we also compare the results obtained using various codes (WIMS D/4), the differences reach 30%.

Studying the temperature coefficient of reactivity is one of the most important tasks for assessment of nuclear safety of NR, therefore the results of such calculations are considered especially significant. The results of neutronics calculations of HTGR are strongly dependent on the nuclear data for graphite. Thereupon benchmark–calculations were carried out using the specialized libraries of nuclear data and thermalization files (TF) prepared for temperatures in the range of 300K-1600K. The results obtained for temperature reactivity coefficient are given below. In these calculations TF was formed on the basis of different initial libraries with the help of program modules that use various theoretical thermalization models.

Table XIII. K_{eff} HTGR for various temperatures and TF

	Keff		
LIBRARY	LIB(MCNP4C)	ENDF/B6	JEF 2.2
METHOD		LEAPR(NJOY)	TERMR(NJOY)
T,K			
300	1.0997±0.0006	1.1008±0.0004	-
400	1.1048±0.0006	1.1062±0.0004	-
500	1.1104±0.0006	1.1117±0.0004	-
600	1.1167±0.0005	1.1176±0.0004	-
700	1.1147±0.0005	1.1176±0.0004	-
800	1.1185±0.0005	1.1284±0.0004	-
1200	1.1159±0.0006	1.1179±0.0004	1.1191±0.0004
1600	1.0768±0.0008	-	1.0921±0.0005

Table XIV. K_{eff} HTGR for T=900, 1000K with various TF

T,K	Keff	LIBRARY	METHOD
1000	1.1294±0.0006	ENDF/B6	TERMR(NJOY)
1000	1.1275±0.0003	ENDF/B6	LEAPR(NJOY)
1000	1.1284±0.0003	JEF 2.2	TERMR(NJOY)
1000	1.1186±0.0004	ENDF/B6	Interpolation: 600,800,1200K
900	1.1169±0.0005	(MCNP4C: 800K)	
900	1.1204±0.0006	(MCNP4C: 1200K)	
900	1.1285±0.0004	ENDF/B6	LEAPR(NJOY)
900	1.1251±0.0006	JEF 2.2	Interpolation: 800,1000,1200K
900	1.1293±0.0005	JEF 2.2	Interpolation: 800,1000K
900	1.1295±0.0004	JEF 2.2	Interpolation: 700,800,1000K

Analysis of the obtained results shows good compliance of K_{eff} for T=300, 400, 500, 600K. There are considerable discrepancies of K_{eff} for the temperatures of 700 and 800K. For the temperature of 1000K there is key non-conformity that leads not only to incorrect quantitative

results but also to qualitative. Further use of TF at 1000K for makefile TF for other temperatures using interpolation techniques also leads to incorrect results for K_{eff}. The resulting non-monotonic character of K_{eff} in the temperature range of 800-1000K is a direct consequence of using incorrect nuclear data TF at 1000K. The given example is indicative by that the similar mistakes in the nuclear data can be exhibited at problem solving incidently and always not express so obviously, and the made conclusions may be erroneous because of incorrectly obtained results.

5 CONCLUSIONS

1. The substantial productivity of precision computing codes can be received only at the indicating of the guaranteed intervals of significances for marked characteristics.

2. Solution of problems using the precision codes with no preliminary studies can lead to incorrect results. Thus benchmark-research becomes of greater importance.

3. There is a necessity to develop a precision calculation techniques. A variety of nuclear safety problems, which are characterized by essentially different neutronics processes, does not allow speaking about universality of precision calculations. However development of technics even for a particular class of problems appears to be an extremely important stage for realization of the precision neutronics calculations.

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