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NUCLEAR PERFORMANCE OPTIMIZATION OF THE BE/LI/TH BLANKET FOR THE FUSION BREEDER*

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ABSTRACT

More rigorous nuclear analysis, including 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 an average U-233/Th ratio of 0.5 a/o average energy multiplication has increased only 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 showing the blankets mechanical design and the cylindrical models used for the nuclear analysis are in Ref. 2.

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 Taczanowski[3] 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 ENDL-based 175 groupdata 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 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 ratio of 4%. The initial round started at a Th v/o of 3% and a Li6/Li ratio of 0.2%.

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METHODS AND RESULTS

In this study the reference Be/Li/Th blanket for the fusion breeder is optimized to maximize specific net fissile breeding (Fnet/M). This optimization was performed by varying the Th-232 volume fraction in the fissile breeding zones and the Li-6 enrichment in the blanket's liquid Li coolant subject to the constraint that the blanket's specific tritium production take on a value of 1.06. The optimization was performed using a simple gradient ascent optimization scheme[11] coupled to the one-dimensional discrete ordinates transport code ANISN.[4]

In order for this optimization to yield credible results, it was necessary to provide ANISN with a good microscopic cross-section set. In the preparation of this cross-section set it was necessary to take into account the effects of two seperate neutronic phenomena. The first of these was blanket heterogeneity. Here, some correction in the cross-section set must be made in order to allow the many discrete 3 cm. Th-Be spheres within the fissile breeding zones to be correctly modeled as homogenized regions. The other less obvious phenomena is neutron resonance self-shielding and absorption. This phenomena is important since several nuclides within the blanket contain resonances in their cross-sections at energies which are prominent in the blanket neutron spectrum.

A prelimary series of calculations were then performed to quantify the significance of these two just described neutronics phenomena. These calculations were performed on a "unit cell" model consisting of a spherical beryllium pebble with a Th snap ring attached, surrounded by spherical annuli of Li and steel sized to give volume fractions as in the fuel zones. The first of these unit cell calculations was performed with the LLNL three-dimensional Monte-Carlo transport code ALICE[5] and a 175 neutron group microscopic cross-section library containing multiband format resonance characterization derived from the ENDL[6] nuclear data library. The major results of this calculation are tabulated in Table 1 under the heading "ALICE exact." The tabulated results of this calculation include T, the specific tritium breeding ratio, (F), the gross fissile breeding ratio, (T+F), the sum of T and F, [Th-232(n,f)], the specific Th-232 fission rate, and (M), the energy multiplication. The next calculation was performed with the LLNL three-dimensional Monte-Carlo code TART,[4] which contains no provisions for using the multiband resonance parameters of the ENDL based 175 group cross-section set. This calculation was performed to help quantify the effects of resonance on the blanket neutronics. The results of this calculation are shown in Table 1 under the title "TART exact." These results show an approximate 25% tradeoff in tritium production for fissile fuel production compared with the first ALICE calculation. This descrepancy is a result of decreased capture of resonance energy neutrons in Th. These significant changes in two important blanket reactions imply that problem specific cross-section resonance corrections must be made in all future neutronic calculations for this blanket. The third unit cell calculation consisted of an ALICE run on a configuration of slightly different geometry. Here the central Be containing cylinderical region was converted to a spherical region of the same volume. With this change the unit cell model is completely spherically symmetric, in anticipation of later unit cell calculations to be performed with the one-dimensional ANISN code. The results of this ALICE calculation appear in Table 1 under the heading "ALICE sphere." A comparison of these results with those from the first ALICE calculation shows a decrease in T of 5% and an increase in F of 10%. The moderate size and opposite sign of these deviations implies that the spherically symmetric unit cell is an acceptable substitute for the original more exact geometry. All ALICE and TART results have statistical uncertainties of 5% or less.

Table 1. Reactions per fusion neutron for 3 v/o Th unit cells.

	T	F	T+F	TH(n,f)	M
ALICE EXACT 0° K	1.32	.576	1.90	.00936	1.55
TART EXACT	1.12	.824	1.95	.00885	1.52
ALICE SPHERE	1.26	.639	1.90	.00939	1.53
ALICE SMEARED	1.25	.877	2.13	.0102	1.65
ANISN (S12) SPHERE	1.38	.878	2.26	.0108	--
ANISN (S12) SMEARED WITH DISADVANTAGE FACTORS	1.37	.886	2.25	.0109	--

A fourth unit cell calculation was performed to quantify the effects of heterogeneity in the unit cell. In this run the unit cell was modeled as a single spherical zone containing a volume fraction weighed homogenized mixture of all materials in the discrete unit cell. The results of this calculation appear in Table 1 under the heading "ALICE smeared." A comparison of these results with those of the original ALICE run shows that the major Th-232 reactions, F and Th(n,f), have increased by 40% and 10% respectively while T and the blanket energy multiplication (M) show increases of 10% and 50%. These noticeable deviations show that the small scale heterogeneities in the blanket fissile breeding zones must be accounted for in the homogeneous modeling of these zones in the full blanket model.

The next two unit cell calculations were performed with the ANISN discrete ordinates code using a microscopic cross-section set derived from MATXS6,[5] a Los Alamos 80 group P4 ENDF/B 4 based library with Bonderenko factors, using the LANL code TRANSX.[9]

The first ANISN unit cell calculation was a repetition of the previously described four zone spherically symmetric unit cell. The results of this 21 interval S12 calculation appear in Table 1 under the heading "ANISN sphere." These results do not include a value for M since the MATXS6 library does not contain kerma factors appropriate for neutron only calculations. The comparison shows that ANISN overestimates the major Th-232 reactions, F and Th(n,f), by 40% and 10% while maintaining a similiar value of tritium breeding. These significant differences in reaction rates may be the combined result of several independent contributing factors. These include differences in the base cross section sets, Monte-Carlo verses discrete ordinates calculational methodologies, and multiband verses Bonderenko resonance approximations.

The second ANISN run was a duplication of the previously described ALICE smeared material unit cell. But this time the cross-section set was modified in an attempt to get overall results similiar to those obtained from the discrete ANISN unit cell calculation. The technique by which these cross-sections were modified is based on the use of disadvantage factors. These factors are the ratios which define the average relative intensity of the flux in a certain zone and energy group to the average flux throughout the cell in that energy group. The cross-sections of each of the materials in the unit cell are then multiplied by the correct set of these factors in order to correct for the flux rises and depressions which occur in the discrete zones. The original ANISN 80 group cross-section set was then modified in this manner using the fluxes obtained in the previously described ANISN discrete zoned unit cell calculation. The results of the homogeneous unit cell calculation performed using these disadvantage factor weighted cross-sections appears in Table 1 under the heading "ANISN S12 Smeared With Disadvantage Factors." As expected, the results of this calculation are very near those obtained in the previous ANISN discrete zoned unit cell calculation.

In the next series of calculations the entire liquid Li cooled blanket was modeled in one-dimensional cylinderical geometry. The materials in the fissile breeding zones of this model were the same as those in the previously described ALICE and ANISN smeared material unit cells except that now one atom % U-233 was added to the fertile Th-232 to simulate the likely situation which would exist when the bred fuel is about to be removed from the blanket for reprocessing.

The first calculations on this model was an ALICE calculation using a room temperature doppler broadened cross-section set which was not modified to take into account heterogeneity. The results of this calculation appear in Table 2 under the heading "ALICE base."

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

	T	F	Fnet	T+Fnet	Th(n,f)	U(n,γ)	U(n,f)
ALICE BASE	1.10	.682	.526	1.63	.0065	.0190	.137
ANISN 80 GP S12	1.17	.676	.500	1.67	--	.0215	.154
ANISN 30 GP S8	1.17	.674	.498	1.67	--	.0215	.154

The next calculation of the entire blanket was an 80 group S12 130 spatial interval ANISN calculation. This run used the previously described disadvantage factor weighted cross-sections in the breeding zones and homogenious resonance self-shielded cross-sections in the other ten blanket zones. The results of this calculation can be seen in Table 2 under the heading "ANISN 80 group S12." The results of this run compare very favorably with those of the previous ALICE calculation. All reactions and calculated quantities agree to better than 5% except the U-233 reactions which are almost 10% higher in ANISN. The results of these calculations are much closer than expected since the small scale heterogeneities are not taken into account in the ALICE cross-sections. The closeness of the results implies that the heterogeneity present in the full blanket model is not as important as it was in the unit cell calculations.

It was next decided that in order to keep the forthcoming ANISN based full blanket optimization calculation from becoming prohibitively expensive, the 80 group library should be zone collapsed to 30 groups using the fluxes from the just described 80 group ANISN calculation.

This collapsed cross-section set was then input into another full blanket ANISN calculation employing a coarser but more economical S8 angular quadrature. The results of this calculation are within 1% of those obtained from the previous 80 group S12 calculation at a savings of over 70% in computation time.

At this point the ANISN based optimization scheme[11] was utilized to search for the breeder zone Th volume fraction and blanket Li-6 enrichment which yields the maximum possible Fnet at a fixed T of 1.06. Fnet optimized at 0.932 at a Th v/o of 15% and an Li6/Li a/o of 4.8%. U(nif) was 0.0633. The performance of this optimum blanket is much better than that of the initial base case (Th = 3 v/o) blanket.

An ALICE run was then performed at the optimum values of Th volume fraction and Li-6 enrichment giving T = 1.15, Fnet = 0.766 and U(nif) of 0.0746. A comparison of the results of this ALICE calculation with those of the ALICE base blanket calculation shows a significant 15% increase in net fissile atom production and a 5% increase in net tritium production. These increases, combined with a decrease in energy multiplication of 50%, result in a 50% increase in Fnet/M, the blanket figure of merit. But the difference between the ALICE results and the equivalent ANISN results is not nearly as small as was seen between ANISN and ALICE at the 3 Th volume % base case. This discrepancy indicates that the 30 group ANISN cross-section set collapsed and resonance self-shielded at 3% Th is not producing valid results for the 15 % Th optimized blanket. Therefore, it is possible that the previously described ANISN based Fnet optimization may not have succeeded in obtaining the values of Th volume fraction and Li-6 enrichment which yield the true optimum in Fnet.

It was therefore decided that a new ANISN cross-section library should be produced in order to obtain accurate results at higher Th volume fractions. This new 80 group library is self-shielded by TRANSX from the master MATXS6 file at a Th volume fraction of 12% and a Li-6 enrichment of 4%. Since new TRANSX runs were necessary, it was decided to attempt to provide some means in the new cross-section library by which ANISN could calculate the net energy multiplication in the blanket. To accomplish this, the Q values (net energy given off per reaction) of several major blanket reactions were input to TRANSX. TRANSX then used this information to produce cross-section information by which ANISN could calculate the net energy produced by these various reactions in the blanket.

To begin the next sequence of calculations, this new cross-section set was input to a discrete zoned spherically symmetric ANISN unit cell with a Th volume fraction of 12% and a Li-6 enrichment of 4%. The fluxes from this discrete unit cell calculation were then used to disadvantage factor weight the new 80 group P4 cross-section set to account for heterogeneities.

After running another TRANSX run to homogeneously self-shield the materials in zones other than those containing fissile breeding material, two 12% Th ANISN S8 full blanket calculations were performed. One of these ANISN runs was performed with 1 atom % U-233 mixed with Th to simulate a blanket at the end of a fuel production cycle. The other run had no U-233 mixed with Th to simulate a fresh beginning of cycle blanket. In addition, two ALICE full blanket calculations were performed to provide a check on the results of these ANISN runs. Comparing of results of these ALICE calculations with those of the equivalent ANISN calculations showed the necessity of performing new resonance self-shielding and unit cell calculations at higher Th volume fractions. The respective ANISN and ALICE results were much closer to one another than they were at the end of the previous Fnet optimization.

The comparison between the new 12% Th ALICE and ANISN calculations at 0 U-233 % were also used to provide ANISN with a means of estimating the specific blanket energy multiplication. This was done by calculating a constant factor when added to the previously described Q value based energy production output of ANISN would yield the same net blanket energy multiplication as did ALICE. This constant factor was then used in all subsequent ANISN calculations to estimate the value of the net energy multiplication.

Finally, we used the ANISN based optimization code to run each of these blankets through a range of Th volume fractions from a minimum of 3% up to the maximum possible value of 58%, which occurs when the Be multiplier is completely removed from the blanket. The two ANISN parametric studies were performed using seperate 10 group cross-section sets obtained from collapsing the new 80 group set over the zone averaged flux spectrums in the respective 80 group ANISN calculations at 12 Th volume %. The major results of these two parametric studies can be seen in Tables 3 and 4 for both the 0% U-233 and and 1% U-233 cases, respectively. Blanket energy multiplication (M) increase with Th volume fraction in a nearly constant manner in the 0% U case while in the 1 a/o U case exhibits a minimum at

Table 3. Summary of ANISN 10 GP Fnet/M optimization of cylindrical model at 0 a/o U-233.

	TH VOL. %	LI-6/LI	T	Fnet	TH(n,f)	M	Fnet/M
1	3.00	.00225	1.04	.575	.00653	1.42	.406
2	8.19	.0105	1.06	.832	.0175	1.55	.536
3	9.46	.0137	1.06	.852	.0202	1.59	.537
4	14.77	.0300	1.06	.888	.0309	1.73	.512
5	25.52	.0698	1.06	.899	.0516	2.01	.447
6	40.00	.121	1.06	.897	.0773	2.36	.380
7	57.99	.152	1.06	.900	.107	2.75	.327
ALICE OPT.	9.46	.0137	1.14	.728	.0198	1.60	.454

Table 4. Summary of ANISN 10 GP Fnet/M optimization of cylindrical model at 1.0 a/o U-233.

	TH VOL. %	LI-6/LI	T	F	Fnet	TH(n,f)	U(n,f)	M	Fnet/M
1	3.00	.00192	1.06	.723	.507	.00702	.188	3.84	.132
2	10.6	.0140	1.06	1.04	.881	.0237	.136	3.40	.259
3	16.6	.0308	1.06	1.03	.915	.0357	.105	3.16	.290
4	20.9	.0448	1.06	1.03	.921	.0443	.0941	3.13	.294
5	26.0	.0615	1.06	1.02	.923	.054	.0873	3.18	.291
6	40.1	.103	1.06	1.02	.926	.0798	.0833	3.47	.267
7	58.0	.124	1.06	1.04	.938	.111	.0963	4.06	.231
ALICE OPT.	20.9	.0448	1.04	.995	.892	.0438	.0916	3.09	.228

∿20 v/o Th. In contrast, the net specific fissile production increases rapidly up to about 10 Th volume % after which it remains approximately constant up to the maximum Th loading. As a result of these variations, the blanket figure of merit, Fnet/M, reaches a maximum value of 0.53 at 9.5 Th volume % and a 1.4% Li-6 enrichment in the case with no U-233. While the 1% U-233 case reaches its maximum Fnet/M of 0.294 at 20.9 Th volume % and a 4.5% Li-6 enrichment.

Lastly, two ALICE calculations were performed for the blanket configurations which yielded the maximum blanket figures of merit in the two just dicussed ANISN parametric studies and are listed at the bottom of Tables 3 and 4.

In comparing ALICE and ANISN Fnet/M optimum results we found that all reactions agree to better than 10%, approximately the same deviation that was observed in the 12 Th volume % comparisons. Therefore, the new collapsed 10 group cross-section sets looks valid at the maximum Fnet/M values for both U-233 blanket loadings. But this conclusion cannot be extended to the entire range of Th volume fractions present in the two parametric studies. A more detailed description of this analysis will be published as Ref. 11.

RESULTS SUMMARY

The results of the final optimization runs shown in Fig. 1 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. 2). Specific net breeding (Fnet/M) is seen to exhibit a broad maximum between 15 and 20 v/o Th of 0.36 (atoms/14 MeV). In a similar study of an ICF blanket, Meier reported specific breeding increasing at least up to 30 v/o Th.[12] Major nuclear parameters of this optimized blanket are listed in Table 5. They include a 3% plenum loss as described in Refs. 1 and 2.

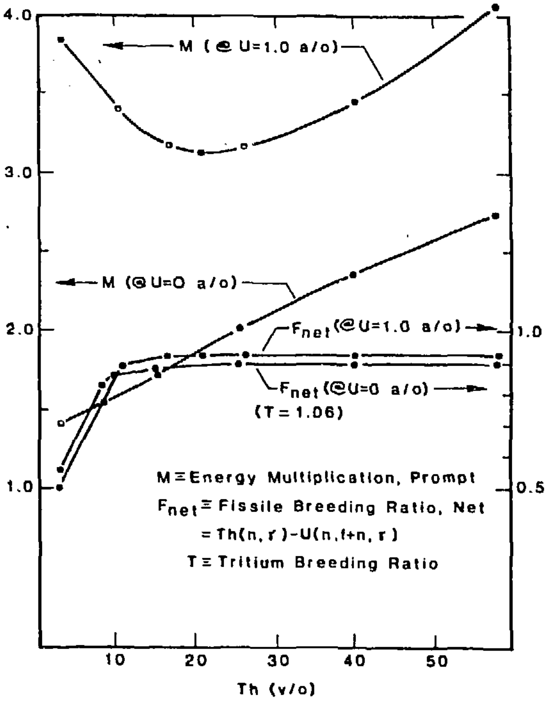

Fig. 1. Net fissile breeding ratio (Fnet) and energy multiplication (M) vs thorium volume fraction.

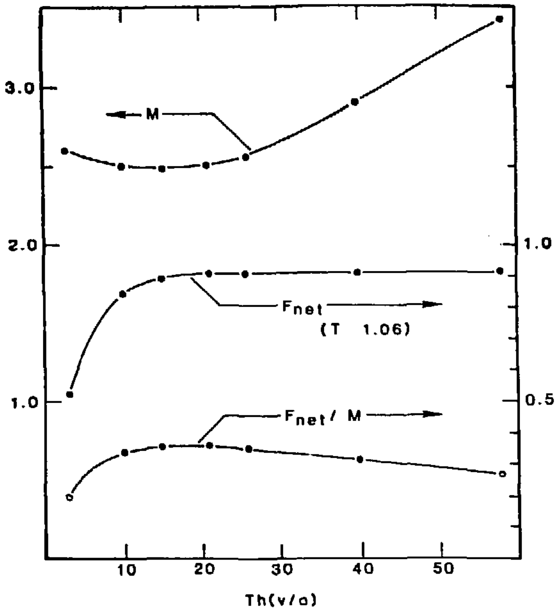

Fig. 2. Equilibrium M, Fnet, and Fnet/M vs Th (v/o) for Th discharge at 1.0 a/o U-233.

Table 5. 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
Li6/Li (a/o)	2.8	2.8	2.8
Fnet	0.83	0.84	0.85
M	1.7	2.5	3.2

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 Fnet 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 Fnet 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.

REFERENCES

1. D. H. Berwald, et al., "Fission-Suppressed Hybrid Reactor - The Fusion Breeder," Lawrence Livermore National Laboratory, UCID-19638 (1982).

2. J. D. Lee, "Nucleonics of a Be-Li-Th Blanket for the Fusion Breeder," Lawrence Livermore National Laboratory, UCRL-88237 (1983); also in *Proc. of the Fifth ANS Fusion Topical Mtg.*, April 1983, *Nuclear Technology/Fusion* Vol. 4, No. 2, Part 3, p. 805, September 1983.

3. S. Taczanoski, "Neutron Flux Shaping in Hybrids for Spent Fuel Regeneration Without Reprocessing," presented at 3rd Intl. Conf. on Emerging Nuclear Energy Systems, Helsinki, Finland, June 1983.

4. W. W. Engle, "ANISN-Multigroup One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering," RSIC CCC-254, June 1973.

5. C. E. Cullen, "Bondarenko Self-Shielded Neutron Cross Sections and Multiband Parameters Derived from the LLNL Evaluated-Nuclear-Data Library (ENDL)," LLNL, UCRL-50400, Vol. 20, 1978.

6. E. F. Flechaty, D.E. Cullen, E. J. Howerton, and J. R. Kimlinger, "Tabular and Graphical Presentation of 175 Neutron-Group Constants Derived from the LLL Evaluated-Nuclear-Data Library (ENDL)," UCRL-50400, Vol. 16, Rev. 2, LLNL, 1978.

7. E. F. Flechaty and J. R. Kimlinger, "TARTNP: A Coupled Neutron-Photon Monte Carlo Transport Code," LLNL, UCRL-50400, Vol. 14, 1975.

8. R. E. Macfarlane, "MATXS: A 80X24 library from ENDR/B 5," February 1984.

9. R. E. Macfarlane, "TRANSX-CTR: A Code for Interfacing XATXS Cross-Section Libraries to Nuclear Transport Codes for Fusion Systems Analysis," February 1984.

10. IMSL library 3, Edition 8.1, "A Mathematical and Statistics Library".

11. J. D. Lee, Special Topics Reports for the Reference Tandem Mirror Fusion Breeder, "Neutronic Issues and Optimization," Vol. 5, LLNL, Livermore, CA, UCID-20166.

12. W. R. Meier, "A High Performance, Suppressed-Fission ICF Hybrid," LLNL, Livermore, CA, UCRL-89274 (1983).