Solution of the OECD/NEA SFR Benchmark with the Mexican neutron diffusion code AZNHEX

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Abstract. The AZTLAN Platform project is a Mexican national initiative led by the National Institute for Nuclear Research of Mexico, which brings together nuclear institutions of higher education in Mexico: the National Polytechnic Institute, the National Autonomous University of Mexico and the Autonomous Metropolitan University, in an effort to take a significant step towards positioning Mexico, in the medium term, in a competitive international level on nuclear reactors analysis and modeling software. The project is funded by the Sectorial Fund for Energy Sustainability CONACYT-SENER and one of its main goals is to build up as well as strengthen the national development of specialized nuclear knowledge and human resources. The AZTLAN platform consists of several neutronics and thermal-hydraulics modules. Among the neutronics tools, the AZNHEX code has been developed. AZNHEX is a 3D diffusion code that solves numerically the time dependent neutron diffusion equations in hexagonal-z geometry. The diffusion solver is based on the RTN0 (Raviart-Thomas-Nédélec of index 0) nodal finite element method together with the Gordon-Hall transfinite interpolation which is used to convert, in the radial plane, each one of the four trapezoids in a hexagon to squares. In order to support and provide reliability to the platform, a stringent verification and validation (V&V) process in which the use of international Benchmarks and Monte Carlo reference solutions has been started. As a part of this V&V activities, results obtained with AZNHEX for the full-core simulations of the two nuclear cores of the OECD/NEA SFR Benchmark (a 1000 MW metallic-fueled and a 3600 MW MOX-fueled) are shown and compared with the ones obtained with the reference Monte Carlo code Serpent. The cross sections sets used in AZNHEX were also generated in a previous step with the Serpent code to maintain consistency between calculations. The obtained Results for k_{eff}, sodium void worth and control rods worth are within reasonable agreement; in the order of tens of pcms. The results presented are not only useful for the verification of AZNHEX, but also these ones help to define a well-tested methodology in order to generate cross section sets for future dynamic calculations with AZNHEX. Based on the results, the strengths and limitations of the AZNHEX code are discussed in the conclusions and a series of improvements have been identified and planned to be implemented.

Key Words: AZTLAN, AZNHEX, Serpent, Verification and Validation (V&V).

1. Introduction

The “AZTLAN Platform” [1] is a joint effort lead by the National Institute of Nuclear Research that gathers the main Mexican public universities which are the National Autonomous University of Mexico, National Polytechnic Institute and the Metropolitan Autonomous University, in an effort to place Mexico in a competitive position on reactor analysis matters.

The Platform consists on the following modules:
- AZTRAN (AZtlan TRANsport): code that solves the neutron transport equation for several

energy groups on 3D Cartesian geometry and steady state (time-dependent version is under development). The code is capable to determine the effective neutron multiplication factor (k_{eff}), angular neutron flux on every point for a given discretization as long as the radial and axial power. Its main use is to perform neutronic studies of fuel assemblies with square cross section such as BWR and PWR.
- AZKIND (AZtlan KInetics in Neutron Diffusion): code that solves the neutron diffusion equation with time dependency in 3D Cartesian geometry, for several energy groups and precursor concentrations of delayed neutrons. It delivers the k_{eff}, and radial and axial power distribution. A module for parallel calculations with AZKIND is currently being under development.
- AZNHEX (AZtlan Nodal HEXagonal): code that solves the neutron diffusion equation in 3D hexagonal lattices for steady and time dependent scenarios. The code delivers k_{eff}, neutron flux and axial and radial power distribution. The capability of the code in cores with hexagonal-z geometry makes it suitable for analysis of systems as the High Temperature Gas-Cooled Reactor (HTGR), the Vadá Vadá Energeticheski Reactor (VVER) or the Liquid Metal Fast Breeder Reactor (LMFBR). This code will be more deeply described in further sections.

The motivation of this work is to compare AZNHEX results against a well-known reference code, in this case SERPENT, as well as the capabilities of the work team in neutron Cross Sections (XS) generation to be used on deterministic codes.

The next sections will describe the codes used, the methodology followed and the results obtained.

2. Description of the codes

2.1 SERPENT

SERPENT [2] is a 2D/3D continuous-energy Monte Carlo reactor physics code with burnup capabilities developed at the VTT Technical Research Centre of Finland and has been distributed by OECD/NEA Data Bank and RSICC since 2009. The applications in which Serpent is suggested by the developers include:

a) Spatial homogenization and group constant generation for deterministic nuclear reactor simulator calculations.
b) Fuel cycle studies involving detailed assembly-level burnup calculations.
c) Validation of deterministic lattice transport codes; among others.
d) Full-core modeling of research reactors, SMRs, and other closely coupled systems.
e) Coupled multi-physics applications.
f) Educational purposes and demonstration of nuclear reactor physics phenomena.

Reason a) and c) make SERPENT an ideal candidate for testing AZNHEX capabilities in nuclear reactor core simulations, as well a for XS generation.

2.2 AZNHEX

AZNHEX [3] is the tool aimed to the design and analysis of cores with hexagonal-z geometry elements. It is based on the numerical solution of the multi-group neutron diffusion equations in 3D for steady state or time-dependent problems [4], [5], [6], for the calculation of the effective neutron multiplication factor k_{eff}, neutron flux, and power distribution. The first step was to apply a Gordon-Hall transformation to each quadrant of hexagonal cross sections (see Figure 1) of all the assemblies in a core as it is described in [7]. With this transformation, the starting multi-group neutron diffusion equations with constant XS are changed to a set of partial differential equations with non-constant coefficients. The next step was to apply the classical Galerkin finite element method using the well-known RTN-0 (Raviart-Thomas-

Nédélec of index zero) nodal approximation to approximate the space dependency of the neutron flux and the precursors concentration as well. To discretize the time-dependency of the final set of ordinary differential equations the theta-method leading to the fully implicit scheme when θ=1 and the semi-implicit when θ=1/2.

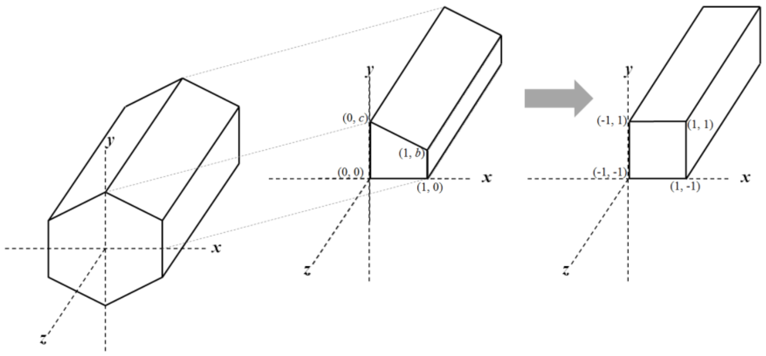

FIG. 1. Coordinates transformation from a 1/4th of hexagon-z cell into square-z cell.

For more information on nodal methods [8][9] and for more on the Gordon-Hall transformation [10][11].

3. Description of Cores

Two cores were treated; one big sized 3600 MW_t MOX-fueled and one medium sized 1000 MW_t metallic-fueled core. The most general features for the core are presented here, for a more detailed description the reader is encouraged to review reference [12].

3.1 3600 MW MOX Fuel Core

The core consists in:

- 453 fuel assemblies (225 in inner zone and 228 in outer zone, see Figure 2).
- 330 radial reflector assemblies.
- 33 control assemblies (24 in primary system and 9 in secondary system).

The Table I shows the main characteristics of the core's assemblies and the Figure 3 shows the geometric layout of the main assemblies. In the case of plenums and axial reflectors are almost identical to the fuel assemblies but, instead of fuel pellet the reflector has a Stainless Steel (SS) pellet and in the case of plenum there is no pellet at all.

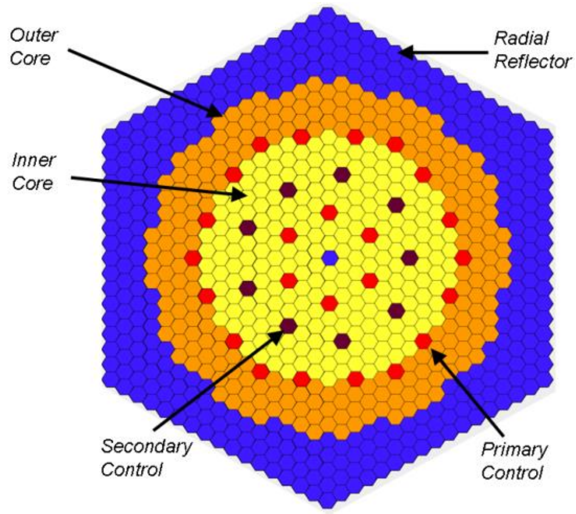

FIG. 2. Layout of the 3600 MW core [13].

TABLE I: Characteristics of 3600 MW core's fuel subassemblies.

Whole Subassembly	Upper Axial Reflector	80.45 cm
	Upper Gas Plenum	10.05 cm
	Active Core Height	100.56 cm
	Lower Axial Reflector	30.17 cm
	Lower Gas Plenum	89.91 cm
Subassembly pitch		21.2205 cm
Subassembly duct outer flat-to-flat distance		20.7468 cm
Subassembly duct wall thickness		0.4525 cm
Number of fuel pins		271
Outer radius of cladding		0.5419 cm
Inner radius of cladding		0.4893 cm
Fuel slug radius		0.4742 cm
Inner central hole radius (helium)		0.1257 cm
Pin to Pin distance		1.1897 cm

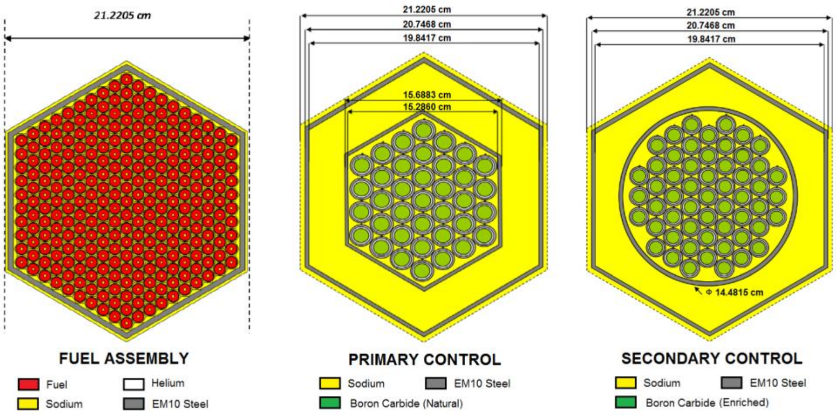

FIG. 3. Layout of the assemblies in the 3600 MW core [13].

3.2 1000 MW Metallic Fuel Core

The core consists in the following elements:

- 180 fuel assemblies (78 in inner core and 102 in outer core, see Figure 4).
- 114 radial reflector elements.
- 66 radial shield elements.
- 19 control subassemblies (15 in primary system and 4 in secondary system).

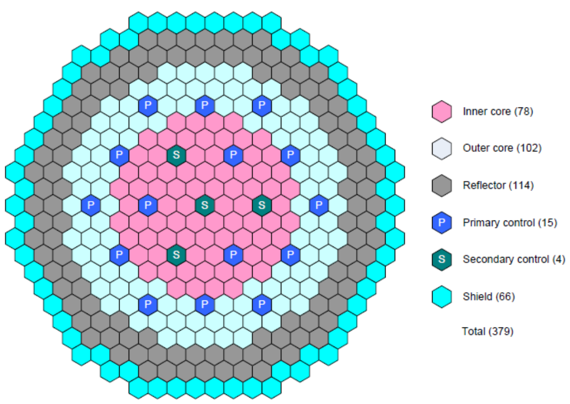

FIG. 4. Layout of the 1000 MW core [13].

As in the later case, the fuel subassembly's main features are summarized in Table II, the Figure 4 shows a cross section of the whole core and the description of each of its elements and Figure 5 shows the cross sections of the main assemblies in the core. As expected, the axial reflector and plenum sections on the core share the same geometric features as the fuel assembly but without the fuel pellet.

TABLE II: Characteristics of 1000 MW core's fuel subassemblies.

Whole Subassembly	Upper Structure	112.39 cm
	Gas Plenum	101.01 cm
	Sodium Plenum	20.06 cm
	Active Core Height	85.82 cm
	Lower Reflector	125.16 cm
	Lower Structure	35.76 cm
Subassembly pitch		16.2471 cm
Subassembly duct outer flat-to-flat distance		15.8123 cm
Subassembly duct wall thickness		0.3966 cm
Number of fuel pins		271
Outer radius of cladding		0.3857 cm
Inner radius of cladding		0.3236 cm
Fuel slug radius		0.3236 cm
Pin to Pin distance		0.8966 cm

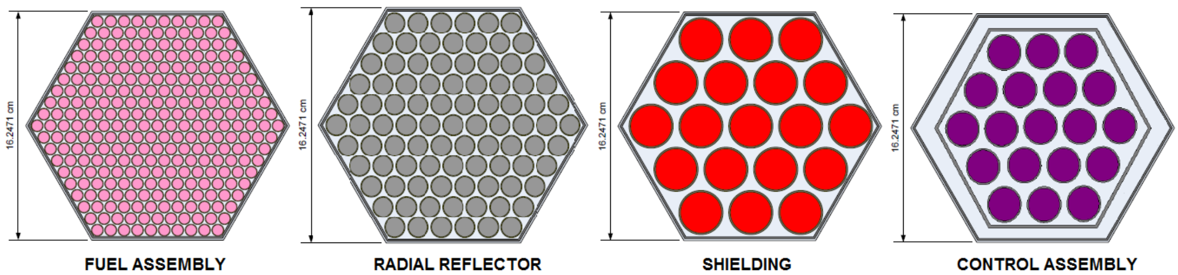

FIG. 5. Layout of the assemblies in the 1000 MW core [13].

4. Methodology for XS Generation

The methodology followed has been previously tasted [13] for XS generation on similar cores in which the way the XS are generated differ on fuel, non-fuel and peripheral fuel, in this section the methodology followed for each of the elements in the core is described.

4.1 Non Fuel Elements

For non-fuel elements, such as radial and axial reflector, Na and He plenums, shielding or control systems the main characteristics on the modeling were:

- 2D model.
- Radial reflection.
- Supercell consists on Non-fuel element surrounded by half of fuel assemblies (see Figure 6).
- 1,000,000 neutron stories per cycle, 330 active cycle, 30 inactive cycles.

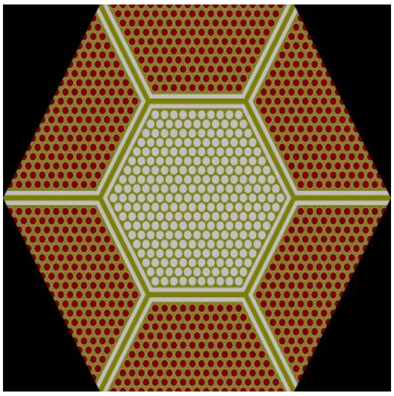

FIG. 6. Layout of the axial reflector supercell of the 1000 MW core.

4.2 Fuel Elements

Considerations made for fuel elements in both inner and outer zones of the core are treated in this section, it is important to note that for the fuel belonging to the most external ring of the outer zone, i.e. the one next to the radial reflector, a special treatment is done which will be described later. The considerations for the fuel are:

- 3D model.
- Radial reflection and no axial reflection.
- Whole active zone simulated at a time (supercell consists in five different axial layers, see Figure 7).
- XS generated for each fuel zone included in the whole active zone.
- 1,000,000 neutron stories per cycle, 330 active cycle, 30 inactive cycles.

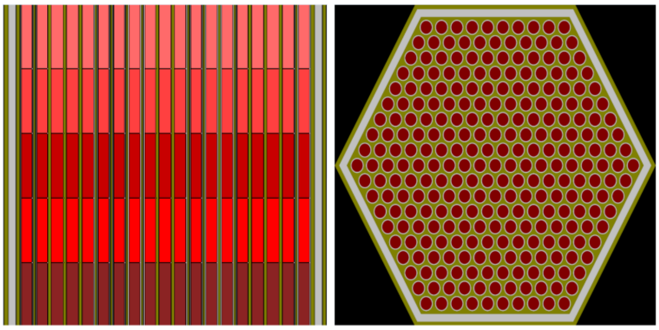

FIG. 7. Side cut (left) and cross section (right) of a given fuel assembly of the 1000 MW core.

4.3 Fuel Elements on the Most External Ring

A special treatment is needed for the most peripheral fuel elements in order to take into consideration the contribution of the reflector on the smothering of the neutron spectrum in that region. The considerations were the following:

- 3D model.
- Radial reflection and no axial reflection.
- Three types of materials included: radial reflector, peripheral (which is in contact with the reflector) fuel and regular fuel (see Figure 8).
- Regular fuel and peripheral fuel are identical but defined as two different materials in order to treat them separately.
- Whole active zone simulated at a time (supercell consists in five different axial layers in the two fuel regions, see Figure 8).
- XS generated only in the fuel region belonging only to the peripheral fuel assemblies.
- 1,000,000 neutron stories per cycle, 330 active cycle, 30 inactive cycles.

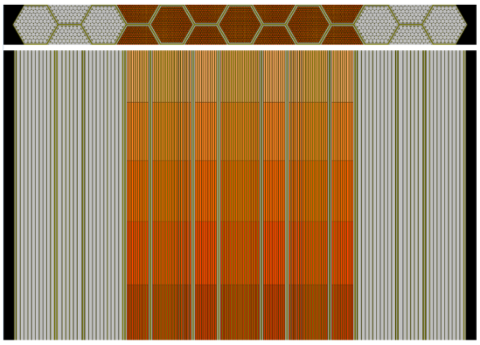

FIG. 8. Side cut (down) and cross section (up) of the supercell used for XS generation on the peripheral fuel assembly of the 1000 MW core.

4.4 Neutron Energy Grouping

As the energy section of diffusion equation is discretized, the neutron energy spectrum has to be discretized into energy groups in order to generate XS for each of them, in this work the energy spectrum was segmented in 24 groups, the upper energy limits of each group are shown in Table III. This segmentation used has been previously used in similar problems [13] by other research teams.

TABLE III: Neutron energy groups limits.

Group	Upper Limit [MeV]	Group	Upper Limit [MeV]	Group	Upper Limit [MeV]
1	2.0000E+01	9	3.0197E-01	17	5.5309E-03
2	1.0000E+01	10	1.8316E-01	18	3.3546E-03
3	6.0653E+00	11	1.1109E-01	19	2.0347E-03
4	3.6788E+00	12	6.7379E-02	20	1.2341E-03
5	2.2313E+00	13	4.0868E-02	21	7.4852E-04
6	1.3534E+00	14	2.4788E-02	22	4.5400E-04
7	8.2085E-01	15	1.5034E-02	23	3.1203E-04
8	4.9787E-01	16	9.1188E-03	24	1.4894E-04

5. Results and discussion

Three cases for simulations were considered: a) Core operating under nominal conditions, b) The core has all the Control Rods (CR) completely inserted, and c) The fuel assemblies have no sodium inside. In the present section the results of the simulations will be presented, as well as a brief discussion on it.

TABLE IV: Results of k_{eff} on the simulated cores.

	1000 MW Metallic Core		**Error* [pcm]**	**3600 MW MOX Core**		**Error* [pcm]**
	SERPENT	**AZNHEX**		**SERPENT**	**AZNHEX**	
Nominal Conditions	1.01989	1.02192	-199	1.01326	1.01157	167
CR inserted 100%	0.92797	0.92358	473	0.95366	0.94998	386
Na voided	1.04114	1.05008	-859	1.02734	1.03549	-794

*Relative error calculated as: $\frac{Serpent-AZNHEX}{Serpent} * 1x10^{5}\ \ pcm$

In Table IV the obtained k_{eff} values for the different simulated cores are shown. As can be seen, the results obtained with AZNHEX show good agreement if are compared with the ones obtained with SERPENT in the case of nominal conditions and with bigger differences in the other cases.

The relative error for results under nominal conditions is only a couple hundreds of pcm, this is a notorious result since given the difference of methodologies followed by the solvers (SERPENT is a stochastic/continuous-energy code and AZNHEX is a deterministic/multi-group code). The operation neutron spectrum of fast reactor is also a factor on these results, since fast reactors have, in general, a longer mean free path, the results are not much affected by the fact that SERPENT considers the heterogeneity of the geometry and AZNHEX treats each region with homogenized XS; in the case of thermal reactors special treatment must be done to take into consideration these heterogeneities.

As mentioned before, in the case of the core with the CR inserted and especially in the case with no sodium in the fuel zones, the discrepancy between codes is considerably bigger than in the nominal conditions. One explanation for this can be that this is an effect of the methodology for XS generation itself, most of the XS were calculated isolated (with the exception of the peripheral fuels where the impact of the neighbor reflector was considered) and no special treatment was used for materials that are next to others. This can become an issue when we have regions with widely different absorption XS next to each other (such as fuel/absorbent vicinity), as in the case of core with the CR inserted; and it can have a much smaller effect in the nominal conditions where the CR are above the active zone where most of the neutronic activity is taking place.

As a further step from this research, a new strategy for XS generation can be implemented where the mention considerations can be taken into account.

6. Conclusions

Based on the numerical results here above given and the discussion about them, it can be concluded that the AZNHEX code is a promising tool to the study of nuclear reactor cores with hexagonal-z geometry. Regarding the numerical results, it is important to point out that the differences are bigger than those taken as references when the core exhibit a localized larger absorption which can be diminished once that discontinuity factors may be included. Nonetheless the fact that differences are less than 200 pcm for smooth scenarios and 800 for non-smooth ones motivates the AZTLAN neutronic team to improve AZNHEX code to obtain better results than the ones here above given and to study its behavior for time-dependent problems.

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