كلية الهندسة بشبرا
FACULTY OF ENGINEERING AT SHOUBRA
ERJ
PRINT ISSN 3009-6049
ONLINE ISSN 3009-6022

ENGINEERING RESEARCH JOURNAL (ERJ)
Volume (52) Issue (4)
October 2023, pp:82-87
https://erjsh.journals.ekb.eg

Core calculations of the Molten Salt Fast Reactor using different computational codes

Montaser Tharwat*[1], R. Y. Sakr[2,3], Nader M. A. Mohamed[1], Abdelfattah Soliman[4] and M. W. Al Dosoky[2]

[1] Department of Reactors, Egyptian Atomic Energy Authority. Egypt
[2] Department of Power Mechanical Engineering, Shoubra Faculty of Engineering, Benha University, Egypt
[3]Department of Mechanical Engineering, College of Engineering, Imam Mohammad Ibn Saud Islamic University.
[4] Egyptian Nuclear and Radiological Regulatory Authority, Egypt
* Corresponding Author
E-mail:mamdouh.aldesoky@feng.bu.edu.eg , rysakr@imamu.edu.sa, mnader73@yahoo.com, ausoliman@kau.edu.sa, m_th_elkady@yahoo.com.

Abstract: This study presents core calculations of the Molten Salt Fast Reactor using different codes. The KENO (one of the SCALE package) code was used at the beginning to calculate the multiplication factor K_{eff} for the benchmark design. After that, the TRITON (one of the SCALE package) was used to find the nuclear constants for the different regions of this design. These nuclear constants were used in the multi-physics code COMSOL to model the reactor and calculate the neutron flux Eigen values of the neutron diffusion equation and then calculate the multiplication factor K_{eff} and get the neutron flux distribution. This distribution was used to make a coupling between the neutronic and the thermal hydraulic of the reactor. The nuclear codes MCNP5 and WIMS were also used in modelling this reactor to calculate K_{eff}. The study showed the differences between the multiplication factor values from each code and compared them by the values from old reference studies and reflected the effect of the selection of the data libraries and the code on the results. It showed also the thermal hydraulic results for the benchmark as modelled by COMSOL.

Keywords: MSFR KENO TRITON MCNP COMSOL.

1. INTRODUCTION

This study is concerned with the nuclear calculations related to the Molten Salt Fast Reactor (MSFR), which is one of the most important types of the fourth generation nuclear power reactors. The reference MSFR which aimed in this study is a 3000 MWth. It has a spectrum of fast neutron with Thorium fuel cycle [1]. The COMSOL code was employed by Cammi et al. [2] for the first time in the study of nuclear reactors in 2007 by developing a specific module for neutronics. COMSOL proved to be a strong useful tool in solving coupled partial differential equations.

Lucotte et al. [3] showed The Thorium Molten Salt reactor without using moderator and its advantages like simplicity, viability, performance in breeding and safety. They showed the important topics should be reviewed like the online control of the composition of the salt and the chemical and the physical properties and the enough safety verification. They also referred to the importance of the analysis of the motion of the precursors of the delayed neutrons.

A presented model that describes the turbulent flow, the turbulent transport of heat and the precursors and the mutually dependent neutron flux was presented by Linden et al.[4]. They showed that if the heat is extracted with the same flow rate, the MSFR transport reaches to the steady state operation passively. During steady state operation a large zone of recirculation is found through the core that causes the appearance of high temperatures which lead to the corrosion of the structural material with high rate. They concluded that different concentrations of precursors would have been detected and the precursors turbulent transport would not been accounted for.

The reference design of the concept of MSFR and the results from different parametric studies were defined and presented by Brovchenko et al.[5]. They have developed a tool for the calculation of the decay heat. They calculated the loss of heat sink transients with a tool based on point kinetics and studied their impact on the salt temperature of the fuel. The calculations of the residual heat are the basis of the draining system design because drainage must happen

for any shut down of the reactor whether in normal conditions or in the conditions of accidents.

Luzzi et al. [6] presented a multi-physics approach for modeling the behavior of the nuclear reactor core and applied this approach to study the Molten Salt Reactors dynamics. They designed a model to predict the velocity and temperature fields, neutron fluxes, and precursor concentrations

Fiorina [7] presented multi-physics modeling for a circulating nuclear fuel in a simple geometry by using COMSOL 3.3. This study was sufficient for primary evaluation of the thermal and physical behaviors of the system and showing the way for further complex study with realistic geometry.

Siemer [8] pointed out the reason that the concept of this reactor represents the most encouraging reactor in the fourth generation nuclear reactors. He mentioned causes like relatively simplicity, cheapness for building and operating, sustainability of the fuel cycle, relatively simplicity and cheapness of the radio waste management, benign accident consequences, no need for Uranium enrichment facilities after achieving steady state, and no generation and requirement for huge amounts of transuranic elements. The capabilities of this reactor were illuminated by Lantzos et al. [9] showing the impact of two fuel types on the performance of the burnup. They also investigated the transition from the second mode to the first. They developed a model to perform isotopic evolution calculations in the fertile blanket.

2. The benchmark description

The core is a square cylinder where the nuclear reactions happen inside the flowing salt. The core composition and the parameters are abbreviated in Table 1. The geometry details of the benchmark are illustrated in Fig.1.

The molten salt acts as fuel and coolant in the same time. The core contains a fluoride salt. It is composed of 77.5 molar % of LiF which enriched in ^{7}Li (99.999 at %) and 22.5 molar % of heavy nuclei includes fissile element. The HN fraction is fixed during the reactor evolution, the FPs produced replacing an equivalent proportion of the lithium. The neutronics benchmark emphases on the ^{233}U-started MSFR.

As shown in Table 1, the initial fuel is composed of LiF-ThF_4-$^{233}UF_3$ in this case. The fraction of ^{233}U is adjusted initially to have a critical reactor. The radial reflector is a fertile blanket. It is filled with LiF-ThF_4 with the mentioned fractions. The blanket is surrounded by a B_4C layer for absorbing the remaining neutrons. The reflectors are made of a Ni-based alloy with density equal to 10 g/cm^3. Its composition is shown in Table 2. The density of B4C is 2.52016 g/cm^3.

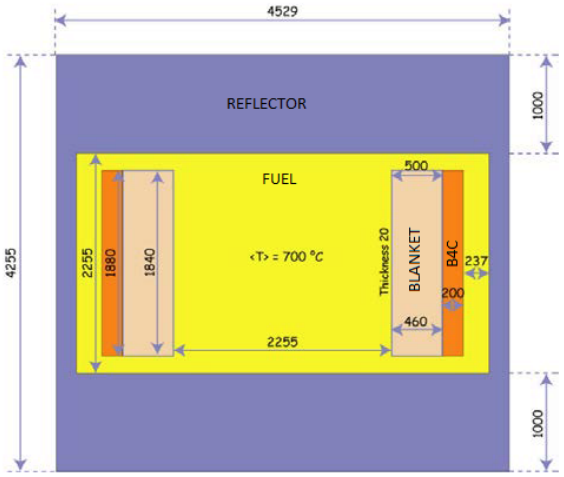

Fig. 1. Model used in neutronic simulation (dimensions in mm). [1]

Table 1. Characteristics of the MSFR simulated on the neutronics benchmark [1]

Thermal power (MWth)	3000
Electric power (MWe)	1500
Fuel initial composition (mol %)	LiF-ThF4-233UF4 with 77.5 % LiF
Blanket initial composition (mol %)	LiF-ThF4 (77.5%-22.5%)
Melting point (°C)	565
Input/output operating temperature (°C)	650 - 750
Initial inventory (kg)	233U-started MSFR Th 38300 233U 5060
Density (g/cm3)	4.1249
Core dimensions (m)	Radius: 1.1275 Height: 2.255
Volume of the Fuel Salt (m3)	18 9 out of the core 9 in the core
Volume of the Blanket Salt (m3)	7.3
Total cycle of the fuel salt in the system	4.0 s

Table 2. Composition (%) of the Ni-based alloy used in simulation [1]

Ni	W	Cr	Mo	Fe	Ti	C
79.432	9.976	8.014	0.736	0.632	0.295	0.294

Mn	Si	Al	B	P	S
0.257	0.252	0.052	0.033	0.02	0.004

3. Calculation tools

This study used different codes for modelling the MSFR. The KENO code was used in the beginning to calculate the multiplication factor K_{eff} for the benchmark of the MSFR. Then, the TRITON code was used to find the nuclear constants. These nuclear constants were used in the multi-physics code COMSOL to model this reactor and calculate the neutron flux Eigen values of the neutron diffusion equation and then calculate the multiplication factor K_{eff}. After that, COMSOL was used to get the neutron flux distribution. This distribution was used to calculate the reactor temperature distribution and the fuel salt velocity distribution by making a coupling between the neutronics and the thermal hydraulic using the turbulent model k-ε. The computational codes MCNP5 and WIMS were also used in modelling this reactor to calculate K_{eff} .

The nine-group diffusion equation and the six-group delayed neutron equation (Equations. 1, 2) [13] can be presented as follows:

$$\frac{1}{v^g}\frac{\partial \phi^g}{\partial t} + \frac{u}{v^g}\cdot\nabla\phi^g - \nabla\cdot D^g\nabla\phi^g + \left[\Sigma_a^g + \sum_{g'=1,\neq g}^{9}\Sigma_s^{g\to g'}\right]\phi^g = \sum_{g'=1,\neq g}^{9}\Sigma_s^{g\to g'}\ \phi^{g'} + \frac{1}{k}\left(1-\beta_{eff}\right)x_\rho^g\sum_{g'=1}^{9} v\,\Sigma_f^{g'}\,\phi^{g'} + \sum_{i=1}^{6}x_i^g\,\lambda_i c_i \quad (1)$$

$$\frac{\partial Ci}{\partial t} + u\cdot\nabla C_i + \lambda_i c_i = \frac{1}{k}\beta_i\sum_{g=1}^{9} v\,\Sigma_f^g\,\phi^g \quad (2)$$

The left and the right hand sides in the two equations define the loss and the production mechanisms, respectively. The subscripts a, s, and f refer to absorption, scattering, and fission, respectively. The superscript g is the number of the energy groups of the neutrons and i is the precursor. v^g is the neutron speed of group g (cm/s), ϕ is the neutron flux (n/cm^2/s). D is the diffusion constant (cm), Σ is the macroscopic removal cross section (cm^{-1}), x is the fraction of the delayed neutrons, v is the average number of neutrons produced by fission induced by a neutron, λ is the decay constant (s^{-1}), β is the fraction of the produced delayed neutrons, C_i is the precursor concentration (cm^{-3}), and u is the fuel's velocity vector (cm/s).

3.1. SCALE calculations

The Scale code package is used in modelling and simulation in the design and analysis of the nuclear safety. It gives a comprehensive, validated and verified tool for different nuclear analysis purposes. KENO and TRITON codes were selected from the SCALE package to be used for the MSFR benchmark to calculate the multiplication factor by KENO and find the nuclear constants by TRITON. The concentrations are given by molar fractions. Therefore, the mass fractions were calculated to use them in the KENO and TRITON input files. The nine neutron energy groups used in EVOL project calculations have been used again in the TRITON calculations [1]. The previous step was repeated with different temperatures to find the nuclear constants as a function of temperature using Excel.

3.2. COMSOL calculations

The first step was done by COMSOL is introducing the nuclear constants extracted from TRITON calculations in the COMSOL file to solve the neutron diffusion equation. From COMSOL, the Eigen values that solves the diffusion equation for the flux were calculated and then the neutrons flux distribution and the multiplication factor K_{eff} were determined. The neutron flux distribution was used as a heat source in the turbulent model k-ε. This model was used to make a coupling between the neutronics and the thermal hydraulic. After that, the temperature distribution was calculated for the reactor regions and the velocity was calculated for the fuel salt.

3.3. WIMS calculations

WIMS is used for performing 2D lattice calculations, typically for generating the homogenized parameters of the reactor physics. WIMS was used in modeling the benchmark MSFR core to calculate the multiplication factor K_{eff}.

3.4. MCNP5 calculations

MCNP is one of the most common general-purpose nuclear codes. It can be used in different transport modes. MCNP5 was used with the same geometry and with the operation temperature conditions to calculate the multiplication factor. These calculations were done using the library ENDFB-7.

4. Results and discussion

Table 3 shows the delayed neutrons precursors data for the six groups. These data were extracted from the TRITON output file. The values are close to the reference values from the EVOL project [1] because the same neutron energy groups were used in the two studies. These values were used in the neutron source term in COMSOL.

Table 3. The delayed neutrons precursors data for the six groups using TRITON for the benchmark

β	0.00029 1483	0.0006 66053	0.0007 65932	0.0011 4085	0.0003 27382	0.00013 7248
λ	0.01249 81	0.0359 455	0.1376 58	0.3180 67	1.2197 2	3.15227

Table 4. Shows the values of the multiplication factor K_{eff} calculated by the different codes and libraries in this study compared with the reference values from previous studies. The data of this study are shown in red colour with (*) and the values of the reference studies are shown in black colour without (*). From this table we can notice that the multiplication factor K_{eff} from COMSOL is K_{eff} = 1.0065. This value shows that the initial fuel composition leads nearly to a critical reactor ($K_{eff} \approx 1$).

Fig. 2. Shows the benchmark as modelled by COMSOL. The neutron flux distribution is shown in 2 D, 3 D, and profile curve in Fig. 3, Fig. 4, and Fig. 5 respectively. It shows that the maximum neutron flux value is 9.33×10^{19} ($n/m^2.s$).

Table 4. The values of K_{eff} from the different codes and libraries compared with the reference values, current study data are shown in red colour with (*).

Code name and library	WIMS, WLUP *	WIMS, ENDF-B7 *	WIMS [11]	POLIMI SERPENT, ENDF-B7 [1]	LPSC, ENDF-B.6 [1]	COMSOL *	KENO, SCALE, ce_v6_endf *	MCNP5 *
Keff	1.108646	1.010355	1.06650	0.98301	1.02141	1.0065	1.0103	0.98349

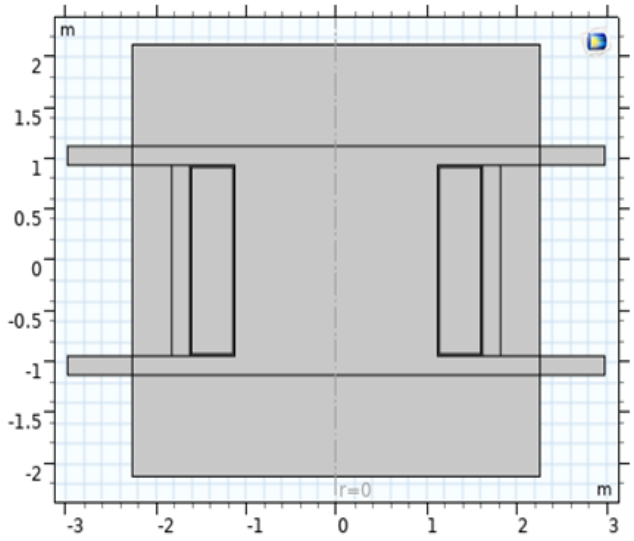

FIG. 2. MSFR as modelled by COMSOL

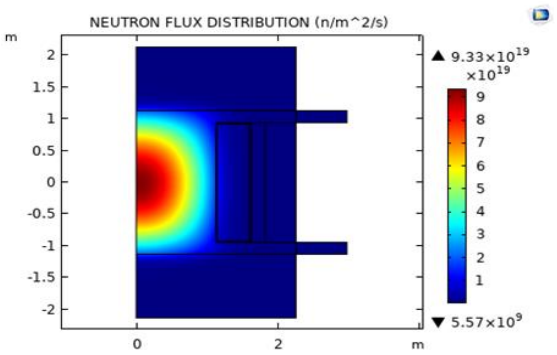

Fig. 3. 2D Flux distribution as modeled by COMSOL.

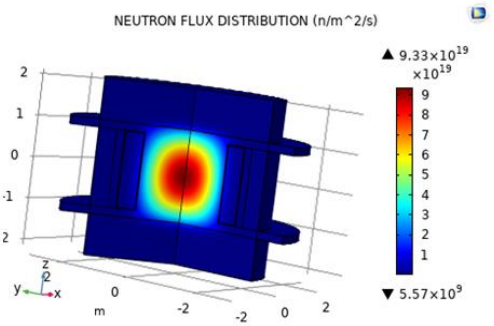

Fig. 4. 3D Flux distribution as modeled by COMSOL.

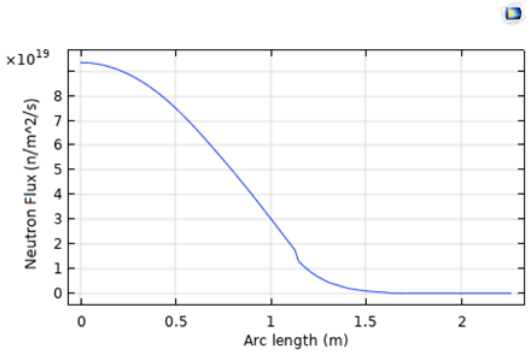

Fig. 5. Flux distribution as modeled by COMSOL with Centre cutline.

By using KENO from the SCALE package in modelling MSFR, the value Keff = 1.0103. Fig. 6. Shows the benchmark of the MSFR as modelled by KENO.

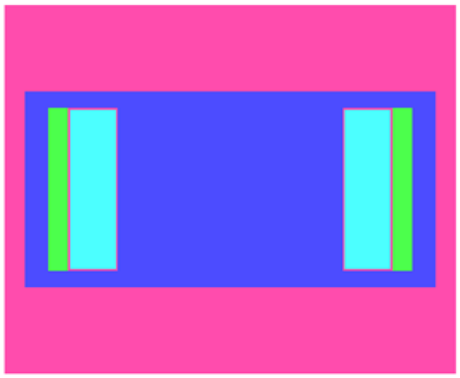

FIG. 6. The benchmark of the MSFR as modelled by KENO

By using MCNP5 with the library ENDFB7 in modelling MSFR, the value K_{eff} is equal to 0.98349. It is noticed that this result is more close to the result POLIMI SERPENT with ENDFB7 library. This result reflects the effect of using the same data library. Fig. 7 Shows the benchmark of the MSFR as modelled by MCNP5.

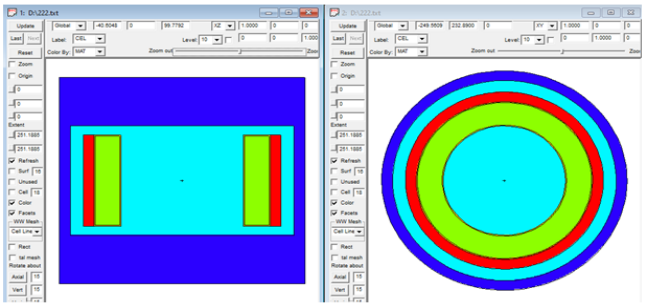

FIG. 7. The benchmark of the MSFR as modelled by MCNP5

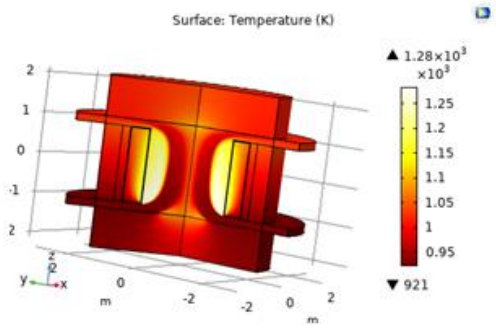

FIG. 8. The benchmark temperature distribution as modeled by COMSOL.

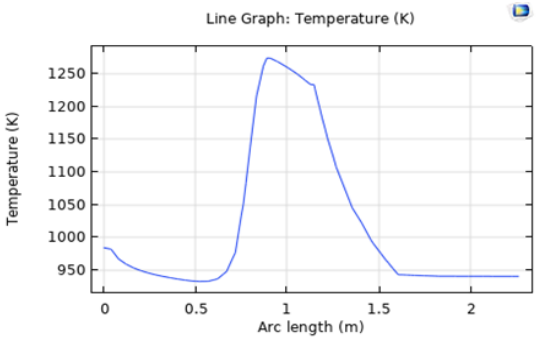

FIG. 9. The benchmark temperature distribution as modeled by COMSOL with cutline in the maximum temperature zone.

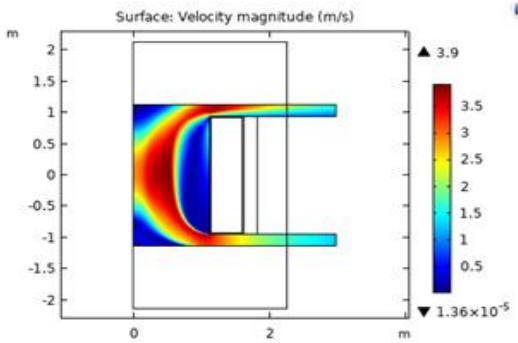

FIG. 10. The benchmark velocity distribution as modeled by COMSOL.

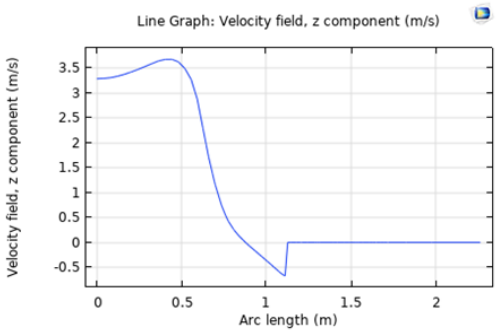

FIG.11. The benchmark velocity distribution as modeled by COMSOL with Centre cutline.

From results, it can be noticed that the results from WIMS with the library ENDF-B7 are very close to the results from KENO with ce_v6_endf because they are versions of the same library. Therefore, the differences of the two versions are very small. The results from COMSOL with the library ENDF-B7 is more close to the critical reactor case because the nuclear constants were calculating by TRITON, which is very accurate in selecting the suitable neutron energy groups.

The thermal hydraulic results generated by COMSOL coupling are shown through Fig. 8, Fig. 9, Fig. 10, and Fig. 11. The maximum temperature is 1280 K and the maximum velocity is 3.9 m/s. This maximum temperature value is high compared with the outlet core temperature because of the fuel salt recirculation phenomenon, which causes regions of hot spots. These regions of high temperature values are disadvantages in the benchmark design because they may cause corrosion in the structural materials and decrease the reactor life. The delayed neutrons fraction may be decreased by the hot spots. This decrease is not desirable in the reactor safety because it leads the reactor in the direction of prompt critical catastrophic case.

5. Conclusion

The codes WIMS, COMSOL, KENO and MCNP5 were used successfully in modelling MSFR to calculate the multiplication factor k_{eff} and adjust the criticality of the reactor. The effect of the selected library is very important. So, it must be carefully taken into consideration before using in the MSFR modelling. For each code there is a suitable library which gives an accurate result. For example, In case of using WIMS the library WLUP is not accurate, while using ENDFB-7 library the result is very close to KENO result. The code TRITON was used successfully in calculating the nuclear constants for the reactor. The calculations show that COMSOL is a very good tool in the coupling between neutronic and thermal hydraulic calculations. The MSFR benchmark design shows hot spot regions. These regions of high temperature may cause

problems in safety like structural material corrosion and decrease in the value of the delayed neutrons fraction. These problems must be solved by changing the benchmark design to modified design with lower maximum temperature values.

Acronyms and abbreviations

MSFR Molten Salt Fast Reactor
MCNP Monte Carlo N-Particle
EVOL Evaluation and Viability Of Liquid fuel fast reactor system
HN Heavy Nuclides
FP Fission Product

Nomenclature

K_{eff} effective multiplication factor
β delayed neutron fraction
λ decay constant

REFERENCES

[1]. Mariya Brovchenko et al., Optimization of the pre-conceptual design of the MSFR, Evaluation and Viability of Liquid Fuel Fast Reactor System EVOL, 2013.
[2]. A. Cammi et al., Modelling of Circulating Nuclear Fuels with COMSOL Multiphysics, Proceedings of the COMSOL Users Conference Grenoble, 2007.
[3]. E. Merle-Lucotte et al., Optimization and simplification of the concept of non-moderated Thorium Molten Salt Reactor. International Conference on the Physics of Reactors, 2008.
[4]. E. van der Linden, Coupled neutronics and computational fluid dynamics for the molten salt fast reactor featuring a physical description of the precursor transport in liquid turbulent nuclear fuels, Master Thesis, 2012.
[5]. M. Brovchenko et al., Preliminary safety calculations to improve the design of Molten Salt Fast Reactor, 2012.
[6]. lelio luzzi et al, Multi-Physics approach to the modelling and analysis of Molten Salt Reactors, Nova science publishers, inc., new york, 2012.
[7]. Carlo Fiorina, The Molten Salt Fast Reactor as a Fast-Spectrum Candidate for Thorium Implementation, 2013.
[8]. Darryl D. Siemer, Why the molten salt fast reactor (MSFR) is the "best" GenIV reactor, 2014.
[9]. Ioannis Lantzos et al., Molten Salt Fast Reactor: Shift from burner to breeder, Moving on to the Thorium era, Master thesis, 2016.
[10]. J.R. Deen and W. L. Woodruff and C.I. Costescu, WIMS-D4M user manual REV. 0, 2001.
[11]. Ben Lindley, Developments within the WIMS reactor physics code for whole core calculations, 2017.
[12]. John R. Lamarsh, Anthony J. Baratta, Introduction to Nuclear Engineering, Third Edition, 2001.
[13]. D. H. Daher et al., Simulation of a molten salt fast reactor using the COMSOL multiphysics software, 2020