Comparison of PWR – burnup calculations with SCALE 5.0/TRITON other burnup codes and experimental results

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Abstract

The increasing tendency towards fuel lifetime extension in thermal nuclear reactors led to the need of validation of the evaluation tools for burnup calculations. In this study two deterministic codes with different transport solvers are compared and validated by experimental and statistical results.
KAPROS/KARBUS uses the classical deterministic First Collision Probability method which provides the cylindrized Wigner-Seitz cell. In SCALE5.0/TRITON/NEWT the Extended Step Characteristic method is applied. In a first step the two codes are compared with experimental results from the KWO-Isotope Correlation Experiment up to 30 MWD/kg HM burnup. Therefore two pin cell calculations are analyzed by comparison of important heavy isotope vectors. With deviations lower than 0,1‰, the results are very good.
In addition further validation at higher burnup (< 80 MWD/kg HM) is provided by comparison of the two deterministic codes by PWR UO_2 fuel assembly calculations. For reference the Monte Carlo based burnup code MONTEBURNS is used.
Reasons for result differences are analyzed and discussed. Especially the influence of cross section data and processing is shown.

Keywords: SCALE5, TRITON, KAPROS, MONTEBURNS, KWO-ICE, burnup

1. Introduction

One of the common ways to generate relevant data for fuel unit cells is based on one dimensional cylindrized Wigner-Seitz unit cells while preserving the unit cell volume of the original square or hexagonal array. The KAPROS system [1] uses this classical approach utilising the collision probability method.
Another more complex but also more accurate way is to represent the geometry of the problem with a flexible cell structure to give a better approximation of both rectangular and curved geometries inside the unit cell. Such a geometric solution was established in the transport program NEWT which is part of SCALE 5.0 [2]. NEWT uses the Extended Step Characteristic Method [3] in which the neutron probability transfer is constrained to characteristic lines.
The first step in this study compares these two deterministic methods with experimental results from the KWO-isotope correlation experiment [7] by pin cell burnup calculations. The results are evaluated by comparison of corresponding important heavy isotope vectors.
Pursuing the analysis, KAPROS, SCALE5/TRITON and the Monte Carlo code MONTEBURNS are compared by 18x18-24 (24 water holes) PWR UO_2 assembly [5], with 4 w/o U-235 enrichment, burnup calculations. Therefore KAPROS uses the two dimensional transport solver TWODANT [9] in combination with homogenized unit cells while the SCALE5/TRITON/NEWT method stays the same as in the pin cell calculation. The results are examined due to k_{inf} and important heavy isotope vectors.

2. Short description of the transport and burnup calculation methods in NEWT, KAPROS and MONTEBURNS

Conventional discrete ordinate codes can only handle regular geometries like (R, Z), (X, Y), (X, Y, Z), (R, θ, Z). NEWT which applies the Extended Step Characteristic method [3], can perform a completely arbitrary problem grid by using a polygonal grid structure instead of an orthogonal grid structure. The only regulation is that the cells are only allowed to own a non re-entrant polygonal shape. The number of these polygons is not limited.

A classic discrete ordinate method is used in KAPROS/KARBUS. KARBUS applies the First Collision Probability (FCP) method (Bonalumi Method [4]). The problem geometry in the FCP method is represented by a structured grid which only provides a single geometrical shape of grid meshes. In the Wigner-Seitz cell calculation in KARBUS the appropriated geometrical form of the meshes to represent the geometrical problem are rings. The advantage of the FCP method applied in KARBUS in contrary to the ESC method applied in NEWT is that in the FCP method a neutron can move from each point to each point of the geometric problem while in the ESC method a neutron can only move along characteristic lines.

In Figure 1 the pin cells of both deterministic codes are shown as applied in the experiment recalculation. In the KAPROS/KARBUS model the pin cell is divided into 16 fuel zones, 3 clad zones and 4 moderator zones to a total of 23 cylindrical meshes (not all meshes are indicated in the KAPROS/KARBUS pin cell in figure 1).

In SCALE5.0/TRITON/NEWT the pin cell is divided into 9 zones, 8 consisting of 3 polygonal meshes each (one mesh for each material) and one zone consisting of one mesh (the middle fuel zone) to a total of 25 meshes.

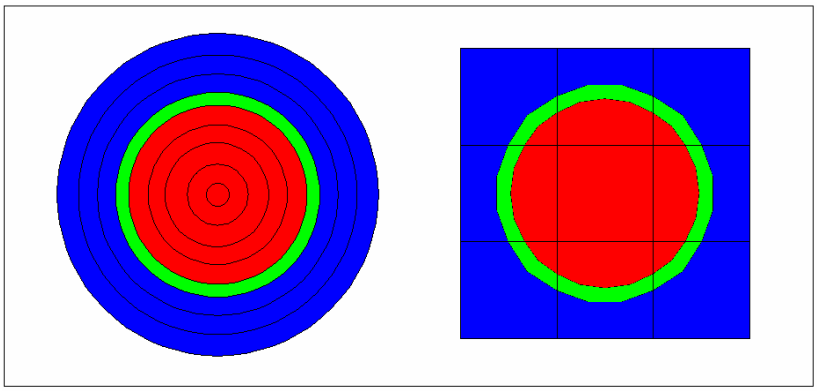

Figure 1: Basic pin cell meshes used in KARBUS (left) and NEWT (right)

The radial boundary conditions were specified as reflective, while the length of the pin was infinite, so the problem can be seen as infinite in radial and axial direction. Both deterministic calculations have been performed with S_n order of 8 and a convergence criterion of 10^{-5} for k_{inf}. The cross section libraries used are ENDF/B 5 (44 groups) in the SCALE 5.0/TRITON and ENDF/B 6.5 (69 groups) in the KAPROS/KARBUS calculation.

Both codes KAPROS and TRITON are using burnup modules which are based on ORIGEN from Oak Ridge National Laboratorium, USA. The module BURNUP [1] which is used in KAPROS is a proceeding development from KORIGEN [10] which is based on ORIGEN. In TRITON [2] ORIGEN-S is provided which is a further development from ORIGEN too.

3. The KWO - Isotope Correlation Experiment and the corresponding pin cell calculations

The pin cell configurations have been taken from the final report of the isotope correlation experiment at the nuclear power plant of Obrigheim [7]. The material composition in the fuel is UO_2 with 3,1 w/o enrichment of U-235. The clad consist of Zircaloy-4. The boron concentration in the moderator (water) changes during burnup as well as there are several reactor down times included in the experiment. Figure 2 shows the boron density history. Figure 3 tabulates the power time steps. The maximum fuel rod power is P=219,6 W/cm. The volume ratio of moderator to fuel is $V_m/V_f = 1{,}494$.

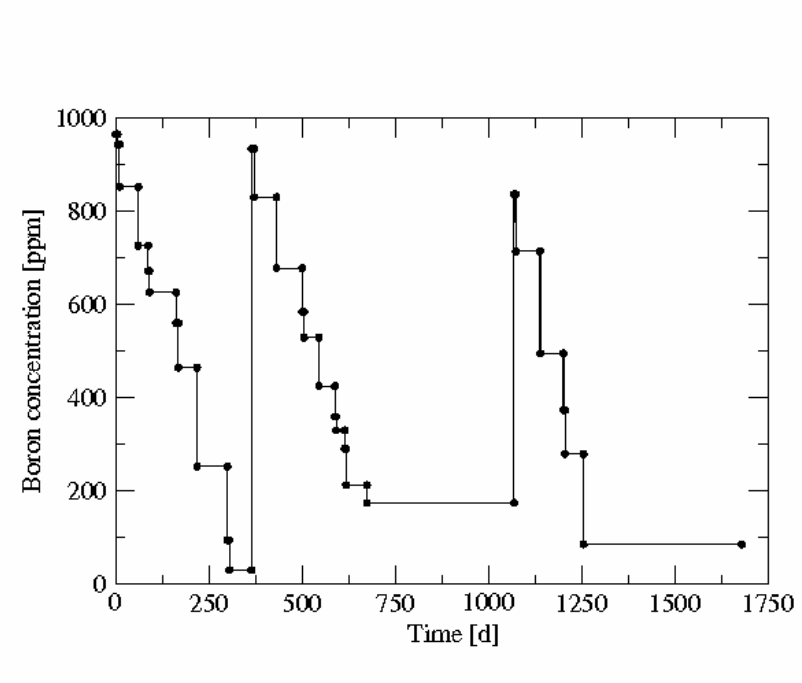

Figure 2: Boron concentration of KWO - ICE

Time [d]	Power [%]
5,8	100
1	0
79,6	100
2	0
33,5	100
41,5	0
131,5	100
5,8	0
36,9	100
28	0
126,9	100
9,2	0
84,7	100
3,5	0
23	100
3	0
60	100
13,8	87
380	0
246,7	100

Figure 3: Power time steps of KWO - ICE

Figures 4, 5 and 6 show very good agreement between the calculated and the measured isotopic distributions. Figure 4 indicates that both codes overestimate the U-238 consumption which is in accordance with the enlarged production of Pu-239 in both codes. Figure 5 shows a slightly exalted burning of U-235 in both codes to the experimental results. Figure 6 presents a little higher converting of Pu-239 to Pu-240 which accords with the little increased Pu-239 inventory. The deviations of the Pu-241 results are hardly visible but the very small overestimation of the codes fit again to the differences of the other isotopic vectors. All these differences are slightly higher than the calculation accuracy (10^{-5}) and though it is not feasible to associate these differences to certain reasons.

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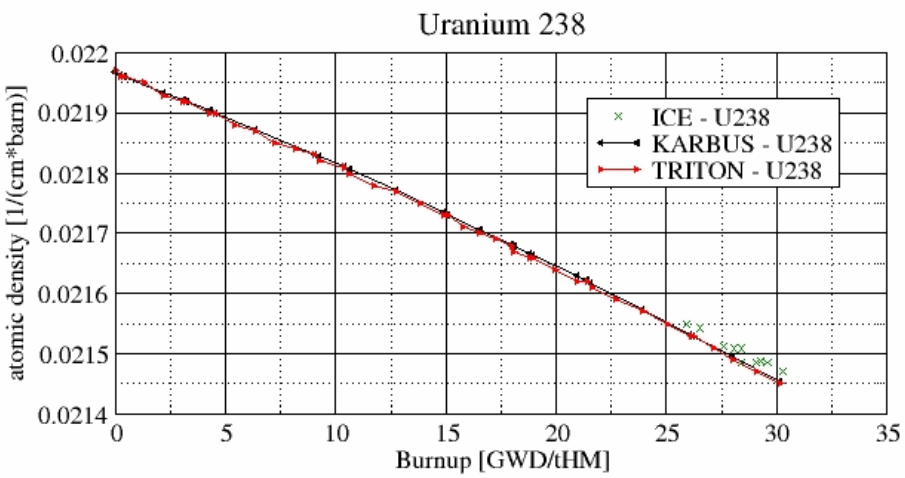

Figure 4: Uranium 238 inventory of the KAPROS/KARBUS and SCALE5/TRITON burnup calculations compared with the experimental results

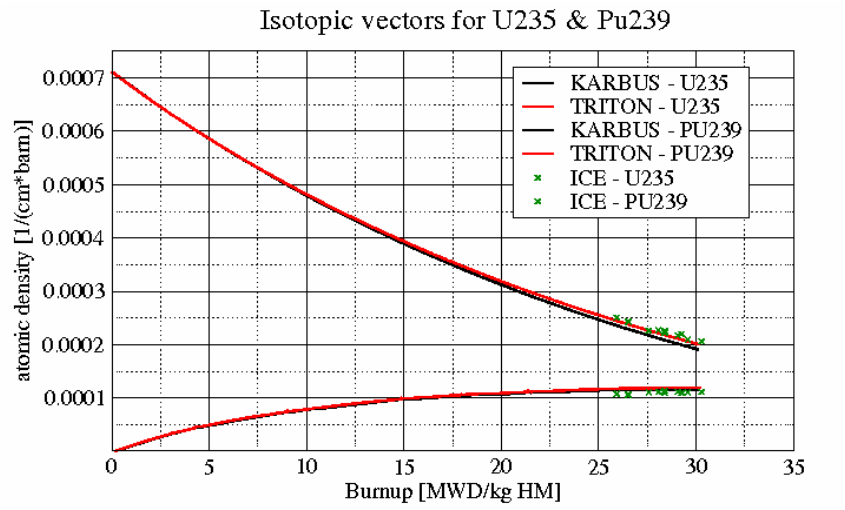

Figure 5: Uranium 235 and Plutonium 239 inventory for the KAPROS/KARBUS and SCALE5/TRITON burnup calculations compared with the experimental results

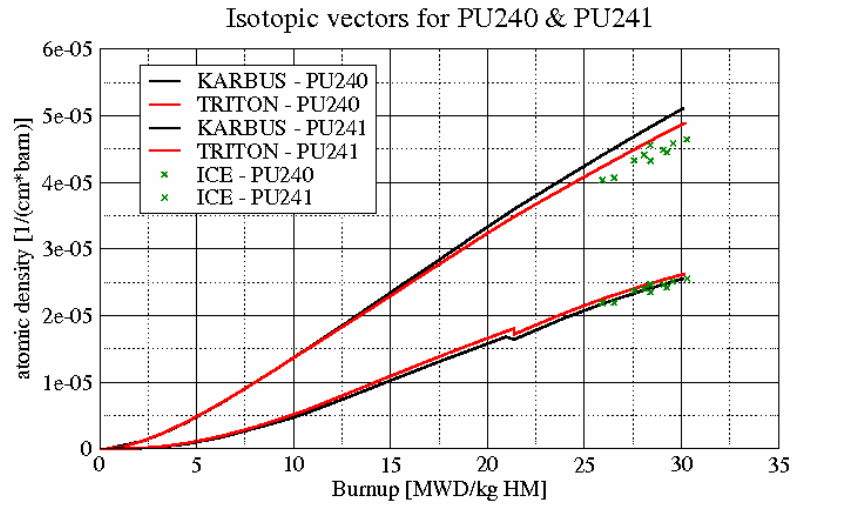

Figure 6: Plutonium 240 and Plutonium 241 inventory for the KAPROS/KARBUS and SCALE5/TRITON burnup calculations compared with the experimental results

4. Further validation with PWR assembly calculations

For further validation KAPROS and SCALE5/TRITON are compared by PWR assembly burnup calculations. For reference the Monte Carlo based code MONTEBURNS [6] is applied. MONTEBURNS calculates burnup with ORIGEN 2.1, while the transport calculations are performed by the Monte Carlo code MCNP4C.

The specifications for the PWR assembly calculations are taken from reference [5]. The 18x18-24 PWR assembly consists of 300 square lattice fuel rods and 24 water holes. Figure 7 shows the assembly geometry. Due to symmetry only one quarter of the assembly was calculated. The volume ratio of moderator to fuel in the fuel rods is V_m/V_f = 1,564. The material composition in the fuel is UO_2 with 4 w/o enrichment of U-235. The clad consist of Zircaloy-4. The boron in the water stays constant at 500 ppm over burnup. The boundary conditions are reflective, so the system is infinite in radial direction.

The modelling of the assembly problem was done by rod wise homogenization in KAPROS/KARBUS while the two dimensional transport calculations for KAPROS were done by TWODANT, which is part of DANTSYS 3.0 [9]. The SCALE5/TRITON transport calculation was done by the two dimensional transport module NEWT using 3299 calculation cells in total. The deterministic calculations were done with a SN order of 6 and convergence criteria of 10^{-5}. The Monte Carlo calculations in MONTEBURNS have been provided with a standard deviation of 10^{-3}.

The used libraries are the ENDF/B 5 (44 groups) library in the SCALE5/TRITON and the ENDF/B 6.5 (69 groups) library in the KAPROS/KARBUS/TWODANT calculation. In MONTEBURNS a mixture of ENDF/B 5, 6 and 6.5 was used.

The calculation time of TRITON (ca. 10h, on a 3 GHZ, UNIX PC) was approximately half of the KAPROS time, the number of groups respected. The MONTEBURNS calculation time depends very strong on the chosen standard deviation (in this study: 10^{-3}, calculation time ca. two weeks). Therefore the calculation time was enlarged approximately by a factor of 35 to the TRITON calculation duration. Determination of the exact calculation time is difficult due to the different accuracy parameter (e.g. number of cells in NEWT) but it seems obvious that the characteristic method is faster than the classical approach of KAPROS while the biggest disadvantage of Monte Carlo methods still seems to be time consumption.

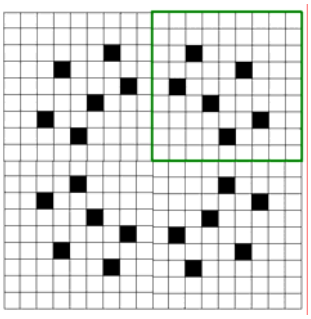

Figure 7: Assembly geometry, the calculated quarter is signed green

All assembly calculations have been performed up to a burnup of 80 MWD/kg HM.

Figure 8 shows the good agreement of the three codes but there are also small differences visible in the progress of the curves. Especially the Monte Carlo curve seems to fluctuate a little bit between the deterministic curves. A part of this fluctuation can be caused by the standard deviation (up to ±20 % of the differences of k_{inf} in Figure 9). Evaluation reasons for these deviations may be the different treatment of the fission product inventory, resonance shielding, data processing and the spectral deviation of the neutron flux used at higher burnup

in the Monte Carlo code but not in the deterministic tools. The two deterministic results show that the KAPROS curve has a slightly higher reactivity loss at the beginning of burnup but then tends to a flatter progression than the TRITON curve does, crossing it at ca. 25 MWD/kg HM. This may be an isotopic effect again. The consumption of U235 and U238 is a little bit smaller in KAPROS than in TRITON. Therefore less U-238 is converted to Pu-239 (as shown in Figure 11). A possible reason is that in KAPROS the neutron losses (due to absorption cross section data) are smaller than in TRITON and thus the reactivity loss during burnup is relatively decreased. The MONTEBURNS results in Figure 10 and 11 confirm the influence of the cross section data and processing at higher burnup. Again a higher consumption of Uranium 238 and Uranium 235 than in KAPROS is shown which fits with the higher conversion of Uranium 238 to Plutonium 239 and the resulting reactivity changes.

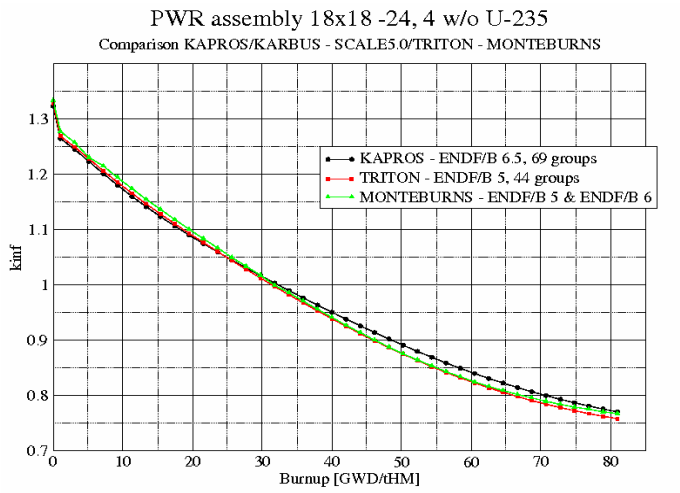

Figure 8: k_{inf} against burnup for the three assembly calculations

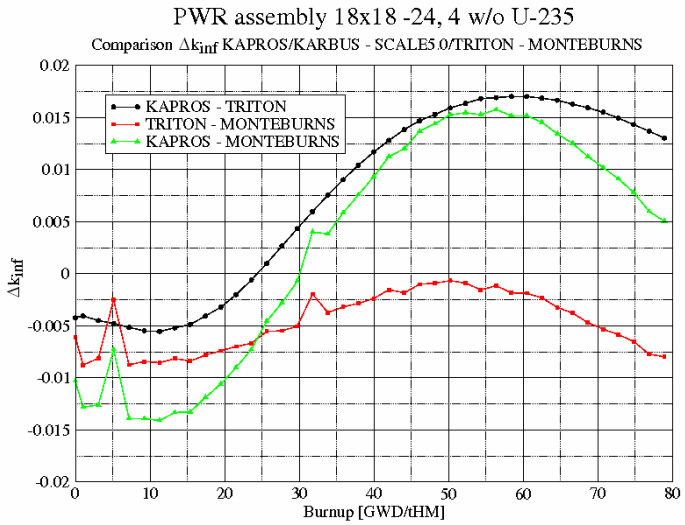

Figure 9: Δk_{inf} against burnup for the three assembly calculations

The maximum deviations of Δk_{inf} shown in Figure 9 at BOL are smaller than 0,8 % (KAPROS-MONTEBURNS) and smaller than 1,7 % (KAPROS-TRITON) at 80 MWD/kg HM.

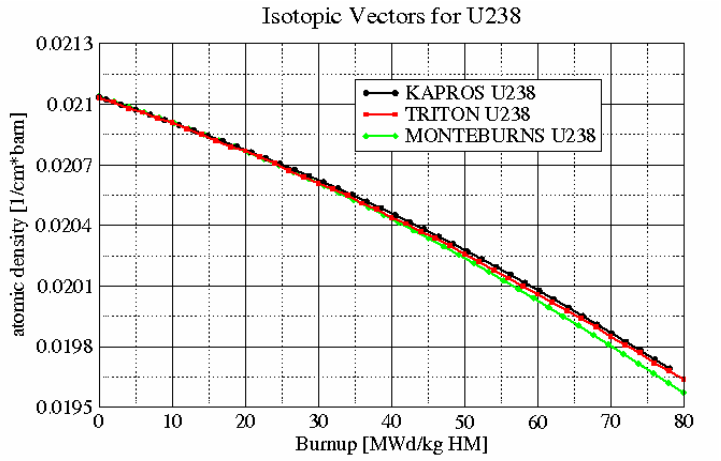

Figure 10: Isotopic Vectors for Uranium 238 for the three calculations

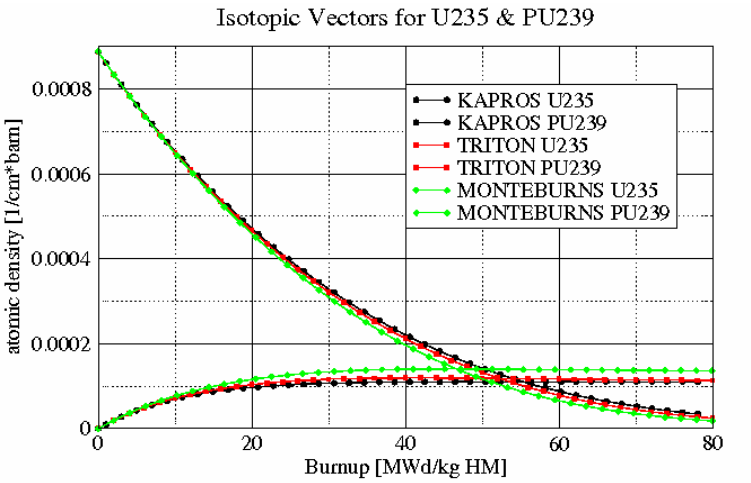

Figure 11: Isotopic Vectors for Uranium 235 and Plutonium 239 for the three calculations

7. Summary and outlook

The KAPROS and the SCALE5/TRITON system were both validated at pin cell level with experimental results and with stochastical results at subassembly level.

The recalculations of the KWO – Isotope Correlation Experiment show very good agreement of both deterministic codes with the experiment up to 30 MWD/kg HM. The very small deviations show that the classical Wigner-Seitz cell in KAPROS/KARBUS and the Extended Step Characteristic method in SCALE5/TRITON/NEWT provide accurate results.

Subassembly calculations have been performed for a PWR UO_2 assembly for further validation at higher burnup (up to 80 MWD/kg HM). The two deterministic codes, KAPROS/KARBUS developed at FZK, Karlsruhe and TRITON/NEWT a new option in the SCALE 5.0 standard code for LWR licensing, have been validated using the MONTEBURNS Monte Carlo based code system. The differences between KAPROS and MONTEBURNS grows from ca. 0,7% at BOL to a maximum of ca. 2% during burnup. Between

SCALE5.0/TRITON and MONTEBURNS the differences amount ca. 0,5 % at BOL and 0,8% at EOL.
For further validation the different data bases and the differences in the data processing e.g. the treatment of the resonance shielding and the fission spectra should be considered. In addition spectral deviation of the neutron flux should be analyzed, especially at higher burnup. Another point is the different treatment of neutron scattering between deterministic and stochastic codes due to data processing. Among other deviations, up to 220 pcm for scattering in water were shown by Litaize [11] recently.

8. References

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