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Python tool for parametric modeling and simulation of a generic SMR reactor core with Thorium-Uranium fuel.

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1. Introduction

In this work we tried to build a python-based tool to investigate the critical configuration for an SMR core reactor, based on a NuScale model (MASLWR)[1] as a generic model. The python tool will generate the corresponding geometry of 24 square fuel assembly, with 17x17 fuel pin for each assembly as is shown in Fig. 1. The fuel is made from a homogeneous mixture from UO_2 and ThO_2 within a Zircalloy-4 cladding. The whole fuel pin with cladding are presents in a light water as moderator within a square cell. Core barrel and Primary vessel cylinder, are made both from stainless-steel. Detailed characteristics of the reactor are given in Table 1 below.

In the aim to achieve criticality calculation and obtention of some neutron parameters, namely neutron flux and reaction rates, the standards of the widely used code MCNP [2] are adopted here and included in the python scripts to generate the corresponding input file. In the same way it is possible to execute the Monte-Carlo code in automatic way by means of the python code, read the output file to check the $k_{eff}(enr_{U5})$ value and look for the corresponding U5 enrichment to obtain a critical core. It was also possible by means of plotting libraries in python (matplotlib) to represent graphically the neutron flux spectrum, spatial flux distribution and reaction rates (fission and gamma-capture). In parallel, a similar work is underway using the opensource Monte-Carlo code, namely OpenMC [3].

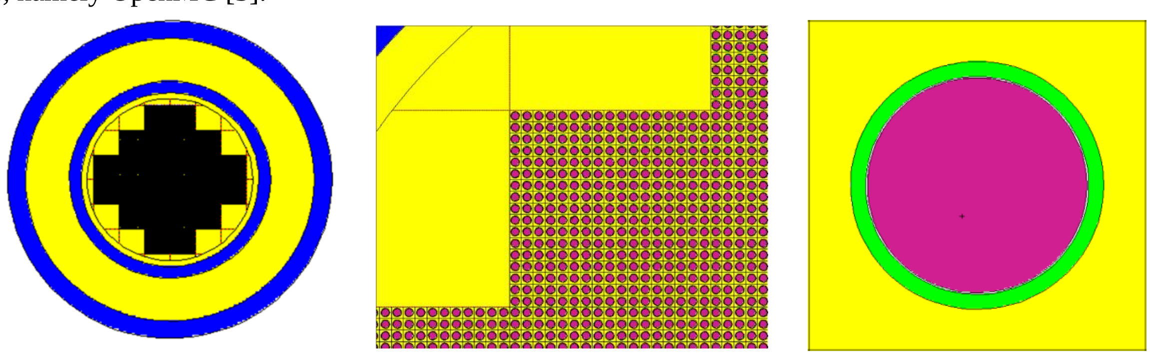

Figure 1: From left to right (a) The axial cross section of the reactor, (b) The fuel assembly (17x17), (c) The fuel cell (Pin, cladding and moderator)

It should be noticed that fuel mixture is considered with volume approach, where:

$$V_{UO2}[\%] + V_{ThO2}[\%) = 100\% \quad (1)$$

By considering both oxydes and resulting fuel as incompressible material, the fuel density is given by:

$$\rho_{fuel}[g/cc] = V_{UO2}[\%] \times \rho_{UO2} + V_{ThO2}[\%] \times \rho_{ThO2} \quad (2)$$

Table 1. Characteristics of the nuclear reactor core elements

Element/parameter	Value	Element/parameter	Value
Fuel pin diameter	0.8259 cm	Active fuel height	100 cm
Cladding Inner diam.	0.8379 cm	Core barrel Inn/Out height	136.70/176.70 cm
Cladding outer diam.	0.9522 cm	Prim. Vess. Inn/Out height	305.50/365.50 cm
Pin pitch	1.2626 cm	ρ_{UO2}	10.60 g/cc
Core Barrel Inner diam.	150.00 cm	ρ_{ThO2}	9.86 g/cc
Core Barrel Outer diam.	170.00 cm	ρ_{Z-4}	6.56 g/cc
Prim. Vess. Inner diam	244.00 cm	ρ_{SS}	7.76 g/cc
Prim. Vess. Outer diam	274.00 cm	ρ_{Wtr}	1.0 g/cc

2. Methodology

As is shown in Fig.2, we build a based python [4] code (MCNP_Input_Generator.py) to generate a typical MCNP input file corresponding to the NuScale model. Then, the criticality prospector code, will invoke MCNP_Input_Generator.py program to generate the corresponding configuration input file and execute the MCNP simulation. At the end of each simulation is possible to read and then read the output file and check the multiplication factor value k_{eff}(with its standard deviation). At this stage, a decision loop is set up to continue the calculation if criticality is not obtained, by modifying the input file (U5 enrichment value is taken here as a variable) and recalculate the k_{eff} until the value of this factor is obtained within the tolerance interval, defined in this study to be $0.99500 \leq k_{eff} \leq 1.00500$. The criticality prospecting will be stopped when the U5 enrichment corresponding to critical situation is obtained.

3. Results and Discussion

Several configurations were simulated corresponding to the six values of V_{ThO2}[%]. The needed U5 enrichment to reach criticality is prospected and for each situation it is possible to get the average neutron flux spectrum, spatial flux distribution and reaction rates. Initially, MCNP simulations were carried out with 5000 neutrons/cycle with 50 inactive cycles and 100 active cycles to get rapidly close to the critical situation. With this choice, each simulation took about 4 minutes of time machine calculation. Once low precision criticality results are obtained, finest calculations are conducted with 20000neutrons/cycle with 400 active cycles. The criticality calculation results are recapitulated in Table2.

Table 2. Needed U5 enrichment corresponding to critical configuration

Configuration	V_{UO2}[%]	V_{ThO2}[%]	Critical enr_{U5}[%]	Number of Iterations
1st Configuration	99	1	**8.6**	4
2nd Configuration	75	25	**14.6**	6
3rd Configuration	67	33	**16.6**	2
4th Configuration	50	50	**23 .6**	7
5th Configuration	33	67	**34.6**	11
6th Configuration	25	75	**45.6**	11

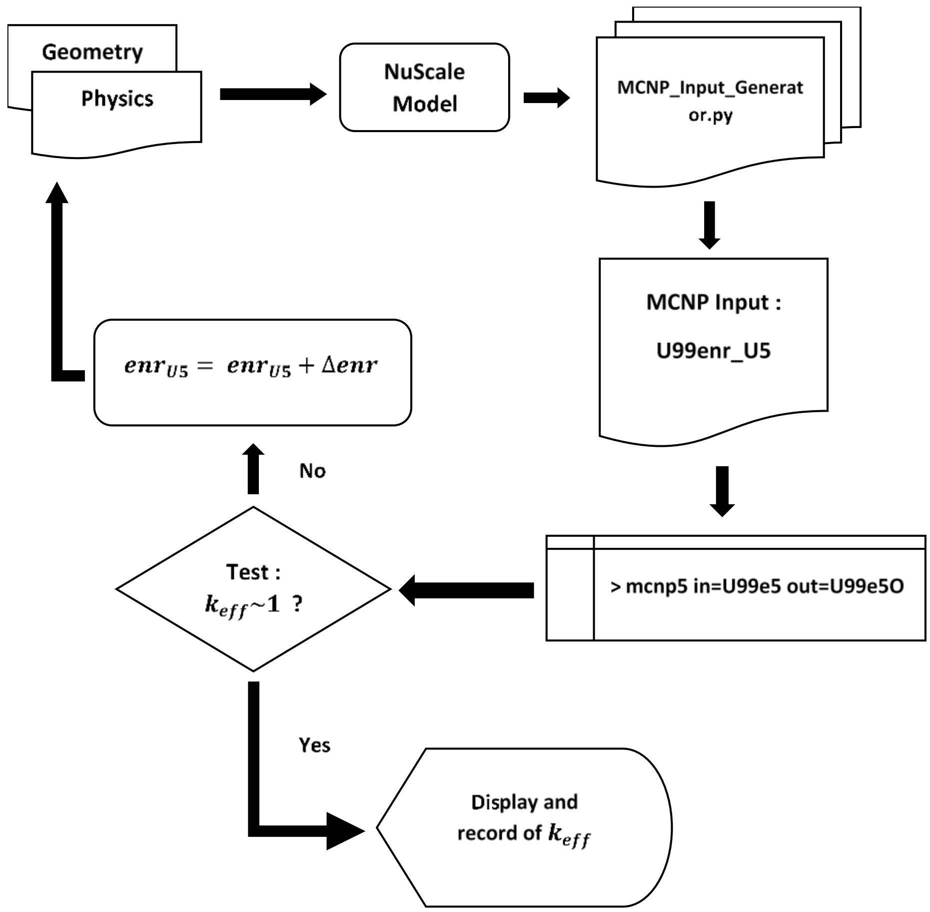

Figure 2. The flowchart diagram of the python code to investigate critical configuration

For each configuration, the neutron flux spectrum is obtained from the F4 tally (normalized flux) multiplied the conversion factor S given by:

$$S = \frac{P[MW] \times 10^6 \times \nu[n]}{Q[MeV.n_{src}{}^{-1}] \times 1.602 \times 10^{-13}[J.MeV^{-1}]}$$

In our case a fission induced thermal power of $1MW$ is considered as a reference value (power unit for nuclear reactor) to define a conversion factor of $S = 7.62 \times 10^{16}$

Thus, we can obtain the physical flux as follows: $\Phi[n.cm^{-2}.s^{-1}] = S \times F4$.

Fig. 3 shows the flux spectrum averaged on all the fuel volume in the reactor core. All the configurations present the same allure of the flux spectrum with a slight shoulder on the left for the first configuration where fuel it is made essentially from UO_2. The flux spectrum presents an epithermal dominance with less thermal contribution. The integral contribution may be obtained from the output file, where more than 60% of epithermal neutrons are involved in the fission reaction chain, where thermal neutron presents less than 30% and the rest is induced from fast neutrons.

By using FMSEH tally it was also possible to obtain the spatial distribution of some neutronic parameters on the central cross-section to the reactor (at Z = 0 with a thickness of 10cm). As it is shown in Fig. 4, spatial distribution -corresponding to 6th configuration ($V_{ThO2} = 75\%$)- of neutron flux, fission reaction rate and capture reaction rate are produced from FMESH files and graphically interpreted by using Matplotlib python's library.

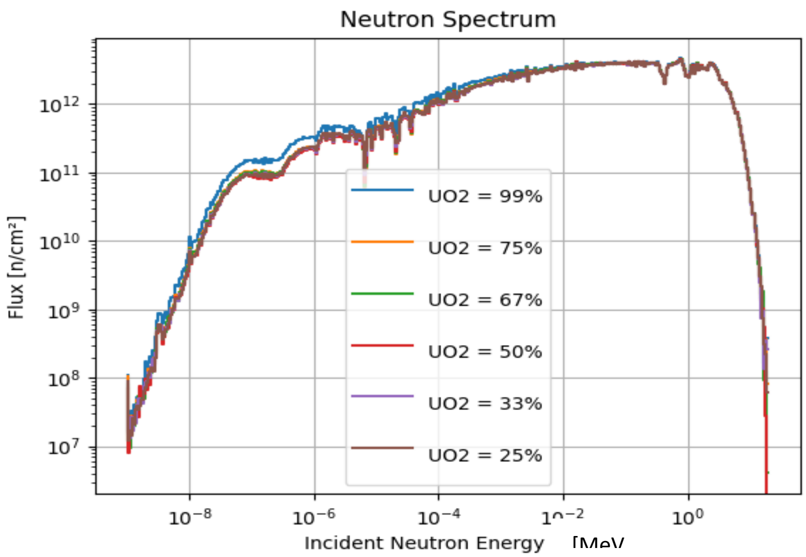

Figure 3. The neutron flux spectrum for six configurations simulated with MCNP

Fig. 4 shows that the neutron flux is mainly central and the fission and capture rate are well correlated to this flux. We can also see that the inner surface of the core barrel is well irradiated with neutron flux and experienced a high rates of neutron capture in the first centimeters.

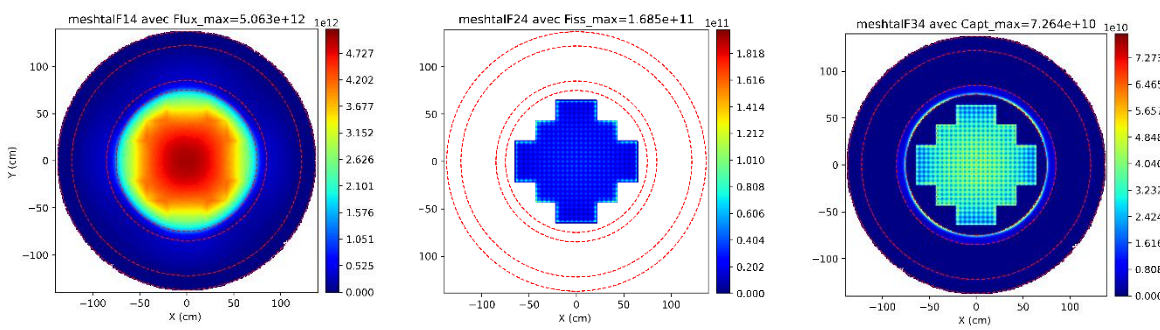

Figure 4. Spatial distribution of (from right to left): Neutron Flux, Fission reaction Rate and Capture reaction rate

4. Conclusions

This word was conducted as a project for students in Master degree, to learn and master coding with python programming language and take benefits from its capabilities and wide range of librairies and modules, freely available. Hence, it was possible to generate formatted file, execute third-party code and read output files, including a decision loop to investigate a specific situation as a function of a given parameters (U5 enrichment in this case). Modelling and simulation results may indicate some interesting features of using fuel made from a mixture of UO_2 and ThO_2. More results should be provided by another Monte-Carlo Code (OpenMC) to compare results and explore more features of the python native code.

References

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[3] Official Python Website: https://python.org