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Validation against experimental data of the INVAP calculation line for Mo-99 production from LEU plates

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ABSTRACT

INVAP's nuclear design team participates in the continuous improvement and validation process of its calculation line in a collaborative working environment. Besides the benefits of this validation effort, the participation in this kind of exercises enhances the qualification and training of INVAP analyst's staff, promoting the internal transfer of know-how.

The specific scope of this paper is to present the approach developed by the INVAP nuclear design team to validate four different calculation methodologies (MCNP, Serpent, SCALE, and CONDOR-CITVAP) against the IPEN-CNEN benchmark, which is based in experimental data available from IPEN/MB-01 reactor. The main experimental data available are the Mo-99 activities from 10 LEU U-Al_x mini-plates and gold activation measurements.

The paper describes the main characteristics of the experimental measurements available and the results of the INVAP's neutronic calculation line applied.

The agreements between the measured and experimental Mo-99 activities were about 6% in average for the four calculation methodologies.

1 Introduction

The IPEN/MB-01 reactor is a low power research facility located in Brazil. The proposed benchmark extends the experimental data previously available [1] by including specific experiments that consider configurations with heavy water and fission Low Enriched Uranium

(LEU) mini-plates.

Accordingly, the IPEN-CNEN proposal expands the original experiments and configurations, including next to the core a heavy water reflector box which contains a light water hole, where two irradiation configurations are measured and grouped in the following cases:

a. A case with 10 LEU mini-plates for molybdenum production inside a holder, where final activity of ^{99}Mo in the central zone is provided.
b. A case with the holder containing only one dummy (pure Al alloy) plate, where five Au-Al foils where placed and the final ^{197}Au (n,g) saturation activity is provided.

This benchmark represents an interesting analysis case for INVAP's nuclear design team as far as it covers a series of relevant aspects, such as:

a. Provides experimental data for ^{99}Mo production by fission in standard LEU mini-plates, placed in a configuration similar to several INVAP reactor designs [2] (such as OPAL[3], RMB [4] or RA-10 [5]).
b. Provides saturation reaction rates for foils in a configuration that includes a heavy water reflector box, similar to several INVAP reactor designs.
c. Provides high quality data for the configurations discussed in this document, and for the original critical configuration [1].

2 Experimental Description

The benchmark geometric model for the IPEN/MB-01 configuration is shown in Figure 1. A rough description of the core comprises a square array of 28×26 positions immersed in water, a heavy water box and the holder for the U-Al$_x$ mini-plates.

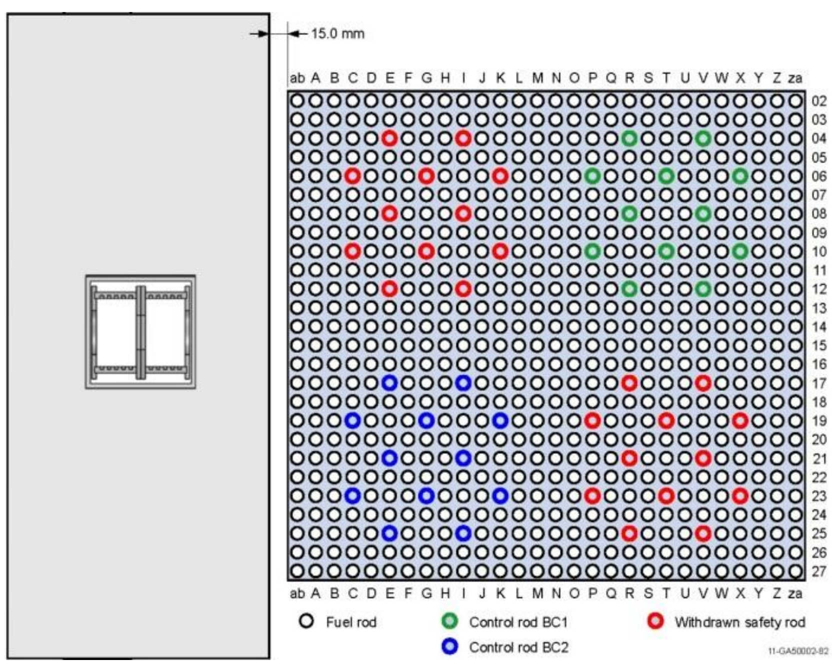

Figure 1. Upper view showing the heavy water reflector box in the west face of the reactor core; this representation also shows the square hole in the reflector box where the mini-plates holder is inserted.

Figure 2 shows an upper view of the holder inside the water box, while Figure 3 shows the relative position of the mini-plate with Au-Al foils in the holder device, and a scheme of the foil distribution along the mini-plate.

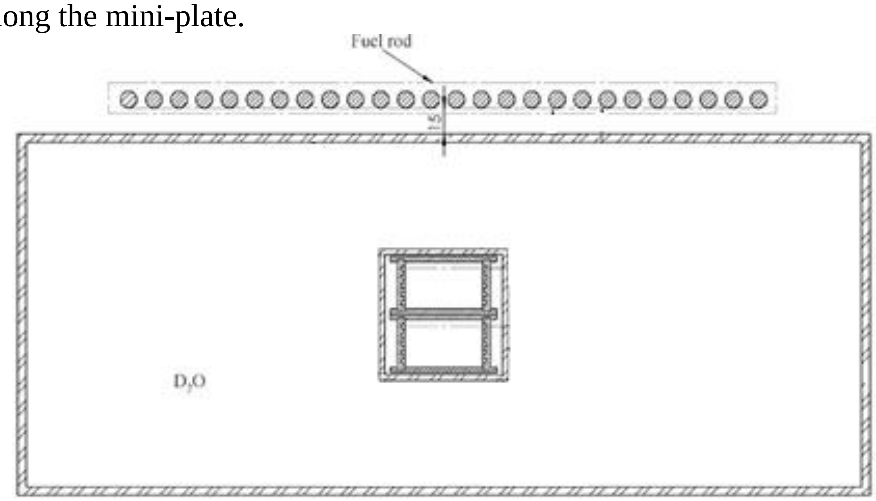

Figure 2. Upper view of the reflector box with the holder device in position and relative distances to the core.

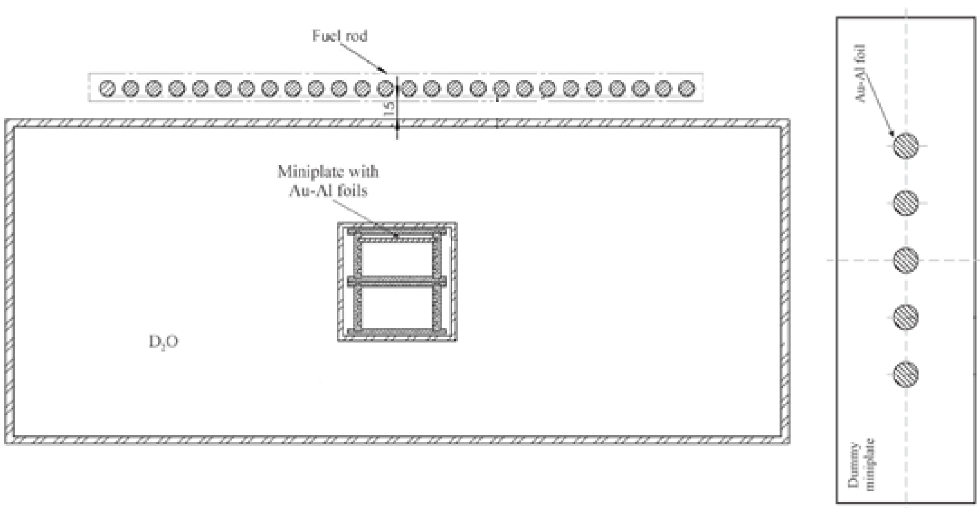

Figure 3. Upper view of the reflector box with the holder device in position and a simplified description of the position of the Au-Al foils in the mini-plate.

The specifications to complete the models and the as-built measurement data are given in [1]. From an operational point of view in the course of the experiments, the control rods critical positions were BC1 = 48.42% withdrawn and BC2 = 50.00% withdrawn, while the safety banks were totally withdrawn.

3 INVAP's Neutronic Calculation Line

As far as the calculation process is concerned, INVAP's nuclear design team has developed an integrated approach that considers the analysts and the methodology as a key part of the calculation process. Thus, the development of this benchmark contributes to improve several aspects of the team skills and capabilities, including:

a. The know-how transfer between participants that enhances the training and knowledge of the INVAP participant's staff.
b. The validation and verification of calculation and modeling capabilities, by means of the development of independent design models using the stated methodology.
c. The improvement of well-established procedures for the qualification of computational tools and users.
d. The encouragement of know-how transfer in the area of innovative methods in research reactors that in turn will lead to the reduction of user effects, which are usually identified as implementation errors or inaccurate modeling assumptions introduced by the users.

INVAP´s neutronic calculation line [6] is composed by a combination of in-house developed codes and utilities, together with several nuclear data libraries and well-known third-party codes as can be seen in Figure 4.

The approach of INVAP's calculation line is, on one hand, having a fast-methodology (namely CONDOR-CITVAP cell-core scheme) to develop main core design and fuel management calculations; and on the other hand count with 3-D, state-of-the-art, continuous energy Monte-Carlo codes (such as MCNP or Serpent) that are mainly used for ex-core device design, independent verification and detailed flux calculations.

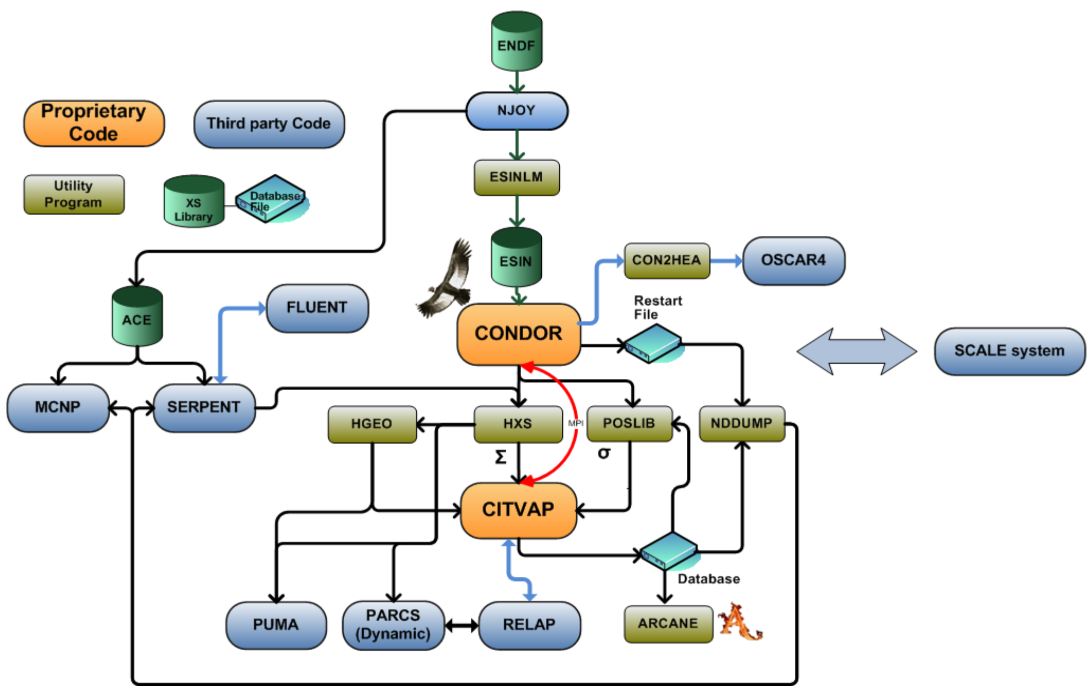

Figure 4. INVAP's neutronic calculation line

INVAP proposal for the development of the IPEN/MB-01 benchmark consisted on the employment of the different approaches from Figure 4 that consider not only the diverse paths shown, but also diverse specialists for each path. Accordingly, the alternatives are presented in, Table 1 where the main calculation scope, codes and analysts are described.

Table 1. INVAP proposed neutronic analysis alternatives for IPEN/MB-01 benchmark

#	Calculation scheme	Nuclear Data Used	Calculation results to be presented	Analyst
1	CONDOR 2.7.01 + CITVAP 3.9.04	ESIN2001 69g	^{99}Mo activity for mini-plates using power by plate and analytical approach	*Facundo Boschetti*
		HELIOS 190g	Saturation reaction rate in ^{197}Au(n,g) in Al foils	
2	Serpent 2.1.28	ENDF/B VII.0	^{99}Mo activity for mini-plates using the code capabilities Saturation reaction rate for ^{197}Au(n,g) in Al foils	*Diego Ferraro*
3	SCALE 6.1.2: KENO-VI + COUPLE + ORIGEN-S	v7-238g Xs + AMPX (JEFF-3.0/A)	^{99}Mo activity for mini-plates using power by plate and auxiliary inventory code Saturation reaction rate in ^{197}Au(n,g) in Al foils	*Hernán Meier*
4	MCNP5.1.60 + ORIGEN-S	ENDF/B VII.0 + AMPX (JEFF-3.0/A)	^{99}Mo activity for mini-plates using flux by plate and auxiliary inventory code Saturation reaction rate for ^{197}Au(n,g) in Al foils	*Manuel Zegarra*

4 Results for Critical Experiment

In order to perform a preliminary verification of the model, the cases 1 to 5 from [1], are presented in this document for all the methodologies. In Table 2 the results are presented.

Table 2. Validation of the neutronic calculation line against critical benchmarks for the IPEN/MB-01

Critical case	**Calculated reactivity [pcm]**			
	CONDOR-CITVAP (ESIN2001 69g)	**Serpent 2.1.28 (ENDF/B VII.0)**	**KENO-VI (v7-238g)**	**MCNP5 (ENDF/B VII.0)**
Case 1	-358	231 ± 5	*93±8*	341 ± 2
Case 2	-372	227 ± 5	*92±9*	304 ± 2
Case 3	-495	256 ± 5	*71±9*	322 ± 2
Case 4	-501	267 ± 5	*74±8*	331 ± 2
Case 5	-469	282 ± 5	*92±8*	350 ± 2
Average	***-439***	***253***	***84***	***330***

5 Results for mini-plate ^{99}Mo production case

The proposed IPEN/MB-01 critical configuration for this experience was reproduced by diverse alternatives and analysts, accordingly to the INVAP integrated approach for neutronic calculations described in Section 3. In Table 3, the offset in reactivity to the critical position for the different approaches for the ^{99}Mo production case is presented.

Table 3. Reactivity offset from critical position for the different calculation approaches

Critical case	Calculated reactivity [pcm]			
	CONDOR-CITVAP (ESIN2001 69g)	Serpent 2.1.28 (ENDF/B VII.0)	KENO-VI (v7-238g)	MCNP5.1.60 (ENDF/B VII.0)
Critical Configuration with holder and 10 mini-plates	-569	-95 ± 6	-170±3	-92 ± 2

From Figure 5 to Figure 7, the 2D cell and 3D core models for the deterministic methodology employed by INVAP in research reactors design are presented. In Figure 8 the 3D core model for MCNP5; this model is similar in all the Monte-Carlo methodologies employed.

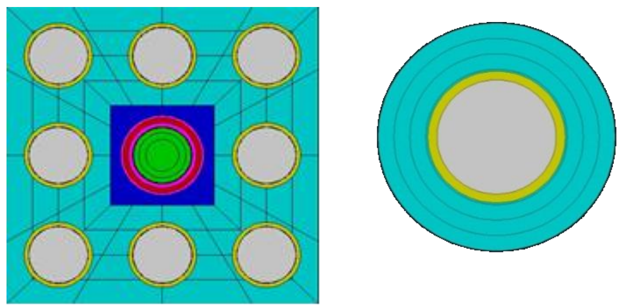

Figure 5. On the left cell model for CR inserted in the core and on the right cell model for fuel rod homogeneization.

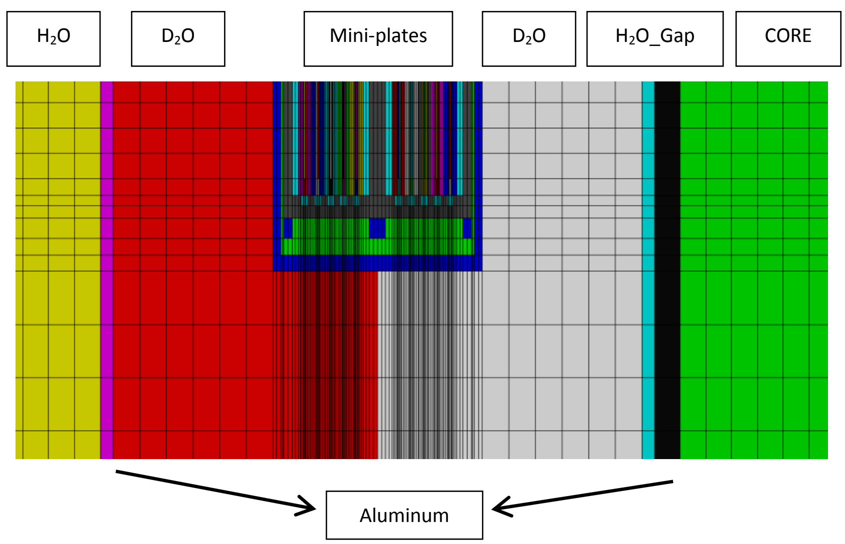

Figure 6. Cell model for heavy water reflector box and LEU mini-plates homogeneization for CITVAP.

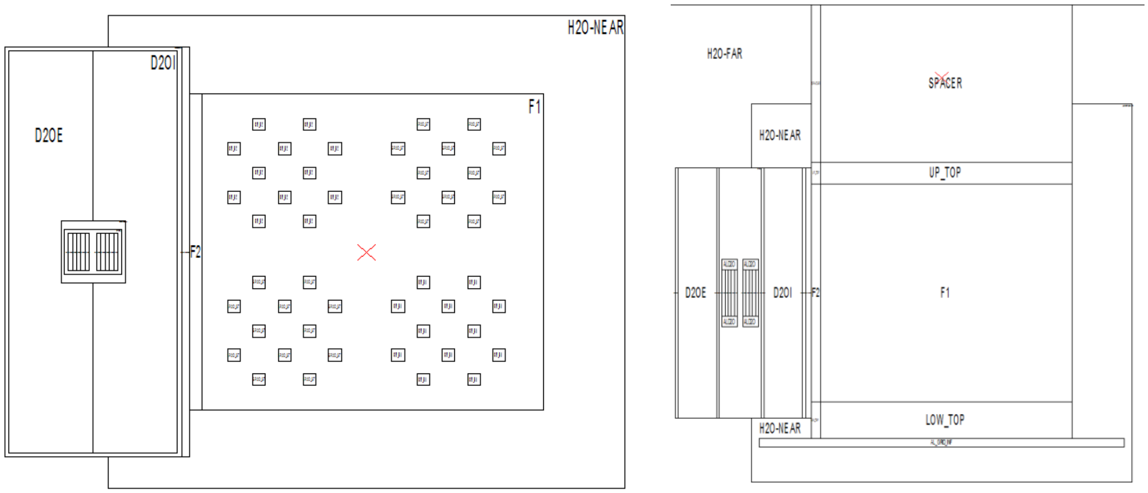

Figure 7. CITVAP 3D core level models. On the left, x-y plot of model at centre of active length; on the right x-z of model at centre of core.

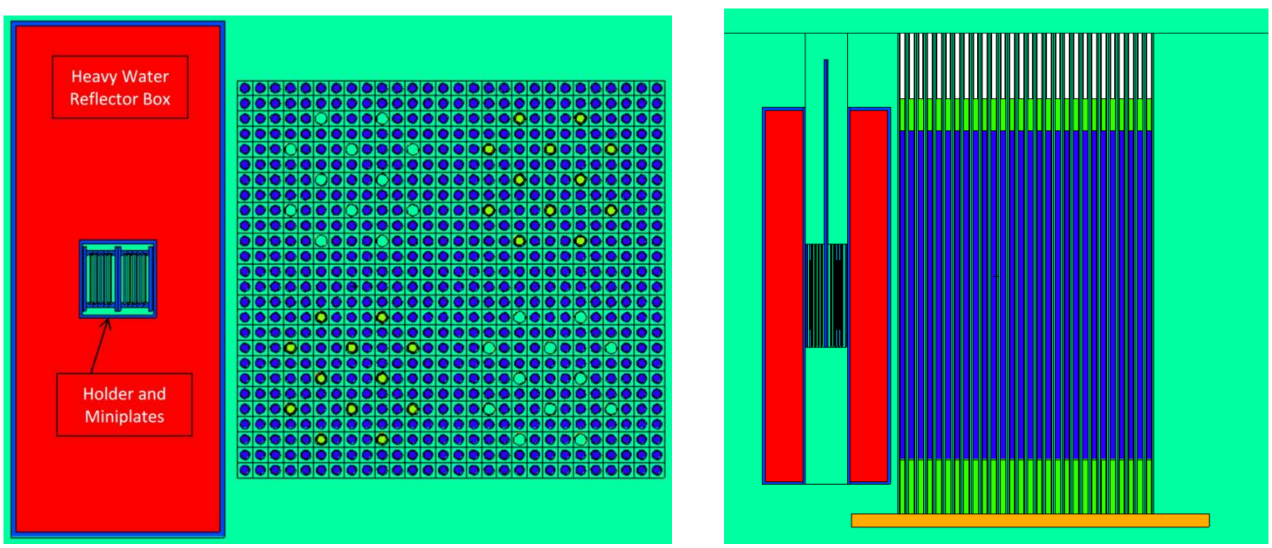

Figure 8. MCNP5 3D core models. On the left, x-y cut of the core including the heavy water reflector box and holder with mini-plates. On the right, the x-z cut of the core.

The results obtained for ^{99}Mo activation are summarized in Figure 9 and Table 4 where it can be seen that a fairly good agreement against experimental data reported is observed.

Regarding maximum differences, it should be noted that:

a. The maximum global absolute average error, defined as the average of the absolute differences for all mini-plates and calculation alternatives, is as low as 6%
b. The maximum absolute error for the total activity is 4.7%
c. These values change to 5% and 3.5 % respectively, if the mini-plate number 9 is not considered.

Table 4. Comparison of alternative calculation for ^{99}Mo activity for mini-plates against experimental values.

Mini-plate	Calculated activity [Bq]				Experimental (measured IPEN) [Bq]	Max (C-E)/E [%]
	CONDOR-CITVAP	Serpent 2.1.28	Power activation SCALE 6.1	MCNP5 + ORIGEN		
1	9.46E+04	9.22E+04	9.46E+04	9.68E+04	8.90E+04	8.8
2	8.35E+04	8.04E+04	8.31E+04	8.39E+04	8.00E+04	4.9
3	7.72E+04	7.25E+04	7.51E+04	7.61E+04	7.30E+04	5.8
4	7.36E+04	6.83E+04	7.04E+04	7.18E+04	6.90E+04	6.7
5	7.34E+04	6.80E+04	6.99E+04	7.01E+04	7.10E+04	4.3
6	6.61E+04	6.27E+04	6.46E+04	6.54E+04	6.50E+04	3.6
7	6.20E+04	6.09E+04	6.02E+04	6.10E+04	6.10E+04	1.6
8	6.06E+04	5.65E+04	5.89E+04	5.96E+04	6.00E+04	5.8
9	6.14E+04	5.89E+04	5.89E+04	6.07E+04	5.30E+04	15.8
10	6.50E+04	6.30E+04	6.21E+04	6.53E+04	6.40E+04	2.9
Total	***7.17E+05***	***6.83E+05***	***6.98E+05***	***7.11E+05***	***6.85E+05***	***4.7***
Total*	***6.56E+05***	***6.25E+05***	***6.39E+05***	***6.50E+05***	***6.32E+05***	***3.5***

**Mini-plate 9 is not considered*

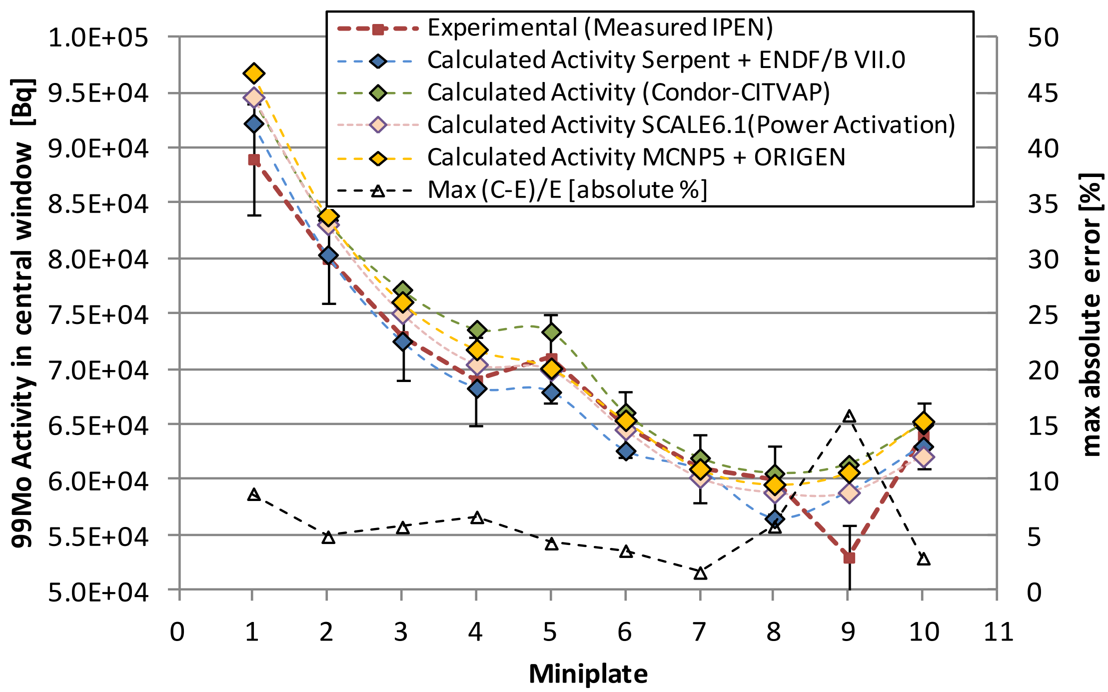

Figure 9. Overall ^{99}Mo calculation alternatives comparison against experimental values

6 Results for ^{197}Au (n,g) RR experience

In Table 5 the offset in reactivity to the critical position for the different approaches for the ^{197}Au (n,g) RR case.

Table 5. Reactivity offset from critical position for the different calculation approaches.

Critical case	Calculated reactivity [pcm]			
	CONDOR-CITVAP (ESIN2001 69g)	**Serpent 2.1.28 (ENDF/B VII.0)**	**KENO-VI (v7-238g)**	**MCNP5.1.60 (ENDF/B VII.0)**
Critical Configuration with holder and 1 dummy mini-plate for foils	-548	-76 ± 6	-157±3	-85 ± 2

Finally, the results obtained for ^{197}Au(n,g) reaction rates are summarized in Figure 10 and Table 6, where it can be seen that the agreement with the reported experimental data is not good as for ^{99}Mo case. Regarding maximum differences, it should be noted that:

a. The maximum global absolute average error, defined as the average of the absolute differences for all the foils and calculation alternatives, is around 13%.
b. The maximum absolute error for the total reaction rate is 12.4%

Table 6. Comparison of alternative calculations for foils ^{197}Au (n,g) RR against experimental values

Foils	Calculated RR [1/s]				Experimental [1/s]	Max (C-E)/E [%]
	CONDOR-CITVAP	***Serpent 2.1.28***	***SCALE 6.1***	***MCNP5***		
1	1.21E+05	1.23E+05	1.18E+05	1.24E+05	1.27E+05	7.5
2	1.27E+05	1.22E+05	1.24E+05	1.30E+05	1.36E+05	10.7
3	1.29E+05	1.22E+05	1.19E+05	1.35E+05	1.40E+05	15.3
4	1.32E+05	1.24E+05	1.19E+05	1.30E+05	1.42E+05	16.0
5	1.34E+05	1.27E+05	1.26E+05	1.30E+05	1.46E+05	14.0
Total	***6.43E+05***	***6.18E+05***	***6.06E+05***	***6.49E+05***	***6.91E+05***	***12.4***

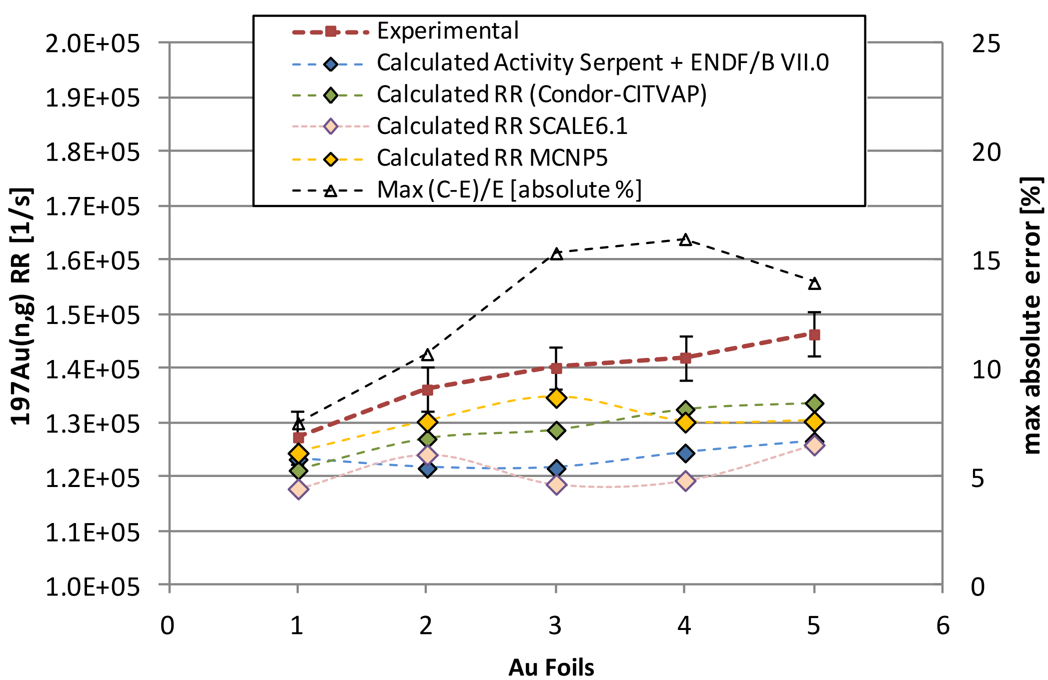

Figure 10. Overall calculation alternatives for ^{197}Au (n,g) RR comparison against experimental values

7 Conclusion

The proposed IPEN/MB-01 reactor extended benchmark was developed with the aim of evaluating alternative calculation approaches that considers not only diverse codes, nuclear data and calculation approaches but also diverse specialists and modelling criteria.

This benchmark represents an interesting case of analysis for INVAP's nuclear design team since it provides the opportunity of developing calculation comparison with high quality experimental data for ^{99}Mo production by fission in standard LEU mini-plates placed in a heavy water reflector zone.

This configuration represents a standard INVAP´s design for ^{99}Mo production (such as those in OPAL, RMB, RA-10). The obtained results showed a very good agreement with the reported experimental values, both regarding reactivity calculations and activation results. In general, ^{99}Mo activity calculation has shown to be more accurate than Au foils reaction rate calculations. In particular, some discrepancies have been observed in mini-plate number 9, which should be further analysed.

Finally, it should be noted that the combination of the main INVAP design tools, the developed calculation methodology, and the analyst's modelling skills were capable to obtain accurate results for all the main parameters proposed in this benchmark.

8 References

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9 Acknowledgment

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