

Analyses of Integral and MOX Critical Experiments to Qualify PARAGON2 Predictions*

Mohamed Ouisloumen

Westinghouse Electric Company LLC
Cranberry Twp., Pennsylvania 16066, USA

ouislom@westinghouse.com

ABSTRACT

This paper presents the qualification of the newly developed Westinghouse lattice physics code PARAGON2. PARAGON2 uses high energy resolution in the solution of the transport equation. The objective of this paper is to demonstrate that PARAGON2 accurately predicts the integral and critical experiments. The integral experiments are used to assess PARAGON2 predictions of fine neutronics parameters such as: resonance integrals and radial profiles of reactions rates, isotopics, and burnup for depleted pellets. The integral experiments considered are: the Hellstrand's, TRX, and the PIE experiments. For critical experiments, this paper will focus only on VENUS-2 MOX critical experiment.

The results obtained for the integral experiments clearly show the good predictions of PARAGON2 with the resonance scattering model which are close to measurement. The PARAGON2 predicted capture reaction rates, temperature coefficients, burnup and isotopic profiles match the measured values both in shape and magnitude. VENUS-2 reactivity prediction is in excellent agreement with the critical measurement value. Also, the standard deviations of measured minus predicted pin-wise fission reaction rates are very good (i.e. $\leq 2\%$) for both individual assemblies and the whole core.

KEYWORDS: PARAGON2, Critical Experiments, MOX

1. INTRODUCTION

This paper presents the second part of the qualification of the newly developed Westinghouse lattice physics code PARAGON2 [1]. The use of high energy resolution in the solution of the transport equation is the main characteristic of PARAGON2. The objective of this paper is to demonstrate that PARAGON2 accurately predicts the integral and critical experiments. The good predictions of these types of experiments are paramount prerequisites to the regulatory licensing of a lattice neutron transport code. The standard deviations of the measured minus predicted pin-power distribution of the critical experiments play a major role in the evaluation of the peaking factor safety limits used in core design applications. The integral experiments are used to assess the PARAGON2 predictions of fine neutronics parameters such as resonance integrals, radial profile distribution of reactions rates, and radial distribution of the isotopic concentrations for burned fuel. PARAGON2 with cross section libraries using either the resonance scattering model or asymptotic [2] model will be used in these analyses to contrast the differences of these two physics models.

For the integral experiments, the Hellstrand's experiment described in Ref. [3], the TRX experiment described in Ref. [4], and the Post Irradiation Examination (PIE) experiment described in

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Ref. [5] will be analyzed. For oxide and metal fuel compositions, the $^{238}_{92}\text{U}$ capture reaction rates, as a function of fuel temperature and as a function of surface to mass ratio of the fuel pellet, will be assessed using the Hellstrand's experiments. The experimental radial $^{238}_{92}\text{U}$ resonance capture profile for UO_2 , U-Metal and U-Zr pellets, from the TRX experiment will also be analyzed. The PIE experiment will be used to evaluate PARAGON2 predictions of the burnup profile, uranium profile, and plutonium profile within the fuel pellet. The discharge average burnup of the UO_2 sample in this experiment is 74.5 GWd/t and the burnup of the peripheral region was estimated at about 150 GWd/t.

For critical experiments, this paper will focus only on VENUS-2 MOX critical experiment described in Ref. [6]. This experiment was configured with UO_2 and MOX 15x15 fuel assemblies with the intent of analyzing the MOX/ UO_2 spectral interactions. PARAGON2 criticality (k_{eff}) prediction will be assessed using the measured axial buckling. The fission reaction rates distribution will be directly compared to measured values.

A brief overview of PARAGON2 lattice code is presented in Section 2. For interested readers, the references contain abundant descriptions of PARAGON2 theory and algorithms. Sections 3 and 4 present the modeling and results of the integral and MOX critical experiments. The paper ends with the conclusions in Section 5.

2. OVERVIEW OF PARAGON2 LATTICE PHYSICS CODE

The development of PARAGON2 is founded on first principle physics models which permits the avoidance of weak approximations in the solution algorithms of the transport equation. The objective is to come up with a state of the art lattice physics code that can improve the predictions in current operating plants, and at the same time produce a code capable of modeling the next generation of fuel products that are currently in research phase; such as the accident tolerant fuel. With this strategy, it becomes possible to develop a code that can be used for any type of fuel assembly regardless of the complexities of its geometry design and material compositions.

The advanced methods used in PARAGON2 are computationally intensive. To offset this inconvenience, parallel computing algorithms were introduced throughout the code using the shared-memory multi-core processing OpenMP directives. The shared-memory approach is suitable for the kind of applications that PARAGON2 will be used for in core design analysis. With a modest computing power (few nodes with ~ 120 GB RAM and couple dozens of cores per node), one can easily achieve the required running time for few-group cross-sections generations, used in core simulators.

The main new improvements incorporated in PARAGON2 are summarized as follows:

- PARAGON2 uses the ultra-fine energy mesh cross-sections library (UFEML) with 6064 energy groups. The library will eventually contain all the isotopes available in ENDF/B7.1 basic nuclear data repository. This new library has been extensively benchmarked against Monte Carlo continuous energy solution for all types of fuel assemblies, currently in use, and against critical experiments and measured plants data. It is important to note that the cross-sections of this library are processed through NJOY Ref. [7] code and are used, as they are, from the source without any adjustment.
- All the scattering matrices of the isotopes in UFEML are based on the anisotropic resonance scattering model described in Ref. [2], except for hydrogen in water and the graphite as addressed in Ref. [2].
- The depletion chains in PARAGON2 have been extended to track 116 fission products and 25

actinides. In the point of view of the memory management and the running time performance of the code, these detailed depletion chains are a challenging problem for UFEML method.

The collision probability and interface current methods were used in the flux solution as described in Ref. [2].

3. INTEGRAL EXPERIMENTS

3.1. Hellstrand's Experiments

3.1.1. Description of the Experiments

The Hellstrand's experiments for measuring $^{238}_{92}\text{U}$ resonance integral (RI) were performed in a Swedish heavy water reactor. Fuel rods samples of uranium metal or uranium oxide were placed in a cadmium covered oven and irradiated in the central channel of the reactor. These experiments are described in details in References [3], [8] and [9]. The capture of neutrons in $^{238}_{92}\text{U}$ gives rise to $^{239}_{93}\text{Np}$. By measuring the $^{239}_{93}\text{Np}$ activity, a quantity proportional to the neutron capture in $^{238}_{92}\text{U}$ is obtained. The capture rate measured by the experiment is primarily in the resonance energy range. The RI ($^{238}_{92}\text{U}$ capture rate) needs to be normalized for comparison among different sample temperatures. The measured epithermal flux outside the sample was used to normalize the RI to the unit epithermal flux. The detailed information of the reactor core were not important in evaluating the resonance integrals, because the idea of the experiment was to create a $\frac{1}{E}$ spectrum outside of the sample. The amplitude of the flux that relates to the core configuration is not important because RI is normalized to the unit $\frac{1}{E}$ epithermal flux Ref. [10].

3.1.2. Modeling and Results

In Reference [10], a simplified model that mimics the $\frac{1}{E}$ flux surrounding the fuel sample was developed. This same model is also adopted in this study. Thus, a two-dimensional 3x3 assembly blocks (with 7x7 pins per assembly) are modeled in PARAGON2. The center block contains the fuel cell sample and the other cells of this block are moderator cells (without fuel). The flux in this moderator of this central region is used for normalization of the reaction rate as suggested in Reference [10]. Both uranium metal and oxide samples are modeled using heavy water as the moderator. As suggested in References [3] and [10], the energy domain for the epithermal capture $^{238}_{92}\text{U}$ reaction rates is chosen to be [0.39eV, 110keV].

The temperature coefficients were simulated for the 0.4 cm sample radius for both uranium oxide and metal. Fuel temperatures were varied from 300K to 1500K. The following formulas from Ref. [8] were used to compute the Hellstrand experimental resonance integral values:

$$\begin{cases} \text{UO}_2 & RI = RI_0[1 + 0.00824(\sqrt{T} - \sqrt{T_0})] \\ \text{U-metal} & RI = RI_0[1 + 0.00642(\sqrt{T} - \sqrt{T_0})] \end{cases} \quad (1)$$

Where, RI is the $^{238}_{92}\text{U}$ capture resonance integral for fuel temperature T and RI_0 is the corresponding value for the temperature $T_0 = 300\text{K}$.

Figure 1a and 1b show the $^{238}_{92}\text{U}$ predicted PARAGON2 resonance integrals compared to the Hellstrand experimental values. PARAGON2 results using the resonance scattering model (RSM) fit better the experiments (especially for U-metal case). Using RSM, PARAGON2 coefficient values are 0.0085 vs. experiment value of 0.0082 (± 0.0006) for UO_2 and 0.0059 versus experiment

value of 0.0064 (± 0.0005) for uranium metal case. As expected the asymptotic results get deviated from the experiment as the fuel temperature increases. The good agreements of PARAGON2 with experiment show the importance of the resonance scattering model and the fine energy mesh in predicting the temperature coefficients and Doppler effect. The uranium metal results show larger deviations compared to oxide case. This discrepancy is most likely attributed to the inaccuracy of the measurement as explained in Ref. [9].

References [3], [8] and [9] contain also the absolute $^{238}_{92}\text{U}$ capture resonance integral correlated to the $\sqrt{\frac{S}{M}}$, where $\frac{S}{M}$ is the surface to mass ratio of the fuel pellet in cm^2/g . The experimental correlations are given by the following formulas:

$$\begin{cases} \text{UO}_2 & RI(\text{barns}) = 4.15 + 26.6\sqrt{\frac{S}{M}} \\ \text{U-metal} & RI(\text{barns}) = 2.95 + 25.8\sqrt{\frac{S}{M}} \end{cases} \quad (2)$$

Note that the equation for the metal case has been obtained from Ref. [8]. This formulation is a correction of the one published in Ref. [3] and it has been obtained after conduction of new, more precise experiments. PARAGON2 with RSM was used to model different fuel rod sizes. The experiment fuel temperature is assumed to be 300K. Figures 1c and 1d show the comparison of PARAGON2 results against the experiments for both oxide and metal fuels. Good agreement between experimental values and PARAGON2 predicted values is seen in these figures. The slopes of the PARAGON2 predictions are very close to the experimental ones for both fuel types. This analysis provides a proof that PARAGON2 does actually predict accurately the resonance integral for all fuel rod sizes and for heavy fuel density (such as metal fuel).

3.2. TRX Experiment - Radial $^{238}_{92}\text{U}$ Resonance Capture Distribution

3.2.1. Description of the Experiment

The relative $^{238}_{92}\text{U}$ resonance neutron capture per atom was measured for cylindrical, 0.387-in diameter rods of uranium metal, UO_2 (density 10.5 g/cm^3) and U-Zr alloy (74.9 w/o U, 25.1 w/o Zr) placed in a water hole in the TRX critical facility. In all cases the uranium was enriched to 1.3% $^{235}_{92}\text{U}$. The density of $^{238}_{92}\text{U}$ atoms in each alloy was the same as in the UO_2 fuel. The measurement techniques are similar to the ones used in Hellstrand's experiments including measurement for the radial distribution of the $^{238}_{92}\text{U}$ resonance capture. The experiments and results are described in Reference [4].

3.2.2. Modeling and Results

The references available for this experiment have little information for a detailed modeling. Therefore, a single pin cell was modeled in PARAGON2. Since the geometry of the TRX experiment is hexagonal, and PARAGON2 cannot handle this geometry, the square cell modeled is developed by preserving the fuel to moderator ratio. Small volume rings are used at the measurement points to simulate the foils used in the experiments.

Figures 2a, 2b and 2c give the comparison between the measured relative $^{238}_{92}\text{U}$ capture resonance reaction rates for UO_2 , uranium metal and U-Zr fuel pellets. These figures show good PARAGON2 predictions of the radial reaction rates distributions for all fuel types. The consistency of the results, across all fuel types, confirms the accuracy of PARAGON2 fine energy mesh model to predict detailed micro reaction rates. The accurate radial reaction rates distribution is important for fuel integrity analysis as well as for reactivity predictions during the fuel depletion.

3.3. PIE Experiment - Isotopics and Burnup Radial Distributions

3.3.1. Description of the Experiment

To assess PARAGON2 predictions of the radial distributions of the burnup and major actinides concentrations (uranium and plutonium) within the pellet, the Post Irradiation Examination (PIE) experiments, described in References [11] and [5], will be considered. The discharge average burnup of the UO_2 sample in this experiment is ~ 74.5 GWd/t and the burnup of the peripheral region was estimated at about 150 GWd/t.

3.3.2. Modeling and Results

The same pin cell model used in Reference [11] is also used here to compute the radial distribution of the burnup and isotopic concentrations. However, a finer spatial meshing (45 equal volume rings), within the pellet, is used to better simulate the profile variations of different parameters. The pin cell was depleted up to the discharge burnup. The power history provided in Reference [5] was used in the depletion.

In Figure 3a, the spatial burnup distribution obtained with PARAGON2 is compared to PIE measurements reported in Reference [5]. PARAGON2 accurately predicts the measured burnup including the peak at the pellet periphery. Figures 3b and 3c show the uranium (U) and the plutonium (Pu) spatial concentrations, respectively, within the pellet. Uranium concentration decreases rapidly in peripheral region. On the other hand, Pu concentration increases rapidly in peripheral region. PARAGON2 does predict accurately the profile variations of these actinides.

4. VENUS-2 EXPERIMENT

4.1. Description of the Experiment

The VENUS critical facility is a PWR mock-up zero power critical reactor located at SCK-CEN in Belgium (Reference [6]). The central part of the VENUS-2 MOX core consists of UO_2 fuel pins with MOX fuel pins loaded on the periphery of the core. The VENUS-2 core consists of twelve 15x15 sub-assemblies with a pitch of 1.26 cm and a full core height of 50 cm. Each of the four central assemblies contain 3.3 wt.% ^{235}U enriched UO_2 fuel pins and 10 Pyrex pins. The 8 periphery assemblies contain both UO_2 and MOX fuel, with the 7 internal rows containing 4.0 wt.% ^{235}U enriched UO_2 and the 8 external pins containing MOX fuel (UO_2 -PuO₂) enriched with 2.0 wt.% in ^{235}U and 2.7 wt.% in high-grade plutonium with the major plutonium isotopes. The VENUS-2 experimental data contain fission rates for 121 of the 325 fuel rods in $\frac{1}{8}^{\text{th}}$ of the core. These 121 pins consist of 41 pins with 3.3 wt.% UO_2 , 35 pins with 4.0 wt.%, and 45 pins with 2.0/2.7 wt.% MOX.

4.2. Modeling and Results

VENUS-2 two-dimensional full core was modeled directly in PARAGON2. The PARAGON2 k_∞ was compared to the k_∞ calculated by the Monte Carlo code MCNP for the same configuration. In addition, the axial buckling provided in the references was used with the PARAGON2 reactivity result to calculate k_{eff} . Details for the experiment are provided in Reference [6]. The PARAGON2 k_{eff} obtained is 1.00013 which is in a good agreement with the experiment. PARAGON2 k_∞ is close to MCNP value. The difference in k_∞ between MCNP and PARAGON2 is 192 pcm.

Figure 4 shows the pin fission reaction rates distribution in $\frac{1}{8}^{th}$ of the core. Table I summarizes the relative differences between measured (M) and PARAGON2 (P) computed fission reaction rates, (M/P-1) (%), for the full core and different fuel assembly types. This table shows also the comparison for the whole core and for the measured locations (pins) only. The non-measured values (204 pins) in the whole core were obtained by interpolations (Reference [6]). The uncertainty of the measured data is 1.7% in UO₂ and 2.5% in MOX pins. Table I compares (M/P-1) deltas in percent. The standard deviation (Std) for individual fuel assembly types is small and within a maximum of 1.8% (especially if only measured locations are considered). The standard deviation for the whole core is slightly larger and the maximum absolute error is within 7.45% (or 4.3% for measured pins only). The standard deviations of all the differences are within 1σ or 2σ of the measurement uncertainties.

Using a global normalization, the averages of the differences for individual assemblies show an over-prediction of MOX rods (periphery) and an under-prediction in the UO₂ rods (a slight tilt). This trend is also clearly visible in Figure 4, where M-P is plotted using global normalization. This same trend in predictions is also observed in the aggregate simulation results obtained by different codes and libraries presented in Reference [6]. Overall PARAGON2 results are very similar to other deterministic and Monte Carlo codes results described in References [6] and [12]; especially, the codes using same cross-sections library ENDF/B.VII.

5. CONCLUSIONS

A new lattice physics code, PARAGON2, was developed and is currently under validation and qualification for licensing submittal and future core design applications. The new code is based on first physics principles such as high energy resolution, new anisotropic resonance scattering model, and detailed depletion chains. PARAGON2 is now part of the Westinghouse core design code systems PARAGON2/ANC.

PARAGON2 lattice physics code was used in this paper to model integral and MOX critical experiments. The results obtained show an excellent agreement with measurements for both integral and critical experiment data. PARAGON2 predicts, with high accuracy, the temperature coefficients and the capture resonance integral. The intra-pellet profiles of the burnup, the isotopic concentrations, and the capture resonance integrals are also accurately predicted for all fuel types and fuel geometries. The criticality as well as the pin-power distribution for MOX experiment are accurately predicted. Of particular interest, this paper shows the importance of the implementation of the Resonance Scattering Model to correctly predict the Hellstrand's measured resonance integrals as a function of the fuel temperature.

Table I: VENUS-2 Measured vs. predicted pin-wise fission reaction rates in %

	Measured locations Only				All locations			
	Whole Core	MOX 2.0/2.7 wt%	UO ₂ 4 wt%	UO ₂ 3.3 wt%	Whole Core	MOX 2.0/2.7 wt%	UO ₂ 4 wt%	UO ₂ 3.3 wt%
Max	3.68	3.68	2.49	2.38	4.29	3.95	3.76	4.29
Min	-4.34	-3.86	-4.34	-3.48	-7.45	-3.83	-7.45	-3.58
Std	1.62	1.79	1.65	1.37	1.73	1.87	1.83	1.41

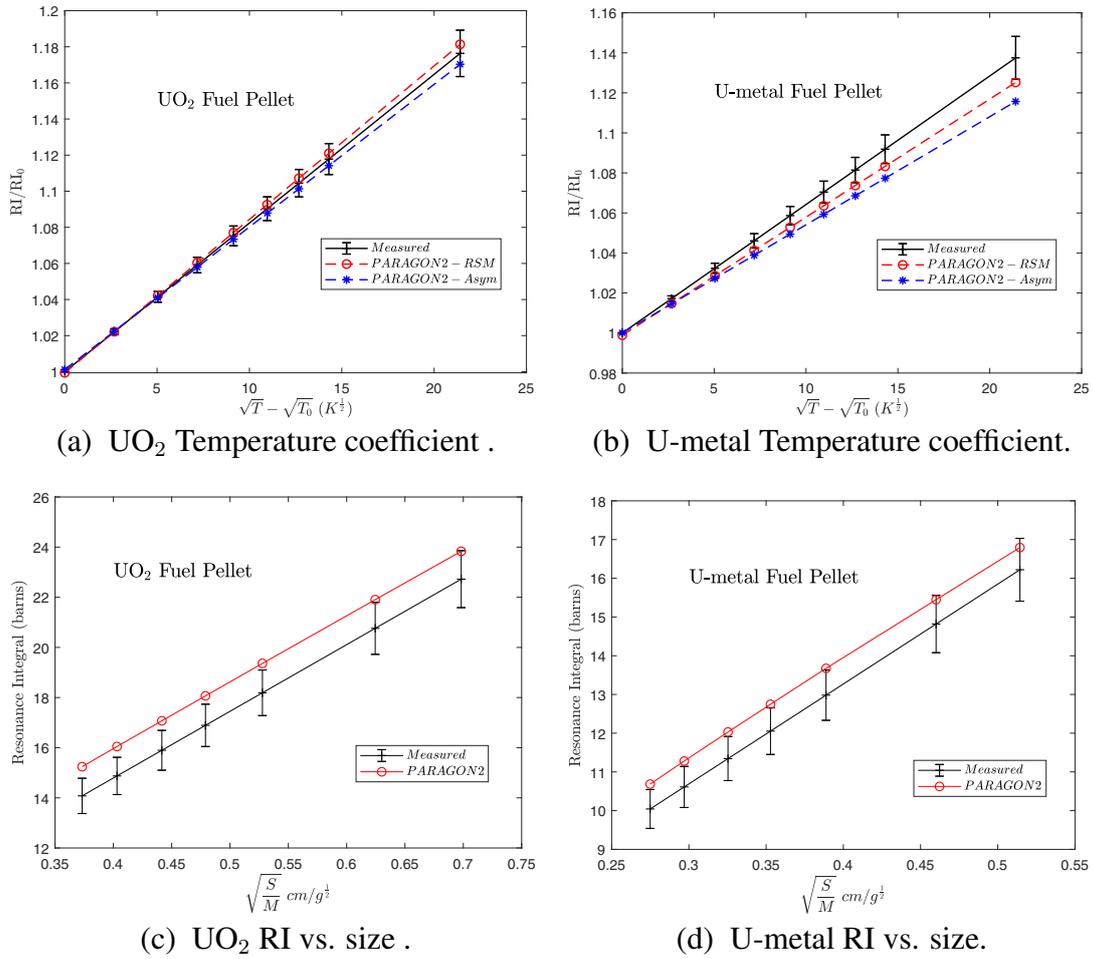


Figure 1: Hellstrand Experiment - U238 Resonance Integral vs. Temperature and Pellet Size.

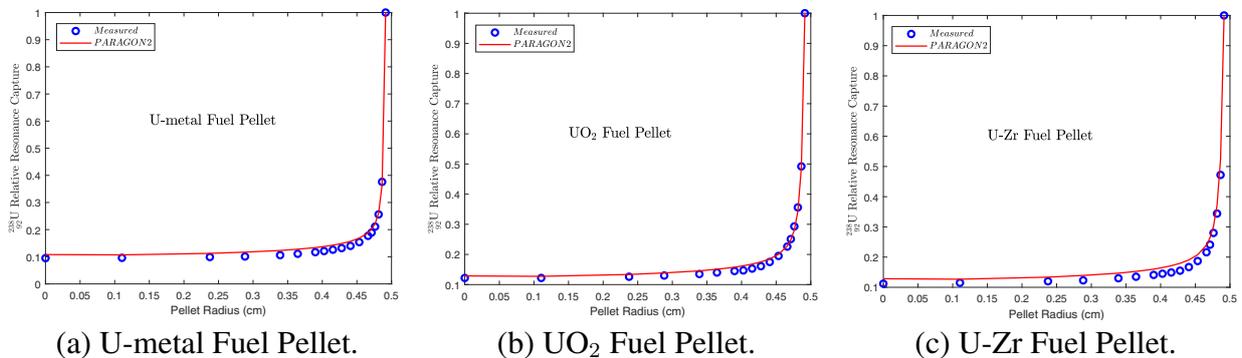


Figure 2: TRX Experiment - U238 Spatial Resonance Capture Distribution.

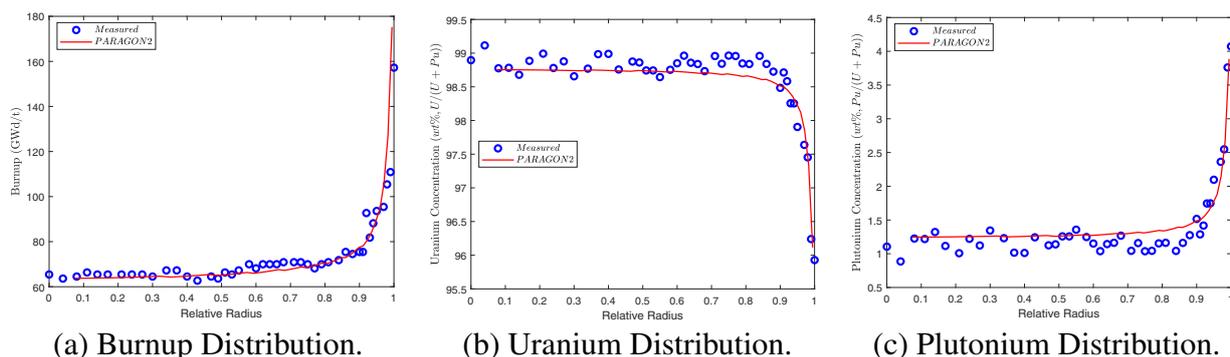


Figure 3: UO₂ Radial Pellet Distribution of Burnup, Uranium and Plutonium Concentrations

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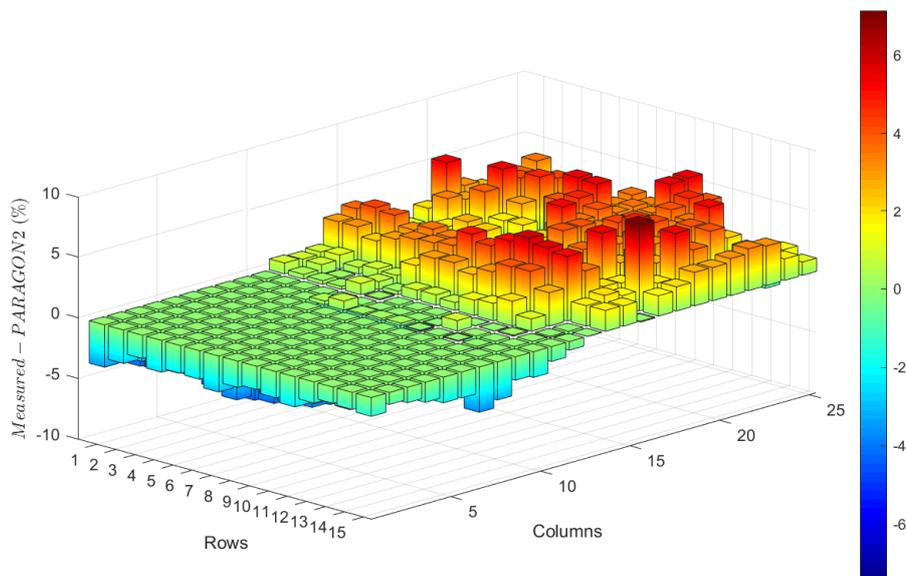


Figure 4: VENUS-2 Experiment: Measured and PARAGON2 Fission Reaction Rates Differences (MOX, UO₂ 4 wt% & 3.3 wt% are in columns: 1 to 8, 9 to 15 and 6 to 25, respectively)

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