Participation of Mexico in the OECD/NEA SFR Benchmark using the Monte Carlo code Serpent

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Abstract. In 2014, Mexico was honored with its acceptance as an observer member in the Technical Working Group on Fast Reactors of the IAEA. Afterwards, the Mexican participation in the fast reactors activities augmented when in 2016 the Mexican Team was accepted in the UAM SFR Benchmark of the OECD/NEA. The first technical specifications of the mentioned Benchmark consisted of four sodium-cooled fast reactors (3600 MWt metallic-fueled, 3600 MWt MOX-fueled, 1000 MWt carbide-fueled, and 1000 MWt MOX-fueled). The code selected for the full-core simulations was the Finnish Monte Carlo code Serpent version 2.1.20 and the calculations were performed using two different cross sections libraries, namely JEFF 3.1.1 and ENDF/B7.0. The geometry, material composition and Monte Carlo solution parameters used are briefly described in this paper together with the main results obtained by the Mexican team. Quite good agreement (in the order of tens of pcms) for results of k_{eff}, sodium void worth, and delayed neutron fraction was observed when comparing with the ones obtained by other participants that followed the same methodology (code and evaluated data libraries). Larger deviations were found when comparing with different methodologies, but in general the calculated solutions were reasonably close to the averaged results reported in the Benchmark. The use of the Monte Carlo code Serpent fulfills two objectives; firstly, to get confidence in the obtainment of reference solutions; and secondly, to generate homogenized cross sections to be used within the currently development of the Mexican neutron diffusion code for hexagonal-z geometry AZNHEX, which is part of the AZTLAN platform: Mexican platform for analysis and design of nuclear reactors. The participation of Mexico in this OECD/NEA Benchmark strengthens the Mexican fast reactors knowledge and allows the country to contribute more actively to the international efforts in the field.

Key Words: OECD/NEA SFR, Serpent, Monte Carlo.

1. Introduction

A first version of the UAM SFR Benchmark of the OECD/NEA was published in which four fast reactor cores are treated. The objective of the Benchmark is to simulate the mentioned cores and compare the results obtained by different participant institutions.

Eleven institutions were involved in the Benchmark:

- Argonne National Laboratory (ANL) from United States.
- Commissariat à l'Énergie Atomique et aux énergies alternatives (CEA Cadarache and Sacley) from France.
- Centre for Energy Research (CER-EK) from Hungary.
- Energy and Sustainable Economic Development (ENEA) from Italy.

- Helmholtz Zentrum Dresden Rossendorf (HZDR) from Germany.
- Institute of Nuclear Technology and Energy Systems (IKE) from Germany.
- Japan Atomic Energy Agency (JAEA) from Japan.
- Karlsruhe Institute of Technology (KIT) from Germany.
- Centre d'Étude de l'énergie Nucléaire (SCK•CEN) from Belgium.
- University of Illinois at Urbana Champaigne (UIUC) from United States.

The intention of the novel fast reactors research group in Mexico, was to test the full core calculation capabilities by participating in the mentioned Benchmark. The code selected for these calculations was the Monte Carlo Finnish code Serpent version 2.1.26 [2] with cross section libraries JEFF 3.1.1[3] and ENDF/B7.0 [4].

The reported results included:

- Core's effective multiplication factor.
- Sodium void worth (defined as the reactivity change between normal operation and operation without sodium in the active core).
- Effective delayed neutron fraction.

After this brief introduction, the four core models from the benchmark will be defined followed by the implementation on the code and, to finish, results will be shown including conclusions.

2. Definition of models

Four nuclear cores are treated:

- 3600 MW carbide-fueled core.
- 3600 MW MOX-fueled core.
- 1000 MW metallic-fueled core.
- 1000 MW MOX-fueled core.

Due to space limitations, the material compositions of each component are not shown in this paper but can be easily consulted in [1].

2.1 3600 MW Carbide Core

Figure 1 shows the 3600 MW carbide core. The core is divided into two fuel zones (inner and outer), two control systems (primary and secondary) and a radial reflector zone. Figure 1 also shows the axial configuration of the assemblies that form the core. The radial reflector consists of hexagonal blocks of a homogeneous mixture 26% Na 74% SS EM10 (% vol). The fuel assembly consists in two axial reflector zones, two gas plenums and a fuel zone divided into 5 fuel subzones each with different fuel composition. The control assembly consists of control rods in a position above the active zone; the rest of the assembly is a sodium-filled channel.

The Table I shows the geometric features of the core's components.



FIG. 1. Description of 3600-CAR core (left) and assemblies' axial description (right).

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	Axial	Gas	Fuel	Primary	Secondary	Sodium
	Reflector	Plenum		Control	Control	Channel
Assembly pitch (cm)	20.9889	20.9889	20.9889	20.9889	20.9889	20.9889
F-F external face of	20.2641	20.2641	20.2641	20.2641	20.2641	20.2641
external channel (cm)						
F-F internal face of	19.3591	19.3591	19.3591	19.3591	19.3591	19.3591
external channel (cm)						
F-F external face of	N/A	N/A	N/A	15.6883	N/A	N/A
internal channel (cm)						
F-F internal face of	N/A	N/A	N/A	15.2860	N/A	N/A
internal channel (cm)						
External diameter of	N/A	N/A	N/A	N/A	14.8838	N/A
internal channel (cm)						
Internal diameter of	N/A	N/A	N/A	N/A	14.4815	N/A
internal channel (cm)						
Number of pins	469	469	469	37	55	N/A
Cladding external	0.7908	0.7908	0.7908	2.2953	1.6443	N/A
diameter (cm)						
Cladding internal	0.6940	0.6940	0.6940	2.0948	1.5417	N/A
diameter (cm)						
Pellet diameter (cm)	0.6638	N/A	0.6638	1.8404	1.4079	N/A
Pellet material	SS	He	(U,Pu)C	Nat B ₄ C	Enriched	Na
	EM10				B ₄ C	
Temperature	743 K	743 K	1260 K	743 K	743 K	743 K

TABLE I: Geometric characteristics of 3600-CAR core elements.

2.2 3600 MW MOX Core

Figure 2 shows the 3600 MW MOX core. As it can be seen, the core layout and configuration are very similar to 3600-CAR, the core is divided into two fuel zones, it has two control systems and a radial reflector zone. In the center there is a solid SS hexagonal block identical to the radial reflector assemblies. The axial configuration of the assemblies is also described in Figure 2 and Table II.



FIG. 2. Description of 3600-MOX core (left) and assemblies' axial description (right).

	Axial	Gas	Fuel	Primary	Secondary	Sodium
	Reflector	Plenum		Control	Control	Channel
Assembly pitch (cm)	21.2205	21.2205	21.2205	21.2205	21.2205	21.2205
F-F external face of	20.7468	20.7468	20.7468	20.7468	20.7468	20.7468
external channel (cm)						
F-F internal face of	19.8418	19.8418	19.8418	19.8418	19.8418	19.8418
external channel (cm)						
F-F external face of	N/A	N/A	N/A	15.6883	N/A	N/A
internal channel (cm)						
F-F internal face of	N/A	N/A	N/A	15.2860	N/A	N/A
internal channel (cm)						
External diameter of	N/A	N/A	N/A	N/A	14.8838	N/A
internal channel (cm)						
Internal diameter of	N/A	N/A	N/A	N/A	14.4815	N/A
internal channel (cm)						
Number of pins	271	271	271	37	55	N/A
Cladding external	1.0838	1.0838	1.0838	2.2953	1.6443	N/A
diameter (cm)						
Cladding internal	0.9786	0.9786	0.9786	2.0948	1.5417	N/A
diameter (cm)						
Pellet diameter (cm)	0.9484	N/A	0.9484	1.8404	1.4079	N/A
Pellet material	SS	He	$(U,Pu)O_2$	Nat B ₄ C	Enriched	Na
	EM10				B_4C	
Temperature	743 K	743 K	1500 K	743 K	743 K	743 K

TABLE II:	Geometric	characteristics	of 3600-MOX	core elements.
			01 0 0 0 0 11 0 11	•••••••••••••••••

2.3 1000 MW Metallic Core

Figure 3 and Table III show the main characteristics of the 1000-MET core components. One important thing to mention at this point is that the lower axial reflector and the upper structure are identical. Also the lower structure is made of hexagonal blocks of a homogeneous mixture of 70/30 (volumetric %) of sodium and SS-316 Steel.



FIG. 3. Description of 1000-MET core (left) and assemblies' axial description (right).

	Low Refl	Radial	Radial	Fuel	Na/He	Control	Sodium
	/ Up Str	shielding	Reflector		Plenum	System	Channel
Assembly pitch	16.2471	16.2471	16.2471	16.2471	16.2471	16.2471	16.2471
F-F external face of	15.8123	15.8123	15.8123	15.8123	15.8123	15.8123	15.8123
external channel (cm)							
F-F internal face of	15.0191	15.0191	15.0191	15.0191	15.0191	15.0191	15.0191
external channel (cm)							
F-F external face of	N/A	N/A	N/A	N/A	N/A	14.2140	N/A
internal channel (cm)							
F-F internal face of	N/A	N/A	N/A	N/A	N/A	13.4208	N/A
internal channel (cm)							
Number of pins	271	19	91	271	271	7	N/A
Cladding external	0.77134	3.35875	1.55130	0.77134	0.77134	4.72126	N/A
diameter (cm)							
Cladding internal	0.64720	2.85549	N/A	0.64720	0.64720	4.57801	N/A
diameter (cm)							
Pellet diameter (cm)	0.64720	2.85549	N/A	0.6472	N/A	4.57801	N/A
Pellet material	SS HT-9	Nat B ₄ C	SS HT-9	U,Pu	Na/He	Enriched B ₄ C	Na
Temperature	705 K	705 K	705 K	807 K	705 K	705 K	705 K

TABLE III: Geometric characteristics of 1000-MET core elements.

2.4 1000 MW MOX Core

As before, Figure 4 and Table IV show the geometry description of the core's component. As in the case of 1000-MET core, the lower axial reflector and the upper structure are identical and the lower structure is a homogeneous mixture of 70/30 (volumetric %) of sodium and SS-316 Steel.



FIG. 4. Description of 1000-MOX core (left) and assemblies' axial description (right).

	Low Refl	Radial	Radial	Fuel	Не	Control	Sodium
				ruei	DI DI	Control	Cl
	/ Up Str	shielding	Reflector		Plenum	System	Channel
Assembly pitch	16.2471	16.2471	16.2471	16.2471	16.2471	16.2471	16.2471
F-F external face of	15.8123	15.8123	15.8123	15.8123	15.8123	15.8123	15.8123
external channel (cm)							
F-F internal face of	15.0191	15.0191	15.0191	15.0191	15.0191	15.0191	15.0191
external channel (cm)							
F-F external face of	N/A	N/A	N/A	N/A	N/A	14.2140	N/A
internal channel (cm)							
F-F internal face of	N/A	N/A	N/A	N/A	N/A	13.4208	N/A
internal channel (cm)							
Number of pins	271	19	91	271	271	7	N/A
Cladding external	0.78565	3.3588	1.55130	0.78565	0.78565	4.72126	N/A
diameter (cm)							
Cladding internal	0.66431	2.8555	N/A	0.66431	0.66431	4.57801	N/A
diameter (cm)							
Pellet diameter (cm)	0.66431	2.8555	N/A	0.66431	N/A	4.57801	N/A
Pellet material	SS HT-9	Nat B ₄ C	SS HT-9	$(U,Pu)O_2$	He	Enriched B ₄ C	Na
Temperature	705 K	705 K	705 K	1300 K	705 K	705 K	705 K

TABLE IV: Geometric characteristics of 1000-MOX core elements.

3. Implementation of models in Serpent

The models previously described were simulated in Serpent, the version used was 2.1.20. Two cross section (XS) libraries were used for the calculations: JEFF 3.1.1 and ENDF/B7.0. Some considerations were done in order to ease the modeling in the code such as temperature selection, both XS libraries by default work with 600 K, 900 K, 1200 K and 1500 K temperatures, intermediate temperatures would imply the generation of new XS sets, in order to avoid this extra step the material temperatures were adjusted as described in Table V.

TIBLE (Temperatures used in the models in Serpenti								
	Axial	Structure	Radial	Radial	Fuel	Na/He	Control	Sodium
	Reflector		shielding	Reflector		Plenum	System	Channel
3600-CAR	600 K	600 K	600 K	600 K	1200 K	600 K	600 K	600 K
3600-MOX	600 K	600 K	600 K	600 K	1500 K	600 K	600 K	600 K
1000-MET	600 K	600 K	600 K	600 K	900 K	600 K	600 K	600 K
1000-MOX	600 K	600 K	600 K	600 K	1200 K	600 K	600 K	600 K

TABLE V: Temperatures used in the models in Serpent.

The Figures 5 to 8 show radial and axial views for all the four cores treated in this paper.



FIG. 5. 3600-CAR core model in Serpent.



FIG. 6. 3600-MOX core model in Serpent.



FIG. 7. 1000-MET core model in Serpent.



FIG. 8. 1000-MOX core model in Serpent.

Every core was simulated four times; one flooded with sodium and other with no sodium on the active part; and with both XS libraries, JEFF 3.1.1 and ENDF/B7.0.

4. Implementation of models in Serpent

In this section the results of the effective neutron multiplication factor (k_{eff}), delayed neutron fraction (β) and the sodium void fraction are presented. In order to measure the accuracy of the obtained results, the solutions are compared with the ones reported in the Benchmark obtained with similar methodologies (Monte Carlo + JEFF or ENDF/B) as well as the average reported in the Benchmark, see Tables VI to VIII.

ID	XS Library	Code	3600-MOX	3600-CAR	1000-MET	1000-MOX
ANL-2	ENDFB 7.0	MCNP5	1.00750	0.99970	1.02420	1.02230
ANL-3	JEFF 3.1	MCNP5	1.01370	1.00850	1.03730	1.03030
CEA-10	JEFF 3.1.1	TRIPOLI-4	1.01970	1.01220	1.04290	1.03530
ENEA	ENDFB 7.0	MCNPX	1.01080			
HZRD	ENDFB 7.0	SERPENT	1.01040			
JAEA-3	JENDL 4.0	MVP	1.01390		1.03400	
JAEA-5	JENDL 4.0	MVP/Diff			1.03400	
CEN-1	ENDFB 7.1	MCNPX/ALEPH2.5				1.02560
CEN-2	JEFF 3.1.2	MCNPX/ALEPH2.5				1.03480
UIUC-1	JEFF 3.1.1	SERPENT	1.02340	1.02100	1.03590	1.02580
UIUC-2	ENFB 6.8	SERPENT	1.02940	1.02780	1.03800	1.02370
UIUC-3	ENDFB 7.0	SERPENT	1.01930	1.01560	1.02690	1.02000
IKE-1	JEFF 3.1	MCNP 5			1.04260	
IKE-2	JEFF 3.1	MCNP 5			1.03740	
ININ-1	JEFF 3.1.1	SERPENT 2.1.20	1.03428	1.00913	1.04140	1.03303
ININ-2	ENDFB 7.0	SERPENT 2.1.20	1.02965	1.00326	1.03226	1.02719
		AVERAGE	1.01380	1.00900	1.03550	1.02870
		±SD	0.00405	0.00620	0.00780	0.00620

TABLE VI: Results of k_{eff} for all cores.

TABLE VII: Results of void worth for all cores.

ID	XS Library	Code	3600-MOX	3600-CAR	1000-MET	1000-MOX
ANL-2	ENDFB 7.0	MCNP5	2033	2289	2238	2002
ANL-3	JEFF 3.1	MCNP5	2078	2312	2273	2050
CEA-10	JEFF 3.1.1	TRIPOLI-4	1963	2122	1858	1621
ENEA	ENDFB 7.0	MCNPX	1940			
HZRD	ENDFB 7.0	SERPENT	1860			
JAEA-3	JENDL 4.0	MVP	2009		2164	
JAEA-5	JENDL 4.0	MVP/Diff			2164	
CEN-1	ENDFB 7.1	MCNPX/ALEPH2.5				1760
CEN-2	JEFF 3.1.2	MCNPX/ALEPH2.5				1789
UIUC-1	JEFF 3.1.1	SERPENT	1559	1465	1032	1508
UIUC-2	ENFB 6.8	SERPENT	1696	1911	1251	1642
UIUC-3	ENDFB 7.0	SERPENT	1569	1750	1128	1526
IKE-1	JEFF 3.1	MCNP 5			2257	
IKE-2	JEFF 3.1	MCNP 5			2520	
ININ-1	JEFF 3.1.1	SERPENT 2.1.20	1554	1698	1831	1562
ININ-2	ENDFB 7.0	SERPENT 2.1.20	1544	1688	1844	1566
		AVERAGE	1937	2120	2024	1831
		±SD	158	225	407	228

TABLE VIII: Results of β for all cores.

ID	XS Library	Code	3600-MOX	3600-CAR	1000-MET	1000-MOX
ANL-2	ENDFB 7.0	MCNP5	360	365	330	326
ANL-3	JEFF 3.1	MCNP5	354	378	332	335
CEA-10	JEFF 3.1.1	TRIPOLI-4	370	377	343	334
ENEA	ENDFB 7.0	MCNPX	352			
HZRD	ENDFB 7.0	SERPENT	361			
JAEA-3	JENDL 4.0	MVP	363		339	
JAEA-5	JENDL 4.0	MVP/Diff			339	
CEN-1	ENDFB 7.1	MCNPX/ALEPH2.5				315
CEN-2	JEFF 3.1.2	MCNPX/ALEPH2.5				344
UIUC-1	JEFF 3.1.1	SERPENT	371	382	350	337
UIUC-2	ENFB 6.8	SERPENT	360	367	335	324
UIUC-3	ENDFB 7.0	SERPENT	358	368	335	326
IKE-1	JEFF 3.1	MCNP 5			352	
IKE-2	JEFF 3.1	MCNP 5			341	
ININ-1	JEFF 3.1.1	SERPENT 2.1.20	371	379	343	333
ININ-2	ENDFB 7.0	SERPENT 2.1.20	359	368	334	323
		AVERAGE	367	382	345	333
		±SD	13	16	10	15

Given the results shown in Tables VI to VIII, it can be seen that good agreement was found between the local results (ININ-1 and ININ-2) and the results obtained by other institutes following similar methodologies, particularly the values marked in green. It was observed that the temperature change used to make it coincide with the default XS libraries temperatures did not have an important effect on the results tendency, since most of our results are in a region around the ones obtained by others. Nevertheless, XS generation for the required exact temperature can improve the results.

5. Conclusions

One of the goals of participating in the Benchmark is to test the capabilities and experience of the Mexican group on fast reactor simulation. Based on the results reached, it can be concluded that the fast reactor sub-group owns capabilities to participate in these kind of exercises.

Serpent is a very appropriate tool for full core calculations and XS generation that does not require much hardware power and with parallel calculation capabilities; taking advantage of multicore processors when possible.

Numerically, the results are in the order of the ones obtained by other institutes following similar methodologies, which gives confidence in the results obtained by the methodology here followed. The participation of Mexico in these kinds of exercises helps to improve the capabilities of the research group involved, this experience will be used in the developing and testing of the new domestic nuclear code platform called "AZTLAN Platform".

6. Further Work

Further steps will include the calculation of reactivity changes due to fuel temperature changes and the reactivity change due to control rods insertion; and the same results after an operation cycle.

Another further goal is the generation of cross sections with Serpent for the use in a domestic deterministic code for hexagonal-geometry reactors called AZNHEX [5] which is part of the AZTLAN Platform [6], a Mexican multi-institutional effort for domestic nuclear reactor analysis code development.

7. Bibliography

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