

MONTE CARLO CALCULATION FOR VARIOUS ENRICHMENT LITHIUM
COOLANT USING DIFFERENT DATA LIBRARIES IN A HYBRID REACTOR

Hacı Mehmet ŞAHİN^{a*}, Şenay YALÇIN^b, Taner ALTINOK^c and Adem ACIR^a

^aGazi Üniversitesi
Teknik Eğitim Fakültesi
Makina Eğitimi Bölümü
Teknikokullar, Ankara 06503, TURKEY

^bBahçeşehir Üniversitesi
Mühendislik Fakültesi
Beşiktaş, İstanbul, TURKEY

^cKara Harp Okulu,
Savunma Bilimleri Enstitüsü,
Ankara 06654, TURKEY

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* Corresponding author:
Office phone: 00-90-312-202 86 06
Fax: 00-90-312-212 43 04
E-Mail: mesahin@gazi.edu.tr

ABSTRACT

The main objective of this study is to compare the effect of the natural lithium and lithium with different enrichments between 10 % and 90 % on neutronic parameters; such as tritium breeding ratio (TBR), displacement per atom (DPA) and gas production using the different data libraries (ENDF/B.V, ENDF/B.VI and CLAW IV). Therefore, the natural lithium and different enrichment lithium were used as a moderator in an experimental hybrid reactor for the calculation of the nuclear parameters. Neutronic calculations were performed by recent Monte Carlo Neutron-Particle Transport code MCNP5 version 1.40 for a 14.1 MeV (D,T) fusion driver under a neutron wall load of 2.25 MW/m^2 (10^{14} n/s). TBR values in the blanket for all investigated cases were obtained greater than the minimum requirement (TBR>1.05). Considering radiation damage limits (100 DPA and 500 appm/FPY) for structural materials, the FW replacement will be needed every 2.1 and 3.5 years for DPA and He-production, respectively.

Key Word: Hybrid reactor, radiation damage, tritium breeding ratio (TBR).

1. INTRODUCTION

In the 21st century, world energy needs have increased dramatically because of world population growth; the sustainable developing and the continuing improve living standards. Today, combustion fossil fuel provides 88% of the world's energy [1]. However, barriers of fossil fuel utilization include limited supply, pollution, CO₂ emissions, thought to be responsible for global warming, etc. In addition, they have storage problems and require a large plant to produce high levels of energy. Therefore, energy requirement of the future is nearly impossible to be met by the conventional methods of present-day energy production [2]. Hence, there has been the world's energy need that is less environmental impact, abundant and continuous. In this respect, nuclear fusion is safe, clean and unlimited energy source particularly the abundant fusion fuel, contrary to fission fuel and conventional fuels. Besides, it has environmental advantages compared to other energy sources. But, the commercial pure fusion reactors have not been expected to run in the short period. Because the fusion reactor have many problems such as plasma instability, high material damage, high radiation, sensitive fluid jet design, high driver power and other complex problems [3-5]. Thus, a fusion-fission reactor namely hybrid reactor would be an appropriate solution for some of these problems. Furthermore, the aim of the hybrid reactor is to improve the neutronic and economical performances of fusion reactors by means of higher energy production and/or significant fissile fuel breeding. Some advantages and main structure of the hybrid blanket has been given in earlier works [6-9].

The fusion-fission (hybrid) is basically a combination of the fusion and fission processes. A line neutron source in a cylindrical cavity simulates the fusion plasma chamber. The latter is surrounded by a first wall (FW). In this concept, the FW is surrounded with a blanket made of the fertile materials to convert them into fissile materials by transmutation through the capture of the high yield fusion neutrons. In a hybrid reactor system, a fusion breeder can produce up to 30 times more fissile fuel than a fission breeder per unit of energy [7, 10]. In addition, some of the bred fissile material burns in the hybrid blanket. Another potential of a hybrid reactor is to burn up minor actinides with the help of high energetic fusion neutrons. Besides, there have been the rejuvenation capability of the LWRs and Canada Deuterium Uranium Reactor (CANDU) spent fuels in the hybrid reactors. To improve the neutronic performance of the hybrid blanket with low radiation damage in the FW by various moderator materials has been investigated [11]. The radiation damage for FW structural material of fusion chamber occur displacements per atom (DPA) and gas production in the metallic lattice, mainly through (n,p) and (n,α) and to some extent through (n,d) and (n,t) reactions. In addition, the FW structure of fusion chamber in the hybrid reactor exposed to the high heat loads, the highest neutrons, gamma-ray and energetic particle fluxes together with alternating mechanical stress pattern. These events will limit the lifetime of the FW structure of the fusion reaction chamber. The hybrid reactors have been investigated by several studies [12-20].

A liquid zone has been suggested to protect the FW of a fusion reactor from a direct exposure to the fusion products to extend the lifetime of the FW, namely 30 years [21-25]. The important parameter in hybrid reactors is burned the nuclear waste material and

breed fissile fuel in the blanket of the reactor by the high energetic neutron. However, when using liquid zone between plasma and solid FW, the high neutron flux will be kept in the liquid zone before reaching the fuel zone. Therefore, a liquid zone does not use in the hybrid reactors. Thus, the lifetime of the dry FW material in the hybrid reactor will dramatically reduce and it will be replaced every year.

In hybrid reactors, one of the most important parameters is the selection of the suitable coolant to improve its neutronic performance remarkably and also to breed sufficient tritium for a self sustaining operation as well as to transfer nuclear heat out of the blanket. The working fluid in the fusion reactors, particularly deuterium-tritium (DT) driven fusion reactors, must contain a lithium compound to breed sufficient tritium amount. The main tritium breeders are natural lithium, $\text{Li}_{17}\text{Pb}_{83}$, Flinabe, Flibe, etc. The most important properties of tritium breeders would be summarized as: high breeding properties, low melting point, high boiling point, high thermal conductivity, low density, low vapor pressure, high chemical stability, no tritium solubility, low viscosity, low cost. It can be found more details in the literatures [11, 26]. Considering this properties, a suitable material in the candidate liquid coolants is natural lithium for tritium breeding. Moreover, the operation temperature required for the natural lithium is between 180.5 °C (melting point) and 1342°C (boiling point). Therefore, the natural lithium obtains a wide range for the operation temperature of the working fluid [27].

In this study, the natural lithium and lithium with different enrichment between 10% and 90% were used as a moderator, which is the nuclear heat transfer out of the fuel zone and contributing of the tritium breeding ratio (TBR). Neutronic calculations were

performed by recent Monte Carlo Neutron-Particle Transport code MCNP5 version 1.40 [28] for a 14.1 MeV (D,T) fusion driver under a neutron wall load of 2.25 MW/m² (10¹⁴ n/s).

The main objectives of this study are followed as below:

1. Presentation of the effect of the natural lithium and different enrichment lithium for tritium breeding capability,
2. Investigation of the neutronic parameters such as TBR in the blanket and radiation damage; DPA and He-production (n, α) as a lifetime of one full power year (FPY) in the FW,
3. Using the different data libraries for comparing neutronic parameters.

2. NUMERICAL CALCULATIONS

Calculations were conducted using a (D,T) fusion neutron driver for the hybrid reactor. The temporal neutronic performance of the hybrid blanket have been evaluated for the NWL of 2.25 MW/m² by full reactor power (plant factor PF=100%). Hence, this corresponds to the fusion neutron flux of 10¹⁴ (14.1 MeV) n/cm²s at FW for conventional (D,T) driven hybrid reactor.

2.1. Geometrical model for neutronic calculations

The basic structure of the hybrid blanket adapted from previous studies [10-22, 29-32] to this work, shown in Figure 1. A line neutron source in a cylindrical cavity simulates the fusion plasma chamber in this concept. The latter is surrounded by a FW in which

various materials would be used. In this study, a stainless steel (SS304) was considered as FW and fuel cladding material, given in Table 1. In the fissile zone, a typical LWR spend fuel which contains natural uranium dioxide (UO_2) in hexagonal geometry as 10 rows having pitch length=1.25 cm in the radial direction was used. The fuel zone is considered to be cooled with natural and different enrichment lithium which contributes to tritium breeding ratio, at the same time, as a working fluid for the nuclear heat transfer out of the fuel zone. The coolant to fuel volume fraction is $V_c/V_f = 2$. Under consideration of the volume for the fuel cladding material also, the coolant occupies a volume fraction of 62.6% in the fuel zone. The radial reflector is made of Li_2O for production of tritium (T) and graphite in a sandwich structure. This measure reduces the neutron leakage drastically and leads to a better neutron economy [8, 9].

2.2. Calculation tools

The neutron transport calculations were carried out with Monte Carlo Methods, using the widely known three-dimensional particle transport code MCNP, the most recent version MCNP5 1.4 [28]. MCNP5 allows an authentic geometrical description limited only with available computational power and uses the built-in most recent continuous energy nuclear and atomic data libraries. The primary source of nuclear data used by MCNP code is evaluations from the Evaluated Nuclear Data File (ENDF) system [33]. ENDF/B-V and ENDF/B-VI are the Evaluated Nuclear Data Files, a US effort coordinated by the National Nuclear Data Center at Brookhaven National Laboratory [34]. Furthermore, the evaluations are updated periodically by evaluators from all over the world. ENDF/B-V [35] and ENDF/B-VI [36], in which the neutron energy regimes are from 10^{-11} MeV to 20 MeV for all isotopes and up to 150 MeV for some isotopes,

are the most recent data available. On the other hand, activity cross-section data library CLAW-IV [37] for atomic displacement cross-sections of the FW structural materials was used for both evaluating DPA values and the gas generations.

3. RESULTS AND DISCUSSIONS

3.1. Tritium Breeding Ratio

The DT driven fusion-fission (hybrid) reactor should contain lithium as a fusion fuel source material, there two main contributors to tritium breeding, namely coolant in the fuel zone and in the sandwich structure of the blanket, which Li_2O zones locate at outer of the fuel zone. High enrichment lithium (^6Li) increases the tritium production and neutron absorption, and also allows a lower neutron leakage fraction out of the blanket of the hybrid reactor. In the coolant zone, there is a higher neutron spectrum, this leads to a higher neutron multiplication in the coolant. Tritium production in the coolant increases with increasing enrichment ratio of ^6Li . On the other hand, in the Li_2O zones, there is a lower neutron spectrum, therefore, this reduces tritium production in those zones. Nevertheless, total TBR values in the hybrid reactor increase with increasing enrichment ratio due to breeding of higher tritium production in the coolant zone. The contribution of ^7Li in the coolant and the sandwich structure of the blanket to tritium production is rather modest. Main contribution to tritium production comes from ^6Li . Total TBR becomes self-sufficient for all investigated cases. For a self sustaining fusion reactor, a $\text{TBR} > 1.05$ will be required. The TBR values were calculated 1.15, 1.16 and 1.10 for the ENDF/B-V, ENDF/B-VI and CLAW-IV cross-section data libraries at

natural lithium, respectively. While the TBR values increase with enrichment of ${}^6\text{Li}$, the TBR values reach 1.32, 1.30 and 1.38 at 90 % enrichment of ${}^6\text{Li}$, seen in figure 2.

3.2. Radiation Damage

In a fusion-fission (hybrid) reactor, the FW will be exposed to plasma particles and electromagnetic radiation. Moreover, the FW will be suffered from irradiation by 14 MeV neutrons for DT driven systems. The high energy neutrons will cause atomic displacement via displacement cascades and gas productions various nuclear reactions within structural materials. The radiation damage will limit life time of the FW material. Design concepts for fusion energy reactors indicate a life time of FPY for the FW structure. This means that every year first wall material must be replaced [5, 11, 18, 24, 25, 27].

3.2.1. Gas Production

All hydrogen isotopes, produced by (n,p), (n,d), (n,t) reactions will diffuse out of the metallic lattice or form metal hybrids. Therefore, H-production values could not take into consideration of the material damage criterion of the fusion reactors. Though, calculations of the hydrogen production in the FW were made for three different data libraries; ENDF/B-V, ENDF/B-VI and CLAW-IV. The H-production values were obtained 833.9, 735.2 and 717.9 appm/FPY for the ENDF/B-V, ENDF/B-VI and CLAW-IV at natural lithium, respectively. The H-production values decrease rather

quietly with increasing enrichment of ${}^6\text{Li}$, and they reach 815.8, 725.1 and 701.3 appm/FPY at 90 % ${}^6\text{Li}$.

On the other hand, α -particles will remain in metal and produce helium gas bubbles. The highest He-production values were found 264.6, 235.5 and 238.6 appm/FPW for natural lithium using the ENDF/B-V, ENDF/B-VI and CLAW-IV, respectively. Similar to H-production values, He-productions decrease rather quietly with increasing enrichment of ${}^6\text{Li}$, and they reach 260.8, 232.6 and 234.2 appm/FPY at 90 % ${}^6\text{Li}$, seen in figure 3. References [38, 39] have suggested a helium limit of 500 atomic parts per million [appm]. When this limit was considered as criteria for helium production in the FW structure, the FW replacement will be needed every 2.1 years for all investigated cases.

3.2.2. Atomic Displacement

Displacement of the atoms from their lattice sites as a result of collisions with highly energetic fusion neutrons, called displacement per atom (DPA). The DPA is the fundamental process of radiation damage in metals. It can be found a great number of research studies [5, 11, 18]. In nuclear reactors, the DPA is caused by scattering of fast neutrons; on the contrary, thermal neutrons do not cause atomic displacement.

In the FW, after 1 year operation period as DPA/FPY using CLAW-IV cross-section data library, the highest value 29.66 was found for natural lithium while the lowest value 26.56 was for 90 % ${}^6\text{Li}$. Figure 4 shows DPA values as a function of enrichment

of ${}^6\text{Li}$. One can see that the DPA values decrease with enrichment of ${}^6\text{Li}$. In the literature, two different DPA limit have been proposed for stainless steel of structural material in the FW: DPA=165 [38, 39] and DPA=100 [21, 40]. In this study, a conservative radiation damage limit of 100 DPA was selected for DPA calculations. Then, the FW will be replaced every 3.5 years.

5. SUMMARY AND CONCLUSIONS

The main conclusions can be summarized as follows:

1. The most recent version MCNP5 1.4 code with three different data libraries (ENDF/B-V, ENDF/B-VI and CLAW-IV) was applied successfully for the evaluation of the neutronic parameters of a hybrid reactor. Obtained results indicated in a good agreement with previous studies [4, 5, 11, 18, 24, 25, 27].
2. The TBR values were calculated 1.15, 1.16 and 1.10 for the ENDF/B-V, ENDF/B-VI and CLAW-IV cross-section data libraries at natural lithium, respectively. While the TBR values increase with enrichment of ${}^6\text{Li}$, the TBR values reach 1.32, 1.30 and 1.38 at 90 % enrichment of ${}^6\text{Li}$.
3. H-production values could not take into consideration due to all hydrogen isotopes produced by (n,p), (n,d), (n,t) reactions which will diffuse out of the metallic lattice or form metal hybrids.

4. The highest He-production values were found 264.6, 235.5 and 238.6 appm/FPW for natural lithium using the ENDF/B-V, ENDF/B-VI and CLAW-IV, respectively. He-productions decrease rather quietly with increasing enrichment of ${}^6\text{Li}$, and they reach 260.8, 232.6 and 234.2 appm/FPY at 90 % ${}^6\text{Li}$. When the limit of 500 appm was considered as criteria for helium production in the FW structure, the FW replacement will be needed every 2.1 years for all investigated cases.

5. The highest value 29.66 was found for natural lithium while the lowest value 26.56 was at 90 % ${}^6\text{Li}$ for 1 year operation period as DPA/FPY. A was selected for DPA. Then, the FW will be replaced every 3.5 years for a radiation damage limit of 100 DPA.

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FIGURE CAPTURE

Figure 1. Cross sectional view of the investigated blanket

Figure 2. TBR values in the blanket versus ${}^6\text{Li}$ enrichment of the coolant using three data libraries

Figure 3. Gas productions in the first wall versus ${}^6\text{Li}$ enrichment of the coolant using three data libraries

Figure 4. DPA value in the first wall versus ${}^6\text{Li}$ enrichment of the coolant

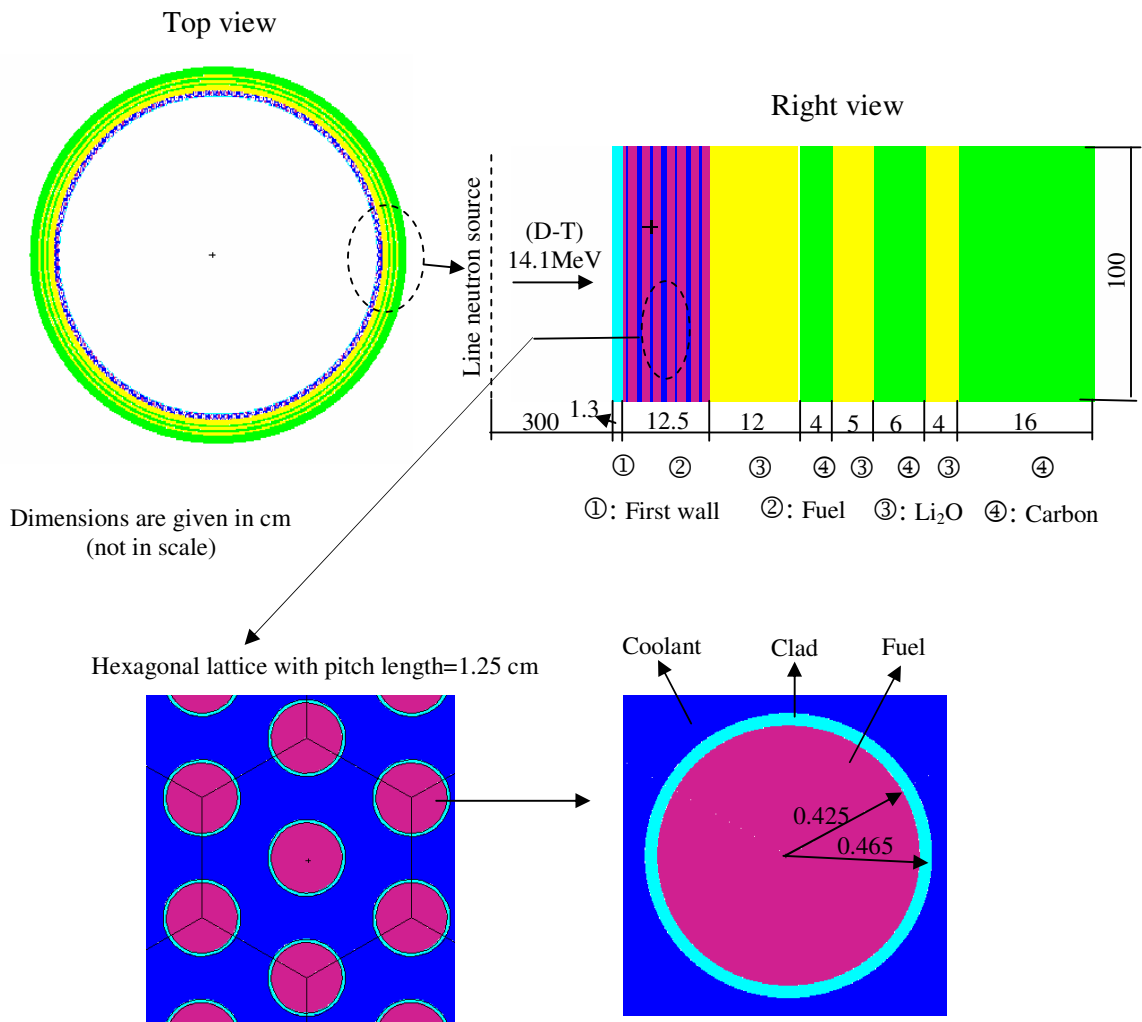


Figure 1. Cross sectional view of the investigated blanket.

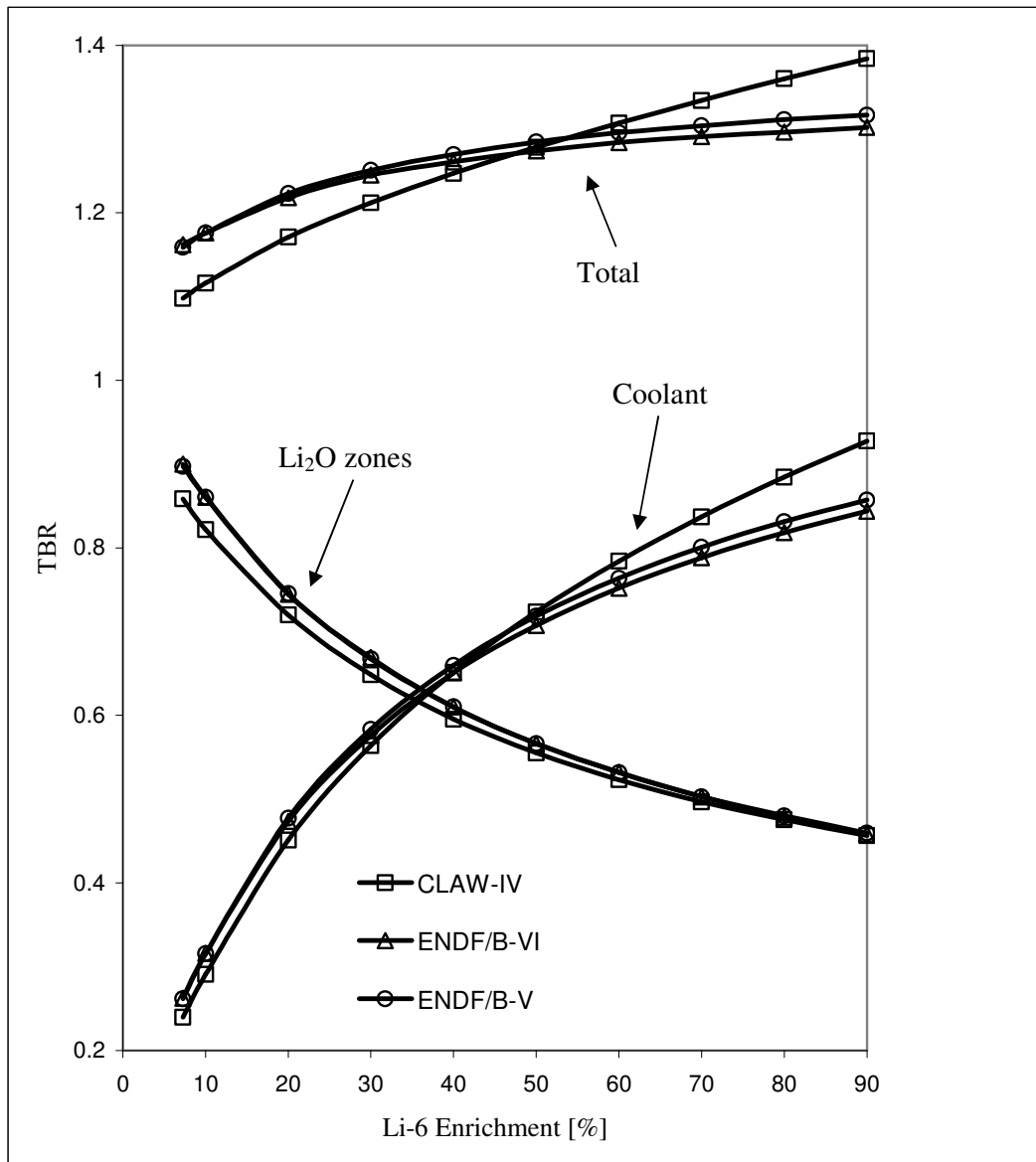


Figure 2. TBR values in the blanket versus ⁶Li enrichment of the coolant using three data libraries

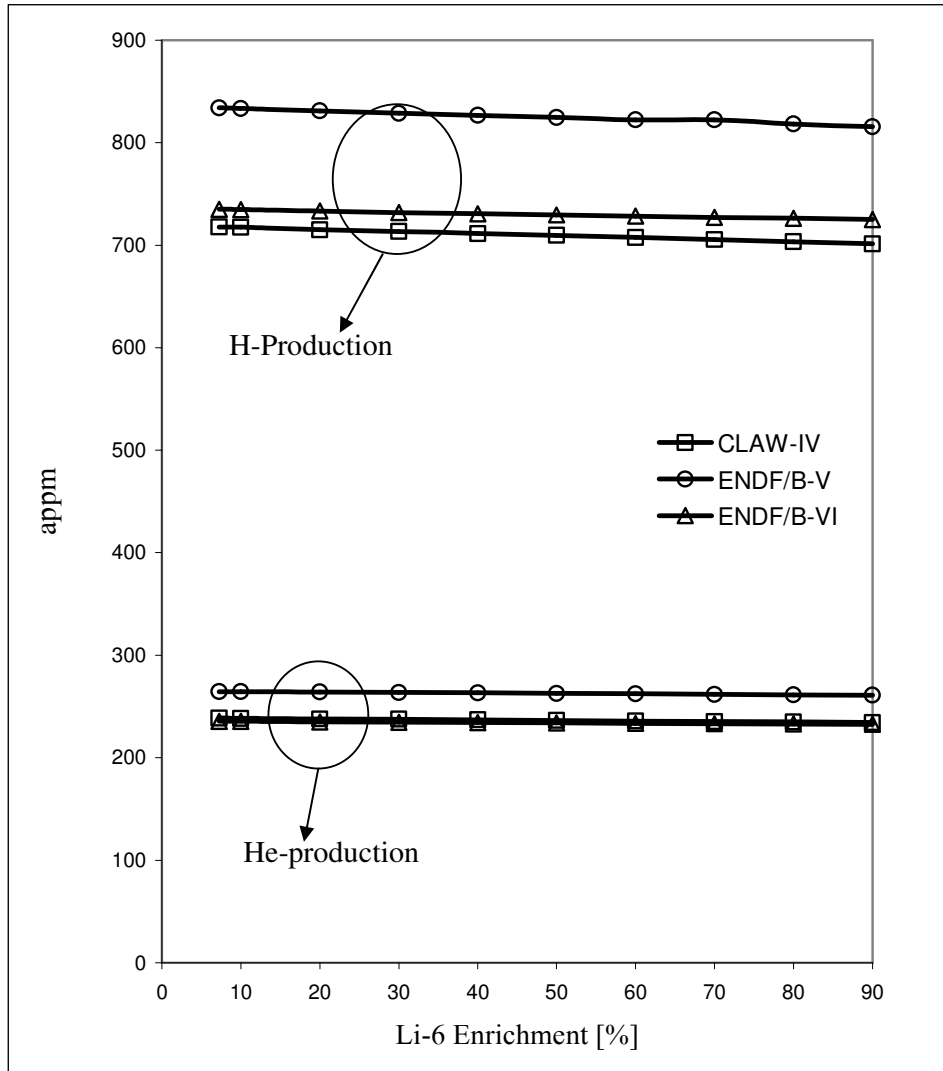


Figure 3. Gas productions in the first wall versus ${}^6\text{Li}$ enrichment of the coolant using three data libraries

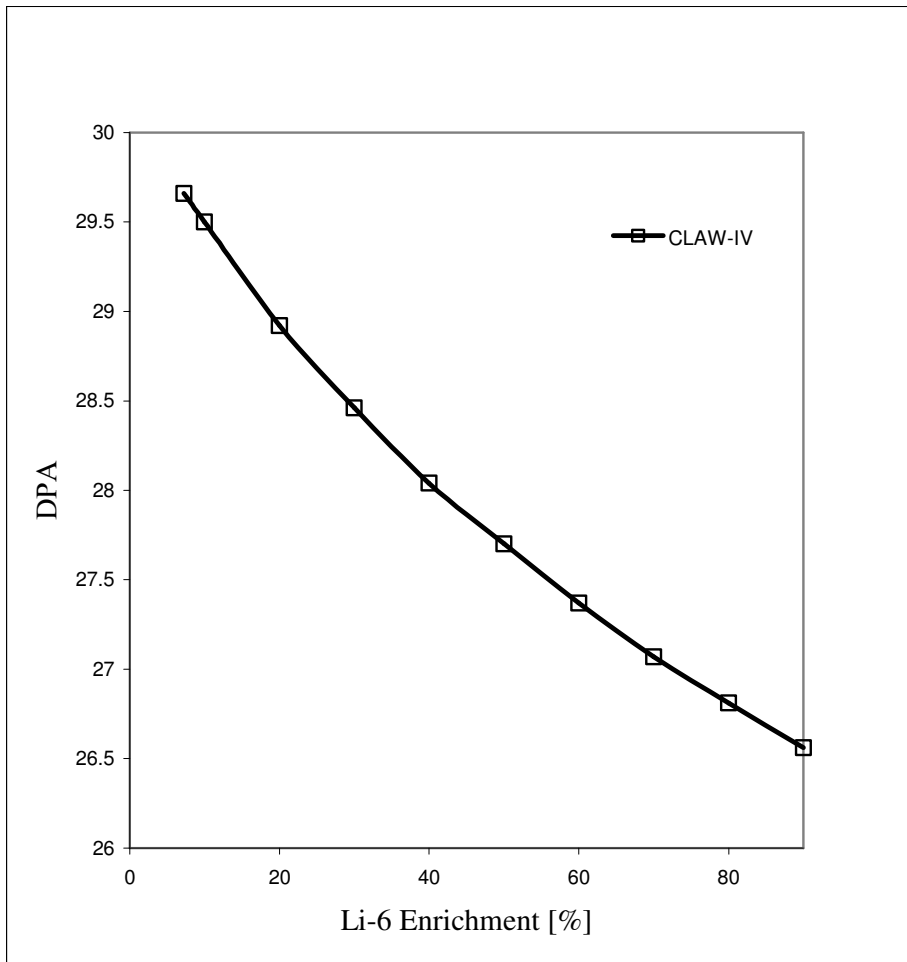


Figure 4. DPA value in the first wall versus ${}^6\text{Li}$ enrichment of the coolant

Table 1. Atomic densities of the blanket materials.

Material	Density(g/cm ³)	Zone	Nuclide	Nuclei Density (10 ²⁴ /cm ³)
UO ₂	8.76	Fuel	²³⁵ U	1.39600E-4*
			²³⁸ U	1.94080E-2
			O	3.91040E-2
SS304 Stainless Steel	7.94	First wall	C	6.94934E-5
			Si	8.68667E-4
			P	3.90900E-5
			Cr	1.65048E-2
			Mn	1.73733E-3
			Fe	5.93951E-2
			Ni	8.25234E-3
Natural-Li	0.53	Moderator (coolant)	⁶ Li	3.52301E-3
			⁷ Li	4.28935E-2
(Enrichment of ⁶ Li)			⁶ Li	4.64165e-3
10%			⁷ Li	4.17749e-2
20%			⁶ Li	9.28330e-3
			⁷ Li	3.71332e-2
30%			⁶ Li	1.39250e-2
			⁷ Li	3.24916e-2
40%			⁶ Li	1.85666e-2
			⁷ Li	2.78499e-2
50%			⁶ Li	2.32083e-2
			⁷ Li	2.32083e-2
60%			⁶ Li	2.78499e-2
			⁷ Li	1.85666e-2
70%			⁶ Li	3.24916e-2
			⁷ Li	1.39250e-2
80%			⁶ Li	3.71332e-2
			⁷ Li	9.28330e-3
90%			⁶ Li	4.17749e-2
			⁷ Li	4.64165e-3
Li ₂ O	2.01	Tritium breeding	⁶ Li	6.15831E-3
			⁷ Li	7.49787E-2
			O	4.05685E-2
Carbon	2.26	Reducing neutron leakage	C	1.12800e-1

read as *1.39600.10⁻⁴