Comparative neutronic study for heterogeneous and homogeneous fuel assembly in a lead-cooled fast reactor

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Abstract. ALFRED (Advanced Lead-cooled Fast Reactor European Demonstrator) is a (300 MWth) pool-type reactor with closed hexagonal Fuel Assemblies (FAs) which are divided into two radial zones (inner and outer core zones). In this work two three dimensional (3D-heterogenous and 3D-homogeneous) for inner assembly (IA) and outer assembly (OA) have been designed using MCNPX transport code to simulate the neutronic behavior and to study the fuel performance and the effect of homogenization inside the fuel assemblies. The results of the present work for power distribution and fuel burn-up show good agreement between 3D-homogeneous and 3D-heterogeneous models.

1. Introduction
In 2002, fast spectrum reactor cooled by lead was considered as one of three systems of advanced fast spectrum nuclear reactors by the fourth Generation International Forum (GIF) [1]. Thus, fast spectrum reactors are the most efficient technology for effectively utilizing uranium resources because of the ability of using the uranium stored in spent nuclear fuel to be recycled while providing energy and consequently overs a realistic path forward for achieving energy sustainability consistent with environmental stewardship by introducing an advanced technology for good management of long lived minor actinides and nuclear fission products [2]. Among all fourth generation (Gen-IV) advanced innovative concepts, lead cooled fast reactor (LFR) was considered as one of the brightest prospects concept potentially able to excel in four broad areas which are sustainability, economics, safety and reliability, and proliferation resistance and physical protection [3]. Lead-cooled fast reactor features high temperature operation, low pressure, closed fuel cycle and has the ability to operate on a flexible basis between two modes either as breeder to achieve the net creation of fissile fuel or to convert long lived minor actinides and other radioisotopes with to short lived ones as a transmuter. Because of the unique safety benefits of LFR over other fast reactors, it has bright prospects to be under
development worldwide. At present, Europe's ELFR lead-cooled system [4], Russia's BREST-OD-300 [5], and the SSTAR system concept designed in the US [6] represents the base of the Generation-IV International Forum (GIF) System Research Plan (SRP) for system concepts of lead-cooled fast reactors [5].

ALFRED (Advanced Lead-cooled Fast Reactor European Demonstrator) is one of the most advanced projects in Europe which will play the role of a demonstrator for the ELFR (European lead fast reactor) concept to prove the safety and reliability in all operating conditions, predicted to start its operation in 2025 [7]. Three of the most important steps of this project are the fuel selection, design and optimization. The goal of this work is to design a 3D-homogeneous and 3D-heterogeneous model for both inner fuel assembly (IA) and outer fuel assembly (OA) to study the neutronic characteristics of the 3D-homogeneous concept relative to the 3D-heterogeneous concept with respect to power distributions, $k_{\text{eff}}$, reactivity, fuel burn-up and nuclear fuel transmutation. This study represents the first step for further studies to provide alternative approaches of minor actinides management achieving the best refueling scenario in LFR systems.

2. The description of ALFRED core

ALFRED (300 MW$_{el}$) is a pool-type with small-size. The reactor core is consisting in 171 wrapped hexagonal fuel assemblies (FAs) to form a cylindrical core, together with sixteen positions for twelve control rods (CRs) and four safety rods (SRs), and surrounded by two rows of 108 dummy elements serving as reflector. The 171 Fuel Assemblies (FAs) is divided radially into two zones (inner zone with 57 FAs and outer zone with 114 FAs) with different plutonium enrichments. Each fuel assembly (FA) containing a triangular lattice with 127 fuel pins arranged in it and surrounded by pure lead as coolant. Fig. 1 shows the ALFRED primary system and the layout of the core. The ALFRED core main parameters are presented in Table. 1. The fuel is composed of MOX pellets with theoretical density of 95% and O/M (Oxygen-to-Metal ratio) of 1.97. The U and Pu isotopic vectors have been evaluated considering recovered U and Pu extracted from LWR spent fuel (burnt up to 45 GWD/t, with a 4.5% initial enrichment in $^{235}$U) after a total of 15 years of cooling, 4 of which after reprocessing (so that also the decay of $^{241}$Pu into $^{241}$Am has been taken into account). See Table. 2 for the fuel isotopic composition of uranium and plutonium. The fuel pin design was considered with inner and outer radius (1, 4.5 mm respectively) and active length of 60 cm [7], [9] as shown in Fig. 2. The design parameters of fuel pin is presented in Table. 3. The considered absorber material for control and safety rods is $\text{B}_4\text{C}$ (with 90 at.% of $^{10}$B and density of 2.2 g/cm$^3$).

| Table 1. ALFRED main parameters [9]. |
|--------------------------------------|
| **Main parameters**                  |
| Thermal power (MW)                   | 300                          |
| Fuel assembly concept                | Closed hexagonal.            |
| Coolant                              | Lead                         |
| Inlet temperature of coolant (°C)    | 400                          |
| Outlet temperature of coolant (°C)   | 480                          |
| Mass flow rate of coolant (kg s$^{-1}$)| 26000                       |
| Maximum velocity of coolant (m s$^{-1}$)| < 2.0                       |
| Cladding                            | 15-15 Ti                     |
| Cladding maximum temperature at nominal conditions (°C) | 550 |
Table 2. The isotopic vectors of uranium and plutonium [11].

| Plutonium isotopes | Fraction (wt.%) | Uranium isotopes | Fraction (wt.%) |
|-------------------|----------------|-----------------|----------------|
| $^{238}$Pu        | 2.332          | $^{238}$U       | 0.003          |
| $^{239}$Pu        | 56.873         | $^{235}$U       | 0.404          |
| $^{240}$Pu        | 26.997         | $^{236}$U       | 0.010          |
| $^{241}$Pu        | 6.105          | $^{238}$U       | 99.583         |
| $^{242}$Pu        | 7.693          |                 |                |

3. Modeling and simulation

Two 3D models (3D-heterogeneous and 3D-homogeneous) for both inner fuel assembly (IA) and outer fuel assembly (OA) based on the same design limits and technological constraints have been designed using MCNPX [10] to compare power peaking factor, reactivity parameters, fuel burn-up and masses of fissile inventory. Reflected boundary conditions are assumed for both models (3D-heterogeneous and 3D-homogeneous) to consider interaction of neutrons with other neighboring assemblies in radial direction while the top and bottom boundaries in axial direction are assumed to be free surfaces. MCNPX (Monte-Carlo N-Particle Transport Code) is a general purpose for simulating the interaction of nearly all particles (neutrons, photons and electrons) at nearly all energies with the substance of the system using Monte-Carlo methods. It has the ability to predict the isotopic transmutation of fuel as a function of irradiation time.
Table 3. Design parameters of ALFRED fuel pin [8].

| Design Parameters of fuel pin | Value |
|-------------------------------|-------|
| Type of fuel                  | MOX   |
| (Pu+Am)/(Pu+U+Am) enrichment of inner zone (at. %) | 21.7 |
| (Pu+Am)/(Pu+U+Am) enrichment of outer zone (at. %) | 27.8 |
| Fuel density (%) of theoretical density | 95   |
| O/M                           | 1.97  |
| Fill gas                      | He    |
| Length of upper plenum (mm)   | 120   |
| Length of Active zone (mm)    | 600   |
| Length of lower plenum (mm)   | 550   |
| Outer diameter of cladding (mm) | 10.5  |
| Inner diameter of cladding (mm) | 9.3    |
| Outer diameter of fuel pellet (mm) | 9.0   |
| Inner diameter of fuel pellet (mm) | 2.0   |
| Pin pitch (mm)                | 13.86 |

3.1. Heterogeneous model of fuel assembly

The 3D-heterogeneous model of fuel assembly is consisting of a triangular lattice with 127 fuel pins arranged in it and surrounded by pure lead as coolant. Then, to enclose the 127 fuel pins and form the bundle, a T91 wrapping with suitable rigidity was added. The fuel pin’s design includes a reflector zone that extends 1.0 cm below and above the active length of the fuel (Active zone), as well as an empty plenum zone that extends 12 cm above the higher reflector and 55 cm below the lower reflector providing a confining of the fission the thermal expansion of reflector materials and the fuel as well as the fission gases, after that the reflector extends again for 1.0 cm below the lower plenum and for 6.0 cm above the upper plenum. During the earlier stages of this technology development, Ti-15-15 austenitic stainless steel was proposed as a cladding material in fast reactors [12], so it has been chosen for cladding the fuel pin. See Fig. 3(a) and Fig. 4(a) for axial and radial cross section respectively of the 3D-heterogeneous model of the ALFRED fuel assembly.

Figure 3. Axial cross section of ALFRED FA (a) Heterogeneous model (b) Homogeneous model.
3.2. Homogeneous model of fuel assembly

Fig. 3(b) and Fig. 4(b) show axial and radial cross section respectively of the 3D-homogeneous model of the ALFRED fuel assembly. As shown, all the active zone materials within the wrapped hexagonal T91, including the exterior fuel pins with lead coolant were homogenized into one material. In simulations, the active fuel zone was divided into 12 axial meshes of equal length (5 cm each) to analyze the influence of the homogenization on the axial power distribution. Both inner and outer fuel assemblies has been homogenized in order to investigate the influence of fuel homogeneity on neutronic characteristics and fuel performance. This, in turn, helps to provide confidence in fuel burn-up results estimated using 3D-heterogeneous models.

4. Results and discussion

From a neutronic standpoint, this analysis has been characterized by using ENDF/B-VI.2 cross sections library. It includes nuclides cross sections data such as those of fuel, reflector materials, clad and coolant given at multiple temperatures (e.g. 1200 K, 900 K, 600 K and 293 K). The burn-up of MOX fuel inside the assembly is simulated during a total cycle length of 5 years, which is equivalent to 1825 Effective Full Power Days (EFPD), and the build-up of the masses of U/Pu/MA isotopes have been tracked for each irradiation time interval to compare the results of fuel transmutation within 3D-homogeneous relativeto 3D-heterogeneous model for both inner assembly (IA) and outer assembly (OA). The Dell Precision T5610 with two processors; Intel Xeon processor E5-2600 V2 and ECC RDIMM memory of 32GB and 1866MHz has been used to run MCNPX code with 550 cycles. Every simulation calculation goes with the first 55 cycles skipped before the tally accumulation begins. The total number of neutron source histories used in the calculation are 1000. The run time for burn up of IA lasted for 38 hours for the 3D-homogeneous model and 46 hours for the 3D-heterogeneous model. On the other hand, the run time for burn up of OA lasted for about 36 hours for the 3D-homogeneous model and 44 hours for the 3D-heterogeneous model. The results of the simulation will be discussed as follows: the effects of homogeneity on the power distribution for IA and OA are introduced in Section 4.1; the effects of homogeneity on reactivity parameters and fuel burn-up for both IA and OA are discussed in Section 4.2; comparing of fuel transmutation results between 3D-homogeneous and 3D-heterogeneous models for both IA and OA are presented in Section 4.3.

4.1. Power distribution

For both inner assembly (IA) and outer assembly (OA) the fuel region was divided axially into 12
axial regions of equal volumes and radially into 127 hexagonal of equal volumes. The results of comparison for axial power distribution between 3D-homogeneous and 3D-heterogeneous models for IA are slightly different but achieved the same maximum peak power factor. Fig. 5 shows the axial power peaking factor for 3D-heterogeneous and 3D-homogeneous model of IA and OA. The results of comparison for axial distribution between 3D-homogeneous and 3D-heterogeneous model for OA show a good agreement. It is expected because of the lower initial fissile enrichment of the IA in comparison with OA. On the other hand, Fig. 6 shows that, the 3D-heterogeneous model provides at radial power distribution on both IA and OA when compared with the 3D-homogeneous model.

Figure 5. Axial power distribution for 3D-heterogeneous and 3D-homogeneous models of (a) Inner assembly (IA) (b) Outer assembly (OA).

Figure 6. Radial power peaking factor for 3D-heterogeneous and 3D-homogeneous model of (a) Inner assembly (IA) (b) Outer assembly (OA).
4.2. The effect of homogeneity on fuel burn-up

As shown in Fig. 7 for the $k_\infty$ value as a function of Effective Full Power Days (EFPD) for both the 3D-heterogeneous and 3D-homogeneous models of inner assembly (IA) and outer assembly (OA), the results show that the $k_\infty$ values of 3D-homogeneous assembly is slightly lower than that of 3D-heterogenous for both IA and OA and this is because of the significantly harder spectrum of 3D-heterogeneous model. From a neutronic standpoint, this agreement between the 3D-homogenous and 3D-heterogeneous model can be explained as, for fast neutrons, the length of the elementary lattice pitch is lower than the mean free path of the neutrons.

![Graphs showing the effect of homogenization on $k_\infty$ for (a) Inner assembly (IA) (b) Outer assembly (OA).](image)

**Figure 7.** The effect of homogenization on $k_\infty$ for (a) Inner assembly (IA) (b) Outer assembly (OA).

![Graphs showing peak fuel burn-up for 3D-heterogeneous and 3D-homogeneous models of (a) Inner assembly (IA) (b) Outer assembly (OA).](image)

**Figure 8.** Peak fuel burn-up for 3D-heterogeneous and 3D-homogeneous models of (a) Inner assembly (IA) (b) Outer assembly (OA).

Fig. 8 shows a good agreement between 3D-heterogeneous and 3D-homogeneous models for fuel
burn-up where, the fuel burn-up of the two models has reached 71.8 MWd/kg$_{HM}$ for IA and 71.6 MWd/kg$_{HM}$ for OA at the end of irradiation period (1825 EFPD).

4.3. The effect of homogeneity on fuel transmutation

As shown in Fig. 9(a) and Fig. 9(b), the $^{235}$U mass inventory of 3D-heterogeneous and 3D-homogeneous model shows good agreement for both inner assembly (IA) and outer assembly (OA). As we can see from Fig. 10(a), for IA, the total Pu mass inventory of 3D-homogeneous model is higher than the 3D-heterogeneous models at the end of irradiation time.

On the other hand, for OA, Fig. 10(b) shows a good agreement between 3D-heterogeneous and
3D-homogeneous model for the total mass inventory of Pu isotopes. This is because the results indicate that, the destruction rate of fertile Pu isotopes ($^{239}$Pu and $^{241}$Pu) of 3D-homogenous model is lower than of 3D-heterogenous model for IA. This indicates that the destruction rate of fertile nuclides (except $^{242}$Pu) of 3D-heterogeneous model is higher than of 3D-homogeneous model for IA due to the low enrichment of Pu in IA relative to Pu enrichment in OA. See Fig. 11 and Fig. 12.

**Figure 11.** Mass inventory of Pu isotopes of inner assembly (IA) for (a) 3D-heterogeneous model (b) 3D-homogeneous model.

**Figure 12.** Mass inventory of Pu isotopes of outer assembly (OA) for (a) 3D-heterogeneous model (b) 3D-homogeneous model.
Fig. 13 shows good agreement between 3D-heterogeneous and 3D-homogeneous model for both IA and OA with irradiation time for $^{241}$Am. Also, you can see how Fig. 14 and Fig. 15 show good agreement for the MA-isotopes mass inventory with irradiation time for both IA and OA.

**Figure 13.** $^{241}$Am mass inventory for 3D-heterogeneous and 3D-homogeneous models of (a) Inner assembly (IA) (b) Outer assembly (OA).

**Figure 14.** MA mass inventory of inner assembly (IA) for (a) 3D-heterogeneous model (b) 3D-homogeneous model.
Figure 15. MA mass inventory of outer assembly (OA) for (a) 3D-heterogeneous model (b) 3D-homogeneous model.

5. Conclusion

Two models (3D-heterogeneous and 3D-homogeneous) for both inner fuel assembly (IA) and outer fuel assembly (OA) have been designed using MCNPX to study homogenization effect on power peaking factor, $k_\infty$, fuel burn-up and the fuel isotopic transmutation. Both 3D-homogeneous and 3D-heterogeneous designs were based on the same design assumptions and constraints. Firstly, the 3D-homogeneous model can be employed as a beginning steps for validation and verification calculations rather than 3D-heterogeneous model by observation that it saves about 18% of run time for burn-up simulation for both IA and OA. The neutronic analysis shows close behavior between the two models of axial power distribution for both IA an OA which has a peak of (1.09). On the other hand, the 3D-heterogeneous model provides at radial power distribution on both IA and OA when compared with the 3D-homogeneous. There is no effect of homogenization on the fuel burn-up of for both IA and OA at the end of burn-up time (1825 EFPD). The results of fuel transmutation for IA show that the destruction rate of fertile nuclides ($^{235}\text{U}$, $^{239}\text{Pu}$, $^{241}\text{Pu}$) of 3D-homogeneous model is lower than of 3D-heterogeneous model. This characteristic would allow the 3D-homogeneous model to have a longer fuel operating cycle than the 3D-heterogeneous model. The results show close behavior for the transmutation rate of MA for 3D-homogeneous model relative to the 3D-heterogeneous model for both IA and OA.

References
[1] DOE, U. S. (2002). A technology roadmap for generation IV nuclear energy systems.
[2] Waltar, A. E., Todd, D. R., & Tsvetkov, P. V. (Eds.). (2011). Fast spectrum reactors. DOI 10.1007/978-1-4419-9572-8. Springer Science & Business Media.
[3] Zohuri, B. (2020). Nuclear Reactor Technology Development and Utilization (pp. 61-120). Woodhead Publishing.
[4] Alemberti, A., Carlsson, J., Malambu, E., Orden, A., Cinotti, L., Struwe, D., ... & Monti, S. (2011). Journal of nuclear science and technology, 48(4), 479-482.
[5] Zrodnikov, A. V., Toshinsky, G. I., Komlev, O. G., Stepanov, V. S., & Klimov, N. N. (2011). Journal of Nuclear Materials, 415(3), 237-244.
[6] Smith, C. F., Halsey, W. G., Brown, N. W., Sienicki, J. J., Moisseytsev, A., & Wade, D. C. (2008). *Journal of Nuclear Materials*, 376(3), 255-259.

[7] Grasso, G., Petrovich, C., Mattioli, D., Artioli, C., Sciora, P., Gugiu, D., ... & Mikityuk, K. (2014). *Nuclear Engineering and Design*, 278, 287-301.

[8] Luzzi, L., Cammi, A., Di Marcello, V., Lorenzi, S., Pizzocri, D., & Van Uffelen, P. (2014). *Nuclear Engineering and Design*, 277, 173-187.

[9] Grasso, G., Petrovich, C., Mikityuk, K., Mattioli, D., Manni, F., & Gugiu, D. (2013). *Proceedings of Fast Reactors and Related Fuel Cycles, Vol. 2: Safe Technologies and Sustainable Scenarios (FR13)*, Paris.

[10] Pelowitz, D. B., Durkee, J. W., Elson, J. S., Fensin, M. L., Hendricks, J. S., James, M. R., ... & Verbeke, J. M. (2011). Los Alamos National Lab.(LANL), Los Alamos, NM (United states).

[11] Sobolev, V., Malambu, E., & Abderrahim, H. A. (2009). *Journal of Nuclear Materials*, 385(2), 392-399.

[12] Bortot, S., Cammi, A., Lorenzi, S., Ponciroli, R., Della Bona, A., & Juarez, N. B. (2013). *Nuclear Engineering and Design*, 265, 1238-1245.