Verification of the neutron diffusion code AZNHEX by means of the Serpent-DYN3D and Serpent-PARCS solution of the OECD/NEA SFR Benchmark

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Abstract. AZNHEX is a neutron diffusion code for hexagonal-z geometry currently under development as part of the AZTLAN project in which a Mexican platform for nuclear core simulations is being developed. 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. The main objective of this work is to test the AZNHEX code capabilities against two well-known diffusion codes DYN3D and PARCS. In a previous work, the Serpent Monte Carlo code was used as a tool for preparation of homogenized group constants for the nodal diffusion analysis of a large U-Pu MOX fueled Sodium-cooled Fast Reactor (SFR) core specified in the OECD/WPRS neutronic SFR benchmark. The group constants generated by Serpent were employed by DYN3D and PARCS nodal diffusion codes in 3D full core calculations. A good agreement between the reference Monte Carlo and nodal diffusion results was reported demonstrating the feasibility of using Serpent as a group constant generator for the deterministic SFR analysis. In order to verify the under-development solver inside AZNHEX, the same Serpent generated cross sections sets for each material were exported to AZNHEX format for four different states (as in DYN3D and PARCS): a) a reference case in which the multiplication factor (k_{eff}) is the compared value, b) the Doppler constant (K_D), c) the sodium void worth, and d) the total control rod worth. Additionally, the radial power distribution was also calculated. The results calculated with AZNHEX showed also a quite good agreement in the direct comparison with DYN3D (-66 pcm in k_{eff}) and PARCS (-109 pcm in k_{eff}) and therefore against the Serpent reference solution (-194 pcm in k_{eff}). As AZNHEX is still under development further improvements will be implemented and new tests will be carried out, but so far, the results presented here give confidence in the development.

Key Words: AZTLAN Platform, AZNHEX Hexagonal Code, DYN3D, PARCS.

1. Introduction

A huge interest on developing reactor analysis tools for hexagonal geometry reactors have been increasing lately due to the current development of GEN-IV systems which include fast reactors with this geometry.

Even though Monte Carlo-based (MC) codes have the advantage of very trustworthy results with the capability of modeling complex geometries, they have the disadvantage of being very computational intensive.

It is a reality that with time, the computer power shall be more powerful and cheaper, so that MC can be more widespread used; nevertheless, in developing countries is still hard to get the computer power required for its use on very intensive problems.

In Mexico, the AZNHEX code, a neutron diffusion solver for hexagonal-z geometry, is currently under development and it is part of the Mexican platform for analysis and design of nuclear reactors: AZTLAN platform. The objective of this paper is to compare the performance of AZNHEX against the deterministic codes DYN3D and PARCS, and the MC code SERPENT, as part of the verification process of AZNHEX.

2. Description of the codes

In this section, all the codes used in this paper will be briefly explained. The idea is for the reader to have a basic knowledge of the codes operation, capabilities and limitations. As a large amount of information is available about PARCS, DYN3D, and Serpent codes in the literature, the focus will be on the domestic code AZNHEX.

2.1 PARCS

PARCS is a deterministic 3D code developed at Purdue University and endorsed by the United States Nuclear Regulatory Commission. Its capabilities [1] include:

- Multi-group diffusion and Simplified P3 (SP3) solvers.
- Time-dependent solutions for transients and burnup.
- Treatment of Cartesian and hexagonal geometries.
- Transient simulation capabilities.
- Corrections for control rod treatment.
- Decay heat and Xe/Sm treatment

Cross Sections (XS) sets must be given to PARCS for a calculation.

2.2 DYN3D

The code DYN3D is another deterministic 3D code originally developed for Light Water Reactors (LWR) but extended for Sodium Fast Reactors (SFR) [2, 3]. Its capabilities are very similar to those of PARCS. Thermal-hydraulic modules have been implemented for one-phase and two-phase coolant flow treatment. As well as PARCS, XS for the specific problem need to be generated prior to the use of DYN3D.

2.3 Serpent

Serpent is a 2D/3D Monte Carlo reactor physics code with burnup capabilities developed at VTT Technical Research Centre of Finland. The developers [4] suggest its use on (among other uses):

- Spatial homogenization and group constant generation for deterministic reactor simulator calculations.
- Validation of deterministic lattice transport codes.

As can be deduced, Serpent meets the right requirements for XS generation for the verification and validation of the newly developed code AZNHEX.

2.4 AZNHEX

The code AZNHEX is part of the "AZTLAN Platform" project [5], a joint effort led by the National Institute of Nuclear Research of Mexico (ININ) that gathers the main public universities in Mexico which are the National Autonomous University of Mexico (UNAM), National Polytechnic Institute (IPN) and the Metropolitan Autonomous University (UAM), in an effort to put Mexico in a competitive position on reactor analysis matters.

AZNHEX [6] is a novel tool aimed to the design and analysis of cores with straight hexagonal prisms. It is based on the solution of the diffusion equations in 3D for steady state or time-dependent problems, for the calculation of the effective neutron multiplication factor k_{eff}, neutron flux and power distribution.

2.4.1 Theoretical basis of the code AZNHEX

The nodal methods for nuclear reactor analysis were developed in the late 70's, and are in general, a way to obtain an approximate solution of a function , in this case the scalar flux, by a continuous polynomial function on each cell of a discretized domain. In a nodal method, every cell is characterized by a set of Legendre moments of the unknown function [7], the whole cells give shape to the core and the physical properties can be homogenized on each cell. In the Figure 1 it can be seen the representation of a cell where *L*, *R*, *N*, *F*, *B* and *T* stands for Left, Right, Near, Far, Bottom and Top faces, and C is used to denote the cell.

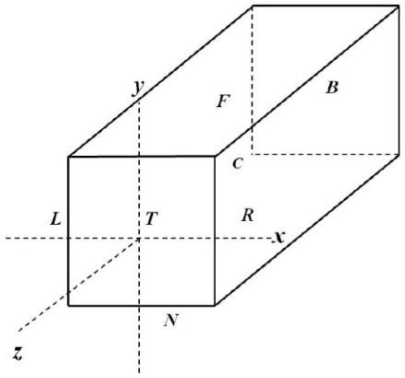

FIG. 1. Representation of a cell in rectangular coordinates.

The method RTN-0 (Raviart-Thomas-Nédelec order 0) is the simplest one of this family and is used in the code AZNHEX; with order 0 the number of unknowns is 7: one for each face moment and one for the cell moment, with order 1 the number of unknowns is 32: 4 per face and 8 per cell. To determine the total number of unknowns which are the average fluxes on each face and in the cell, this method uses the discretization of the domain implicitly made by the discretization of the diffusion equations.

The nodal base functions defined by Legendre polynomials are used then to approximate globally the neutron flux, thus resulting in an approximation $\varphi(x, y, z)$.

The core geometry considered here has two main disadvantages that make difficult the application of nodal methods: it is not tensorizable and it cannot be divided into straight hexagonal prisms which cross section be smaller hexagons than the original ones; one option in order to tackle these difficulties is to use a transformation of the hexagonal cross section of each prism into straight prisms which cross sections are squares in order to apply the known nodal methods.

The idea behind this is to map each one of the quarters of each hexagon to a square using the Gordon-Hall blending method [8] [9] as seen in Figure 2. Applying the mentioned method, a whole cell is then turned into four straight prisms which cross sections are squares as seen in Figure 3.

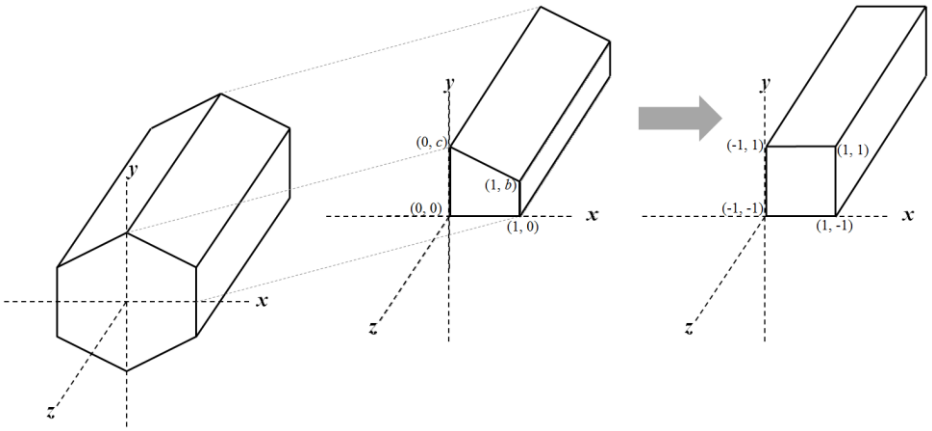

FIG. 2. Coordinates transformation from one quarter of straight hexagonal prism in one with a square cross section.

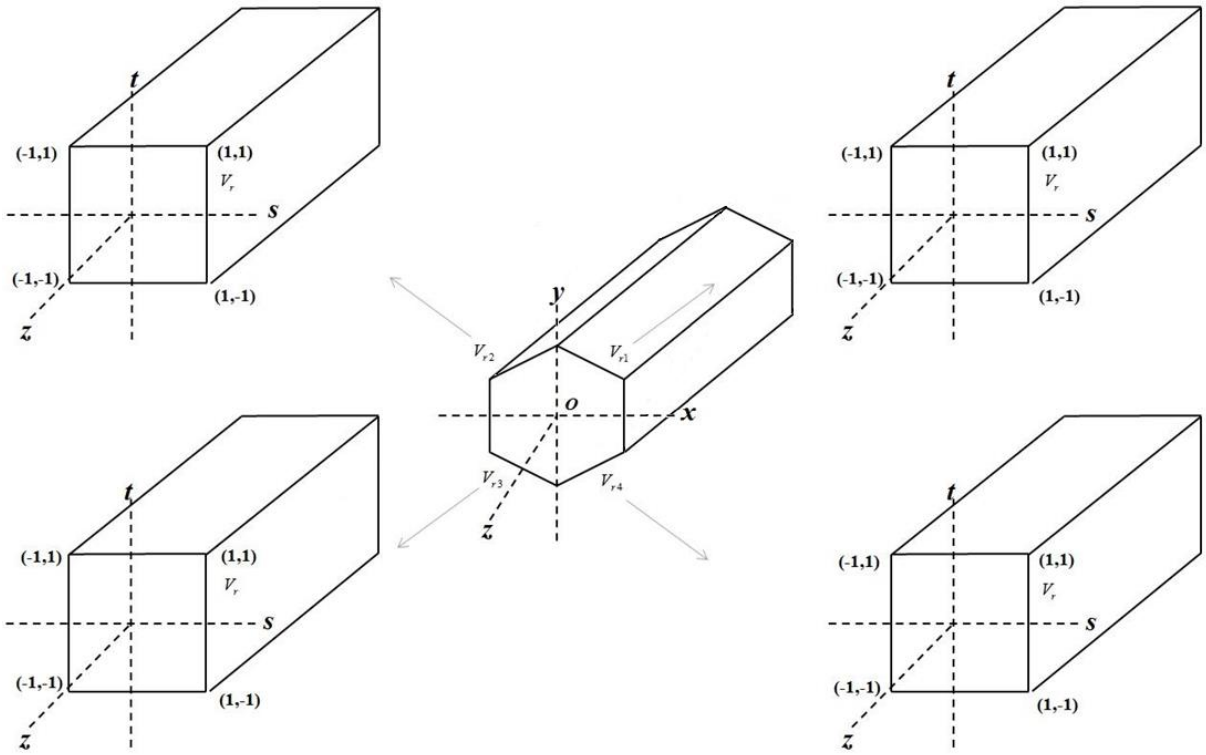

FIG. 3. Transformation of a straight hexagonal prism cell into four straight prisms with square cross sections.

The Figure 4 shows how an array of straight hexagonal prism elements is transformed into an array of straight square prisms, where every straight square prism contains four smaller straight square prisms (not shown in the Figure).

The intention of this section is not to derive the whole mathematical analysis but only to show the basics of the nodal methods as well as the Gordon-Hall blending method. If the reader is interested in read a deeper analysis, we strongly suggest to go to the referenced work [6][7][8].

For the energy dependence, the code is based on the multigroup theory consisting in separate the whole energy spectrum, and the XS are replaced by a mean value in each segment instead of a continuous value. Information about the multigroup theory and the discretization of a domain can be found in reference books [10], [11] and [12] and will not be treated here.

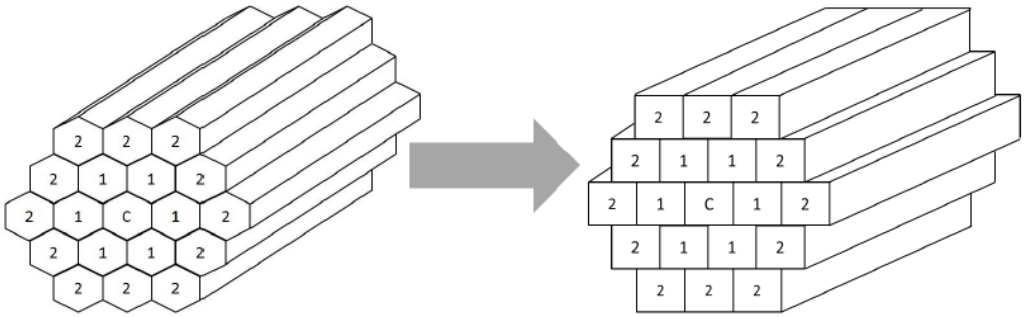

FIG. 4. Transformation of an array of cell elements.

3. Description of the Simulation

In this section a description of the case under study is given in a brief manner.

3.1 Main features of the core

The reactor simulated is a 3600 MW_t MOX-fueled core as defined in the SFR Benchmark Task Force of OECD/NEA Working Party on Reactor Systems (WPRS) [13]. It consists of 225 inner and 238 outer fuel assemblies, surrounded by 330 radial reflector assemblies as shown in Figure 5. The core also contains two independent control systems (CS) with different boron enrichment. Every fuel assembly contains 271 helium bonded fuel pins in the active zone, with steel pellets in the axial reflector region. The Figure 6 shows a cross section of the fuel and control assemblies and the Tables I and II describes the fuel assemblies and control systems.

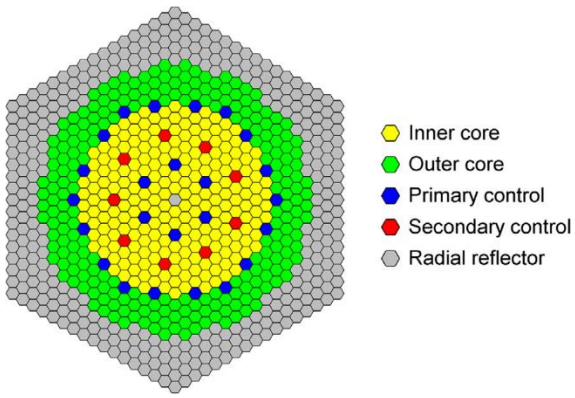

FIG. 5. Layout of the treated core [13].

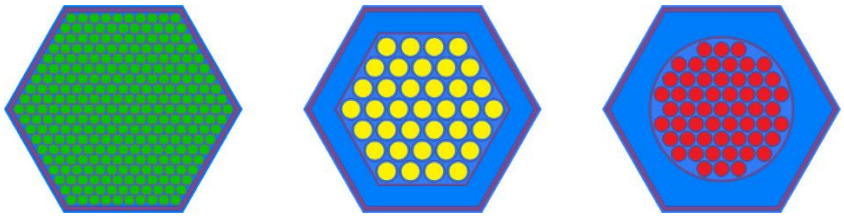

FIG. 6. Cross section of the fuel (left) Primary CS (center) and Secondary CS (right) [13].

TABLE I: MAIN CHARACTERISTICS OF THE FUEL SUBASSEMBLY.

Total sub-assembly height, cm	311.16
Lower gas plenum height, cm	89.92
Lower axial reflector height, cm	30.17
Active core height, cm	100.56
Upper gas plenum height, cm	10.06
Upper axial reflector height, cm	80.45
Sub-assembly pitch, cm	21.22
Outer duct width (flat-to-flat), cm	20.7468
Inner duct width (flat-to-flat), cm	19.8418
Number of fuel pins	271
Outer cladding radius, cm	0.5419
Inner cladding radius, cm	0.4893
Fuel pellet radius, cm	0.4742
Pellet material	$(U,Pu)O_2$
Central hole radius, cm	0.1257
Pin pitch, cm	1.1897

TABLE II: MAIN CHARACTERISTICS OF THE CONTROL SYSTEMS.

	Primary CS	**Secondary CS**
Ext. Duct Outer Width, cm	20.7468	20.7468
Ext. Duct Inner Width, cm	19.8418	19.8418
Int. Duct Outer Width, cm	15.6883 (flat-to-flat)	14.8838 (diameter)
Int. Duct Inner Width, cm	15.2860 (flat-to-flat)	14.4815 (diameter)
Number of pins	37	55
Outer cladding radius, cm	1.1476	0.8222
Inner cladding radius, cm	1.0474	0.7709
Pellet radius, cm	0.9202	0.7039
Pellet material	B_4C (19.9 wt% B-10)	B_4C (90.0 wt% B-10)
Pin pitch, cm	2.4438	1.7519

3.2 Cross Sections considerations

The XS for all the deterministic codes were generated using the MC code Serpent, as mentioned previously this is one of the features of the code. For the XS generations some considerations were done depending on which material is being calculated:

- For fuel assemblies that are not part of the most external fuel ring, the XS were generated

using 3D models radially reflective and axially black, for a more realistic treatment the whole assembly (with its five axial layers) was considered instead of a by-fuel treatment.

- For the outermost fuel assemblies, a special treatment is used where a layer of radial reflector is considered, also in a 3D model with radial-only reflection.

- For non-fuel elements a 2D model with radial reflection was used, where a supercell contains also some fuel surrounding the non-fuel assemblies.

A 24-energy group scheme as shown in Table III was used.

TABLE III: SEGMENTATION OF THE ENERGY SPECTRUM.

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

In Serpent calculations for XS generations 1500 active cycles were used and 200 skipped with 640,000 neutron histories per cycle, giving a total of 960 million of active neutron histories.

4. Results and discussion

The parameters to be compared between the codes are four:

- k_{eff}: Effective neutron multiplication factor.
- K_D: Doppler constant.
- $\Delta\rho_{Na}$: Sodium void worth.
- $\Delta\rho_{CR}$: Control rod worth.

In order to calculate the Doppler constant two reactivities need to be calculated, one at nominal conditions (1500 K) and one at perturbed conditions (3000 K), and it is calculated as:

$$K_D = \frac{\rho_{per} - \rho_{nom}}{\ln \frac{T_{per}}{T_{nom}}}$$

The sodium void worth is calculated as the difference in reactivity due to the extraction of all the sodium (void) in the active zone and the reactivity on nominal conditions:

$$\Delta\rho_{Na} = \rho_{void} - \rho_{nom}$$

The control rod worth is calculated by the difference between the reactivity in nominal conditions and its value when al CR are inserted:

$$\Delta\rho_{CR} = \rho_{CR} - \rho_{nom}$$

Given the later explanation of how the parameters are calculated, the results of the Serpent and the three deterministic codes are shown in Table IV. Table V shows the differences in absolute value when comparing AZNHEX against the other three codes.

TABLE IV: RESULTS OF CORE SIMULATIONS.

	Serpent	**DYN3D**	**PARCS**	**AZNHEX**
k_{eff}	1.01070	1.00940	1.00984	1.00873
K_D (pcm)	-852	-867	-868	-878
$\Delta\rho_{Na}$ (pcm)	1864	1951	1945	2019
$\Delta\rho_{CR}$ (pcm)	-6046	-6173	-6227	-6046

TABLE V: DIFFERENCES IN PCM (ABSOLUTE VALUE) AZNHEX VS OTHER CODES.

	AZNHEX vs Serpent	**AZNHEX vs DYN3D**	**AZNHEX vs PARCS**
k_{eff} (pcm)	194.9	66.37	109.9
K_D (pcm)	26	11	10
$\Delta\rho_{Na}$ (pcm)	155	68	74
$\Delta\rho_{CR}$ (pcm)	0	127	181

As requested in the benchmark specifications, the comparison between Serpent and deterministic codes was made for the power in the main diagonal [13, 14] and the evaluated results are presented in Figure 7. The radial power distribution predicted with AZNHEX is in a very good agreement with the reference MC solution calculated with Serpent and with the other two deterministic codes (DYN3D and PARCS).

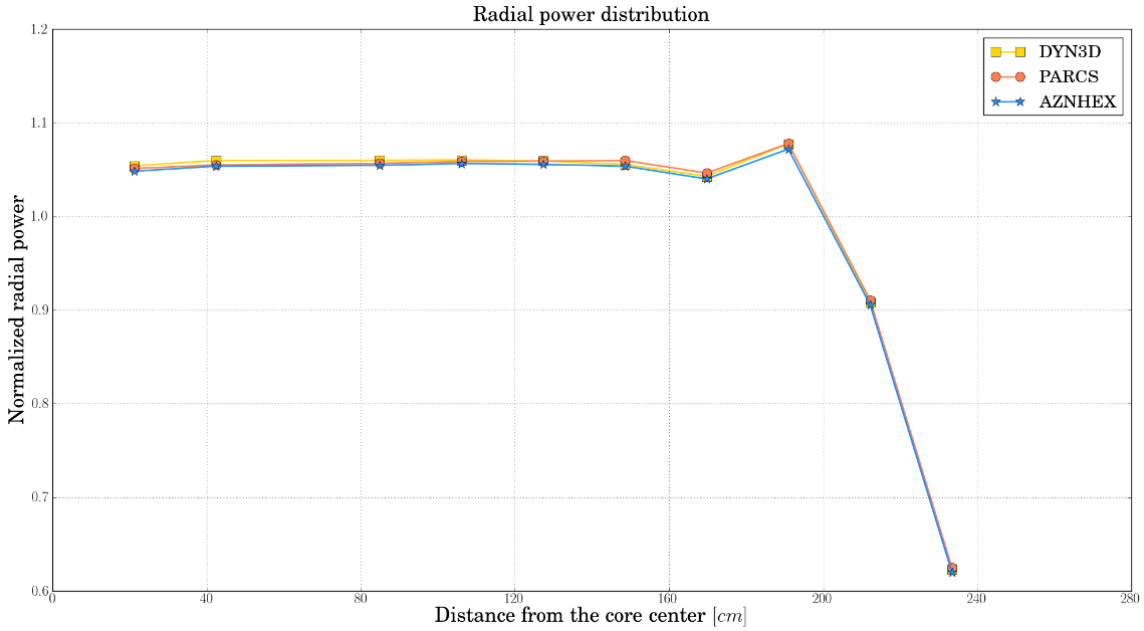

FIG. 7. Comparison of radial power distribution.

The integral results between Serpent-DYN3D and Serpent-PARCS are very similar and were already compared and discussed in [14], thus, discussion will focus in the differences of AZNHEX against the other codes. It should be noted that since AZNHEX does not include the SP3 solver, the comparison between the three deterministic codes was limited to the diffusion solutions.

In general, the results obtained with AZNHEX show also very good agreement. The differences in k_{eff} of AZNHEX vs. DYN3D and AZNHEX vs. PARCS are 66 pcm and 109 pcm respectively and 194 when comparing directly with Serpent. These results are considered acceptable and give confidence that the methodology of the solver inside AZNHEX is well implemented.

In the other compared parameters similar values in pcm were obtained. It is worthy to mention that the value of $\Delta\rho_{CR}$ calculated with AZNHEX is exactly the same as Serpent although differences of 127 and 181 pcm were found when comparing with DYN3D and PARCS respectively. Same values on direct reactivity calculations are generally not expected as the methodologies are different (stochastic vs deterministic) nevertheless as this coefficient is a difference instead of the absolute value, it is possible to have equal values although the deviations in a direct comparison could be higher.

Regarding the normalized radial power in the main diagonal, the AZNHEX code result is in concordance with the other deterministic codes with just small differences.

5. Conclusions

In general, the AZNHEX results showed some higher discrepancy from Serpent than DYN3D and PARCS, however, such discrepancy can be considered acceptable for a novel development. It can be concluded that the AZNHEX obtained results compared very well against the other well validated and known codes DYN3D and PARCS and also while comparing against the stochastic code Serpent. The resulting differences are small enough to consider the comparison a success, but there is still work to do in order to further verify and validate the AZNHEX code.

The performance of the domestic code AZNHEX encourages and motivates the development team to keep on in this direction and to contribute to the AZTLAN platform in order to achieve the objective to put Mexico in a competitive place in nuclear analysis worldwide.

6. Acknowledgements

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