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TANDEM MIRROR FUSION BREEDER
NEUTRONIC ISSUES AND OPTIMIZATION

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PREFACE

This report is the 5th of 6 volumes directed towards the resolution of special topics associated with a reference fission-suppressed tandem mirror fusion breeder reactor design developed during 1981-82. A complete list of the special topics reports follows:

Volume 1: Liquid Metal MHD Pressure Drop Effects in the Packed Bed Blanket by T. McCarville, D. Berwald, and C. P. C. Wong.

Volume 2: Reactor Safety Assessment by I. Maya, C. G. Hoot, C. P. C. Wong, K. R. Schultz, J. K. Garner, S. J. Bradbury, W. G. Steele, and D. H. Berwald.

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Volume 5: Neutronics Issues and Optimization by J. D. Lee and B. R. Bandini.

Volume 6: Materials Compatibility Issues and Experimental Results by J. H. DeVan and P. Torterelli.

Earlier nuclear analysis was carried out without resonant self-shielding included and without optimization of thorium to beryllium ratio. The resonant self-shielding effect reduced breeding somewhat but increasing the thorium volume fraction more than overcame this decrease and the breeding ratio increased by 36%. Energy multiplication also increased.

Further work is required to more fully explore the potential operating envelope.

SPECIAL TOPICS REPORTS FOR THE REFERENCE TANDEM MIRROR FUSION BREEDER

NEUTRONIC ISSUES AND OPTIMIZATION

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ABSTRACT

More rigorous nuclear analysis, including the treatment of resonance self-shielding effects coupled with an optimization procedure, has resulted in improved performance of the Be/Li/Th blanket. Net U-233 breeding ratio has increased 36% (to 0.84) while at a U/Th ratio of 0.25 a/o energy multiplication has increased 12% (to 2.1) compared with earlier results.

INTRODUCTION

The conceptual design and analysis of fissile-fuel-producing blankets for fusion reactors is the principal activity of the Fusion Breeder Project. In FY82 we developed and analyzed a conceptual design of a blanket containing Be pebbles (~ 50 v/o) for neutron multiplication, Li (~ 40 v/o) for tritium breeding and cooling, Th (~ 3 v/o) for U-233 breeding, and steel structure (~ 7 v/o).^{1,2} The Th is in the form of inserts or snap rings attached to each Be pebble. Figures 1 and 2 show the blankets mechanical design and the cylindrical models used for the nuclear analysis.

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Fig. 1. Reference fusion breeder (with tandem mirror driver).

BED MATERIAL VOLUME FRACTIONS

<u>MATERIAL</u>	<u>VF</u>
Th+U-233	.03x.98=.029
Be	.57x.98=.55
Li	.40(.2% Li 6)
Fe	.02

Fig. 2. Cylindrical model - geometry and composition.

This paper reports on additional work done to improve the nuclear analysis and optimize the nuclear performance of this blanket. The improvements made in the nuclear analysis are the following: (1) include resonance self-shielding effects as suggested by Taczanowski³ and others and (2) generate and use resonance and spatial self-shielding, corrected cross-section sets for 1-D blanket calculations.

Nuclear performance is optimized by varying the Th volume fraction (trading Be for Th) to maximize specific breeding [ratio of net fissile (atom) breeding to energy generation]. This is done at U to Th ratios of 0 and 1% and a tritium breeding ratio (T) of 1.06. The 1% upper U/Th ratio is a reasonable compromise between low U content, giving low energy multiplication (M), and high U content, giving low cost reprocessing. T is kept constant by varying the Li^6/Li^7 ratio.

The methods and data used to perform this analysis and optimization include ANISN, a 1-D discrete ordinate transport code used with the LANL 80 neutron group nuclear data library, MATXS6 that is based on data from both ENDF/B4&5 and includes Bonderenko factors for resonance correction. The LLNL Monte Carlo code ALICE (a version of TART that includes resonance effects), coupled with an ENDF-based 175 group data library, was also used to compare with the ANISN results. Optimization was done with a linear programming-based code developed at Penn State University. This optimization code uses ANISN as a subroutine.

The procedure used consisted of generating cross sections corrected for resonance and spatial self shielding with a spherical 1-D unit cell, collapsing the group structure, then running the optimization code to find out how net fissile atom breeding (F_{net}) and blanket energy multiplication (M) vary versus Th v/o. At each point the optimization code varies the Li^6/Li^7 ratio to keep T at 1.06. This procedure was repeated twice to reduce the difference between the point where the cross-section resonance correcting and collapsing is done and the point of optimum performance. The final round started at a Th v/o of 12% and a Li^6/Li^7 ratio of 4%. The initial round started at a Th v/o of 3% and a Li^6/Li^7 ratio of 0.2%.

METHODS AND RESULTS

In this study, the reference liquid Li cooled tandem mirror fusion hybrid blanket^{1,2} is optimized for maximum U-233 fissile fuel production per incident 14.1 MeV fusion neutron. This optimization of the hybrid blanket was accomplished by varying two blanket design quantities. The first of these quantities is the Th to U volume fraction within the multiplier zones. The second is the Li-6 enrichment in the blanket's Li coolant. The production of U within the blanket is obtained by subtracting all blanket fissile fuel consuming reactions (U-233 (n,gamma) and U-233 (n,fission)) from the primary fissile production reaction (Th-232 (n,gamma)). This quantity is then maximized by adjusting the two blanket variables while maintaining the blanket tritium production [Li-6 (n,alpha) + Li-7 (n,n')] at a constant value of 1.06 atoms per fusion neutron.

This optimization was performed on a one dimensional cylindrical neutronics model of the hybrid blanket, as shown in Fig. 2. The mechanics of the procedure were performed using an iterative gradient ascent optimization routine, Appendix A, coupled to the one-dimensional discrete ordinates transport code ANISN.⁴

In order to achieve realistic answers from ANISN based optimization scheme, a good microscopic cross section set had to be developed that was especially tailored for this problem. There were two significant factors which had to be taken into account when this cross section set was created. The first of these factors was blanket inhomogeneities. This is a result of the fuel zones containing discrete 3 cm Be-Th spheres being modeled as homogeneous fuel zones. The small scale neutron flux variations through the discrete geometry of Be multiplier, Th fuel, and Li coolant present in the actual hybrid blanket must also be accounted for in producing the cross sections for the 1-dimensional ANISN based blanket optimization. This was done in order for calculated reaction rates in the homogeneous model to be representative of those in the actual blanket. The other factor which had to be taken into account was neutron resonance self-shielding and absorption. This comes as a result of many resonance nuclides in the blanket coupled with the blankets neutron energy spectrum.

In order to more carefully study the effects of resonance self-shielding and absorption on the neutronics of the problem while eliminating the blanket's heterogeneous nature, a simple model of a single Be-Th sphere within the blanket was created. A diagram of this 'unit cell' model can be seen in Fig. 3. The geometry of this was created as follows. The radius of the Be-Th sphere was set at 1.5 cm, the actual radius of these components. This sphere was then cut by a cylinder to divide it into a Be region and a Th region. This cylindrical-spherical geometry was chosen as the most correct means of representing the actual Be ball surrounded by a Th snap ring. Next the 1.5 cm. radius sphere was surrounded by a spherical shell containing the Li coolant. This shell was in turn surrounded by another shell containing the steel structure within the fuel zone. The radii of the cylinder within the 1.5 cm. sphere and of the outer boundaries of the Li coolant and structural steel shells were chosen to maintain the actual volume fractions of these materials within the blanket fuel production zones. The fuel material volume fractions used were those obtained from the LLNL blanket design project.¹ They are Be 57 vol. %, Th 3vol. %, Li 40 vol. %, and Fe steel 2 vol. %. In order to realize these volume fractions in the unit cell model, the radius of the Be cylinder was set at 1.392 cm, the outer radius of the Li coolant region was set at 1.787 cm, and the outer radius of the steel region and of the entire cell was set at 1.799 cm. The model was completed by making the outer spherical surface a reflecting boundary and by placing a thin shell 14.1 MeV isotropic fusion neutron source near the outer edge of structural steel shell. The material contents of these four zones can be summarized as follows. The central cylinder is made up of pure Be-9 at normal density. The annulus between this cylinder and the 1.5 cm radius spherical boundary is made up of pure Th-232 at normal density. No U-233 is included in this Th zone because of the belief that thermal fission of U-233 would be greatly over emphasized in this cell with reflective boundary conditions. The third zone, the spherical shell containing Li coolant, is made up of Li at normal density with Li-6 in the Li-6 to Li-7 nuclide mixture depleted to 0.2 atom %. This is the Li enrichment described in the previous LLNL model.^{1,2} Finally, the outermost steel shell is made up of normal density ferritic steel which is made up of natural Fe, Cr, and Mo at mass fractions of 96.75%, 2.25%, and 1.0%, respectively.

Fig. 3. Exact 3-D unit cell of Be/Li/Th fuel zones.

These initial unit cell calculations were performed using the LLNL three dimensional Monte-Carlo codes TART and ALICE⁷ and a 175 neutron group cross section library based on the ENDL (6) cross section library. ALICE is a special version of the basic TART code which uses a multi-band treatment for treating the resonance effects in some nuclei.⁵

The first of the previously described unit cells to be run was an ALICE case using the 175 group ENDL library in which no doppler broadening of the multi-band resonance cross sections was performed. The major results of this calculation are shown in Table 1 under the heading 'ALICE exact OK'. The tabulated results first include T, the tritium breeding ratio, which is the sum of all Li-6 (n,alpha) and Li-7 (n,n') reactions. Next is F, the U-233 production ratio, which is just the Th-232 (n,gamma) reaction since no U-233 is included in the cell. Third is the sum of T and F. Fourth is the fission rate within the Th-232. Next is M, the ratio of energy produced in the cell per unit energy emerging from the 14.1 MeV neutron source. Finally are four columns showing the percentage breakdown of the aforementioned unit cell energy production within each of the zones within the unit cell. In the next unit cell calculation ALICE is again used to model the same cell except that now a form of the 175 group is used in which doppler broadening of the multi-band resonance parameters has been performed for a room temperature thermal agitation. The results of this calculation appear on Table 1 under the heading 'ALICE exact room temp.'. The major differences between this run and the previous run are an approximately 5% rise in the Th-232 (n,gamma) reaction and a 5% drop in the Th fission reaction. This was expected because doppler broadening enhances the Th-232 (n,gamma) reaction which takes place as a result of resonance absorption in Th. This increase in neutron loss in the Th then causes fewer neutrons to be available for fission in Th. The other reactions and the unit cell energy production are only affected to a small degree by this doppler broadening of cross sections.

In the third unit cell calculation, TART instead of ALICE is used to calculate the reactions in the unit cell. This calculation whose results appear in Table 1 under the heading 'TART exact', shows the effect of

Table 1. Reactions per fusion neutron for base case liquid LI unit cells.

	T	F	T + F	Th (n,f)	M	E _{Be} (%)	E _{Th} (%)	E _{LI} (%)	E _{FE} (%)
ALICE EXACT 0°K	1.322	0.576	1.898	0.0094	1.549	26.5	21.5	38.7	13.2
ALICE EXACT ROOM TEMP.	1.319	0.617	1.936	0.0090	1.548	25.8	22.1	38.7	13.4
TART EXACT	1.123	0.824	1.947	0.0088	1.518	25.5	27.1	34.9	12.6
ALICE SPHERE 0°K	1.264	0.640	1.903	0.0094	1.534	25.8	23.2	37.8	13.1
ALICE SMEARED 0°K	1.252	0.877	2.128	0.0102	1.652	-	-	-	-
ANISN S12 SPHERE HETEROGENEOUS SELF-SHIELDING	1.377	0.878	2.255	0.0108					
ANISN SPHERE NO SELF-SHIELDING	1.025	1.287	2.312	0.0108					
ANISN SPHERE HOMOGENEOUS SELF-SHIELDING	1.748	0.456	2.204	0.0108					
ANISN SMEARED NO DISADVANTAGE FACTORS	1.365	0.896	2.260	0.0108					
ANISN SMEARED WITH DISADVANTAGE FACTORS	1.368	0.886	2.254	0.0109					

resonance self-shielding and absorption on the reactions within the unit cell. Not accounting for resonances has a significant effect on the results of the unit cell calculation. Table 1 shows a 20% decrease in tritium production and a 30% increase in U-233 production when resonance effects are not included. These discrepancies are a result of the detailed inter-relationship between resonance self shielding and absorption on those reactions whose cross sections are large at resonance neutron energies. In addition, the sum $T + F$, the Th fission rate, and the energy multiplication factor M change only slightly while some of the energy production shifts from the Th zone to the Li zone. These rather large changes in the important blanket reactions T & F , imply that resonance self shielding and absorption are significant factors in this design and therefore must be taken into account if accurate results are expected from these calculations.

In the fourth unit cell calculation, the model was changed somewhat. Here the central cylinder containing Be was converted to a sphere. This change also converts the Th annular zone to a spherical shell. Keeping the volume fractions of the various materials within the unit cell the same as previously, the radius of this innermost spherical boundary was set at 1.474 cm. This modification of the more exact unit cell was made to cause the unit cell to be completely spherically symmetric in anticipation of later calculations on this unit cell with the 1-dimensional ANISN code. This spherically symmetric calculation was performed in ALICE using the original non-doppler broadened 175 group library. A comparison of these results titled 'ALICE sphere Ok' with the original non-doppler broadened ALICE exact unit cell calculation can be seen in Table 1. Upon comparing these results, one can see that the change in model decreases T by about 5% and increases F by about 10% leaving the other quantities approximately constant. These reaction rate differences, while noticeable, are not extremely large, meaning that the totally spherical unit cell geometry is an acceptable substitute for the original more exact geometry.

The final unit cell which was run in ALICE was a single zone spherical unit cell whose outer radius and source distribution were the same as the exact unit cell. This single zoned cell contained a homogeneous mixture of the materials within the discrete zoned cell weighted by their respective geometric volume fractions within the discrete cell. This cell was created to see the effect of the actual fuel region heterogeneities on the neutronics within the blanket. This homogenized model was then run in ALICE using the original non-doppler broadened 175 group library. A comparison of these results titled 'ALICE smeared 0k' with the original non doppler broadened exact unit cell calculation can be seen in Table 1. These results show that the major Th reactions, Th-233 (n,gamma) and Th-232 (n,fission), have increased by about 40% and 10% respectively. They also show that T has decreased by about 10% and that blanket energy multiplication has increased by over 5%. These results show that heterogeneity is important. Therefore, these small scale heterogeneities must be taken into account when the fuel zones are modeled homogeneously in the large cylindrical model of the blanket.

Next these same unit cells were run using the ANISN 1-dimensional discrete ordinates transport code. The cross sections for these ANISN calculations were created with the Los Alamos National Laboratory code package TRANSX-CTR.⁹ This code package contains many options including Bonderenko resonance self shielding. The TRANSX package contains several fine group microscopic neutron libraries. The library chosen for use with these fusion blankets was an 80 neutron group library known as MATXS6.⁸ This library was collapsed from ENDF-B 4 using a fusion breeder/fast reactor flux spectrum. This library contains the isotopes and group structure which are very well suited to fusion blanket calculations. In addition, this library contains extensive tabulations of self shielded cross sections which incorporate listings for a wide variety of material temperatures and background cross sections.

The first of these ANISN unit cell calculations was an 80 group run on the completely spherically symmetric liquid Li base case unit cell described above. For this calculation, the heterogeneous resonance self shielding option

was employed in the TRANSX cross section production run. In this self shielding option a finite neutron escape cross section is input for each zone in the unit cell. The results of this initial ANISN calculation can be seen in Table 1 under the title 'ANISN sphere heterogeneous self shielding'. This output contains only listings for tritium breeding, U-233 production, Th fission, and the sum of T and F. No energy deposition related output is included because the MATXS6 library contains energy deposition factors which are not appropriate for neutron only transport calculations. In addition, some energy deposition factors within the ENDF-B 4 & 5 master libraries have been found to be in error, causing these same factors within MATXS6 to be in error. Returning to the output it can be seen in Table 1 that this ANISN calculation yields a value of tritium breeding within about 2% of that calculated in the initial ALICE exact unit cell calculation. But, the values of Th-232 fission and Th-232 (n,gamma) seem to be more in line with the results of the ALICE smeared material unit cell cases than any of the discrete ALICE unit cell runs. This apparent matchup of results may be coincidental, the combined result of many factors. These include differences in cross section sets, ENDL vs ENDF-B master libraries, Monte Carlo vs discrete ordinates calculational methodologies, and differences between the Bonderenko and multi-band resonance approximations. On the other hand, these results may actually mean that the fluxes within the Th region of the ANISN unit cell are too high as a result of some modeling drawbacks inherent in the ANISN calculations. These drawbacks may include such things as limited angular and spatial intervals for neutron flux.

The next ANISN unit cell calculation was performed using the same geometry but using no resonance self shielding corrections when creating the cross section set. The results of this calculation can be seen in Table 1 under the title 'ANISN sphere no self shielding'. Here the effects of removing self shielding are approximately the same as when TART was used instead of ALICE in the Monte Carlo unit cell calculations. Namely, T dropped by about 30% and F rose by 30%. As before, Th fission and the sum of T and F remained relatively constant. Comparing these two ANISN unit cells further dramatizes and reinforces the significant effect that resonance self shielding and absorption has on the reactions in this hybrid blanket environment.

A third ANISN unit cell was run to study the effects of excessive resonance self shielding. In this run, the results of which are tabulated in Table 1 under the title 'ANISN sphere homogeneous self shielding', the homogeneous resonance self shielding option was employed in producing cross sections with TRANSX. This option assumes that each of the zones in the unit is of infinite extent, with no possibility of neutron escape. This assumption tends to greatly over correct the cross sections for resonance self shielding effects. The results of this calculation tend to substantiate this viewpoint. Here tritium production increases by about 30% over the heterogeneously self shielded case while the Th-232 (n,gamma) reaction decreases by over 40%. As expected, these results are the exact opposite of those encountered when self shielding was removed. Again, as expected, the Th fission rate and the sum of T and F remained approximately constant as the resonance calculation type was varied. Next, an ANISN calculation was run to study the effects of the actual unit cell heterogeneity on the calculated results. Here, as in the the ALICE calculations, a single zone spherical model was created. In this zone was placed a smeared combination of the materials in the unit cell zones weighted by the volume fraction of its respective zone in the total cell. The cross sections used in this calculation were those used in the initial ANISN unit cell calculation, which were produced with the heterogeneous resonance self shielding option of TRANSX. The results of this calculation are shown in Table 1 under the title 'ANISN smeared no disadvantage factors'. These results are within a few percent of those obtained in the original ANISN discrete zone unit cell calculation. In addition, these results are also very near those obtained with the equivalent ALICE smeared material unit cell calculation. These results lend one to believe that somehow the unit cell heterogeneity has more of an effect when an ALICE Monte Carlo run is performed than when an ANISN discrete ordinates calculation is performed. This result as yet remains unexplained.

To exactly compensate for the effects of cell heterogeneities in the homogeneous fissile production zones of the full blanket calculation, a cross section manipulation technique was borrowed from lwr calculational methodology. This technique revolves around the use of spatial advantage/

disadvantage factors. These factors are an attempt to account for the spatial flux depressions and rises in the various zones of the unit cell for each of the 80 neutron energy groups. These factors are ratios which define the average relative intensity of the flux in a certain zone and group to the average flux throughout the cell in that energy group. The cross sections for each of the materials in the unit cell are then multiplied by the correct zonal set of these factors to emphasize materials which actually have higher fluxes within them and to de-emphasize materials which are in lower flux regions. This technique was then performed on the heterogeneously self shielded unit cell cross sections using the fluxes obtained in the first ANISN unit cell calculation. Since the fluxes in this calculation were relatively flat with respect to cell radius, the advantage/disadvantage factors were generally within a few percent of unity for all groups and zones. Next, another ANISN smeared material unit cell calculation was performed using these weighted cross sections. As expected, the results of this calculation, shown in Table 1 under the title 'ANISN smeared material with disadvantage factors', are very near those obtained in the previous smeared unit cell calculation. But the disadvantage factors do have some effect in bringing the tritium production and U-233 production reactions slightly closer to the values obtained in the discrete zone unit cell ANISN calculation. Use of these disadvantage factor weighted cross sections have little effect on the rate of Th-232 fission.

In the next series of calculations, the entire blanket was modeled in one-dimensional cylindrical geometry using the model shown in Fig. 2. The materials in the fissile production zones of this model were the same as those used in the base case unit cells, except that now U-233 is added to the Th-232 fertile material at 1 atom% to simulate the situation which exists when the bred fuel is about to be removed from the blankets for reprocessing.

The first run on this model was an ALICE calculation, whose cross sections were not modified for heterogeneity considerations. The results of this calculation are tabulated in Table 2 under the title 'ALICE base 0k'. This table, in addition to including the same reaction rate information as in

Table 2. Reactions per fusion neutron for base case liquid LI cylindrical model
(at 1 a/o U)

	T	F	F _{net}	T+F _{net}	Th(n,f)	U(n,γ)	U(n,f)	F _{net,eff}	$\frac{F_{net,eff}}{M}$
ALICE BASE 0°K	1.10	0.682	0.526	1.63	0.0065	0.0190	0.137	0.566	0.171
ANISN 80 GP S12	1.17	0.676	0.500	1.67	--	0.0215	0.154		
ANISN 30 GP S12 ALL CROSS SECTIONS	1.17	0.676	0.500	1.67	--	0.0215	0.154		
ANISN 30 GP S8 7-F,5-ST	1.17	0.674	0.498	1.67	--	0.0215	0.154		

the unit cell runs, contains listings of the two important U-233 reactions, U-233 (n,gamma) and U-233 (n,fission). Also included is Fnet, the net fissile fuel production, which is the Th-232 (n,gamma) reaction minus the U-233 loss reactions, (n,gamma) and (n,fission). Even though the cross sections for this ALICE calculation have not been weighted with unit cell disadvantage factors to correct for fuel zone heterogeneities, the results of these whole blanket ALICE calculations are very applicable to the study. This deduction can be made since the ANISN discrete unit cell calculations show that the flux in the unit cell is very flat, resulting in fuel disadvantage factors very near unity. This cross section weighting, therefore, has little effect on the results of the homogenized fuel zone cylindrical blanket calculations.

The next run on the entire blanket was an ANISN calculation. This run was an 80 group - S12 calculation which used the unit cell disadvantage factor weighted cross sections in the the fissile fuel producing regions. For the materials in the other regions, the cross sections were produced by a TRANSX run using the homogeneous resonance self shielding option. The results of this ANISN calculation can be seen in Table 2 under the title 'ANISN 80gp. S12'. The results of this run compare very well with the initial ALICE calculation. All reactions and calculated quantities agree to better than 5%. The largest discrepancies are in the two U-233 reactions where the ANISN results are approximately 10% higher than the ALICE results.

The ANISN run just mentioned was also used to collapse the 80 group MATXS6 library to a more compact and economical 30 group library. The neutron energy boundaries for this group structure can be seen in Table 3. This 80 group collapsing run produced a separate set of cross sections for each microscopic material in each zone. For example each of the four fissile production zones had a separate 30 group cross section set. The next ANISN run for the cylindrical blanket model used all of these separate 30 group material cross sections in their respective zones. The output of this run, performed with the same S12 quadrature set as the the 80 group run, can be seen in Table 2 under the title 'ANISN 30 group S12 all cross sections'. The results of this run are almost identically the same as those obtained in the 80 group run.

Table 3. Upper group energy boundaries for
30 GP neutron cross section library.

Group	Upper boundary (eV)
1	2.000×10^7
2	1.492×10^7
3	1.350×10^7
4	1.191×10^7
5	1.000×10^7
6	7.788×10^6
7	6.065×10^6
8	4.724×10^6
9	3.679×10^6
10	2.865×10^6
11	1.738×10^6
12	1.353×10^6
13	1.194×10^6
14	8.208×10^5
15	4.979×10^5
16	3.020×10^5
17	8.652×10^4
18	2.479×10^4
19	5.531×10^3
20	1.234×10^3
21	4.540×10^2
22	1.670×10^2
23	6.144×10^1
24	2.260×10^1
25	8.315×10^0
26	5.043×10^0
27	3.059×10^0
28	1.125×10^0
29	4.140×10^{-1}
30	1.523×10^{-1}

Next, to avoid the input/output cost of using such a lengthy 30 group cross section set, an ANISN run was performed which used a shortened version of the previously mentioned cross section set. In this run cross sections collapsed in fissile production zone #7 were used in all four fissile production zones. In addition, all structural steel zones used cross sections collapsed in steel zone #5. All other zones continued to use the cross sections which were collapsed in them. The output of this run, which used a coarser S8 angular quadrature set, can be seen in Table 2 under the title 'ANISN 30 group S8, 7-F, 5-ST'. The results of this run are within 1% of those calculated with the 80 group run, but were obtained using only about 1/3 of the computation time.

At this point the ANISN based optimization code was utilized to search for the fissile production zone Th volume fraction and Li-6 enrichment which would yield the maximum possible U-233 production at a tritium breeding ratio of 1.06 and a U-233 atom fraction of 1% in Th. A simple eight step summary of this optimization can be seen in Table 4. This table lists for each step the input variables, Th volume fraction and Li-6 enrichment, as well as the output quantities T, F, and Fnet. As seen in this tabulation, Fnet reaches a maximum value of 0.9317 with a T of 1.06 at a Th volume fraction of 14.96 and a Li-6 enrichment of 0.04794. This optimum point is much better neutronically than the base case (Th = 0.03 volume fraction) results of T = 1.17 and Fnet = 0.5.

Once this Fnet optimization was performed by the ANISN based method, three ALICE cylindrical blanket model runs were performed to verify that the optimum Fnet was actually reached. One ALICE run was at the optimum Th volume fraction and Li-6 enrichment of 14.96 and 0.04974 while the other runs were at Th volume fractions well above and below the optimum points. In these runs the Li-6 enrichment was kept at 0.04794 while the Th volume fractions were set at 0.12 and 0.18, respectively. The results of these three ALICE calculations and a more detailed description of the 30 group ANISN run at Fnet optimum can be seen in Table 5. A careful comparison of these Fnet optimum results and the results of the cylindrical base case calculations in Table 5 reveals many facts about the blanket Fnet optimization. First the ALICE run at the base case is compared to the equivalent ALICE calculation at the ANISN defined Fnet

Table 4. Summary of ANISN 30 GP Fnet optimization of liquid LI cylindrical model.

	Th volume percent	$\frac{\text{Li-6}}{\text{LI}}$	T	F	F _{net}
1	3.520	0.0017	1.054	0.817	0.605
2	4.812	0.0029	1.059	0.939	0.744
3	6.309	0.0059	1.059	1.001	0.843
4	7.917	0.0119	1.059	1.016	0.895
5	10.29	0.0238	1.059	1.013	0.922
6	12.63	0.0363	1.060	1.008	0.930
7	14.96	0.0479	1.060	1.003	0.932
8	16.48	0.0551	1.061	1.001	0.932

Table 5. Reactions per fusion neutron for F_{net} optimum liquid LI cylindrical model.

	T	F	F_{net}	$T+F_{\text{net}}$	$Th(n,f)$	$U(n,\gamma)$	$U(n,f)$	$F_{\text{net,eff}}$	$\frac{F_{\text{net,eff}}}{M}$
ANISN OPT. 30 G,S8	1.060	1.003	0.932	1.992		0.0082	0.0633		
ALICE OPT.	1.148	0.850	0.766	1.914	0.0315	0.0098	0.0747	0.854	0.312
ALICE BEFORE OPT. $Th = 0.12$ VF	1.208	0.781	0.711	1.919	0.0251	0.0081	0.0615	0.859	0.348
ALICE AFTER OPT. $Th = 0.18$ VF	1.077	0.910	0.819	1.896	0.0382	0.0102	0.0813	0.836	0.289

optimum. Here the two important U-233 removal reactions approximately double while the U-233 production reaction, Th-232 (n,gamma), rises by about 20%. The net fissile production therefore rises by about 15%. The tritium production of the blanket at the same time rises by about 5%. Since the tritium production in both calculations differs from the preferred value of 1.06, a more useful comparison of the net fissile production of the two cases can be made by defining a value $F_{net,eff}$ in which all tritium production in excess of 1.06 is converted directly to U-233 production. A comparison of these $F_{net,eff}$ values shows that the blanket fissile production should rise by approximately 50% if the Th volume fraction is raised to 15% from 3%. Another promising result can be seen upon comparing the blanket energy multiplication factors from the two ALICE runs. This comparison shows that the energy multiplication actually decreases by about 20% when the blanket Th loading is increased by a factor of five. The previously mentioned increase in $F_{net,eff}$ and the decrease in M combine to yield a 60% increase in the blanket figure of merit $F_{net,eff}/M$, at the ANISN described optimum point. But it can also be seen from these two tables that the ANISN results at the optimum point are not nearly as close to the ALICE results at that point as was the case in the base Th = 3 volume% calculations. This result may imply that the 30 group ANISN cross section set developed from TRANSX in which resonance calculations were performed for the Th = 3 volume % case, may not yield valid results at a Th volume fraction of 15%. Supporting this viewpoint are the two other ALICE calculations whose results are listed in Table 5. These ALICE runs were at Th volume fractions of 12 and 18%, approximately 20% above and below the optimum point. The Li-6 enrichment for these runs remained at the optimum value of 4.8%. The results of these two bracketing runs show that the blanket energy multiplication and the reaction rates only change by a small degree with this fairly substantial change in Th content. But these results show that neither $F_{net,eff}$ nor $F_{net,eff}/M$ peak at the so-called optimum point of Th = 15 volume %. Both of these important blanket parameters are higher in the 12 volume % Th fraction blanket. Therefore it is probably safe to assume that the ANISN based optimization scheme has not found the true optimum in F_{net} .

Since the base case developed 30 group ANISN cross section library has been shown not to yield good results at high Th volume fractions, it was decided that a new library should be produced by TRANSX which would yield more accurate results at higher Th volume fractions. It was decided to produce this new library from TRANSX at a Th volume fraction of 12% and a Li-6 enrichment of 4%. These values were chosen because this value of the Th volume fraction was the point at which the maximum $F_{net,eff}/M$ in the previously described ALICE runs occurred. In addition, this point was chosen because it was assumed that the Th volume fraction would be lower when an economic rather a purely neutronic optimum is searched for. Since new TRANSX resonance self shielding calculations were to be run at this new point, it was decided to attempt to provide some means in the new cross section library by which ANISN could calculate the energy multiplication in the blanket. To do this the Q's (energy produced per reaction in MeV) of several of the major blanket reactions in the blanket were input to TRANSX. These reactions included Fe (n,gamma), Be (n,2n), Li-6 (n,alpha), Li-7 (n,n'), Th-232 (n,gamma), U-233 (n,gamma), Th-232 (n,fission), and U-233 (n,fission). From this information TRANSX created a cross section set which ANISN subsequently used to calculate the net energy produced in the blanket by these reactions.

To begin these new calculations, TRANSX was first run in the heterogeneous self shielding mode to create a new 80 group resonance self shielded library. This library was first used for a liquid Li blanket unit cell similar to previous unit cells except with a wider Th shell and a smaller Be sphere, corresponding to Th and Be volume fractions of 12% and 46%, respectively. Next the ANISN run which used this new cross section set was run. The results of this new ANISN unit cell calculation can be seen in Table 6. The listings in this table are the same as those for the previous ANISN unit cells with the addition of a listing for blanket energy production. Upon comparing this unit cell calculation to the similar calculation at the Th = 3 volume % base case it can be seen that the tritium production remains approximately unchanged while the unit cell Th reactions increase strongly. The fluxes in this ANISN calculation were then input into the previously described disadvantage factor cross section weighting program to produce a

Table 6. Reactions per fusion neutron for Th = 12 Vol.% liquid LI
ANISN unit cell.

	T	F	T + F	Th (h,f)	Energy (MeV)
ANISN Th = 12	1.331	1.100	2.431	0.0417	30.9
ANISN Th = 12 SMR	1.331	1.101	2.432	0.0417	30.9

cross section set in which unit cell heterogeneities have been taken into account. Again the flux profiles in the unit cell were very flat, causing the disadvantage factors to be all within a few percent of one. In the next calculation, these disadvantage factor weighted cross sections were fed into an ANISN smeared material spherical unit cell in which all cell materials were combined into one homogeneous mixture in proportion to their volume fractions in the discrete unit cell. The results of this calculation, which can also be seen in Table 6 under the title 'ANISN Th = 12 smr', are almost exactly the same as those for the previously mentioned discrete calculation. This result shows the accuracy inherent in homogeneizing cross sections with the disadvantage factor method.

The next calculations which were performed were two ANISN 80 group S8 cylindrical blanket model calculations. These calculations were performed at a Th volume fraction of 12% and a Li-6 enrichment of 4% using the previously described unit cell disadvantage factor weighted cross sections in the fissile production zones and new homogeneously self shielded TRANSX cross sections in the other zones. One of these ANISN calculations was performed with 1 atom % U-233 mixed with Th to simulate a blanket at the end of a fuel production cycle. The other was a run with no U-233 mixed with Th which simulated a beginning of cycle blanket. The results of these two calculations can be seen in Table 7 under the respective titles 'ANISN 80,U = 1' and 'ANISN 80,U = 0'. To provide a check on the results of these runs, ALICE cylindrical model calculations were performed with the same values of Th volume fraction and Li-6 enrichment at both U-233 atom fractions in Th of 1% 0%. The results of these calculations can be seen in Table 7 under the titles 'ALICE U = 0' and 'ALICE U = 1'. These calculations, even though they in no way account for heterogeneous unit cell effects, should be comparable to the previously mentioned ANISN calculations since the flat fluxes in the ANISN unit cell calculations show heterogeneity to be unimportant. A quick comparison of the results of these ALICE calculations with the equivalent ANISN results reveals that performing new resonance self shielding calculations in TRANSX at a Th volume fraction of 12% was a necessity. It can be seen that the ANISN and ALICE results are now much closer than they were at the end of the previous

Table 7. Reactions per fusion neutron for Th = 12 vol% liquid LI cylindrical model.

	T	F	F _{net}	T+F _{net}	Th(n,f)	U(n,γ)	U(n,f)	M	$\frac{F_{net}}{M}$
ANISN 80,U = 0	1.240	0.715	0.715	1.954	0.0253	-	-	1.658	0.432
ANISN 80,U = 1	1.293	0.771	0.681	1.974	0.0259	0.012	0.079	2.691	0.253
ALICE U = 0	1.086	0.742	0.742	1.828	0.0255	-	-	1.658	0.448
ALICE U = 1	1.118	0.815	0.876	1.994	0.0257	0.010	0.070	2.345	0.373
ANISN 10,U = 0	1.247	0.709	0.709	1.956	0.0252	-	-	1.658	0.428
ANISN 10,U = 1	1.299	0.767	0.676	1.975	0.0259	0.0113	0.0793	2.692	0.251

Fnet optimization. The results, in both the $U = 0\%$ and $U = 1\%$ cases now differ in approximately the same magnitude and direction as did the ANISN-ALICE cases at the $Th = 3$ volume % base case. The ANISN-ALICE comparison at $U = 0\%$ was also used to provide ANISN with a means to estimate the blanket energy multiplication. From these runs a constant factor was determined which when added to the previously described Q-value reaction rate cross section built into the the TRANSX cross sections would give the same blanket energy multiplication in ANISN as was obtained in ALICE. This factor was then used in the $Th = 15$ ANISN run and in the yet to be described ANISN based Fnet optimizations at 0 and 1 atom % U-233 to provide estimates of the blanket energy multiplication. A comparison of the $Th = 12$ volume fraction results for the $U = 0\%$ and $U = 1\%$ runs can be made at this point. Both blanket configurations are seen to have approximately the same rates of tritium production and Th fission. The $U = 1$ blanket has an almost 10% higher rate of Th (n,gamma) reactions. But this blanket ends up with a 5% lower net fissile production as a result of the U-233 consuming reactions in the blanket. The major difference between these blankets is in greatly increased (60%) blanket energy multiplication in the $U = 1\%$ case. In this configuration the U-233 fission adds a great deal to the energy production within the blanket. The smaller multiplication in the $U = 0$ blanket also causes the blanket figure of merit F_{net}/m to be much more favorable in the $U = 0$ blanket than in the $U = 1$ blanket.

The two 80 group 12 Th volume % ANISN calculations were also used for another purpose. They were used to collapse the 80 group cross section set to two respective 10 group libraries to be used for Fnet optimization of the $U = 1$ and $U = 0$ blankets. The group structure of these new 10 group libraries can be seen in Table 8. These two collapsed cross section sets were first tested in calculations which were the same as the collapsing runs. The results of these 10 group S8 calculations can be seen in Table 7 under the respective titles 'ANISN 10,U = 1' and 'ANISN 10,U = 0'. These results are seen to be within a few percent of their respective more time consuming 80 group calculations. Therefore the 10 group cross sections which contain zone dependent collapsed cross sections in all zones except for only zone #5

Table 8. Upper group energy boundaries for
10 GP neutron cross section library.

Group	Upper boundary (eV)
1	2.000×10^7
2	1.492×10^7
3	1.350×10^7
4	1.000×10^7
5	3.679×10^6
6	8.208×10^5
7	2.479×10^4
8	1.670×10^2
9	3.059×10^0
10	1.523×10^{-1}

collapsed steel cross sections and zone #7 collapsed fuel material cross sections, can be used in ANISN to accurately predict blanket reaction rates in an economical fashion.

These newly collapsed 10 group cross sections were next used in the ANISN based optimization scheme to maximize F_{net} in both the $U = 0$ and the $U = 1$ blankets. This was done by varying the Th volume fraction and the Li-6 enrichment while maintaining a constant tritium production of 1.06. Results of these two seven step parametric studies performed using the optimization scheme are listed in Tables 9 and 10 and plotted in Figs. 4 and 5. These studies, at U-233 atom percents in Th of 0 and 1, cover all feasible Th volume fractions from a low of 3% to a high of 58% in which all Be in the blanket is removed. In both these studies Th fission and blanket energy multiplication increase with Th volume fraction in a slow constant manner. F_{net} increases rapidly up to approximately 10 volume % Th from which it remains approximately constant up to the upper limit of 58%. Thus the blanket figure of merit, F_{net}/M is seen to reach a maximum of 0.5366 in the $U = 0$ atom % blanket at a Th volume fraction of 9.5% and a Li-6 enrichment of 1.4%. The $U = 1$ atom % blanket reaches its maximum F_{net}/M of 0.294 at a Th volume fraction of 20.9% and a Li-6 enrichment of 4.5%. These optimum F_{net}/M values are about 20% higher than the respective values of F_{net}/M obtained in the Th = 12 volume % ANISN cross section collapsing runs. The actual increases are probably much much less than 20% since the collapsing runs had higher tritium production rates than did the parametric studies. It can be seen that the new optimum calculation for the $U = 1\%$ blanket yields much the same reaction rates as did the optimum of the previous F_{net} blanket optimization. Finally, as a comparison for the newly obtained F_{net}/M optimum 10 group ANISN calculations, ALICE runs were performed at the optimum points for both the $U = 0$ atom % and the $U = 1$ atom % blankets. The results of these calculations can be seen in Tables 9 and 10, respectively. Upon comparing these runs to the ANISN optimums, it can be seen that all reactions agree to better than 10%, which is about the same deviation which was observed at the Th = 12 volume % ANISN-ALICE comparisons. Therefore, it can be seen that the 10 group cross section sets are still valid at the optimum F_{net}/M points both at $U = 0$ atom % and $U = 1$ atom %. Further TRANSX

Table 9. Summary of ANISN 10 GP Fnet/M optimization of U-233 = 0 atom% liquid LI cylindrical model.

	TH VOL. (%)	$\frac{\text{LI-6}}{\text{LI}}$	T	Fnet	TH(n,f)	M	$\frac{\text{Fnet}}{\text{M}}$
1	3.000	0.0023	1.042	0.575	0.0065	1.415	0.406
2	8.194	0.0105	1.059	0.832	0.0175	1.552	0.536
3	9.461	0.0137	1.059	0.852	0.0202	1.588	0.537
4	14.77	0.0300	1.059	0.888	0.0309	1.734	0.512
5	25.52	0.0698	1.059	0.899	0.0516	2.013	0.447
6	40.00	0.121	1.060	0.897	0.0773	2.360	0.380
7	57.99	0.152	1.061	0.900	0.1065	2.754	0.033
ALICE OPT.	9.461	0.014	1.140	0.728	0.0198	1.601	0.454

Table 10. Summary of ANISN 10 GP Fnet/M optimization of U-233 = 1 atom% liquid LI cylindrical model.

	TH VOL. (%)	LI-6 LI	T	F	Fnet	TH(n,f)	U(n,f)	M	Fnet M
1	3.00	0.0019	1.061	0.723	0.507	0.0070	0.1875	3.843	0.132
2	10.63	0.0140	1.059	1.038	0.881	0.0237	0.1362	3.398	0.259
3	16.55	0.0308	1.060	1.034	0.915	0.0357	0.1050	3.158	0.290
4	20.92	0.0448	1.061	1.027	0.921	0.0443	0.0941	3.132	0.294
5	25.99	0.0615	1.061	1.022	0.923	0.0540	0.0873	3.175	0.291
6	40.11	0.1033	1.061	0.019	0.926	0.0798	0.0833	3.472	0.267
7	57.95	0.1239	1.060	1.042	0.938	0.1108	0.0963	4.056	0.231
ALICE OPT.	20.92	0.0448	1.039	0.995	0.892	0.0438	0.0916	3.093	0.288

Fig. 4. Net fissile breeding ratio (F_{net} and energy multiplication (M) vs thorium volume fraction.

Fig. 5. Li-6 "enrichment" vs Th volume fraction for a tritium ratio of 1.06.

resonance self shielding calculations at new Th volume fractions are therefore unnecessary.

RESULTS SUMMARY

The results of the final optimization runs shown in Fig. 4 can now be used to determine the Th v/o at which to operate this blanket to optimize nuclear performance. For example, at a 1 a/o U-233 in Th discharge concentration, equilibrium nuclear parameters are determined by linear interpolation and plotted vs Th v/o (Fig. 6). Specific net breeding (F_{net}/M) is seen to exhibit a broad maximum between 15 and 20 v/o Th of 0.36 (atoms/14 MeV). Major nuclear parameters of the optimized Be/Li/Th blanket are listed in Table 11. They include a 3% plenum loss as described in Refs. 1 and 2. In a similar study of an ICF blanket, Meier reported specific breeding increasing at least up to 30 v/o Th.¹¹ We have yet to determine the reasons for this difference.

If the U/Th concentration at EOL (discharge enrichment) is reduced to 0.5 a/o, $M(ave)$ drops 15% to 2.1 and $M(EOL)$ drops 22% to 2.5 while F_{net} remains nearly constant. The ultimate choice of discharge enrichment and Th content will require a fusion breeder--fission burner system economic optimization. If such an optimization drives the Th content very far away from the 12 v/o Th where the cross-section sets were generated, additional iterations of this nuclear analysis will be required. Also, if inner zone Th exposure time is found to optimize at less than about 150 days, Pa-233 n,gamma will start to become important and should be included in the F_{net} calculation.

These results are encouraging in that the combined effects of resonance correction, and optimization with the correct T breeding, is a 36% increase in net fissile breeding compared to the initial calculations. The average net breeding in the optimum 15 v/o Th case is 0.84 compared to 0.62 for the original case. Blanket energy multiplication (M) is estimated to vary between 1.8 at 0 a/o U to 3.2 at 1 a/o U.

Fig. 6. Equilibrium M , F_{net} , and F_{net}/M vs Th (v/o) for Th discharge at 1.0 a/o U-233.

Table 11. Optimized blanket parameters (with
 $T = 1.06$ and $U/Th = 1.0$ a/o at EOL)

Parameter	BOL	AVE.	EOL
Th (v/o)	15	15	15
L_{16}/L_i (a/o)	2.8	2.8	2.8
Fnet	0.83	0.84	0.85
M	1.7	2.5	3.2

APPENDIX 1

The following is a discussion of the optimization procedure used in obtaining the optimum allowable values of Th volume fraction and Li-6 enrichment which give the maximum value of F_{net} in the 14 zone liquid Li cylindrical model.

The optimization procedure used basically is an automated iterative gradient ascent technique. The technique operates as follows. First, the quantity being optimized (in this case F_{net}) and any constraints on the system (in this case requiring a tritium breeding ratio of 1.06) must be found as linear functions of the control variables (in this case $R = Th/Be$ and $L = Li-6/Li$) in the vicinity of the guessed initial values of the control variables (R_0, L_0). These functions, called the objective function and the constraint equations/inequalities, respectively, are then obtained from the results of several ANISN 1-dimensional discrete ordinates calculations. The first calculation takes place with the control variables set at their initial values. Next, calculations must be done with each of the control variables being slightly perturbed in turn by a fixed fraction of the initial value of the variable as specified in the input. From each of these respective calculations expressions for objective function and each of the problem constraints are determined. For example, the objective function for F_{net} is determined by subtracting the total number of U-233 fissions and U-233 n, γ s in the blanket from the number of Th-232 n, γ reactions in the blanket. The tritium breeding constraints is determined by summing the total number of tritons produced by neutron bombardment of Li-6 and Li-7. These values of the objective function and the constraint function at the starting point and at the points where each of the control variables are perturbed in turn can then be used to obtain a linear objective function and linear constraint functions in the neighborhood of the starting point. This was done through the use of a first Taylor's series expansion. Thus, the linear objective function is now:

$$F(x,y) = (F1-F0)/(X1-X0) * (X-X0) + (F2-F0)/(Y2-Y0) * (Y-Y0) + \dots$$

where

- F_0, X_0, Y_0 = values of the objective function F and the control variables X, Y at the starting point.
- F_1, X_1 = values of objective function F and control variable X when X is perturbed.
- F_2, Y_2 = values of objective function F and control variable Y when Y is perturbed.

The linear constraint functions can then be written as:

$$A(x,y) = (A_1-A_0)/(X_1-X_0) * (X-X_0) + (A_2-A_0)/(Y_2-Y_0) * (Y-Y_0) + \dots$$

where

- A_0, X_0, Y_0 = values of constraint A and control variables X, Y at the starting point.
- A_1, X_1 = values of constraint A and control variable X when X is perturbed.
- A_2, Y_2 = values of constraint A and control variable Y when Y is perturbed.

Here the constraint function $A(x,y)$ can either be equal to, less than or equal to, or greater than or equal to an input constraint.

Now these linearized objective and constraint functions can be input to a commonly used linear programming routine, such as described in Ref. 10. This routine will choose, if feasible, the values for all control variables X, Y , etc. such that the objective function F is maximized and all constraints A, B , etc. are fulfilled. Upper and lower limits must be placed on each of the control variables in the optimization in order to force the solution to a region where the linearized objective and constraint functions are valid. These limits are input as plus or minus a set of fraction of the initial values of each of the control variables. These fractions are usually set equal to those used for the perturbations from the initial points which were employed in calculating the linear objective and constraint functions. After the new values of the control variables are chosen by the linear programming routine to maximize the objective, the optimization process must be repeated. The new values of the control variables now become the new initial point.

Again, discrete ordinates calculations are done at this initial point and for perturbations of each of the control variables. The values of the objective and of the constraints are once again obtained from these runs, thereby allowing linear objective and constraint functions to be computed. Next, the linear programming routine is used to find new values of the control variables which cause a maximum increase in the objective. This iterative process is then repeated over and over again until the objective no longer increases between iterations. At this point the global optimum of the objective has been reached. The values of the control variables at this point are then the values of these variables which will cause the objective to take on its largest value.

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