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Space Dependent Study of Fast Neutron Spectra and Tritium Production Rate in a Fusion Reactor Blanket of Li₂O

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Study of spatial spectra and tritium breeding ratio (TBR) in a lithium blanket play a crucial role for the successful operation of a Fusion reactor. In this paper, we have reported the results for the space-dependent fast neutron spectra and tritium production rate (TPR) in cylindrical assemblies of Li₂O. The multigroup diffusion equation has been solved using eigenfunction expansion method. The obtained results for scalar spectra, total flux and TPR in Li₂O are compared with corresponding values for natural Li. The space dependent scalar spectrum in Li₂O has been compared for different configurations (slab, sphere and cylindrical). We find that the shapes of the curves are almost similar, though the neutron flux is found to be highest in the case of cylindrical assembly. This suggests a larger value of total TBR for a cylindrical geometry. Further, the study of space variation of total flux for Li₂O and natural Li shows that there is not much change in the shapes and numerical values, however, it falls sharply near the boundary end surface of the assembly for Li₂O as compared to natural Li near the boundary end.. The calculated results of spatial distributions of TPR for ⁶Li (n, \alpha)t and ⁷Li (n, n'\alpha)t reactions are compared with experimentally obtained results for cylindrical slab assemblies. and it is found that agreement is fairly good, both in the case of ⁷Li and ⁶Li.

Keywords: Lithium oxide; Blanket; Tritium Production Rate; Tritium Breeding Ratio

1 Introduction

Lithium bearing blankets in a futuristic Fusion reactor have been a subject of interest for the past several decades, and continuing efforts are being made to study the neutron energy spectra and achieve a suitable value of Tritium Breeding Ratio (TBR) in various assemblies of Li compounds.

For a steadfast, safe and self sufficient operation of a DEMO (DEMOnstration) power plant as a futuristic Fusion Reactor, the critical parameter is Tritium Breeding Ratio and equally important is the study of neutronic spectra related to design and safety analysis of the reactor. Tritium is not available in abundance as a natural resource that may be used as fuel in a fusion reactor; however, it can be created in the blanket enclosing the fusion chamber by a reaction between neutrons and lithium. This makes it important to successfully recover generated Tritium in the breeding blanket. Also, it must be ensured that Tritium Breeding Ratio (TBR) attainable in the blanket should be sufficiently high for covering the entire Tritium required for the fusion reactor for its reliable operation.

Variety of factors influence the value of TBR such as choice of breeding material, geometrical models, reactor layout and neutronic calculations¹. Matsura et al.² suggested evaluation method for TBR using Neutron Transport equation. Studies of Tritium Breeding Ratio with He cooled Lithium Lead Fusion blanket have also been reported by Indah Rosidah et al.3. Their calculations (based on MCNP program) showed that neutron flux produced by this simulation from breeding blanket of Pb-Li does not leak and the production of tritium would be optimal. Sadhegi et al.⁴ have suggested an appropriate model for an advanced breeding blanket of future TOKAMAK fusion reactor with solid breeder (Li₄SiO₄) material in the form of pebble beds, ferritic steel as structural material, and Beryllium as neutron multiplier. They studied TBR, and concluded that ⁶Li should be enriched to 40% for the proposed design. Roux et al.⁵ presented a summary of experimental results for ceramic breeder materials and suggested Li2O as the most attractive ceramic breeding material. Recent studies on Fusion blanket, with lithium based oxide ceramics as tritium breeding material, have also recommended Li2O as an excellent material in the breeder zone⁶.

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Hence, keeping in view about the above mentioned factors, a suitable material such as Li₂O was chosen to calculate TPR in a cylindrical slab and neutronic spectra for different geometrical shapes was calculated using a simple calculational tool of eigenfunction expansion method^{7,8}.

Lithium is the most favorable element to breed tritium, though its physical and chemical forms have not been fully specified so far. In the past few decades, continuing efforts to choose a suitable material for a fusion blanket, so as to achieve the optimal value of 1.05 for Tritium Breeding ratio (TBR); have led to the studies on many Li compounds and alloys. In early studies on blanket materials, Li2O was proposed as a ceramic solid tritium breeding material^{9,10}. As pointed out by Sugiyama *et al.*¹¹ several benchmark integral experiments were carried out in simple cylindrical geometries of various assemblies of Li2O, and Li2O with a graphite reflector or a Be neutron multiplier. A collaborative program (on fusion blankets) between Japan Atomic Energy Research Institute (JAERI) and U.S department of atomic energy (DOE) focused its attention on tritium breeding capabilities of Li2O. As a result of this joint venture, spatial distributions of tritium production rates and neutron spectrum were measured and compared with a variety of calculational results^{12,13}. Most of the earlier experiments on Li blankets adopted a spherical geometry due to simplicity of the model. However, in such a spherical system, the neutron target structure was treated as part of experimental assembly. Moreover, it was found that the distribution of neutrons emitted from the target was not symmetrical but had a large dip for the direction tangential to the target plane¹⁴. Hence, a cylindrical slab geometry was considered to be a better choice for the test blanket module.

Maekawa *et al.*¹⁵ determined the TPR distributions in two assemblies. These were the pseudo-spherical assembly (r = 30 cm) of Li₂O with a graphite reflector and a 40 cm thick cylindrical slab of Li₂O (r = 31.4cm).The measured results were compared with transport calculations. It was found that in Li₂O-C assembly, the calculated values of TPR agreed well with the measured values, except near the target. This discrepancy was attributed to the fact that near the target, the source neutron spectrum below 1 MeV was strongly affecting the TPR distributions from ⁶Li (n, α)t reaction. However, fairly good agreement between measurements and calculations for TPR distributions from ⁷Li, ⁶Li and natural Li were obtained for the cylindrical assembly of Li₂O.

Further, Maekawa et al.¹⁴ carried out integral experiments on a Li₂O cylindrical assembly. The size of the assembly was 63 cm (diameter) by 61 cm (length).Besides, the measurements of neutron spectra and TPR from ⁷Li and ⁶Li, certain fission rates and reaction rate distributions were also obtained. Several measuring techniques were used in the experiment and the results obtained were compared with transport calculations. In order to examine the effect of including a Be neutron multiplier, Nakamura et al.¹³ carried out experiments to measure TPR and neutron spectra in the same assembly of Li₂O with a Be layer placed in front of the breeder and also sandwiched between two breeder regions. A considerable increase in TPR from ⁶Li (n,α) t reaction was observed in the breeder region around the Be zone. The measured TPR distributions were found to agree well with the calculated ones except near the zone boundaries.

Angular neutron fluxes leaking from the surface of the pseudo-cylindrical slabs of Li₂O were measured as functions of slab thicknesses and leaking angles by Oyama *et al.*¹⁶.The experimental results were compared with Monte Carlo calculations, with a view to examine the data in JENDL-3PR1,3PR2 and ENDF/BV data files.

TPR was also measured and calculated for a Li₂O assembly (60 cm length x 60 cm diameter) by Santoro *et al.*¹⁷. To stimulate the first wall (*i.e.* breeder region alone) and the coolant materials, they considered four additional configurations where layers of stainless steel and/or polyethylene in various thicknesses and configurations were placed in front of the Li₂O assembly.

It is clear from the above brief survey of studies of Li₂O blankets that the main thrust has been on the new integral experiments which can assess the crosssection information from ⁷Li (n,n' α)t and ⁶Li (n, α)t reactions and various combinations of Li₂O with other materials have been explored. The quantities measured in these experiments are mainly TPR and neutron energy spectra (in the blanket or leaking out from the assemblies) which are then compared with calculations using the transport codes.

Generally, for TBR estimations, high fidelity Monte Carlo simulations are used to minimize the uncertainties due to neutronic calculations. However, it was thought to be interesting to test the validity of a simple model of eigenvalues and eigenfunctions approach, for calculating TPR and TBR in cylindrical assemblies of Li₂O. Hence, here we report the results of a detailed space-dependent study of fast neutron spectra and TPR in a cylindrical slab of Li₂O using 27-group data-set of BARC-892.The scalar spectra and the spectrum averaged quantities like TPR and total flux were obtained for Li₂O and compared with the corresponding values for natural Li. Also, the scalar spectrum in Li₂O has been compared for slab, spherical and cylindrical configurations. The results for TPR from ⁷Li and ⁶Li in two cylindrical assemblies, having a radius of 31.4 cm and lengths of 40 cm and 61 cm respectively , were found to agree well with the experimental and calculated results of Maekawa *et al.*^{14,15}. The results reported by Santoro *et al.*¹⁶ for a 60 cm right cylindrical assembly of Li₂O were also found to be in good agreement with the present results.

2 Method of Calculations

In the steady-state, the multigroup diffusion equation for a cylindrical assembly with a point source located at the center of front face of the assembly (Fig 1.), isotropically emitting S^i neutrons per unit time is given as :

$$-D^{i}\left\{\frac{d^{2}}{dr^{2}}+\frac{1}{r}\frac{d}{dr}+\frac{d^{2}}{dz^{2}}\right\}\phi^{i}(r,z)+\sum_{i}^{t}\phi^{i}(r,z)=\sum_{j=1}^{N}\sum_{s}^{j\to i}+S^{i}\dots(1)$$

One can expand $\phi^i(r, z)$ in terms of the complete set of eigenvalues k_n^2 and the associated eigenfunctions ϕ_n^i as :

$$\phi^{i}(r,z) = \sum_{n} J_{0}(\alpha_{0},r) \phi^{i}_{n}(a_{n}e^{-k_{n}z} + b_{n}e^{k_{n}z}) \qquad \dots (2)$$

where, $J_o(\alpha_o, r)$ is the Bessel's function of zeroth order and α_o is the first zero of the Bessel's function. Using Eq. 2, for z > 0, the Eq. (1) can be written in the form:



Fig. 1 — A cylindrical assembly.

$$-D^{i} \left[-\alpha_{0}^{2} + k_{n}^{2} \right] \phi_{n}^{i} + \sum_{t}^{i} \phi_{n}^{i} = \sum_{j=1}^{N} \sum_{s}^{j \to i} \phi_{n}^{j} \qquad \dots (3)$$

where, $\alpha_0^2 = \left\{\frac{2.405}{R}\right\}^2$ for a cylinder with radius R. The eigenvalue equation thus becomes:

 $k_{n}^{2}\phi_{n}^{i} = \sum_{i=1}^{N} P_{j}^{i}\phi_{n}^{j} \qquad \dots (4)$

where,
$$P_j^i = -\frac{\sum_{s}^{j \to i}}{D^i}$$
 for $j < i$
 $= 0$ for $j > i$
 $= \left| \sum_{t}^i + D^i \alpha_0^2 - \sum_{s}^{j \to i} \right| / D^i$ for $j = 1$...(5)

If one considers the axial variations (along z direction) only, then one may write,

$$\phi^{i}(r,z) = \phi^{i}(z) = \sum_{n} \phi^{i}_{n}(a_{n}e^{-k_{n}z} + b_{n}e^{k_{n}z}) \qquad \dots (6)]$$

Using the extrapolated end-point boundary condition,

$$\phi^{l}(r,z) = 0 \qquad \dots (7)$$

where, $\tilde{z} = z + 0.71 \bar{\lambda}_{tr}$ is the axial dimension of the cylinder while $\bar{\lambda}_{tr}$ is the mean value of the transport mean free path.

$$b_n = -a_n e^{-2k_n \widetilde{z}} \qquad \dots (8)$$

Then, substituting (8) in (7); it becomes;

$$\phi^{i}(z) = \sum_{n} \phi^{i}_{n} a_{n} e^{-k_{n} z} (1 - e^{-2k_{n}(\tilde{z} - z)}) \qquad \dots (9)$$

Using the initial condition;

$$\phi^i(z=0) = \phi^i_o \qquad \dots (10)$$

 a_n 's can be expressed as

$$a_{i} = \frac{\phi_{o}^{i} - \sum_{n=1}^{i=1} \phi_{n}^{i} a_{n} (1 - e^{-2k_{n}\widetilde{z}})}{(1 - e^{-2k_{i}\widetilde{z}})} \dots (11)$$

The total flux can then be calculated using the relation,

$$\phi(z) = \sum_{i} \phi^{i}(z) \qquad \dots (12)$$

Also, Tritium Production Rate (TPR) is defined as,

$$TPR = \frac{\sum_{TP} \delta^{i}}{\sum_{i} \delta^{i}_{o}} \qquad \dots (13)$$

Thus, for the atom density $N = \{p N_{avg} / A\}$ of ⁷Li and ⁶Li, we have obtained TPR distributions as $\frac{\text{TPR}}{N}$

in units of TPR/⁷Li ,⁶Li atom/(source neutron/cm²). Then, TBR is given by the integration of TPR over the volume of the cylinder.

3 Results and Discussions

Following the procedure outlined above, the results have been obtained for space dependent neutron spectra in Li₂O cylindrical assemblies and compared with spectra in lithium assembly at various distances. We have also discussed the results in different type of assemblies (slabs, cylinder, and sphere). The space variation of total flux for Li₂O and Li is discussed. The variation of space dependent TPR is also discussed.

3.1 Space dependent Spectra

In Fig. 2, we have shown the variations of neutron

spectra $\phi(z, E) = \frac{\phi^i(z)}{dE^i}$

with energy at various distances inside a cylindrical slab of assembly of Li₂O. The following features may be noted from this figure:

1. The peak near the source energy disappears beyond ~ 10 cm as the high energy neutrons rapidly



Fig. 2 — Spatial variations of neutron spectra in cylindrical slab assemblies of Li₂O.

slow down to lower energies due to (n,p),(n,2n) and (n,α) reactions from ⁷Li, ⁶Li and O.

2. The small peak at 3.2 MeV corresponds to the inelastic threshold of O. It is present only at a distance very close to the source plane ($\sim 2 \text{ cm}$) and is missing at distances further away from it.

3. At all distances, there is a pile up of neutrons at 0.6 MeV corresponding to the inelastic threshold of natural Li. (This corresponds to the 'trapping effect').

4. The sharp dip at 0.3 MeV is due to the resonance present in the total cross-section of Li_2O , arising from resonances in the elastic cross-section values of ⁷Li and ⁶Li at this energy.

5. In the energy range 0.1MeV- 0.7keV, there is a continuous increase in the flux with a decrease in energy. This steep hike in the curve is seen to be more at larger distances from the source plane. This may be attributed to the fact that the slowing down process in this energy region is due to the slower process of elastic scattering and the elastic cross section values remain almost constant in this energy range for ⁷Li, ⁶Li and O.

6. Below 0.7 keV, the flux starts decreasing with a decrease in energy, as the absorption cross sections of 6 Li rise to very high values in the energy region 0.7 keV-0.025 eV.

The space-dependent spectra for natural Li and Li₂O have been compared in Fig 3, at 10 and 50 cm from the source plane. One may note that the peak at the source energy which disappears at small distances away from the source for the case of Li₂O(Fig 2),is



Fig. 3 — Space dependent spectra in cylindrical slab assemblies of Li₂O and natural Li at 10 cm and 50 cm from the source plane.

present even at 50 cm in the case of natural Li. Also, we notice that in the case of natural Li, there is a continuous decrease below 0.1 MeV unlike the case of Li₂O, where the fall in the flux with the decrease in energy was observed below 0.7 keV. This difference in behavior of low energy spectra in Li₂O are much 'softer' than natural Li at all distances.

In Fig 4, we have compared the space dependent energy spectra for the case of 1-m³ slab, a 1-m right cylindrical and a 1-m diam spherical assemblies. It is clear from this figure that the shapes of the curves are almost similar; though the neutron flux is found to be highest in the case of cylindrical assembly, suggesting a larger value of (total) TBR, for this configuration.

The space variation of the total flux $\phi(z)$ (defined by Eq.(12)) is shown in Fig. 5 for Li₂O and natural Li. One may note that, even though the spectra in the two cases had different shapes (especially at low energies), there is not much change in the shapes and numerical values of their total flux. Both the curves exhibit a linear behavior in the distance range of 20-40 cm, however, as compared to natural Li, the total flux $\phi(z)$ for Li₂O falls sharply near the boundary end surface of the assembly.

Similarly, the TRR curves (Fig. 6) for Li₂O and natural Li coincide with each other up to ~ 30 cm and thereafter, the fall in the TPR curves becomes more rapid for the case of Li₂O as compared to natural Li.



Fig. 4 — Space dependent spectra in Li₂O for a 1 m cubical, 1 m diameter spherical and 1 m right cylindrical assemblies.

3.2 Comparison with the Experiment

In Figs. 7-12, we have compared the presently calculated results of the spatial distributions of TPR for ⁶Li(n, α)t and ⁷Li(n,n' α)t reactions, with the experimental results obtained by Maekawa *et al.*^{14,15} & Santoro *et al.*¹⁷ for cylindrical slab assemblies of various sizes. It must be mentioned here that all these researchers have considered a D-T neutron source placed at some distance (~ 20 cm) in front of the assembly and hence, they have obtained TPR distributions in units of TPR/⁷Li, ⁶Li atom /source neutron. However, in our calculations, we have



Fig. 5 — Variation of space-dependent total flux $\phi(\mathbf{Z})$ for Li₂O and natural Li in a cylindrical assembly (61 cm length x 63 cm diameter).



Fig. 6 — Variations of space-dependent Tritium Production Rate (TPR) for Li₂O and natural Li in a cylindrical assembly (61 cm length x 63 cm diameter).



Fig. 7 — Space-dependence of Tritium Production Rate (TPR) from ⁷Li in a cylindrical slab assembly (40 cm length x 63 cm diameter) of Li₂O. Presently, calculated results have been normalised with the experimental results of Maekawa *et al.* (1983) at 10 cm from the source plane.



Fig. 8 — Space-dependence of Tritium Production Rate (TPR) from ⁶Li in a cylindrical slab assembly (40 cm length x 63 cm diameter) of Li₂O. The presently, calculated results have been normalised with the experimental results of Maekawa et al. (1983) at 10 cm from the source plane.

considered a point source of neutrons placed at the center (r = 0) of the front face of the assembly (Fig 7) along with the initial condition on the flux defined by Eq.(10). As a result, the presently obtained TPR distributions were studied as TPR/⁷Li, ⁶Li atom/ (source neutron/cm²).Therefore, the present results have been normalized with the experimental results at 10 cm from the source plane.

In Fig 7 and 8, we have shown the spatial variations of TPR in a 40 cm (length) by 63 cm (diameter) cylindrical assembly for ⁷Li and ⁶Li respectively. Also, Fig 9 and 10 show the TPR curve in a 61 cm (length) x 63 cm (diameter) assembly. These curves have been compared with the experimental results reported by Maekawa *et al.*^{14,15} respectively. The homogenized nuclide densities for



Fig. 9 — Space -dependence of Tritium Production Rate (TPR) from ⁷Li in a cylindrical slab assembly (61 cm length x 63 cm diameter) of Li₂O. The presently calculated results have been normalized with the experimental results of Maekawa *et al.* (1986) at 10 cm from the source plane.



Fig. 10 — Space -dependence of Tritium Production Rate (TPR) from ⁶Li in a cylindrical slab assembly (61 cm length x 63 cm diameter) of Li₂O. The presently calculated results have been normalized with the experimental results of Maekawa *et al.* (1986) at 10 cm from the source plane.

⁷Li, ⁶Li and O for present calculations have been tabulated in Table 1.

We find that in the case of ⁷Li, (Fig 7 and 9); the agreement between the experimental and calculated values is poor at the zone boundaries. Also in this case, the calculated values of TPR are found to be higher than the experimental values. This is due to the fact that in the vicinity of the surfaces, both the room returned soft neutron effect and the self-shielding effects are large and the present calculations have not been corrected for these effects.



Fig. 11 — Space-dependence of Tritium Production Rate (TPR) from ⁷Li in a 60 cm right cylindrical assembly of Li₂O. The presently calculated results have been normalized with the experimental and calculated results of Santoro *et al.* (1990) at 10 cm from the source plane.



Fig. 12 — Space-dependence of Tritium Production Rate (TPR) from ⁶Li in a 60 cm right cylindrical assembly of Li₂O. The presently calculated results have been normalized with the experimental and calculated results of Santoro *et al.* (1990) at 10 cm from the source plane.

Figures 11 & 12 show the comparison between the present values of TPR and the experimental and calculated values obtained by Santoro *et al.* (1990) for

Table 1(a) — Homogenized nuclide density for cylindrical assemblies of Li ₂ O, having a radius of 31.4 cm and lengths of 40 cm and 61 cm respectively.	
Nuclide	Nuclide Density(10 ²⁴ atoms/cm ³)
⁷ Li	5.190 x 10 ⁻²
6Li	4.152 x 10 ⁻³
0	
	2.803 x 10 ⁻²
Table 1(b) — Homogenized nuclide density for a 1 m right cylindrical slab assembly of Li ₂ O.	
Nuclide	Nuclide Density(10 ²⁴ atoms/cm ³)
⁷ Li	5.05 x 10 ⁻²
6Li	4.05 x 10 ⁻³
0	2.72 x 10 ⁻²

a cylindrical assembly of 60 cm (length) and 60 cm equivalent diameter of Li₂O. The agreement between the presently calculated results normalized with the experimental results at 10 cm is fairly good both in the case of ⁷Li as well as ⁶Li.

4 Conclusions

Achieving the value of tritium breeding ratio more than unity is of major concern for the sustainable operation of a futuristic fusion reactor. The present study has proposed the material as lithium oxide for tritium breeding and tritium production rate has been studied in detail with comparative results for natural Lithium. Also detailed spatial behaviour of fast neutrons in lithium oxide has been studied. The simple calculations using eigenfunction expansion method has produced results which are found to be in good agreement with the experimental as well as with theoretical results using advanced calculations methods. Encouraging results suggest a cylindrical assembly design for a fusion blanket of lithium oxide. This study can be useful for understanding the spatial behaviour of fast neutrons in various geometrical assembly designs using lithium oxide for the fusion blankets. A simulated space dependent study has proposed the material as lithium oxide for tritium breeding and tritium production rate has been studied in detail with comparative results for natural Lithium.

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