Improvement of Modeling HTGR Neutron Physics by Uncertainty Analysis with the Use of Cross-Section Covariance Information

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Abstract. This work is aimed at improvement of HTGR neutron physics design calculations by application of uncertainty analysis with the use of cross-section covariance information. Methodology and codes for preparation of multigroup libraries of covariance information for individual isotopes from the basic 44-group library of SCALE-6 code system were developed. A 69-group library of covariance information in a special format for main isotopes and elements typical for high temperature gas cooled reactors (HTGR) was generated. This library can be used for estimation of uncertainties, associated with nuclear data, in analysis of HTGR neutron physics with design codes. As an example, calculations of one-group cross-section uncertainties for fission and capture reactions for main isotopes of the MHTGR-350 benchmark, as well as uncertainties of the multiplication factor \( k_{\infty} \) for the MHTGR-350 fuel compact cell model and fuel block model were performed. These uncertainties were estimated by the developed technology with the use of WIMS-D code and modules of SCALE-6 code system, namely, by TSUNAMI, KENO-VI and SAMS. Eight most important reactions on isotopes for MHTGR-350 benchmark were identified, namely: \(^{10}\text{B}\) (capt), \(^{238}\text{U}\) (n,\(\gamma\)), \(\nu_s\), \(^{235}\text{U}\) (n,\(\gamma\)), \(^{238}\text{U}\) (el), natC (el), \(^{235}\text{U}\) (fiss)-\(^{235}\text{U}\) (n,\(\gamma\)), \(^{235}\text{U}\) (fiss).

1. Introduction

This study is carried out in frames of the IAEA Coordinated Research Project “HTGR Reactor Physics, Thermal-hydraulics and Depletion Uncertainties Analysis” [1–6]. The main objective of the Project is elaboration of methodical basis for tracking of propagation of different uncertainties in modeling of neutron physics, thermal-hydraulics and fuel depletion, and development of corresponding computational tool. Special attention is paid to propagation of computational uncertainty in transition from one calculation stage to another. It is assumed that the whole chain of the uncertainty propagation from the basic data, technological uncertainties through different calculation stages will be tested on a number of benchmark exercises.

The main objective of our efforts is the analysis of uncertainties in modeling neutron physics of HTGR with prismatic fuel on the basis of MHTGR-350 benchmark [7] proposed by NEA OECD. One of the goals of this research is to study propagation of uncertainties contained in the libraries of the evaluated nuclear data to group wise microscopic cross-sections used for lattice physics calculations, and further to few-group macroscopic cross-sections used in codes for full scale reactor calculations.
Calculations are performed for two different variants of the specification of the MHTGR-350 benchmark, but obtained results showed that the conclusions drawn in both cases concerning the uncertainties are identical. Therefore, results submitted in this paper relate only to the second variant of the specification [8].

2. Preparation of the 69-group Library of Covariance Information for Main Isotopes
As a rule, WIMS-D is used in NRC “Kurchatov Institute” as a design code for HTGR lattice calculations. WIMS-D uses shielded 69-group cross-sections. Therefore, to track the propagation of the nuclear data uncertainties to the next calculation stage, as input one must have 69-group covariance information (group-wise standard deviations and covariance matrices).

An original code sequence was developed for preparation of 69-group library of covariance information from the basic 44-group binary library of SCALE-6 code. This technology uses the program modules Cadillac and Cognac [9] of SCALE-6 code package, Angelo code [10] and several program modules developed by authors of this work for the purposes of the Project. Generally, the functions of these modules are the following;

1) module Cadillac – extraction of covariance information for one isotope in binary form from the basic binary library of SCALE;
2) module Cognac – conversion of covariance information for one isotope from binary form to a formatted file (COVERX format [11]);
3) module Cognac_Angelo (NRC KI) – preparation of input files for Angelo code;
4) Angelo code – conversion of formatted 44-group covariance information to 69 groups;
5) module Cov_matr-69 (NRC KI) – conversion of 69-group covariance information to a special format.

As a result, we get a separate file for each isotope in this library. This provides a possibility to easily extend the library content and change the number of groups.

Currently this library contains covariance information in the following form: group standard deviations, group correlation matrices, group covariance matrices. The library contains following 11 isotopes and elements: $^{235}\text{U}$, $^{238}\text{U}$, $^{16}\text{O}$, $^{4}\text{He}$, Si-nat, $^{28}\text{Si}$, $^{29}\text{Si}$, $^{30}\text{Si}$, $^{10}\text{B}$, $^{11}\text{B}$.

The use of this library together with design codes allows the automation of the entire process of calculation of uncertainties of neutron-physical calculation.

3. Calculation of One Group Cross-Sections Uncertainties for Main Isotopes and Multiplication Factor Uncertainty

3.1. Model problem
A model of a fuel compact cell of MHTGR-350 reactor (Figure 1) is used for calculation of the one-group cross-section uncertainties for fission and absorption reactions for main isotopes. Geometry of the spherical fuel particle is provided in figure 2 [1, 2].

![Figure 1. Fuel compact cell.](image1)

![Figure 2. Spherical fuel particle.](image2)
The model is considered at the following temperatures states:
1) Cold Zero Power (CZP) – temperature of all materials in a fuel compact cell is 293 K;
2) Hot Full Power (HFP) - temperature of all materials in a fuel compact cell is 1200 K.
Calculation of the fuel compact cell model is performed in two variants:
1) with homogenization of UCO TRISO fuel particles within the zone of a fuel compact (Figure 1), helium gap zone, zone of the block graphite (I-1a);
2) with rigorous modeling of TRISO fuel particles structure (I-1b).
For additional information regarding the compact configuration see [8].

3.2. Code sequence developed for calculation of uncertainties
A special software technology (hereafter referred to as SUW technology) using the 69-group library of covariance information was developed for calculating one-group cross-section uncertainties for main isotopes presented in HTGR neutron physics problems. In application to the MHTGR-350 benchmark it consists of three modules: MHTGR-350_Wd5, Reactions_Cross-sections, and Error_Sigl.

Program module MHTGR-350_Wd5 prepares an input file for WIMS-D and performs WIMS-D run. The real three-dimensional fuel compact cell is replaced by a two-dimensional cluster fuel compact cell with conservation of the mean chord in the fuel (with some correction factor) and mass of each material in the actual three-dimensional fuel compact cell and in three-dimensional cell built from two-dimensional cluster fuel compact cell with the same height. Calculation results of MHTGR-350_Wd5 code are WIMS-D output files containing \( k_\infty \) value for the fuel compact cell and all information necessary for the calculation of many-group microscopic cross-sections of the main isotopes presented in the fuel compact cell.

Results of calculations of the multiplication factor are given in tables 1, 2. Values calculated by SERPENT code [12] taken from [13] are used as reference values. Calculations by SCALE-6.1.2 code package were performed by authors of this paper. In so doing, calculations named ‘Scale-6.1, Keno-VI, 238 MG’ for variant I-1a were carried out by TSUNAMI module, and for variant I-1b – by KENO-VI module with ‘doublehet’ option. Calculations named ‘Scale-6.1, Keno-VI, CE’ were carried out by KENO-VI module with library ‘ce_v7’.

| Code                             | CZP          | HFP          |
|----------------------------------|--------------|--------------|
| Serpent (ENFD-B-VII.0)           | 1.31698 ±    | 1.18245 ±    |
|                                  | 0.00019      | 0.00022      |
| WIMS-D5, WLUP (ENFD/ B-VI.8, CENDL-2.1) | 1.33417 | 1.21093 | 2.41 |
| Scale-6.1, Keno-VI, 238 MG       | 1.31161      | 1.18302      |
| Scale-6.1, Keno-VI, CE           | 1.31857      | 1.18911      |

| Code                             | CZP          | HFP          |
|----------------------------------|--------------|--------------|
| Serpent (ENFD-B-VII.0)           | 1.37060 ±    | 1.24461 ±    |
|                                  | 0.00021      | 0.00023      |
| WIMS-D5, WLUP (ENFD/ B-VI.8, CENDL-2.1) | 1.36180 | -0.64 | 1.24474 | 0.01 |
| Scale-6.1, Keno-VI, 238 MG       | 1.36595      | 1.24443      |
|                                  | -0.34        | -0.01        |
It should be noted the essential overestimation of the fuel compact cell $k_\infty$ value calculated by the WIMS-D5 code in comparison with calculation by SERPENT and SCALE. This fact is a subject for further investigations.

The effect of homogenization of fuel particles and graphite matrix in a fuel compact is provided in table 3 and calculated by the following formula:

$$\delta k_e = \frac{k_{\text{hom}} - k_{\text{het}}}{k_{\text{het}}}$$  (1)

Table 3. Effect of Homogenization.

| Code                        | CZP, % | HFP, % |
|-----------------------------|--------|--------|
| Serpent, ref.               | -3.91  | -4.99  |
| WIMS-D5                     | -2.03  | -2.72  |
| Scale-6.1, Keno-VI, 238 MG  | -3.98  | -4.96  |

Module **Reactions_Cross-sections** uses the WIMS-D output file to calculate 69-group microscopic cross-sections for main isotopes in the fuel compact cell model and 69-group neutron fluxes in materials of the cell.

Module **Error_Sigl** calculates microscopic one-group fission and capture cross-sections for each isotope and their uncertainties in the form of dispersions and standard deviations.

Uncertainties of one-group microscopic cross-sections are calculated using formulas given in [2] which, in their turn, are taken from [14]. We rewrote them in a modified form, which is more correct and less complicated:

$$\Delta^2 = \sum_g \sum_g^G \alpha_{x,g} \alpha_{y,g} \sigma_{x,y}^{(g)} \sigma_{x,y}^{(g)} = \alpha_x^T \sigma(x,y) \alpha_y$$  (2)

where:
- $\Delta^2$ – uncertainty (dispersion) of one-group microscopic cross-sections of type “$y$” connected with uncertainty of cross-sections of type “$x$”;
- $\alpha_{x,g}$ – weighting factor based on data from “$x$” reaction in group $g$;
- $\alpha_{y,g}$ – weighting factor based on data from “$y$” reaction in group $g$;
- $\alpha_{x,y} =$ weighting group vector connected with corresponding reaction;
- upper index “$T$” – transposed vector, i.e. a vector-row;
- $\sigma_{x,y}^{(g)}$ – element of group relative covariance matrix $\sigma(x,y)$ for reactions types “$x$” and “$y$”;
- $\sigma_{x,y}^{(g)}$ – cross-section of corresponding reaction in the group $g$;
- $\Phi_g$ – neutron flux in the group $g$;
- $\Phi_{\text{tot}}$ – sum of group fluxes.

### 3.3. Results of the calculations

The covariance information on reactions available in the SCALE-6 library for $^{235}$U and $^{238}$U is listed below in a symbolic form: $\sigma_t - \sigma_{t\nu}, \sigma_{\gamma\nu}, \sigma_{\nu}, \sigma_{t\nu} - \sigma_{t\nu \gamma}, \sigma_{\gamma\nu}, \sigma_{\nu}, \sigma_{t\nu}, \sigma_{t\nu}, \sigma_{t\nu \gamma}, \sigma_{\gamma\nu}, \sigma_{\nu}, \sigma_{t\nu}, \sigma_{t\nu}, \sigma_{t\nu \gamma}, \sigma_{\gamma\nu}, \sigma_{\nu}$. 

Module **Reactions_Cross-sections** uses the WIMS-D output file to calculate 69-group microscopic cross-sections for main isotopes in the fuel compact cell model and 69-group neutron fluxes in materials of the cell.
Covariance information used in further calculations is marked in bold, i.e. we took into account the matrix diagonal of reaction covariance information. We did not take into account the influence of the elastic scattering covariance information on uncertainties of fission and capture reactions and influence of the fission covariance information on the uncertainties of capture reactions.

Results of the calculations of one-group microscopic cross-sections, their uncertainties (dispersions) and standard deviations for $^{238}$U and $^{235}$U for two states of the fuel compact cell model for variant I-1a are provided in the table 4.

**Table 4.** Values and uncertainties of one-group cross-sections for isotopes $^{238}$U and $^{235}$U, variant I-1a.

|          | U-235  |       | U-238  |       |
|----------|--------|-------|--------|-------|
|          | CZP    | HFP   | CZP    | HFP   |
| $\sigma_c$, barn | 34.2201 | 31.0835 | 4.12395E-02 | 4.13055E-02 |
| $\nu_{\text{tot}}$ | 2.43871 | 2.43885 | 2.72996 | 2.72998 |
| $(\Delta \nu)^2$ | 9.29E-06 | 9.12E-06 | 2.94E-05 | 2.94E-05 |
| $(\Delta \sigma)^2$ | 1.68E-04 | 1.68E-04 | 1.68E-04 | 1.68E-04 |
| $\Delta \nu$, % | 0.15 | 0.15 | 0.61 | 0.61 |
| $\Delta \sigma$, % | 0.3 | 0.3 | 0.5 | 0.5 |
| $\Delta \nu$, % | 1.4 | 1.5 | 1.3 | 1.3 |
| $\Delta \sigma$, % | 1.4 | 1.5 | 1.3 | 1.3 |

Results of the calculations of one-group microscopic cross-sections, their uncertainties (dispersions) and standard deviations for non-fissile isotopes for two states of the fuel compact cell for variant I-1a are provided in the table 5.

**Table 5.** Values and uncertainties of one-group cross-sections for non-fissile isotopes, variant I-1a.

|          | O-nat  |       | Si-nat  |       |
|----------|--------|-------|--------|-------|
|          | CZP    | HFP   | CZP    | HFP   |
| $\sigma_c$, barn | 9.55637E-04 | 9.56137E-04 | 1.20812E-02 | 1.12005E-02 |
| $(\Delta \sigma)^2$ | 2.44E-01 | 2.45E-01 | 4.81E-04 | 4.53E-04 |
| $\Delta \sigma$, % | 49.4 | 49.5 | 2.2 | 2.1 |

|          | C-nat, FCM  |       | C-nat, Block  |       |
|----------|--------------|-------|----------------|-------|
|          | CZP           | HFP   | CZP            | HFP   |
| $\sigma_c$, barn | 2.88391E-04 | 2.70435E-04 | 2.88063E-04 | 2.69184E-04 |
| $(\Delta \sigma)^2$ | 2.93E-03 | 3.25E-03 | 2.74E-03 | 3.28E-03 |
| $\Delta \sigma$, % | 5.4 | 5.7 | 5.2 | 5.7 |
Results of the calculations of one-group microscopic cross-sections, their uncertainties (dispersions) and standard deviations for $^{238}$U and $^{235}$U for two states of the fuel compact cell model for variant I-1b are provided in table 6.

Table 6. Values and uncertainties of one-group cross-sections for isotopes $^{238}$U and $^{235}$U, variant I-1b.

|          | U-235 |          | U-238 |          |
|----------|-------|----------|-------|----------|
|          | CZP   | HFP      | CZP   | HFP      |
| $\sigma_f$, barn | 33.4272 | 30.5008 | 4.10312E-02 | 4.09922E-02 |
| $\sigma_c$, barn | 9.12920 | 8.60040 | 3.14137 | 3.78015 |
| $\nu_{tot}$ | 2.43874 | 2.43891 | 2.73265 | 2.73267 |
| $(\Delta f)^2$ | 9.36E-06 | 9.22E-06 | 2.94E-05 | 2.94E-05 |
| $(\Delta f)^2$ | 1.96E-04 | 2.08E-04 | 1.67E-04 | 1.75E-04 |
| $\Delta f$, % | 0.3 | 0.3 | 0.5 | 0.5 |
| $\Delta c$, % | 1.4 | 1.4 | 1.3 | 1.3 |
| $\Delta \nu$, % | 0.15 | 0.15 | 0.61 | 0.61 |

Results of the calculations of one-group microscopic cross-sections, their uncertainties (dispersions) and standard deviations for non-fissile isotopes for two states of the fuel compact cell for variant I-1b are provided in table 7.

Table 7. Values and uncertainties of one-group cross-sections for non-fissile isotopes, variant I-1b.

|          | O-nat |          | Si-nat |          |
|----------|-------|----------|-------|----------|
|          | CZP   | HFP      | CZP   | HFP      |
| $\sigma_c$, barn | 9.76850E-04 | 9.75014E-04 | 1.23579E-02 | 1.14642E-02 |
| $(\Delta f)^2$ | 2.44E-01 | 2.45E-01 | 4.92E-04 | 4.64E-04 |
| $\Delta f$, % | 49.4 | 49.5 | 2.2 | 2.2 |

|          | C-nat, FCM |          | C-nat, Block |          |
|----------|------------|----------|--------------|----------|
|          | CZP       | HFP      | CZP          | HFP      |
| $\sigma_c$, barn | 2.97546E-04 | 2.78865E-04 | 2.96010E-04 | 2.76416E-04 |
| $(\Delta f)^2$ | 2.77E-03 | 3.06E-03 | 2.58E-03 | 2.86E-03 |
| $\Delta f$, % | 5.3 | 5.5 | 5.1 | 5.3 |

|          | C-nat, Fuel |          |
|----------|------------|----------|
|          | CZP       | HFP      |
| $\sigma_c$, barn | 2.87152E-04 | 2.70533E-04 |
| $(\Delta f)^2$ | 3.08E-03 | 3.39E-03 |
| $\Delta f$, % | 5.8 | 5.8 |

Rather large capture cross-section uncertainty of O-nat attracts attention. In addition, it should be noted that we used covariance information for pair $\sigma_{(n,\gamma)} - \sigma_{(n,\gamma)}$ in calculating $(\Delta c)^2$ because covariance information for $(n,\alpha)$ and $(n,p)$ reactions is not available in the library of SCALE-6 code.
3.4. Selection of the most important neutron reactions for the MHTGR-350 benchmark

Selection of the most important neutron reactions, i.e. reactions whose uncertainties give the largest contribution to the $k_{\infty}$ uncertainty is carried out using one-group formula for $k_{\infty}$ of the fuel compact cell model:

$$k_{\infty} = (v f \sigma_f^5 \rho_{\text{fuel}} + v f \sigma_f^8 \rho_{\text{fuel}}) V_{\text{fuel}} / [(\sigma_f^5 \rho_{\text{fuel}} + \sigma_f^8 \rho_{\text{fuel}} + \sigma_c^5 \rho_{\text{fuel}} + \sigma_c^8 \rho_{\text{fuel}} + \sigma_{\text{Omat}}^\text{Nat} \rho_{\text{fuel}})
+ \sigma_{\text{Cnat}}^\text{Fuel} \rho_{\text{fuel}} V_{\text{fuel}} + \sigma_{\text{Cnat}}^\text{FCM} \rho_{\text{FCM}} V_{\text{FCM}} + \sigma_{\text{Sic}}^\text{Nat} \rho_{\text{Sic}} V_{\text{Sic}} + \sigma_{\text{Cnat}}^\text{Block} \rho_{\text{Block}} V_{\text{Block}}]$$

(4)

Let us introduce the notation for the 11 input parameters:

$$\alpha_i = \left\{ \sigma_5^5, \sigma_8^5, \sigma_c^5, \sigma_c^8, \sigma_{\text{Omat}}^\text{Nat}, \sigma_{\text{Cnat}}^\text{Nat}, \sigma_{\text{Cnat}}^\text{FCM}, \sigma_{\text{Cnat}}^\text{Block} \right\}$$

(5)

Dispersion of cell $k_{\infty}$ connected with uncertainty of input parameter $\alpha_i$ with taking into account one-group covariance $C_{ii}$, can be written as:

$$\delta^{2}k_{\infty,i} = S_{k_{\infty},i} C_{ii} S_{k_{\infty},i},$$

(6)

where $S_{k_{\infty},i}$ - sensitivity coefficients of value $k_{\infty}$ to the change of parameters $\alpha_i$.

$$S_{k_{\infty},i} = \frac{\partial k_{\infty}}{\partial \alpha_i}$$

(7)

$C_{ii}$ are provided in the tables 6-7 as $\Delta^2$.

Below there are the explicit expressions for the sensitivity coefficients $S_{k_{\infty},i}$.

$$S_{k_{\infty},i} = \frac{v f \sigma_f^5 \rho_{\text{fuel}} V_{\text{fuel}}}{k_{\infty}}$$

(8)

where:

$$\gamma = (\sigma_f^5 \rho_{\text{fuel}} + \sigma_f^8 \rho_{\text{fuel}} + \sigma_c^5 \rho_{\text{fuel}} + \sigma_c^8 \rho_{\text{fuel}} + \sigma_{\text{Omat}}^\text{Nat} \rho_{\text{fuel}} + \sigma_{\text{Cnat}}^\text{Fuel} \rho_{\text{fuel}} V_{\text{fuel}} + \sigma_{\text{Cnat}}^\text{FCM} \rho_{\text{FCM}} V_{\text{FCM}} + \sigma_{\text{Sic}}^\text{Nat} \rho_{\text{Sic}} V_{\text{Sic}} + \sigma_{\text{Cnat}}^\text{Block} \rho_{\text{Block}} V_{\text{Block}}$$

(9)

$$S_{k_{\infty},2} = \frac{v f \sigma_f^5 \rho_{\text{fuel}} V_{\text{fuel}}}{k_{\infty}}$$

(10)

$$S_{k_{\infty},3} = \frac{\sigma_f^5 \rho_{\text{fuel}} V_{\text{fuel}}}{k_{\infty}} \left( v_f - k_{\infty} \right)$$

(11)

$$S_{k_{\infty},4} = \frac{\sigma_f^8 \rho_{\text{fuel}} V_{\text{fuel}}}{k_{\infty}} \left( v_f - k_{\infty} \right)$$

(12)

$$S_{k_{\infty},i} = -(\alpha_i \cdot \omega_{i-1} \cdot \gamma^{-1}), \quad i = 5,6,\ldots,15$$

(13)

$$\omega_i = \left\{ \rho_{\text{fuel}} V_{\text{fuel}}, \rho_{\text{FCM}} V_{\text{FCM}}, \rho_{\text{Block}} V_{\text{Block}}, \rho_{\text{Sic}} V_{\text{Sic}} \right\}$$

(14)
Formula for the total dispersion of $k_\infty$ has the form:

$$\delta^2_{k_\infty} = \sum_{i=1}^{\infty} \delta^2_{k_\infty,i}$$ (15)

Comparative calculations of sensitivity coefficients of $k_\infty$ of the fuel compact cell model to the change of input parameters $\alpha_i$ are provided in the tables 8, 9. Sensitivity coefficients are calculated using explicit formulas for variants I-1a, I-1b and by SCALE-6.1.2 code for variant I-1a for CZP and HFP states of the fuel compact cell. Note that SAMS module (SCALE-6) that calculates sensitivity and uncertainties does not work for double heterogeneity problems. Therefore, we do not provide results calculated for variant I-1b by SCALE-6.1.2.

Table 8. Sensitivity coefficients of $k_\infty$ of the fuel compact cell to the change of input parameters $\alpha_i$, CZP.

| $\alpha_i$ | $S_{k_\infty,i}$ | Scale-6.1, Keno-VI, variant I-1a |
|------------|----------------|----------------------------------|
| variant I-1b | variant I-1a | |
| $\nu_5$ | 9.92E-01 | 9.93E-01 | 9.93E-01 |
| $\nu_8$ | 7.35E-03 | 7.21E-03 | 6.64E-03 |
| $\sigma^5_{f}$ | 4.38E-01 | 4.50E-01 | 2.31E-01 |
| $\sigma^8_{f}$ | 3.69E-03 | 3.69E-03 | 3.46E-03 |
| $\sigma^5_{c}$ | -1.51E-01 | -1.50E-01 | -2.04E-01 |
| $\sigma^8_{c}$ | -2.80E-01 | -2.94E-01 | -2.41E-01 |
| $\sigma^{\text{Cnat}}_{c}$ | -1.55E-04 | -1.45E-04 | -1.01E-04 |
| $\sigma^{\text{Cnat}}_{c,\text{Fuel}}$ | -1.52E-05 | | |
| $\sigma^{\text{Cnat}}_{c,\text{FCM}}$ | -2.18E-03 | -2.03E-03 | -2.53E-03 |
| $\sigma^{\text{Cnat}}_{c,\text{Block}}$ | -4.01E-03 | -3.75E-03 | -5.06E-03 |
| $\sigma^{\text{Cnat}}_{c,\text{All}}$ | -4.25E-03 | -3.96E-03 | -4.99E-03 |
| $\sigma^8_{\text{el}}$ | -6.45E-03 | -5.99E-03 | -7.52E-03 |
| $\sigma^{\text{Chat}}_{\text{FCM}}$ | -2.85E-02 | | |
| $\sigma^{\text{Chat}}_{\text{el,FCM}}$ | 5.26E-02 | | |
| $\sigma^{\text{Chat}}_{\text{el,Block}}$ | 1.68E-01 | | |
| $\sigma^{\text{Chat}}_{\text{el}}$ | 2.21E-01 | | |
Table 9. Sensitivity coefficients of $k_\infty$ of the fuel compact cell to the change of input parameters $\alpha_i$, HFP.

| $\alpha_i$ | $S_{k_{\infty,j}}$ variant I-1b | $S_{k_{\infty,j}}$ variant I-1a | $S_{k_{\infty,j}}$ variant I-1a | Scale-6.1, Keno-VI, variant I-1a |
|------------|---------------------------------|---------------------------------|---------------------------------|--------------------------------|
| $v_5$      | $9.92E-01$                      | $9.92E-01$                      | $9.93E-01$                      |                                |
| $v_6$      | $8.04E-03$                      | $7.94E-03$                      | $7.36E-03$                      |                                |
| $\sigma_f^5$ | $4.86E-01$                      | $4.99E-01$                      | $2.57E-01$                      |                                |
| $\sigma_f^8$ | $4.38E-03$                      | $4.42E-03$                      | $4.17E-03$                      |                                |
| $\sigma_c^5$ | $-1.43E-01$                     | $-1.40E-01$                     | $-2.03E-01$                     |                                |
| $\sigma_c^8$ | $-3.38E-01$                     | $-3.54E-01$                     | $-2.93E-01$                     |                                |
| $\sigma_{C_{\text{nat}}}$ | $-1.55E-04$                     | $-1.45E-04$                     | $-1.02E-04$                     |                                |
| $\sigma_{C_{\text{nat}},\text{Fuel}}$ | $-1.43E-05$                     |                                |                                |                                |
| $\sigma_{C_{\text{nat}},\text{FCM}}$ | $-2.04E-03$                     | $-1.90E-03$                     | $-2.54E-03$                     |                                |
| $\sigma_{C_{\text{nat}},\text{Block}}$ | $-3.72E-03$                     | $-3.47E-03$                     | $-5.08E-03$                     |                                |
| $\sigma_{C_{\text{nat}},\text{All}}$ | $-3.97E-03$                     | $-3.70E-03$                     | $-4.97E-03$                     |                                |
| $\sigma_{C_{\text{nat}},\text{el}}$ | $-6.02E-03$                     | $-5.60E-03$                     | $-7.51E-03$                     |                                |
| $\sigma_{C_{\text{nat}},\text{FCM},\text{el}}$ | $-3.08E-02$                     |                                |                                |                                |
| $\sigma_{C_{\text{nat}},\text{Block},\text{el}}$ | $5.64E-02$                      |                                |                                |                                |

Sensitivity coefficients marked in bold have the largest values. Besides, we marked in italic some values to draw attention that corresponding values of sensitivity coefficients calculated by explicit formulas are about two times larger than the values calculated by SCALE-6.1.2.

Comparative calculations of uncertainties (standard deviations $\delta_{k_{\infty,j}}$) of $k_\infty$ of the fuel compact cell to the change of input parameters $\alpha_i$ are provided in the tables 10, 11. In so doing, uncertainties are calculated using the SUW technology for variants I-1a, I-1b and by SCALE-6.1.2 for variant I-1a for CZP and HFP states of the fuel compact cell model.
Table 10. Standard deviations of the $k_e$ of the fuel compact cell model, CZP.

| $\alpha_i$       | $\delta_{k_e,i}$, % | variant I-1b | variant I-1a | Scale-6.1, Keno-VI, variant I-1a |
|------------------|---------------------|---------------|---------------|----------------------------------|
| $\nu_5$          | 1.45E-01            | 1.46E-01      | 2.65E-01      |
| $\nu_6$          | 4.47E-03            | 4.40E-03      | 7.93E-03      |
| $^{235}$U(fiss)  | 1.34E-01            | 1.37E-01      | 6.06E-02      |
| $^{239}$U(fiss)  | 2.00E-03            | 2.00E-03      | 1.82E-03      |
| $^{235}$U(n,\(\gamma\))= | | | |
| $^{235}$U(capture) | 2.12E-01 | 2.11E-01 | 2.59E-01 |
| $^{238}$U(n,\(\gamma\))= | | | |
| $^{238}$U(capture) | 3.62E-01 | 3.81E-01 | 3.24E-01 |
| $^{nat}$O(capt.) | 2.46E-04 | 2.45E-05(n,\(\gamma\)) | 2.22E-04(n,\(\alpha\)) |
| $^{nat}$C(capt)  | 7.66E-03 | 7.17E-03 | 2.22E-04(n,\(\alpha\)) |
| $^{nat}$Si(capt) | 2.19E-02 | 1.82E-02(n,\(\gamma\)) | 1.22E-02(n,\(\alpha\)) |
| $^{238}$U(\(el\)) | | | |
| $^{nat}$C(\(el\)) | | | |
| $^{235}$U(fiss)-$^{235}$U(n,\(\gamma\)) | | | |
| $\delta_{k_e}$, % | 4.65E-01$^a$ | 4.80E-01$^a$ | 4.97E-01$^a$ |

\[a\] - total $k_e$ uncertainty, caused by uncertainty of the input parameters, listed in the second column (9 parameters).

\[b\] - total $k_e$ uncertainty, caused by the uncertainty of all input parameters (reactions) taken into account in calculation performed by SCALE-6 code (83 pairs of reactions).
Table 11. Standard deviations of the multiplication factor of the fuel compact cell model, HFP.

| $\alpha_i$                        | $\delta_{k_{\infty}}$, % | $\delta_{k_{\infty}}$, % | $\delta_{k_{\infty}}$, % |
|-----------------------------------|--------------------------|--------------------------|--------------------------|
|                                   | variantI-1b              | variantI-1a              | Scale-6.1, Keno-VI,      |
| $\nu_1$                           | 1.45E-01                 | 1.45E-01                 | 2.62E-01                 |
| $\nu_2$                           | 4.89E-03                 | 4.86E-03                 | 8.79E-03                 |
| $^{235}$U(fiss)                    | 1.47E-01                 | 1.51E-01                 | 6.65E-02                 |
| $^{238}$U(fiss)                    | 2.37E-03                 | 2.40E-03                 | 2.20E-03                 |
| $^{235}$U(n,\(\gamma\)) = $^{235}$U(capture) | 2.06E-01                 | 2.04E-01                 | 2.56E-01                 |
| $^{238}$U(n,\(\gamma\)) = $^{238}$U(capture) | 4.47E-01                 | 4.70E-01                 | 4.00E-01                 |
| $^{nat}$O(capt.)                   | 2.24E-04                 | 2.45E-03(n,\(\gamma\))  | 2.23E-02(n,\(\alpha\))  |
| $^{nat}$C(capt)                    | 7.18E-03                 | 7.18E-03                 | 1.81E-02(n,\(\gamma\))  |
| $^{nat}$Si(capt)                   | 2.19E-02                 | 2.19E-02                 | 1.33E-02(n,\(\alpha\))  |
| $^{238}$U(el)                      | 8.02E-03                 | 7.39E-03                 | 1.15E-03(n,\(\alpha\))  |
| $^{nat}$C(el)                      | 1.23E-01                 | 1.23E-01                 | 1.28E-01                 |
| $^{235}$U(fiss) - $^{235}$U(n,\(\gamma\)) | 1.01E-01                 | 1.01E-01                 | 1.01E-01                 |
| $\delta_{k_{\infty}}$, %          | 5.34E-01$^a$             | 5.54E-01$^a$             | 5.47E-01$^a$             |
|                                   |                          |                          | 5.79E-01$^b$             |

a – total $k_\infty$ uncertainty, caused by the uncertainty of the input parameters, recorded in the second column (9 parameters).

b - total $k_\infty$ uncertainty, caused by the uncertainty of all input parameters (reactions), taken into account in calculation performed by SCALE-6 code (83 pairs of reactions).

It is should be noted, that names in the first columns of the tables 10, 11 are shown in an abbreviated form. Every reaction name means in fact a couple of identical reactions, for example $^{238}$U(n,\(\gamma\)) means $^{238}$U(n,\(\gamma\)) - $^{238}$U(n,\(\gamma\)).

Analysis of the results, provided in the tables 10, 11, allows us to suggest the following seven parameters as parameters giving the largest contributions to the uncertainty of the multiplication factor:

- $^{238}$U(n,\(\gamma\));
- $\nu_1$;
- $^{235}$U(n,\(\gamma\)) ;
- $^{238}$U(el) ;
- $^{nat}$C(el) ;
- $^{235}$U(fiss) - $^{235}$U(n,\(\gamma\)) ;
- $^{235}$U(fiss).

Note that we included parameter $^{235}$U(fiss) as a candidate for these parameters although in all calculations by SCALE code this parameter is not the one of the most important. We did this because all calculations by SCALE code were carried out only for variant 1a, not taking into account the
double heterogeneity. In the same time, in calculations by SUW technology this parameter is surely one of the most important ones both for variant 1a and for variant 1b. Besides, it should be noted that parameters $^{238}\text{U}(\text{el}), ^{\text{nat}}\text{C}(\text{el}), ^{235}\text{U(fiss)}, ^{235}\text{U(n,}\gamma\text{)}$ give close values of contribution to the uncertainty of multiplication factor ($k_{\infty}$) of the fuel compact cell model.

4. Lattice Physics: Calculation of the Few-Groups Macroscopic Cross-Sections

4.1. Fuel block of the MHTGR-350 benchmark
Fuel block of the MHTGR-350 (Figure 3) in Hot Full Power state [8] is used to calculate few-groups macroscopic cross-sections. Fresh fuel block includes six burnable poison compact in the corners of the block. The problem requires accounting the double-heterogeneity effects, i.e. self-shielding that occurs both within the fuel and the burnable poison. Burnable poison compacts consist of a several thousands of coated particles from B$_4$C with buffer (porous graphite) and PyC layers (dense graphite).

Figure 3. Model of the fuel block.

For additional information regarding the fuel block configuration, please refer to the [8, 13]

4.2. Simplified Model for Fuel Block
For calculation of the fuel block of the MHTGR-350 benchmark we used our experience obtained at elaboration of simplified models for fuel block for GT-MHR [15]. A simplified model for the fuel block of the MHTGR-350 is presented in Figure 4. The basic assumptions for elaboration of this simplified model are the following:

- Three dimensional cell of the fuel compact is replaced by a two dimensional cluster cell of the fuel compact with 52 cylindrical rods.
- Diameter of fuel rods is chosen from condition of equality of mean chord in fuel with some coefficient.
- A cell of the fuel compact is surrounded by materials of the fuel block (graphite and helium), accounted per one cell of the fuel compact.
- There are eight poison rods in surrounding.
4.3. Calculation of $k_\infty$ of a simplified model of the fuel block
Calculation of the $k_\infty$ of the simplified model of the fuel block is performed by WIMS-D5 code (Figure 4). Table 12 shows the $k_\infty$ of the full model of the fuel block presented in Figure 3 calculated by SERPENT code with two presentations of fuel particles in fuel compacts: location in random order and in the regular lattice [13].

| Code                                        | $k_\infty$ | $\Delta k$, % |
|---------------------------------------------|------------|---------------|
| Serpent - random (ENDF-B-VII.0), reference  | 1.05679    | –             |
| Serpent - regular lattice (ENDF-B-VII.0), reference | 1.06120    | 0.42          |
| WIMS-D5, WLUP (ENDF/B-VI.8, CENDL-2.1)      | 1.05928    | 0.24          |

4.4. Values and uncertainties of one-group microscopic cross-sections
Table 13 shows the calculation results of one-group microscopic fission and radiation capture ($n,\gamma$) cross-sections and the number of secondary neutrons per fission, as well as their uncertainties in the form of relative dispersion and standard deviation in % for isotopes $^{235}$U, $^{238}$U for the simplified fuel block model.
Table 13. Values and uncertainties of one-group microscopic cross-sections for isotopes 235U, 238U for the simplified fuel.

|          | U-235             | U-238             |
|----------|-------------------|-------------------|
| σ_f, barn| 36.5367           | 4.14150E-02       |
| σ_c, barn| 9.9340            | 3.89793           |
| νtot,    | 2.43882           | 2.73507           |
| (Δf)^2  | 9.69E-06          | 2.93E-05          |
| (Δc)^2  | 1.72E-04          | 1.69E-04          |
| (Δν)^2  | 2.21E-06          | 3.25E-05          |
| Δf, %    | 0.31              | 0.54              |
| Δc, %    | 1.31              | 1.30              |
| Δν, %    | 0.15              | 0.57              |

Table 14 shows the resulting microscopic one-group capture (including reactions (n,γ), (n,p), (n,α)) cross-sections, as well as their uncertainties in the form of relative dispersion and standard deviation in percent for non-fissile isotopes for the simplified fuel block model.

Note that uncertainties of the absorption cross sections of oxygen and boron isotopes are very large.

Table 14. Values and uncertainties of one-group microscopic cross-sections for non-fissile isotopes for the simplified model.

|          | O-nat             | Si-nat             |
|----------|-------------------|-------------------|
| σ_c, barn| 1.01083E-03       | 1.31777E-02       |
| (Δc)^2  | 2.44E-01          | 5.05E-04          |
| Δc, %    | 49.39             | 2.25              |
|          | C-nat, FCM        | C-nat, Block      |
| σ_c, barn| 3.11093E-04       | 3.08934E-04       |
| (Δc)^2  | 2.44E-03          | 2.21E-03          |
| Δc, %    | 4.94              | 4.70              |
|          | C-nat, Fuel       | C-nat, OKP        |
| σ_c, barn| 3.15565E-04       | 3.08305E-04       |
| (Δc)^2  | 2.83E-03          | 2.19E-03          |
| Δc, %    | 5.32              | 4.68              |
|          | B-10              | B-11              |
| σ_c, barn| 253.469           | 3.79880E-04       |
| (Δc)^2  | 1.92E-02          | 3.43E-01          |
| Δc, %    | 13.85             | 58.53             |
|          | C-nat, BP         |
| σ_c, barn| 3.12322E-04       |
| (Δc)^2  | 2.57E-03          |
| Δc, %    | 5.07              |

Rather large capture cross-section uncertainty of O-nat and B-10 attracts attention.
4.5. Selection of the most important reactions on isotopes of the fuel block model of the MHTGR-350 benchmark

Selection of the most important reactions on isotopes, i.e. reactions whose uncertainties give the largest contribution to the $k_\infty$ uncertainty is carried out using one-group formula for multiplication factor $k_\infty$ of the simplified fuel block model:

$$k_\infty = \left( v_5 \sigma_f^5 \rho_{\text{fuel}} + v_8 \sigma_f^8 \rho_{\text{fuel}} \right) V_{\text{fuel}} / \left[ \left( \sigma_f^5 \rho_{\text{fuel}} + \sigma_f^8 \rho_{\text{fuel}} + \sigma_c^8 \rho_{\text{fuel}} + \sigma_c^8 \rho_{\text{fuel}} \right) V_{\text{fuel}} + \sigma_c \rho_{\text{fuel}} \right]$$

$$+ \sigma_{\text{Okr}} \rho_{\text{Okr}} \Phi_{\text{Okr}} + \sigma_{\text{Block}} \rho_{\text{Block}} \Phi_{\text{Block}} + \sigma_{\text{Clad}} \rho_{\text{Clad}} \Phi_{\text{Clad}} + \sigma_{\text{Nat}} \rho_{\text{Nat}} \Phi_{\text{Nat}} + \sigma_{\text{B}} \rho_{\text{B}} \Phi_{\text{B}}$$

$$+ \left( \sigma_{\text{BP}} \rho_{\text{BP}} \right) V_{\text{BP}} \right]$$

(16)

$k_\infty$ are calculated by the formula (14) with using one-group cross-sections given in Tables 13, 14 is 1.059297, which is very close to corresponding value from table 13.

Let us introduce the notation for the formula (16) input parameters:

$$\alpha_i = \left\{ V_5, V_8, \sigma_f^5, \sigma_f^8, \sigma_c^8, \sigma_c^8, \sigma_{\text{Nat}}^8, \sigma_{\text{Fuel}}^8, \sigma_{\text{Clad}}^8, \sigma_{\text{Block}}^8, \sigma_{\text{Nat}}^8, \sigma_{\text{Fuel}}^8, \sigma_{\text{Clad}}^8, \sigma_{\text{Block}}^8, \sigma_{\text{Okr}}^8, \sigma_{\text{Block}}^8, \sigma_{\text{Clad}}^8, \sigma_{\text{Nat}}^8, \sigma_{\text{Nat}}^8, \sigma_{\text{Nat}}^8, \sigma_{\text{BP}}^8, \sigma_{\text{BP}}^8, \sigma_{\text{BP}}^8, \sigma_{\text{BP}}^8 \right\}$$

(17)

Dispersion of the $k_\infty$ of the fuel block model connected with the uncertainties of the input parameters $\alpha_i$ taking into account one-group covariance $C_{ii}$ (table 13, 14) is calculated by the formula (6). Sensitivity coefficients of the $k_\infty$ to the change of $\alpha_i$ are calculated by the formula (7).

Below there are the explicit expressions for the sensitivity coefficients $S_{k_\infty, i}$.

$$S_{k_\infty,1} = \frac{v_5 \sigma_f^5 \rho_{\text{fuel}} V_{\text{fuel}}}{k_\infty}$$

(18)

where:

$$\gamma = \left( \sigma_f^5 \rho_{\text{fuel}} + \sigma_f^8 \rho_{\text{fuel}} + \sigma_c^8 \rho_{\text{fuel}} + \sigma_c^8 \rho_{\text{fuel}} + \sigma_{\text{Okr}} \rho_{\text{Okr}} \Phi_{\text{Okr}} + \sigma_{\text{Block}} \rho_{\text{Block}} \Phi_{\text{Block}} + \sigma_{\text{Clad}} \rho_{\text{Clad}} \Phi_{\text{Clad}} + \sigma_{\text{Nat}} \rho_{\text{Nat}} \Phi_{\text{Nat}} + \sigma_{\text{B}} \rho_{\text{B}} \Phi_{\text{B}} \right) V_{\text{fuel}}$$

$$+ \sigma_{\text{BP}} \rho_{\text{BP}} \Phi_{\text{BP}} \right]$$

(19)

$S_{k_\infty, i}$, $i=2..4$, are calculated by the formulas (10)-(12).

$$S_{k_\infty, i} = -\left( \alpha_i \cdot \omega_i \cdot \gamma^{-1} \right), \quad i = 5, 6, ..., 15$$

(20)

$$\omega_i = \frac{\left\{ \rho_{\text{Fuel}} \Phi_{\text{fuel}} V_{\text{fuel}}, \rho_{\text{Clad}} \Phi_{\text{clad}} V_{\text{clad}}, \rho_{\text{Block}} \Phi_{\text{block}} V_{\text{block}}, \rho_{\text{Nat}} \Phi_{\text{Nat}} V_{\text{Nat}}, \rho_{\text{B}} \Phi_{\text{B}} V_{\text{B}}, \rho_{\text{BP}} \Phi_{\text{BP}} V_{\text{BP}} \right\}}{\left\{ \rho_{\text{fuel}} \Phi_{\text{fuel}} V_{\text{fuel}}, \rho_{\text{clad}} \Phi_{\text{clad}} V_{\text{clad}}, \rho_{\text{block}} \Phi_{\text{block}} V_{\text{block}}, \rho_{\text{Nat}} \Phi_{\text{Nat}} V_{\text{Nat}}, \rho_{\text{B}} \Phi_{\text{B}} V_{\text{B}}, \rho_{\text{BP}} \Phi_{\text{BP}} V_{\text{BP}} \right\}}$$

(21)

Total dispersion is calculated by the formula (15).

Table 15 provides calculations of sensitivity coefficients of $k_\infty$ of the simplified fuel block model to the change of input parameters $\alpha_i$. Sensitivity coefficients are calculated using explicit formulas.
Table 15. Sensitivity coefficients of $k_\infty$ of the simplified fuel block model to the change of input parameters $\alpha_i$.

| $\alpha_i$ | $S_{k_{\infty i}}$  |
|-----------|---------------------|
| $V_5$     | 9.89E-01            |
| $V_8$     | 6.76E-03            |
| $\sigma_f^5$ | 5.59E-01            |
| $\sigma_f^8$ | 4.14E-03            |
| $\sigma_c^5$ | -1.17E-01           |
| $\sigma_c^8$ | -2.47E-01           |
| $\sigma_{Cnat}^{Onat}$ | -1.14E-04        |
| $\sigma_{C_{c,Fuel}}$ | -1.18E-05        |
| $\sigma_{C_{c,FCM}}$ | -1.65E-03        |
| $\sigma_{C_{c,Block}}$ | -3.10E-03        |
| $\sigma_{C_{c,Okr}}$ | -2.29E-03        |
| $\sigma_{C_{c,BP}}$ | -3.01E-05        |
| $\sigma_{C_{c,All}}$ | -7.20E-03        |
| $B_{10}$  | -1.94E-01           |
| $B_{11}$  | -1.17E-06           |

Table 16 provides uncertainties (standard deviation) of $k_\infty$ of the simplified fuel block model to the change of input parameters $\alpha_i$. Uncertainties are calculated using SUW technology.

Analysis of the results, provided in the tables 10, 11, 16, allows us to suggest the following eight parameters whose uncertainties give the largest contribution to the $k_\infty$ uncertainty of the fuel block model:

- $^{10}$B(capt)
- $^{238}$U(n,\(\gamma\))
- $V_5$
- $^{235}$U(n,\(\gamma\))
- $^{238}$U(e1)
- natC(e1)
- $^{235}$U(fiss)–$^{235}$U(n,\(\gamma\))
- $^{235}$U(fiss).

It is should be noted that $^{10}$B(capt) (((n,\(\alpha\))+ (n,\(\gamma\))) reaction contribution to the $k_\infty$ uncertainty of simplified fuel block model is almost ten times more than the other reactions.
Table 16. Standard deviations of the $k_{in}$ of the simplified fuel block model to the change of input parameters $\alpha_i$.

| $\alpha_i$ | $\delta_{k_{in}}$, % |
|------------|----------------------|
| $\nu_5$    | 1.48E-01             |
| $\nu_8$    | 3.87E-03             |
| $^{235}\text{U}(\text{fiss})$ | 1.75E-01 |
| $^{238}\text{U}(\text{fiss})$ | 2.25E-03 |
| $^{235}\text{U}(n,\gamma)=^{235}\text{U}(\text{capture})$ | 1.54E-01 |
| $^{239}\text{U}(n,\gamma)=^{239}\text{U}(\text{capture})$ | 3.22E-01 |
| $^{nat}\text{O}(\text{capt.})$ | 5.64E-03 |
| $^{nat}\text{C}(\text{capt})$ | 1.98E-02 |
| $^{nat}\text{Si}(\text{capt})$ | 6.83E-03 |
| $^{10}\text{B}(\text{capt})$ | 2.64 |
| $^{11}\text{B}(\text{capt})$ | 6.75E-05 |
| $\delta_{k_{in}}$, % | 2.68 |

5. Conclusions

The main achievements of this work are the following:

- Development of an original 69-group library of covariance information in a special format for main isotopes typical for HTGR. At the moment library contains covariance information for the following isotopes and elements: $^{235}\text{U}$, $^{238}\text{U}$, $^{16}\text{O}$, $^{4}\text{He}$, $^{nat}\text{C}$, $^{28}\text{Si}$, $^{29}\text{Si}$, $^{30}\text{Si}$, $^{10}\text{B}$, $^{11}\text{B}$. The library consists of individual files for each isotope or element, and can be easily extended in the future. The library is planned to be used for estimation of nuclear data uncertainty in calculating HTGR parameters in design calculations.

- Results of uncertainty calculations for one-group fission and capture cross-sections for main isotopes of the MHTGR-350 benchmark and uncertainties of the multiplication factor of the fuel compact model. One-group uncertainties are calculated using the developed SUW code technology and modules of the SCALE-6 code package (TSUNAMI, KENO-IV, SAMS).

- Results of calculations of sensitivity coefficients and standard deviations that allowed to distinguish eight nuclear reactions whose uncertainties give the largest contribution to the multiplication factor uncertainty of the fuel block model:
  - $^{10}\text{B}(\text{capt})$;
  - $^{235}\text{U}(n,\gamma)$;
  - $\nu_5$;
  - $^{235}\text{U}(n,\gamma)$;
  - $^{238}\text{U}(\text{el})$;
  - $^{nat}\text{C}(\text{el})$;
  - $^{235}\text{U}(\text{fiss})-^{235}\text{U}(n,\gamma)$;
  - $^{235}\text{U}(\text{fiss})$.

  It is shown that the main contribution to the multiplication factor uncertainty of the fuel block model makes the reaction $^{10}\text{B}(\text{capt}) ((n,\alpha)+(n,\gamma))$. 
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