Conference Paper

The Influence of Resonance Scattering to the Doppler Reactivity Coefficient

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Abstract

The paper presents the results of an evaluation of the effect of scattering on resonances in calculating the Doppler reactivity coefficient using the data preparation algorithms implemented in the GRUCON processing program. A comparison of the free-gas model with the resonance scattering model and published results of calculations performed using other methods of data preparation is presented. On the benchmark of Mosteller for light water grids with various fuel compositions it was shown that taking into account resonances in the differential cross sections of elastic scattering of uranium-238 leads to a shift of the Doppler reactivity coefficient by ~ 10% towards negative values, thereby increasing the negative feedback with the temperature of the fuel.

Keywords: Doppler effect, reactivity coefficient, resonant scattering, processing

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1. Introduction

When assessing the transient processes in thermal neutron reactors that arise when moving the control rods, an important parameter is the Doppler reactivity coefficient. Unfortunately, the determination of its value is problematic, because, firstly, this parameter is small in view of the fact that the change in reactivity associated with a change in temperature during the transition from zero power to nominal in light water reactors is ~ 1%, and secondly, there is no possibility of direct measuring the Doppler reactivity coefficient. Now, in the analysis of the safety of VVER, the permissible error of this parameter is assumed to be 10%.

Traditionally, the model of free gas used in the calculations includes a contradiction: for neutrons losing energy in a collision, the dependence of the cross section on temperature (in the form of Doppler broadening of resonances) is taken into account, and for neutrons acquiring energy, there is no. In the works of A.Y. Kurchenkov and N.I.

Laletin [1], as well as M. Ouisloumen and R. Sanchez [2], were indicated on the possibility of a significant error in the deceleration of neutrons in collisions at resonances U-238.

In the subsequent works W. Rothenstein, R. Dagan, O. Bouland, V.V. Kolesov developed methods and algorithms for taking into account the Doppler effect in energy-angular distributions of neutrons scattered by resonances [3-7], which were implemented in special editions of the NJOY programs [8] and MCNP [9] for detailed calculations by the Monte Carlo method (via table S (α, β) or direct modeling - the DBRC method). The developed algorithms allow analyzing the criticality in security problems more correctly, taking into account the Doppler effect in differential cross sections. The new computational capabilities of the GRUCON package allow us to perform an independent evaluation of the Doppler reactivity coefficient, which in the last decade, due to the task of increasing the burnup of uranium oxide fuel and using MOX fuel with plutonium isotopes, has increased significantly.

The purpose of this paper is to estimate the error of the Doppler reactivity coefficient based on the Mostell benchmark using algorithms implemented in the GRUCON package.

2. The Doppler effect in cross sections

The thermal motion of the target nuclei affects both the integral cross sections and the energy-angular distributions of the scattered neutrons. To calculate the integral cross-sections in the GRUCON package, the method proposed by D. E. Cullen and C. R. Weisbin [10] is used, in which, under the condition of the non-constant scattering cross section at zero temperature, the following formula is used to calculate the double-differential cross sections in the thermal energy region:

$$\sigma_s^T\left(E\to E',\vec{\Omega}\to\vec{\Omega}'\right)=\frac{1}{v}\int_{allV:v_r>0}v_r\sigma_s\left(v_r,0\right)P\left(v,V\to E',\vec{\Omega}'\right)M^T\left(V\right)dV \quad (1)$$

In Fig. 1-3 shows the influence of the thermal motion of the nuclei on the integral (Fig. 1) and differential - energy distribution (Fig. 2) and the angle (Fig. 3) of neutron scattering cross-sections on U-238 nuclei in the vicinity of resonance 6.67 eV. Allowance for the resonance in the scattering cross section leads to a shift in the energies of the scattered neutrons relative to the distribution obtained in the free-gas approximation, toward the resonance (solid and dashed lines in Fig. 2).

In this paper, to calculate the integral (1) we used the algorithm proposed by M. Malkov and A. Rineiskii, using integration with respect to the velocity distribution of

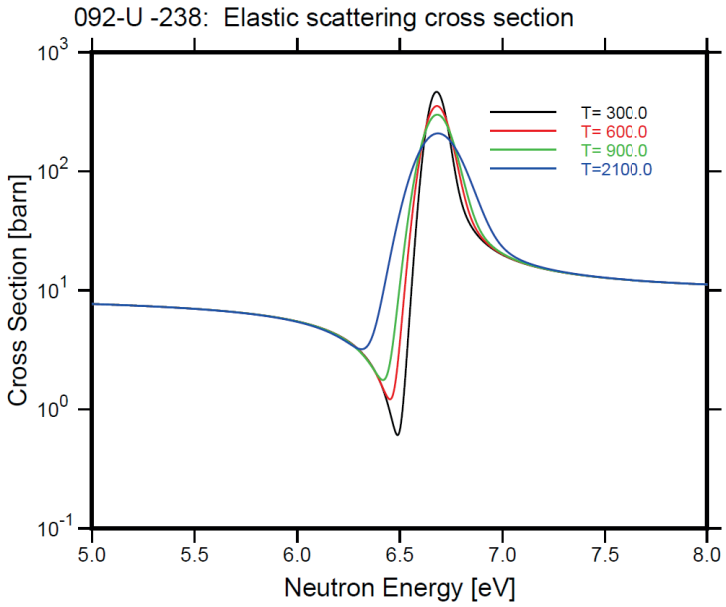

Figure 1: Cross section of the scattering of uranium-238 at temperatures of 300, 600, 900 and 2100K..

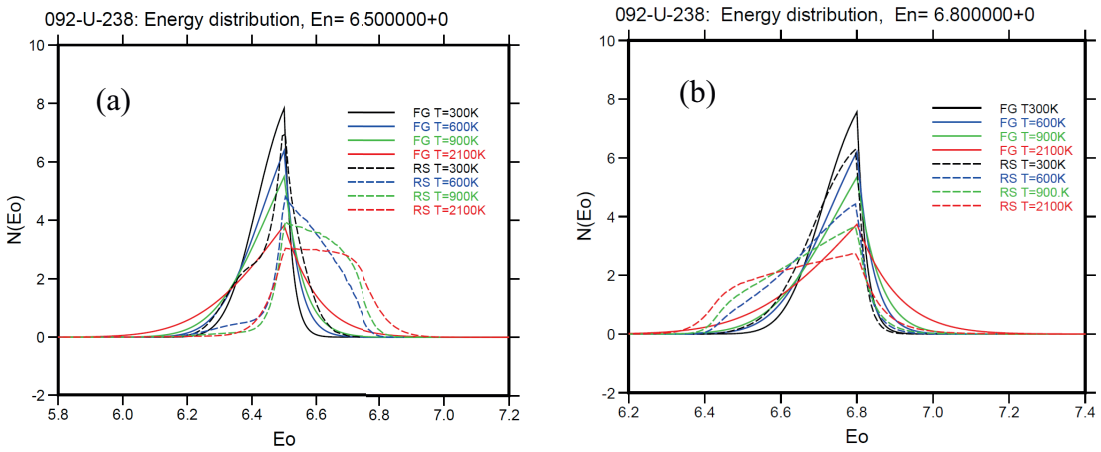

Figure 2: Energy distributions of neutrons scattered on the left (a) and right (b) wings of the resonance of uranium-238 in the free gas approximation (FG) and resonant scattering (RS).

the target nucleus by the Monte Carlo method [11] to take into account the Doppler effect in doubly-differential cross sections. It includes the following steps:

1. For a given neutron energy E, the neutron velocity vector is played out $v = (v_x, v_y, v_z)$ – the neutron velocity before scattering. In modulus it is $\upsilon = \sqrt{\frac{2Ek_1}{m}}$, where m – neutron mass, k_1 – coefficient of energy transfer from eV to Joule, $k_1 = 1.60207 \cdot 10^{-19}$. The direction of the Z axis is chosen in the direction of neutron motion, i.e.: $\upsilon_x = 0; \upsilon_y = 0; \upsilon_z = \sqrt{\frac{2Ek_1}{m}}$;
2. The speed of the movement of the nucleus is played out $v = (v_x, v_y, v_z)$ from the Maxwell-Boltzmann distribution: $P(V,T) = \frac{4}{\sqrt{\pi}}\beta^{3/2}V^2e^{(-\beta V^2)}$, where $\beta = \frac{M}{2k_BT}$, M

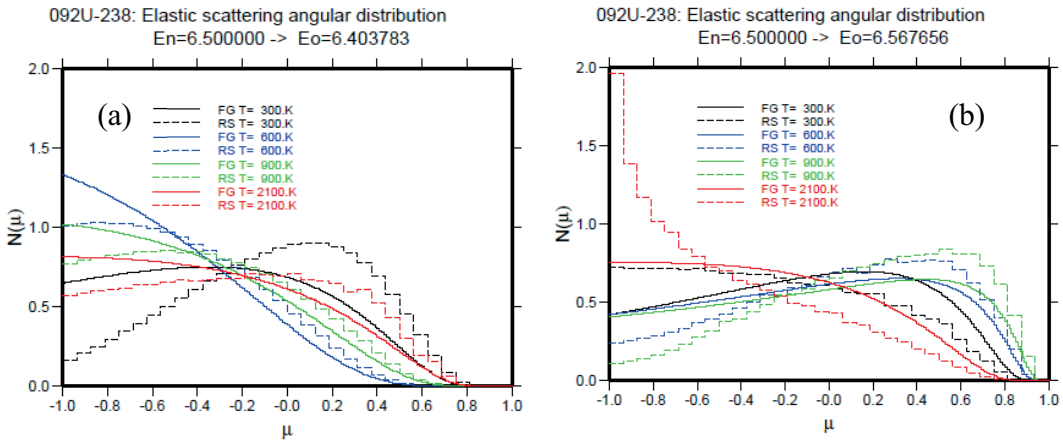

Figure 3: Angular distributions of neutrons scattered on the left (a) and right (b) wings of the resonance of uranium-238 in the free gas approximation (FG) and resonant scattering (RS).

– mass of the nucleus. The components of the core velocity v_x, v_y и v_z have a Gaussian distribution with math expectation of o and variance $\sqrt{\frac{1}{2\beta}}$;

3. The velocity of the center of mass is calculated: $V = \frac{mv+MV}{m+M}$;
4. The transition from the laboratory system to the center of mass system is performed, the core and neutron velocities are recalculated;
5. Isotropic neutron scattering is modeled in the center-of-mass system, a new neutron velocity vector is calculated;
6. The reverse transition to the laboratory system is performed, the neutron velocity vector is calculated in the laboratory system;
7. New neutron energy is calculated $E' = \frac{mv^2}{2k_1}$, where $v' = \sqrt{v'^2{}_x + v'^2{}_y + v'^2{}_z}$;
8. From the previously obtained table of sections at zero temperature, the value σ(*E′*);
9. From the values *E′* and μ pockets numbers are calculated, adding $\frac{v'}{v}\sigma\left(E'\right)$ in the drive;
10. You return to step 2 until the desired statistics.

3. Calculation model

Calculation of the Doppler reactivity coefficient was carried out on the basis of a set of tests developed in 2006 in the Los Alamos laboratory, known as the benchmark of Mosteller. This benchmark was approved by the Joint Committee on Mathematical and

Computational Problems of Reactors Physics and Radiation Protection of the American Nuclear Society and in 2007 an international test was organized on its basis. In total, 44 results of Doppler reactivity calculations were obtained, using various libraries of evaluated data and deterministic and stochastic calculation programs in the traditional free-gas approximation.

The Doppler DC reactivity coefficient was calculated by the formula:

$$DC = \frac{\Delta\rho_{Dop}}{\Delta T_{Fuel}} \quad (2)$$

where ΔTFuel - is the temperature difference between the states of full and zero power;

Doppler reactivity defect, defined as:

$$\Delta\rho_{Dop} = \frac{k_{HFP} - k_{HZP}}{k_{HFP} \times k_{HZP}} \quad (3)$$

where kHFP, kHZP = k∞ for the states of the full power of HFP and zero power HZP.

The computational model consisted of sets of gratings for hot states with zero (HZP) and full (HFP) power corresponding to the lattice of identical fuel cells PWR. The cell layout is shown in Fig. 4.

Fuel cells consisted of four zones: fuel, air gap, shell (natural zirconium), retarder (borated water).

The following fuels were considered:

1. UO_2fuel with enrichment variation from 0.711 wt.% to 5 wt.%;
2. mixed oxide with reactor recycled plutonium (45% Pu239), with the content of $PuO_2$from 1wt.% to 8wt.% (MOXR);
3. mixed oxide with reactor weapon plutonium (93.6% Pu239), with the content of $PuO_2$from 1wt.% to 8wt. % (MOXW).

In the HZP state, the temperature of the fuel, shell and moderator is the same and is 600K. In the HFP state, the fuel temperature is 900K, while everything else remains unchanged.

4. Preparing of ACE Libraries

For calculating k∞, included in the Doppler reactivity coefficient, the MCNP-4c2 program was used with detailed energy tracking. This program requires a library of sections in the ACE format.

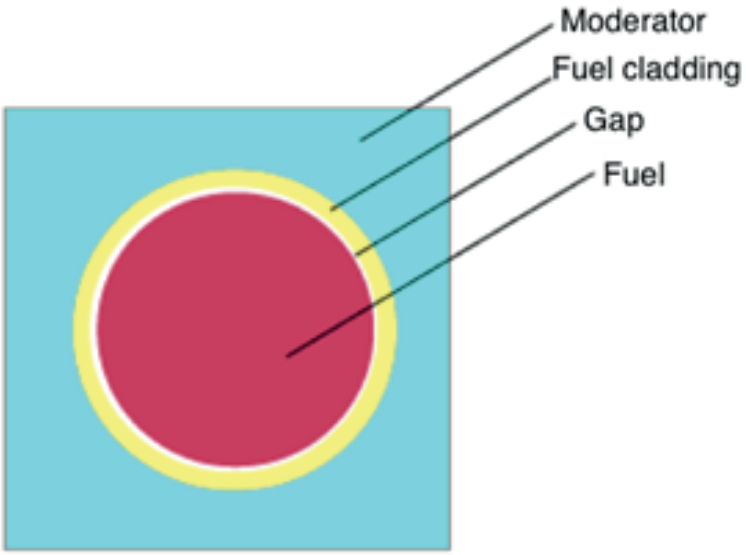

Figure 4: Fuel cell geometry in the Mosteller benchmark.

The ACE files were prepared using the GRUCON package, based on the ENDF / B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1, ROSFOND-2010 and BROND-3.1 evaluation data libraries. In the ACE format, data were obtained for 16 isotopes included in all the specified benchmark materials, as well as S (α, β) data for scattering up to 10 eV for the bound state of hydrogen in water. The S (α, β) data on neutron scattering on U-238 nuclei to 210 eV, obtained in the free-gas model (THXXDS, SXTXDS) and taking into account resonant scattering (SXTXDS), were additionally included in the ACE / ROSFOND-2010 library. The ACE / ENDF / B-VII.1 library was prepared in two versions, using the NJOY program and the GRUCON package.

The resulting set of ACE files was used to verify the determination of the spread of results caused by the initial data and methods of their processing, and to estimate the bias caused by the scattering model.

5. Methodology and results of calculations

To evaluate the effect of resonant scattering on the Doppler reactivity coefficient, three series of calculations were performed.

In the first series - verification - the libraries ACE / ENDF / B-VII.1, prepared using the GRUCON and NJOY programs were used. The second series of calculations was performed with ACE library sets, prepared with the help of GRUCON six world libraries of evaluated data. The influence of the difference in the estimates on the spread of

the Doppler coefficient values was evaluated and compared with the error estimate obtained in the international test.

The third series - calculations with the ACE / ROSFOND-2010 library and S (α, β) tables U-238, prepared in various models - free gas and resonant scattering, in order to estimate the influence of the scattering model. The calculations were carried out according to the MCNP4c2 version with an editorial allowing to take into account the velocity distribution of the target nucleus up to 210 eV.

5.1. Comparison of Estimated Data Libraries

To assess the degree of consistency of the evaluated data from different sources and consistency with the results of the international test, a series of calculations was performed on the data of the national libraries ENDF / B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1, ROSFOND-2010 and BROND- 3.1.

Calculations were carried out in the MCNP program, version 4c, without any special editions, so as to maximally approach the results obtained in the international test. The results of the comparison are presented in Fig.6.

In the same series of calculations, the expected values of DC obtained from a sample of 6 libraries of estimated data were compared), with the results of the international test (Fig. 7).

At the conclusion of this stage, we can draw the following conclusions:

1. The DC values on the library sample are consistent with the test results within one standard deviation.

2. The spread of data on libraries is 3 ÷ 10 times lower than the spread obtained in the international test, which indicates that the error obtained in the international test is due mainly to the difference between calculation methods, and not data. The most significant deviations in DC (~ 10%) are observed for the MOXR fuel composition using the BROND-3.1 library. Presumably they are related to the peculiarity of Pu240 evaluation in this library.

3. The expected value of DC on the library sample runs along the upper border of the error corridor obtained in the international test. On page 7 of the final document of the international test [13] it is noted: "It is somewhat surprising that deterministic programs usually give a more negative Doppler coefficient than Monte Carlo calculation programs. In particular, for three pairs of four, deterministic programs

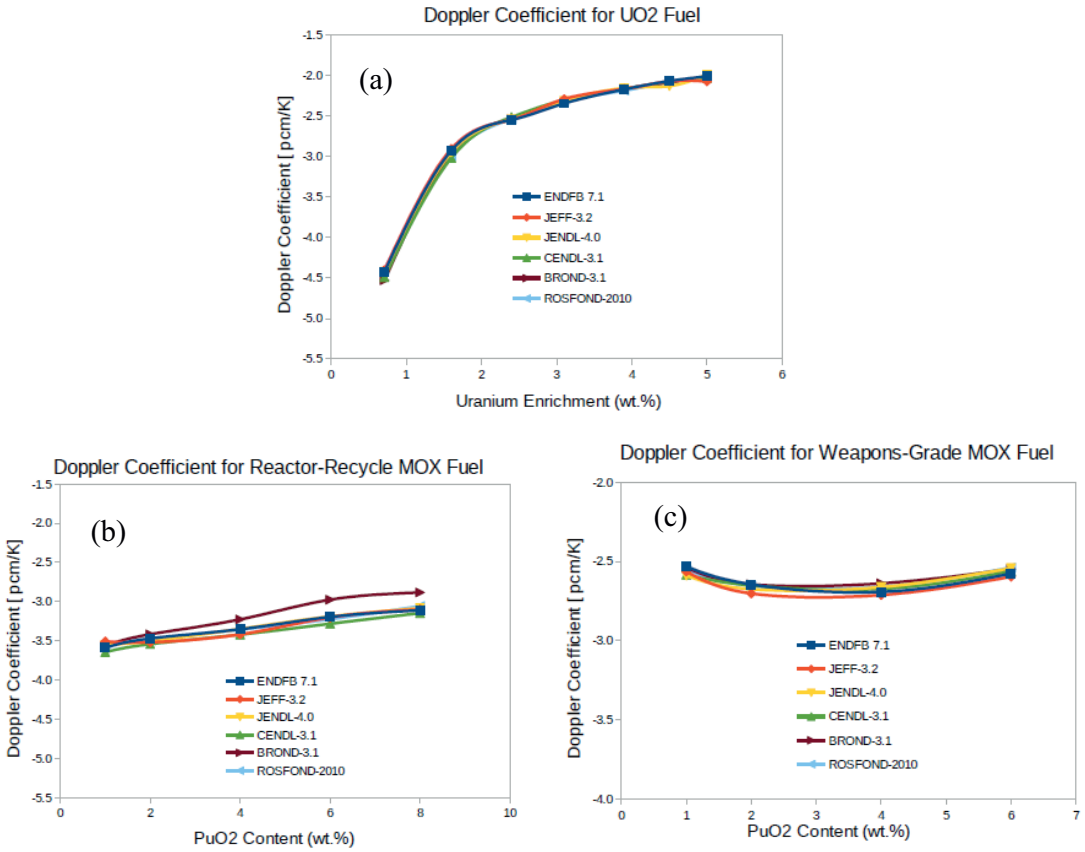

Figure 5: Doppler reactivity coefficients for fuel compositions UO2 (a), MOXR (b) and MOXW (c) obtained in the free gas model on data from various libraries, processed with the GRUCON package.

predict a more negative coefficient than the Monte Carlo programs in all cases, with the differences reaching 24%."

5.2. Comparison of data processing algorithms

To estimate the error in the method of calculating the double-differential cross sections realized in the SXTXDS module, the results of the calculations obtained from the ENDF / B-VII.1 library in the free-gas approximation were compared using various data processing methods: ACE files for fast and thermal neutrons with tables S (α, β) for U-238, prepared by the NJOY / THERMR and GRUCON / SXTXDS modules, ACE files for fast neutrons prepared by NJOY and GRUCON, using the MCNP algorithm for simulating collisions on free gas.

The results are consistent within a statistical error of 3% ÷ 6% (with a statistical error of ~ 0.006% for k∞). The maximum differences are observed between the results obtained with the S (α, β) tables and without them, which is probably connected

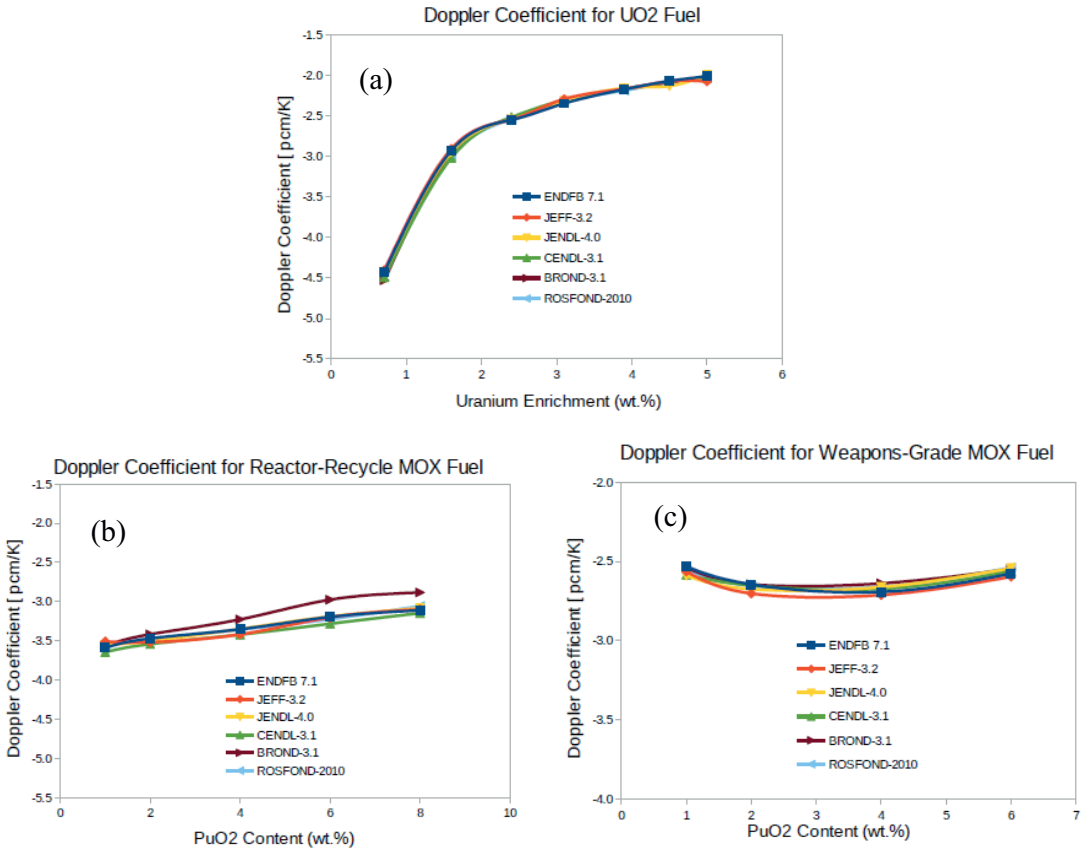

Figure 6: Doppler reactivity coefficients for fuel compositions UO2 (a), MOXR (b) and MOXW (c) obtained from the ENDF / B-VII.1 data in the free gas model using the GRUCON, NJOY, and MCNP data preparation algorithms.

with the algorithm for reducing the cross sections to zero temperature in the MCNP in modeling the scattering by free gas.

5.3. Estimation of the effect of scattering on resonances

The last stage was designed to assess what effect the Doppler reactivity coefficient has on the U-238 resonances. ACE files containing S (α, β) tables prepared by the SXTXDS module from the ROSFOND 2010 library in free-gas and resonance scattering models were used in the calculation. The statistical error of calculations using the free gas model (FG) was ~ 3%, taking into account the scattering by resonances U-238 (RS) ~ 4%. Comparison of the obtained dependences shows that the allowance for scattering at resonances enhances the negative feedback of the neutron multiplication factor with the fuel temperature by 7% ÷ 11% in the transition from zero to full power (Fig. 8a, b, c, left), which confirms the results, obtained on the benchmark of Mosteller B. Becker, R. Dagan, CHM Broeders and G. Lohnert [14] (Fig.8a, b, c, right).

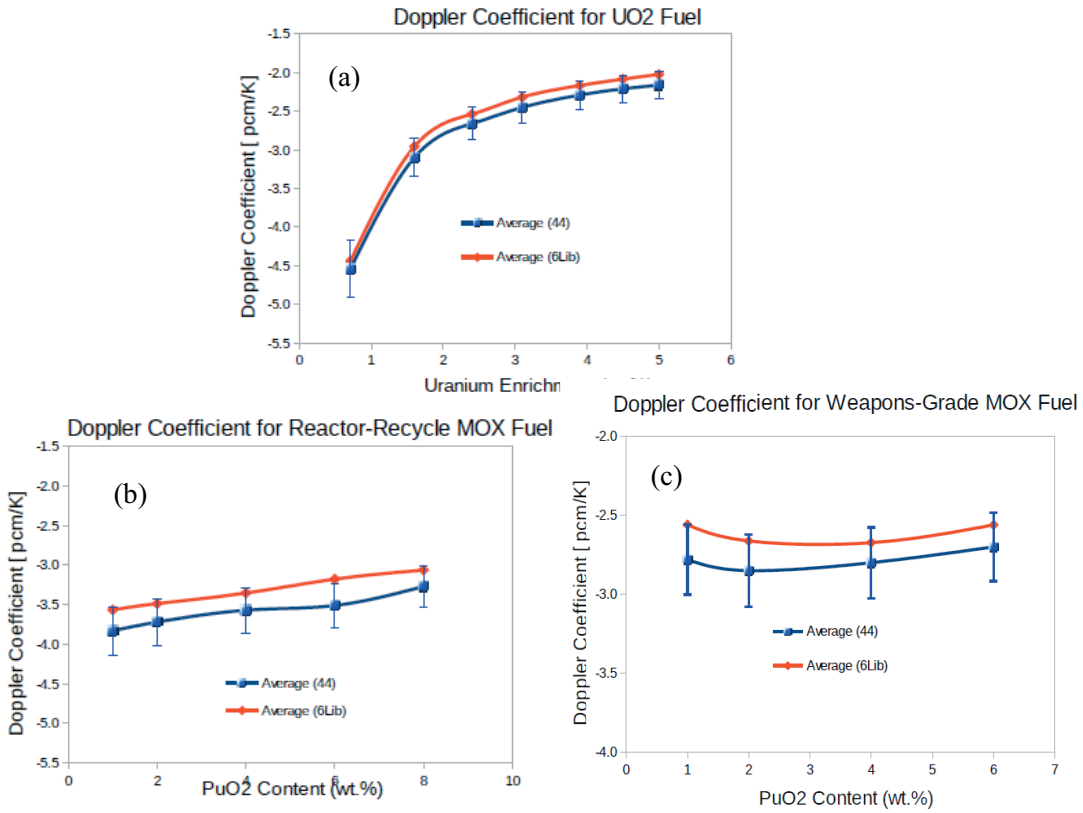

Figure 7: The expected values of the Doppler reactivity coefficients for fuel compositions UO2 (a), MOXR (b) and MOXW (c) obtained in the present work for a sample of 6 libraries of estimated data, compared with the international test estimate [10].

6. Conclusion

The spread of Doppler DC coefficients due to the difference in data from the ROSFOND-2010 libraries, BROND-3.1 ENDF / B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1, with a statistical error due to the use of the Monte Carlo method in 3 -5%, is on average 1-2%. This is significantly lower than the currently accepted 10% allowable limit, which makes it possible to conclude that any of the listed libraries can be used to estimate this value. It is entirely possible that the libraries' agreement is due not so much to the accuracy of the estimated data as to the deficit of independent estimates (at least for key nuclides).

Algorithms for data processing in processing programs NJOY, GRUCON, and built-in MCNP for the free gas model lead to deviations not exceeding 3% of the mean value, which is comparable to the statistical accuracy of the assessment. From this it can be concluded that the error in the processing of the estimated data does not have a significant effect on the DC estimate.

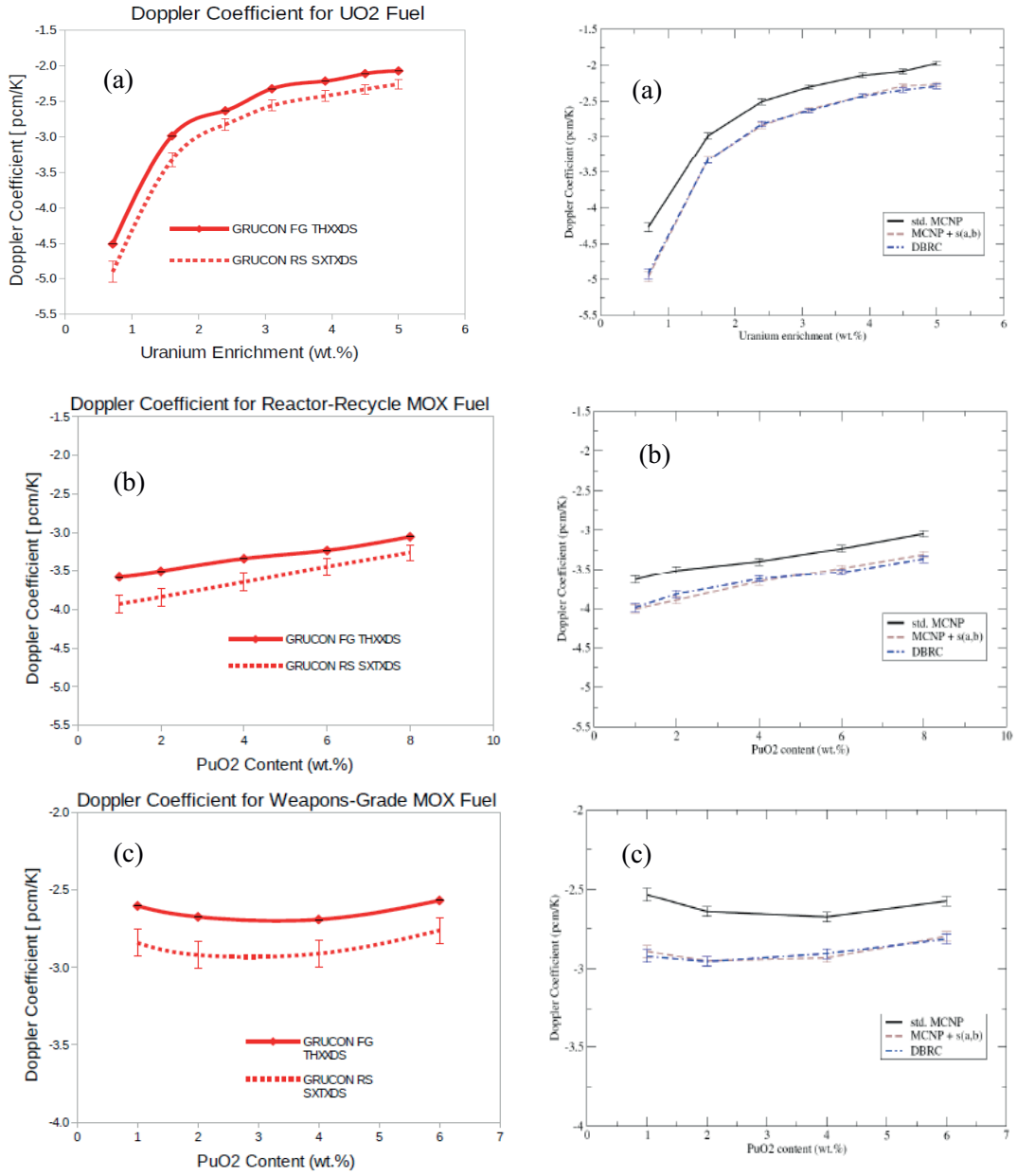

Figure 8: Values of Doppler reactivity coefficients for fuel compositions UO2 (a), MOXR (b) and MOXW (c) for the free gas model (solid lines) and taking into account scattering at U-238 resonances (dashed lines) obtained in the present study. (left) and published in [13] (right).

The error due to the application of the free gas model, traditionally used in nuclear safety problems, is comparable to the permissible value of 10%, leading to a more conservative estimate (to a decrease in the negative feedback).

The estimation of the influence of the scattering effect on U-238 resonances on the Doppler reactivity coefficient for the main fuel compositions used in water-cooled

thermal neutron reactors indicates a systematic shift of ~ 10% towards negative values, which is confirmed by the results of computational studies performed by other authors.

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