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Status Report
LANL - EIR Cooperative Work in the Field of "Nucleonics and Particle Transport in Fusion Reactors"

For Period 1 January 83 to 30 June 84

D.J. Dudziak (LANL), J. Stepanek (EIR)

Published also as Los Alamos National Laboratory Report,
LA-UR-84-3962

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ABSTRACT

The cooperation between LANL and EIR in the field of "Nucleonics and particle transport in fusion reactors started on 1 January 1983.

Reported is the research and development progress in the areas of one- and two-dimensional transport theory (ONEDANT and TRIDENT-CTR), Monte Carlo transport (MCNP), development of the nuclear data processing system NJOY, production of pointwise and groupwise cross-sections, calculations of the LOTUS fusion-fission hybrid blanket experiment and other fusion blanket studies, proposal of the LWHCR-PROTEUS experiment as a calculational benchmark and study of pump limiters.

The report covers the period 1 January 1983 to 30 June 1984.

ZUSAMMENFASSUNG

Die Zusammenarbeit zwischen LANL und EIR auf dem Gebiet des "Nukleonik und Teilchentransport in Fusionsreaktoren" begann am 1. Januar. Berichtet wird über den Fortschritt in Forschung und Entwicklung auf dem Gebiet der ein- und zweidimensionalen Transporttheorie (ONEDANT und TRIDENT-CTR), des Monte Carlo Transports (MCNP), über die Entwicklung des Erzeugungssystems für nukleare Daten NJOY, Produktion der Punkt- und Gruppenwirkungsquerschnitte, Berechnungen des Blanketexperimentes des LOTUS Fusion-Spaltung Hybrid und anderer Studien der Fusionsblankets, Vorschlag des PWR-PROTEUS Experiment als rechnerische Benchmark und Studie des Pumpenlimiters.

Der Bericht überbrückt die Periode 1. Januar 1983 bis 30. Juni 1984.

To the cooperative work contributed:

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1.0 INTRODUCTION

The cooperation between LANL and EIR in the field of "Nucleonics and particle transport in fusion reactors" started on 1 January 1983. The present report represents the first documentation of progress under the agreement.

For a number of years the Swiss Federal Institute for Reactor Research (EIR) has been carrying out an extensive work program related to the field of reactor physics aspects of fission and fusion reactors. As part of this effort, EIR is carrying out a number of tasks that deal with the development and verification of calculational methods for the transport of neutrons and other particles in reactor cores, blankets and shielding.

The Los Alamos National Laboratoy (Los Alamos) has been actively involved in fission and fusion research and development for many years. As part of this work, Los Alamos is developing numerical methods and computer codes for fusion reactor nucleonics, as well as measuring and evaluating nuclear data (both for charged particles and neutrons) applicable to fusion reactor design studies.

The EIR/Los Alamos cooperative agreement is intended to advance the technology related to fusion reactor particle transport analysis methods at both EIR and Los Alamos, through exchange of information, computer codes and data files. Included, by mutual agreement, are possible exchanges of personnel and joint development efforts. With EIR and Los Alamos having mutual interests in nucleonics and particle transport theory, nuclear data, and calculations, both parties agreed in late 1982 to establish the cooperative effort in this field on the basis of the following considerations:

a) Many important and unsolved problems exist in the development of numerical transport methods for the computation of neutral-atom and charged-particle transport in the plasma edge/first wall region, as well as for calculation of sputtering and material damage in the first wall and blankets.

b) Neutron and plasma transport methods are still far from satisfactory for fusion reactors analyses, so that more effort should be invested in their development, and their convergence should be accelerated.

c) The nuclear data processing system has to be extended, especially for better geometry-dependent resonance treatment, and benchmarked by comparisons with Monte Carlo calculations and by analysing fusion and fusion/fission hybrid blanket experiments.

Given the above considerations, EIR increased its efforts to expand its theoretical program, and has supported the Los Alamos program by participating in the solution of coordinated common problems, examples of which are the TRIDENT-CTR and NJOY code developments, analysis methods and data for the LOTUS fusion/fission hybrid experiment, and spallation-neutron source analysis for fusion material technology development.

Under the term of cooperation each institution funds its own activities and personnel, with the exception of sharing transportation costs for personnel exchange. Both parties maintain continual communication on technical developments, and computer code developments are undertaken jointly. Relevant publication are exchanged on a regular basis. Also, each year during an exchange of management personnel an implementation program is drafted for the following year's efforts, as provided for in the Agreement. During this same personnel exchange visit the present progress report was prepared.

2.0 ONE DIMENSIONAL TRANSPORT THEORY: ONEDANT

At the beginning of October 1982, the official CDC 7600 export version of the one-dimensional discrete-ordinates transport code ONEDANT was received from LANL. It is known as the 27 SEP 82 version. It was adapted and tested in the CYBER 170 environment. The bulk of the work concerned communication between small- and large-core memory and external disc storage. For a full description of all modifications please refer to Ref. 4.

To fulfil the request from LANL, this special version of ONEDANT for a CYBER 170 machine was distributed by EIR to NEA in Saclay and to RSIC in Oak Ridge.

ONEDANT is seen from the EIR as the most advanced discrete-ordinates one-dimensional production transport code. Based on LANL and EIR experience with the use of ONEDANT, it was suggested that implemention in the near future of the following options would be very valuable for the users:

a) Print more detailed balance tables, not only for the whole system but also for each particular material zone.

b) Implement a surface source also on the inner boundary in spherical and cylindrical geometries.

c) Implement a collimated surface source which would be treated as a function in addition to the usual source which is integrated by the Gaussian quadrature method (S_N).

d) For a group dependent library tape GRUPXS, ONEDANT requires for library handling much more core than one needs for one energy group. For very large multigroup calculations excessive core has to be reserved. In this case it was proposed to modify the code to enable better utilization of core on CYBER computers.

A large advantage of the S_N method is its simplicity and therefore ready applicability to many different geometries. This is a result of the Gaussian method of quadrature used to integrate the flux over space as well as angle. The method leads to a well converging inner iteration process as the result of the good coupling between the spatial meshes following the angular rays.

On the other hand the Gaussian quadrature method can lead to poor integration over space and therefore to poor coupling between the spatial meshes. Also, the representation of the angular flux dependency through the angular rays is often poor for low S_N approximation.

On the other hand the "Surface flux" method developed at EIR uses the spherical harmonics representation of the angular flux. In comparison to the S_N method the unknown angular fluxes in the S_N directions are replaced by angular flux moments. The advantage is that by such a representation of the angular flux the space variable can be integrated analytically for each particular spatial mesh. Therefore, this method leads to good coupling of spatial meshes even if a low degree of the angular flux representation is used. The "ray effect" is fully removed in this method. A disadvantage of this method is larger mathematical complexity, and therefore a much longer effort is needed to develop this method to an additional geometry in comparison to the S_N method. In EIR the code SURCU was developed on the basis of the surface flux method for slab, spherical and cylindircal one-dimensional geometries, and for x-y geometry. As a part of the LANL-EIR cooperation the surface flux method (SURCU code) will be incorporated into ONEDANT as an option in the next year's program.

In order to give the reader a brief impression of what additional capability can be expected after the implementation of a surface flux method option into the code ONEDANT, both methods are briefly compared below for the three-layer slab, one-energy problem. This problem was defined at the first International Atomic Energy Agency meeting for the coordinated research program on "Transport Theory and Advanced Reactor Calculations", in Swierk, Poland in 1973.

The eigenvalue k_{eff}, is calculated for a three-layer system. One energy group and P_0 neutron scattering are considered. The geometrical system consists of three layers of thicknesses and materials: layer No. 1, material No. 2, thickness 1.8 cm; layer No. 2, material No. 1, thickness 4.95 cm; layer No. 3, material No. 2, thickness 2.4 cm. Boundary conditions: vacuum. Cross-sections are:

Material	No. 1	No. 2
Capture + fission, $\Sigma_0(cm^{-1})$	0.065	0.0195
Scattering $P_0, \Sigma_0(cm^{-1})$	1.200	2.0475
νx fission $\nu\Sigma_f(cm^{-1})$	0.090	0.0000
Total, $\Sigma_t(cm^{-1})$	1.265	2.0600
Scattering P_1, $3\Sigma_{S1}(cm^{-1})$	0.720	3.06075
Scattering P_2, $5\Sigma_{S2}(cm^{-1})$	0.600	3.06075

Whereas SURCU utilizes a Legendre Polynomial expansion of the flux in each space interval both ANISN and ONEDANT use trepezoidal flux approximation. The results indicate a poor convergence of the P_0 spatial approximation in SURCU, while higher Legendre expansions lead to a very fast convergence. Even for a low DP approximation good results are obtained. ONEDANT and ANISN needs much higher S_N approximation caused not so much by the boundary angular flux anisotopy as by the need of accurate spatial integration over angle. The result is a shorter calculational time used by SURCU for the same accuracy of the results as those used by ONEDANT or ANISN. Due to synthetic-diffusion calculation and advanced programming, ONEDANT is faster than ANISN.

For more details about the surface flux one-dimensional method, refer to Ref. 29.

Three-Layer Slab, One-Energy Group, P_0 Order of Scattering

ANISN					ONEDANT				
S_N	M	I	k_{eff}	T (S)	S_N	M	I	k_{eff}	T (S)
4		45	0.99109	5.9	4		45	0.99137	2.0
4		90	0.99130	11.9	4		90	0.99142	2.6
8		45	0.99152	9.0	8		45	0.99179	2.4
8		90	0.99173	21.4	8		90	0.99185	3.3
	1*					1*			
16		90	0.99184	36.5	16		90	0.99193	4.2
16		150	0.99192	98.6	16		150	0.99194	5.9
32		90	0.99190	68.2	32		90	0.99195	6.4
32		150	0.99194	185.0	32		150	0.99196	9.0
SURCU									
N	M	I	k_{eff}	T (S)	N	M	I	k_{eff}	T (S)
1	0	3	0.73742	0.1	2	1	3	0.95771	0.2
3	0	3	0.73742	0.2	2	1	6	0.98810	0.4
1	0	6	0.84330	0.2	2	1	12	0.99160	0.8
3	0	6	0.84322	0.3	3	2	3	0.99188	0.3
1	0	12	0.93248	0.3	3	2	6	0.99196	0.6
3	0	12	0.93194	0.6	3	2	12	0.99197	1.4
1	0	24	0.97376	0.8	4	3	3	0.99196	0.4
3	0	24	0.97299	1.8	4	3	6	0.99197	0.9

Three-Layer Slab, One-Energy Group, Order of Scattering = P_1 and P_2

L	ANISN					SURCU				
	S	M	I	k_{eff}	T (S)	N	M	I	k_{eff}	T (S)
1	4	i*	15	0.91004	2.6	2	1	3	0.93405	0.3
	4		45	0.91041	12.3	3	2	3	0.91129	0.5
	8		45	0.91109	14.7	4	3	3	0.91140	0.7
	16		90	0.91131	97.3	4	3	6	0.91141	1.5
2	4	1*	15	0.91498	2.9	3	1	3	0.93726	0.4
	4		45	0.91535	12.7	3	2	3	0.91610	0.6
	8		45	0.91616	15.6	4	3	3	0.91625	0.9
	16		90	0.91638	167.0	4	3	6	0.91642	1.8

3.0 TWO-DIMENSIONAL TRANSPORT THEORY: TRIDENT-CTR

One of the major tasks for both EIR and LANL under both the 1983 and 1984 agreement implementation programs has been TRIDENT-CTR code development and implementation, and considerable progress has been made. After the initial adaptation of the code to the VAX and CDC Cyber computers at EIR, and the concommitant debugging, a phased program of joint development was initiated. Los Alamos continued to emphasize development and testing of the streaming matrix hybrid method (SMHM), edit capabilities, graphics, inhomogeneous source generation, coupling to the SENSIT-2D sensitivity and uncertainity analysis code, documentation and general code structure improvements. At the same time EIR developed and tested convergence acceleration methods, and helped in general code structure improvements. One anticipated benefit of the cooperation has been the code iteration acceleration and testing at EIR for fission reactor eigenvalue problem, an area in which the code is not frequently being applied at Los Alamos. In August 1983 during a personnel exchange visit, a detailed code exchange protocol was defined, and is being used to coordinate changes to a common reference version of the code. The next general exchange anticipated is for the two programmers responsible for the code to work together at Los Alamos and throughly test a single source code version. Although not a very visible effort, this standardization of programming methods has been a major advance in facilitating efficient and prompt exchange of code improvements.

In September 1983 the NEA Data Bank at Saclay, France, organized a Workshop Seminar on Finite Element Multidimensional Diffusion Codes. EIR supported this workshop by a major number of contributions and also the workshop was carried out under EIR chairmanship. EIR's 3-dimensional finite element diffusion code FINELM was assigned as the major future diffusion code for international exchange at the NEA Data Bank. Even if the main task of this workshop was to give an overview about the existing finite element diffusion codes, the second important task was to describe the possible applicability to transport methods. The TRIDENT-CTR code was the most important representative of the existing finite element transport codes. An overview about the present status and future development of this code was submitted by the authors of this status report (see Ref. 5 in Conclusions). Many participants at the NEA Workshop have shown an interest to obtain this code.

The next major milestone expected in the joint efforts under the agreement is a TRIDENT-CTR Workshop to be held at Los Alamos in October 1984, sponsored by the U.S.D.O.E. Office of Fusion Energy. The Workshop will emphasize the user-oriented aspects of the code, including extensive discussion of computational options, efficient operating strategies, experience in programming applications, and theory of the newer capabilities (e.g., acceleration methods and SMHM). Active participation by EIR personnal is anticipated, including invited lectures on several topics.

We describe below the respective programs of the two institutions, including discussion of TRIDENT-CTR applications to ongoing projects.

3.1 Los Alamos Developments for TRIDENT-CTR:

During the period of the Agreement a major computational option has been added to the TRIDENT-CTR code on an experimental basis; viz. the SMHM implementation*. Coding of the SMHM was completed and has been undergoing testing on several specific streaming problems. At the present time the SMHM appears to provide reasonable results for simple ducts, but for a major complex fusion reactor nucleonic analysis, anomolous results have been discovered at the corner of the void region represented by the streaming matrix. An effort to study and correct this anomoly will be undertaken after the October TRIDENT-CTR workshop. In the meantime, the use of multiple contiguous streaming matrices is being explored for the complex reactor case; viz., an inertial confinement fusion "point" source in a spherical void of radius 2 m, with a cylindrical uranium/Li hybrid blanket surrounding it. To date the streaming matrices have been computed and stored. Transport calculations with the matrices are now underway. Calculation of the matrices has tested options never used before, such as stacking independently computed matrices, and has provided computer time information for comparison with future alternative deterministic streaming methods (e.g., a surface-flux method such as in the SURCU code).

Applications of the SMHM are also planned for the near future in three other areas of programming interest. These should provide further testing and debugging of the SMHM version (number 2.1) of TRIDENT-CTR currently used in the joint Los Alamos/EIR developments. The three applications are, briefly:

- Analysis of the fusion blanket experiments being performed on the 14-MeV source at JAERI in Japan. The analysis is a joint effort of JAERI, the Univeristy of California at Los Angeles (UCLA), and Los Alamos (cf. discussion of UCLA cooperation below).

* The SMHM version of the code is now still experimental, and available only at Los Alamos and EIR. However, it is the reference version for our joint development, and upon successful testing will be released publicly via code centers at RSIC and NEA. That new version with the SMHM, the EIR iteration acceleration methods, and several other features will then be renamed the TRISM code.

TRIDENT-CTR uses

a) Inner iterations as opposed to the direct solution method in FINELM
b) A discontinuous element formulation.

The first condition (a) implies that fine mesh rebalancing pays dividends whereas it brought no advantage in FINELM. The second difference, (b), implies that the smallest unit that we can consider in TRIDENT is a single element.

Originally, we had proposed to extract the (0,0)-th flux moment contained in the array FLUX, form a weighted linear combination to arrive at the average flux and extrapolate this only. TRIDENT-CTR was linear approximations only and the weights at the vertices of the triangle for this approximation are all equal. Hence, it is far more convenient to operate directly on the point values.

$$\phi_{ex}^{(n)} = \omega^{(n)}\phi^{(n)} + (1 - \omega^{(n)})\,\phi^{(n-1)}$$

The $\omega^{(n)}$ are determined according to the Lebedev rearrangement of the Chebyshev sequence of cycle lenth k. In the Chebyshev scheme the $\omega^{(t)}$s are determined by

$$\omega^{(t)} = \frac{1}{1 - \frac{\sigma}{2}\left[\cos\left(\frac{\pi}{2k}\, m^{(t)}\right) + 1\right]}$$

Here σ is the dominance ratio i.e. the ratio λ_1/λ_0 where is the magnitude of the largest eigenvalue and λ_1 is that of the second largest. In the Chebyshev case m(t) is determined by

m(t) = (2 t - 1) where t = 1, 2, 3 ... k. For k = 6; This would
yield m(t) = 1, 3, 5, 7, 9, 11.

The Lebedev rearrangement of this sequence is

m(t) = 3, 9, 5, 7, 1, 11.

The Lebedev scheme uses Chebyshev polynomials of degree k where $k = 2.3^n$ n = 0, 1, 2, ... In our example above we used k = 6. It should be noted that this cycle; contains the subcycle resulting from k = 2.

Similarly a cycle of length 18 would contain the subcycles of lengths 2 and 6. The Chebyshev scheme minimizes the error at the end of a cycle the Lebedev scheme offers error minnima at the ends of subcycles.

In order to estimate the dominance ratio σ we have used

$$\phi^{(0)} = \sum_{i=0}^{N} a_i u_i$$

and

$$\phi^{(n)} = a_0 u_0 + \sum_{i=1}^{N} a_i \left(\frac{\mu_i}{\mu_0}\right)^n u_i$$

$$\approx \phi^{(\infty)} + a_1 u_1 \left(\frac{\mu_i}{\mu_o}\right)^n \quad \text{asymptotically.}$$

Here the U's are the eigenvectors and the a_i's coefficients of the linear combination.

The dominance ratio is then expressed as

$$\frac{\left\| \phi^{(n)} - \phi^{(n-1)} \right\|}{\left\| \phi^{(n-1)} - \phi^{(n-2)} \right\|} \rightarrow \sigma$$

To date we have implemented only a cycle length of six. However, in the final version there will be a single input parameter with values 0, $\pm$ 1, $\pm$ 2, $\pm$ 3 which enables the user to either switch off the Lebedev extrapolation or use extrapolation schemes with cycle lengths 2, 6 or 18 respectively. The positive non-zero values of the parameter indicate that only the scalar flux is extrapolated, whereas, the negative values indicate that all flux moments are to be extrapolated. The decision to do this was based on the claims made in the literature that extrapolation of the higher moments is benificial in cases with strong forward anisotropic scattering. We have tested this out as far as debugging is concerned. However, we have not had the opportunity to test the effect on an appropriate test example. The only anisotropic case run up to now has been our heat reactor with P1 approximation where the higher moments contribution measured in a norm constituted only a few percent when compared with the norm of the scalar flux. Here, there was no change in the number of iterations required to convergence but the eigenvalue and the point fluxes were different in about the fourth significant digit.

(2) For acceleration of the inner iterative process two methods were selected:

(1) nodal equivalent acceleration and
(2) synthetic diffusion method.

Both methods are based on the idea of accelerating the iterations over the system of exact transport equations solving additionally a lower order equation. Use is made of the fact that it is possible to determine such correction parameters in the lower order equation so that this will

reproduce a given exact transport theory solution. Whereas, the nodal equivalent acceleration uses the lowest order of the transport equation, the balance equation, the synthetic-diffusion acceleration is based on the use of "corrected" diffusion equation. The iterative solution of both equations, balance transport as well as the diffusion, are accelerated using the method of asymptotic flux extrapolation applied to the mesh-average flux in each energy group. The nodal equivalent acceleration seems to be simple to implemented into the TRIDENT-CTR code. On the other hand the synthetic-diffusion acceleration needs much more effort. Therefore, the nodal equivalent acceleration was coded inside TRIDENT in the last months with the aim to compare this method with synthetic-diffusion method after an appropriate formalism is developed and implemented into TRIDENT-CTR. The better method will be then retained.

Whereas the nodal equivalent acceleration method is not fully teste. yet, the method of the asymptotic flux extrapolation was built in and succesfully tested. It is applied directly to the mesh-average flux at each energy group at the present time.

This method was outlined by Lyusternik (32) and used by Wagner in the diffusion code GAUGE (23). Later this method was succesfully used by Stepanek in the EIR surface flux transport code SURCU (34) and by Arkuszewski in the hexagonal diffusion code SIXTUS (35).

Its slightly modified form built into TRIDENT-CTR is:

After n-th iteration the mesh-average flux in each energy group is extrapolated using the formula

$$\phi_i^{*(n)} = \phi_i^{(n)} + \Theta^{(n)} \left(\phi_i^{(n)} - \phi_i^{(n-1)}\right),$$

where $\phi_i^{*(n)}$ is the extrapolated flux, $\phi^{(n)}$ is the non-extrapolated flux and $\phi^{(n)}$ is the extrapolation factor. It is derived after each iteration as follows:

$$\varepsilon_i^{(n)} = \left(\phi_i^{(n)} - \phi_i^{(n-1)}\right) / \phi_i^{(n-1)},$$

$$\varepsilon_{max} = \mathrm{Max}_i \left|\varepsilon_i^{(n)}\right|,$$

$$\bar{\varepsilon}^{(n)} = \sum_{i=1}^{N} \left|\varepsilon_i^{(n)}\right|,$$

where N is the number of triangular meshes.

$$\varepsilon'_{max} = \max_i |\varepsilon_i^{(n-1)}|$$

$$\sigma_{max} = \frac{\varepsilon_{max}}{\varepsilon'_{max}} (1 + \varepsilon'_{max}),$$

$$\bar{\sigma} = \frac{\bar{\varepsilon}^{(n)}}{\bar{\varepsilon}^{(n-1)}} (1 + \bar{\varepsilon}^{(n-1)}),$$

$$\tilde{\sigma} = \text{Max} (\sigma_{max}, \bar{\sigma}),$$

$$\hat{\sigma} = \text{Min} (\sigma_{max}, \bar{\sigma}),$$

$$\Theta^{(n)} = \frac{\hat{\sigma}}{1 - \tilde{\sigma}}.$$

The conditions for extrapolation are:

$$n \geq 4,\ \tilde{\sigma} < 1.0,\ \hat{\sigma} > 0.4 \text{ and } \text{Max} (\delta^{(n-1)}) \leq 0.15,$$

where

$$\delta^{(n)} = \frac{\Theta^{(n)} - \Theta^{(n-1)}}{\Theta^{(n-1)}}.$$

In the following, the present status of both the Chebyshev-Lebedev acceleration of the outer iterations and the asymptotic flux extrapolation method to accelerate the inner iterations, is numerically documented using the SAPHIR reactor test case in x-y geometry. This is the test case used to compare the MULTIMEDIUM, TWODANT and SURCU codes in Ref. 36. The calculated problem consists of basically 4x4 meshes and 5 zones, 2 with fissionable material, 2 absorbing zones. Those 4 zones are surrounded by light-water-like zone. Only 1 energy group is considered. The total dimensions of the reactor are 96x86 cm. Just P_0 scattering, S_{16} approximation and 4x4 meshes are considered to demonstrate the efficiency of the both accelerations below. For more details see Ref. 37.

Sn-16 case

Current iteration Total		Unaccelerated case		Current iteration Total		Outer accel. only	
Outer	Inner	k-eff	T(min)	Outer	Inner	k-eff	T(min)
6	60	0.86434	8.46	6	60	0.86434	8.41
7	70	0.87240	9.87	7	70	0.87240	9.81
12	120	0.88885	16.9	12	120	0.89729	16.8
13	130	0.89045	18.3	13	130	0.89815	18.2
18	180	0.89619	25.3	18	180	0.90429	25.2
19	190	0.89706	26.8	19	190	0.90463	26.5
24	240	0.90055	33.8	24	240	0.90708	33.5
25	250	0.90111	34.9	25	250	0.90721	34.9
30	300	0.90339	41.9	30	300	0.90824	42.0
31	310	0.90375	43.3				
36	360	0.90526	50.2				
37	370	0.90550	51.6				
42	420	0.90649	58.6				
43	430	0.90665	60.0				
48	480	0.90731	66.9				
49	490	0.90742	68.3				
50	500	0.90752	69.7				
51	510	0.90761	71.1				
52	520	0.90769	72.5				
53	530	0.90779	74.0				

Current iteration Total		Inner accel. only		Current iteration Total		Both Outer and Inner accel.	
Outer	Inner	k-eff	T(min)	Outer	Inner	k-eff	T(min)
6	60	0.87845	8.62	6	60	0.86434	8.64
7	70	0.88419	10.0	7	70	0.87230	10.1
12	120	0.89563	17.2	12	120	0.94311	17.3
13	130	0.89676	18.6	13	130	0.90439	18.8
18	180	0.90308	25.8	18	180	0.90929	26.0
19	190	0.90454	27.4	19	190	0.90840	27.5
				24	240	0.90885	34.8

4.0 IMPLEMENTATION OF THE MONTE CARLO CODE MCNP ON VAX-780 AT EIR

- MCNP geometry graphics

The linked version of MCNP (file MCNP3.EXE), a pre-release VAX version made available to EIR, ran immediately after installing the code but only for test cases without vacuum regions. The reason was that at this time the G-FLØATING facility was not supported on the VAX at EIR. This linked version also produced poor quality plots as in the enclosed sample cases without labeling.

The DISSPLA graphic system as well as graphic devices (T 4010, VERSATEC and FR 80) are unavailable at EIR. Our system supports instead a device independent system DI-3000 of Precision Visuals Inc. (Boulder, Colorado) with the choice of following devices: VT100 terminal with VT640 screen, LYNWOOD ALPHA terminal with attached matrix graphic printer, T4662 flat plotter, FACIT matrix graphic printer and HOUSTON drum plotter. Both screen devices emulate the T4010 graphic terminal. The DI-3000 system has to be linked before use with a defined device driver, therefore it is impossible, in contrast to CGS implementation, to produce screen and hardcopy plots simultaneously except for the combination of LYNWOOD screen with matrix printer. Line precision hardcopy plots could be obtained in two ways: either by linking the program with a T4662 driver or by producing a DI-3000 metafile and postprocessing it with the output on the HOUSTON plotter.

Having this in mind the DISSPLA and CGS routines have been successfully emulated within a SETUP route by DI-3000 routines, while not a single line of the source code has been changed. The WRAPUP (hardcopy) route which appears to be rather heavily device dependent has not been emulated. At the moment this arrangement has been found quite satisfactory.

Three of the graphic routines referred to in the source code had not been documented: DTEWRT, SETDEV and HWDATA. The two first ones caused little problem, while the meaning of HWDATA has been found from the context of the code. It has been successfully replaced by the LOCATOR input of DI-3000. It is worth while to mention that most of the geometry plot transformations which are presently coded in an explicit form in MCNP can be replaced by very versatile DI-3000 routines. These encompass so-called modelling, viewing and image transformations. Also, the 3-D geometry display could be implemented with the DI-3000 system. This, however, would require profound changes in the source code.

- Other Problems

After installing the G-FLØATING facility the source code has been compiled and linked. The overflow occurring for vacuum regions disappeared and stochastic evaluations of volumes and areas became possible. However, the use of the RMCCS2 unformatted library had caused unexpected problems. The print tables no. 40 and 50 displayed unrealistic either gram or atom densities depending on the entries on cell and material cards. The trouble has been traced back to the AT entry on RMCCS2, which contained unexplained values: 1.2715E+2 for hydrogen (1001.04C) and 5.1072E+11 for oxygen (8016.04C). The reason for this is that the original RMCCS2 library has been produced with MAKXSF compiled in D-FLØATING mode. It has been checked that other nuclides data contained a similar error. The use, however, of the program MAKXSF produced correct values from RMCCS1. The new PMCCS2 library has been produced from RMCCS1. After obtaining a July 1983 version of the NJOY code as well as the documentation on its ACER module, the generation of a new ACER-produced library is planned according to the current needs.

Running tests on fourteen sample inputs delivered with the MCNP code led to discovery of several bugs.

Additional tests were made with the KCODE option. This included the SAPHIR case as published in the Manual of MCNP and SAPHIR benchmark problem based on a synthetic single library specially produced for this case.

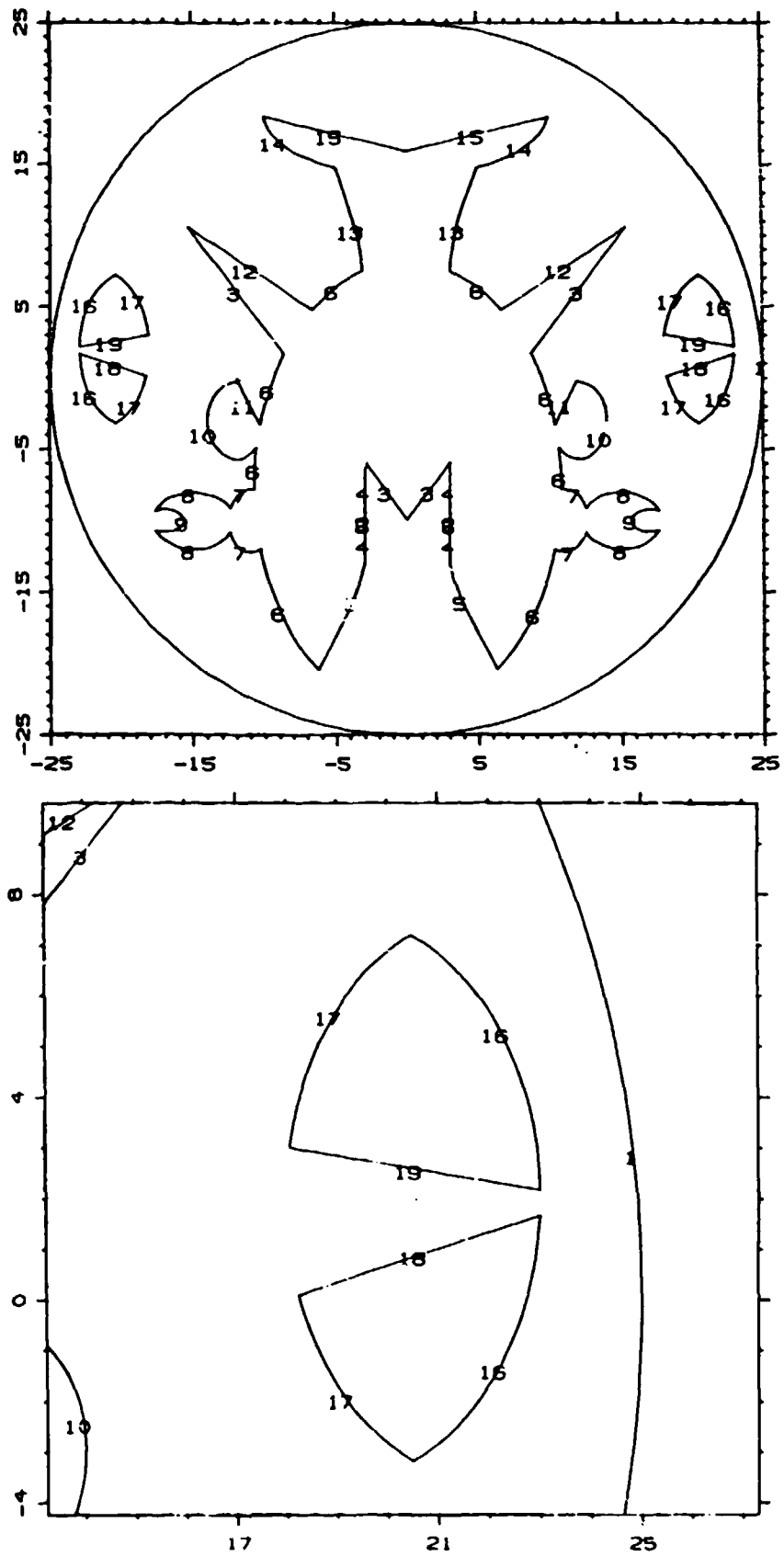
According to information obtained on 6 April 1984 from R. Forster, the above bugs had been corrected in an MCNP Vers. 3 code available at the RSIC, ORNL. Therefore, the new copy of the code was ordered the middle of April 1984 and obtained the beginning of May 1984. The new version of MCNP was installed in May 1984. Because the geometry plot facility has been thoroughly recoded in the new version, a necessity arose to emulate its functions anew with the DI-3000 graphic system. First, an attempt was made to have this task performed at the EIR Computing Center; however, other commitments of the Computing Center programmers did not guarantee a rapid implementation. Therefore, the emulation has been performed without their help. An additional feature has been added to the code; namely, the scaling of plots. The hardcopy of geometry plots is obtained through the DI-3000 metafile facility. An example of the off-line produced hardcopy plot is presented in the next figure.

Thirteen sample cases have been run with reasonable results. All the bugs found in the older version of the code seen to be removed. The sample case TEST14 requests data that are not available (BLUEBIRD library) and has not been run.

The new delivered libraries BMCCS and BMCCSD together with their directory have slightly modified format. The first block has been changed, as well as the ESZ table has been shortened by one word. Therefore, the code ACEDIT (Ref. 38) had to be modified accordingly. However, the location of all parameters in the PREF record could not be established. The new directory format states that all nuclides in BMCCS correspond to the temperature 0.0253 eV; however the data seem to be identical with the old library RMCCS, where some of the nuclides had been listed at temperatures of 900 or 30000 K. This now has to be clarified.

EIR is now going to use MCNP for calculations of HTR streaming effects, fusion blankets, shielding, PROTEUS PDWR experiments (see latter part of this report), etc. For most of those applications the problem of the unshielded unresolved resonance range arose. In contrast to LANL the shielding of the unresolved resonance range is urgent for EIR. Therefore, EIR requested in April 1983 the leader of the Group X-6, W.L. Thompson, to give this task a priority and define the guidelines for the relevant work on the NJOY module ACER as well as for necessary modifications of MCNP. Unfortunately, the Group X-6 had many other priorities, so that incorporation of resonance shielding in the unresolved resonance range would be possible only in about 3 years.

We discussed the consequences for EIR's MCNP reactor applications and the use of MCNP for fast reactor calculations at LANL. R.E. MacFarlane mentioned that it is an old need of the fast reactor community to shield the unresolved resonance range in MCNP. Therefore, it was proposed to develop the needed formalism inside of MCNP at EIR. R.E. MacFarlane will in such a case try to obtain financial support at LANL for his work on ACER. LANL sent the guidelines for this work to EIR at the end of 1983.



Hardcopy plots from DI-3000 metafile. The lower one is obtained with LOCATOR input from the screen.

5.0 NJOY NUCLEAR DATA PROCESSING SYSTEM:

The NJOY cross-section processing system was selected at EIR for future use after a long period of evaluation considering many possible cross-section processing systems. The EIR's requirements for such a system were very broad.

From the very outset one of EIR's main interests has been LWR studies. Later, the cooperative work with General Atomic in the field of GCFR reactors brought the need of data preparation for this reactor type. Since the beginning of the 70's, EIR has cooperated with a German partner on the development of HTR reactors.

Since the French fast breeder reactor PHOENIX is located near the Swiss border, the physics calculations for fast-reactor safety studies have importance for EIR.

The fusion material damage experiment PIREX as well as neutronic fusion-blanket design studies at EIR, which are being performed in cooperation with General Atomic in San Diego and with Los Alamos, lead to requirements to prepare cross-sections important in the fast energy range, such as (n,xn), (n,α), (n,p) etc.

One of the most important requirements was the need to perform detailed analyses of both the fusion-fission blanket experiment LOTUS at the "Institut de Genie Atomique" of the Federal Institute of Technology in Lausanne and our own zero-power reactor experiment PROTEUS with a hexagonal tight-pitch light-water reactor lattice.

The evaluation of cross-section processing systems at EIR has shown that only NJOY can fullfil all of our requirements. This evaluation also showed that NJOY has the best general architecture for the present, as well as future, developments. It has the best basic formalism to reconstruct pointwise data for almost all existing neutron and photon data, including neutron and photon energy deposition and material damage, in both the fast and thermal ranges.

Even the formalism for the production of covariance matrices, important for sensitivity studies, is present.

An important argument for NJOY was also the possibility to produce cross-sections not only for deterministic transport but also for continuous-energy Monte Carlo transport calculations with Los Alamos Monte Carlo Code MCNP.

In July 1982 a tape containing the Los Alamos cross-section processing system NJOY (NJOY 10/81-2) together with four representative test cases was received from the NEA Data Bank.

In May 1984, an FTN5 version of NJOY (6/83) was received from the NEADB. The OVERLAY structure of previous versions has been replaced by segmentation. An attempt has thus been made by the NEADB to minimize machine dependency.

Our initial reactions to NJOY are given in Ref. .

a. New NJOY modules developed at EIR

To this version we have added the following modules.

MICROR	-	to generate cross-section library tapes for resonance-cell codes MICROX-2 (23), MICROX (22) and for resonance-cell-burn-up code MICROBURN (24)
EPLOTR	-	to plot reaction cross-sections from ENDF/B formatted files
CPLOTR	-	to plot the differences between two evaluations of the same reaction
COMBR	-	to combine two ENDF/B formatted files
SEPR	-	to select data associated with a particular temperature and for a particular nuclide
DECAYR	-	to print-out decay data from ENDF/B files . MF=8

- MICROR

One of the main features of NJOY is the use of the "Bondarenko" method to shield the neutron cross-section resonances. This method, as implemented in the GROUPS module, considers a single resonance absorber mixed into a scattering medium with scattering cross-section σ_0 to calculate the neutron resonance flux. The user can use the simple analytical "Bondarenko" flux considering just narrow resonances or to solve the slowing down equation considering exact form of resonances. The condition of narrow resonances has then to be used only in deriving the interpolation formula to interpolate in resulting σ_0 dependent cross-sections for a given mixture of isotopes in the code TRANSX. The heterogeniety of the system is considered using the rational approximation of the neutron probability for a single zone with resonance absorber. It was shown that this method is very efficient and is used in a similar form in many known codes such as EPRI-CELL, WIMS, etc.

The main disadvantage of this method is that the resonance overlap between the resonances of different absorbers can be taken into account only approximately.

For more accurate calculations it is often important to consider the resonance overlap and shielding in a mixture of resonance isotopes by the direct resonance flux calculation using the slowing down equation for the mixture of resonance absorbers.

Therefore, it was decided to develop in a cooperation among EIR, General Atomic in San Diego, and Hochtemperatur Reaktorbau GmbH in Mannheim, Germany, a new NJOY reformatting module MICROR (27) to produce cross-section library tapes FDTAPE (fast), GGFAPE (fast and thermal) and GAR (resonance point library) for resonance-cell codes MICROX-2 (23), MICROX (22) and MICROBURN (24).

The MICROR module uses some modern features offered by the NJOY system, such as calculation of the fission spectra for a given neutron spectrum using prompt fission matrices and adding the delayed neutron portion, transfer of up to 30 different reaction cross-sections (FDTAPE only) etc. The boundary between the resolved and unresolved resonance range can be freely chosen by the user. It is usually about 8000 eV. For practical calculations with the code MICROX-2 this boundary can be set by the user to be lower, if the user wishes to speed up the calculation. The pointwise resonance shielding will be then replaced by "Bondarenko" method above this boundary.

Pointwise resonance cross-sections (GAR data) are prepared by optmized interpolation from pointwise (PENDF) data prepared by the NJOY, RECONR and BROADR modules. Equality of the infinite dilute NJOY resonance integrals calculated using original energy point distribution on the PENDF tape and the equidistant (velocity or lethargy) energy point distribution on the GAR tape is enforced.

The energy point distribution is obtained in NJOY (RECONR and BROADR modules) using the method of cross-section linearization. For a required accuracy of the cross-section reconstruction and of the resonance integrals, this method leads to the smallest number of energy points and to the most efficient point positions. But the distribution of the energy points is irregular over the given energy range. There are more points with a higher density of distribution in the regions with sharp cross-section shapes and fewer points in the parts with more smoother cross-section shapes.

In such a case, the smallest number of energy points enables a quick calculation of the group integrals if just one absorber in a homogeneous scattering medium and the Bondarenko flux-weighting model are considered. If the neutron flux is calculated solving the "slowing down" equation, the method is no longer as efficient as even for just one absorber in a homogeneous medium. Greater problems occur if one considers

- DECAYR

ENDF/B-V Evaluated Nuclear Data Files contain now a large amount of radioactive decay and fission product yield data. These data are usually published by evaluators in many different publications and if they are summarized in a common publication, then incompletely and with large delays. Therefore, the nuclear reactor designers had to invest time to find the required information or they have to use rather old data. The nuclear data processing system NJOY gives now the basis to print these data from ENDF/B formatted files. For this reason a special new NJOY module DECAYR was developed at EIR to print out data in file MF = 8.

By this a way it is now possible to obtain all data which are included onto the newest nuclear data files written in ENDF/B format, such as ENDF/B-V. Those data are very useful for reactor system designers, for scientists working in the field of waste disposal etc. to consider better the possible short as well as long time activities and energy depositions or for applications such as decay heat, depletion and buildup studies, shielding or full integrity.

The experimental scientist can use these data to select the activation foils for a given measurement, for example.

b. Generalisations in NJOY

The generalisations were concentrated to the modules GROUPS and GAMINR in which new neutron and photon group structures were introduced. They are

- 193 GA-neutron group structure which combines the GAM-II 100 group structure in the fast energy range and GA TMER-100 points structure in the thermal energy range

- 400 EIR neutron group structure based on CSEWG 239 group structure in the fast energy range and IKE Stuttgart 126 energy group structure in the thermal energy range. This group structure was additionally modified to consider Hf resonances between 2 and 10 eV, Cr, Fe and Ni resonances, the 3.0 MeV carbon window, etc.

  This group structure should enable accurate calculations of all fusion and fission reactor types.

- 39 LOTUS neutron group structure for fast fusion blanket calculations. This group structure was developed on the basis of the LANL 30 group structure, considering D-T source groups, Th fission structure, oxygen scattering minimum, carbon window, etc. (see chapter 6).

- 100 EIR photon group structure. This structure was developed from the CSEWG 94 group structure.

- 19 EIR photon group structure. This structure is based on the LANL 12 group structure.

c. Reconstruction of the pointwise neutron and photon library

Using the version 6/83 of the NJOY system with all additional modifications up to April 1984, a new pointwise neutron and photon cross-section library was generated (37). It is an important basis for production of any group library using any weighting spectrum and group structure.

The neutron pointwise library includes all generally available ENDF/B-V isotopes. They are supplemented by many ENDF/B-IV JEF-1, IRDF-82 and JENDL-2 isotopes. At the present time included are about 450 stable as well as unstable isotopes important for calculation of the fusion and fusion-fission blanket burn-up including first wall and structural materials. This also enables proper calculation of long and short-lived heat decay and material activities. The presence of the heat and displacement per atom cross-sections enables the required calculation of material heating (neutron and photon) and of material damage.

Generally, the temperature 296°K was used. For the structural isotopes the temperatures 296, 600 and 900°K were taken. For actinides as well as for fission products the temperatures from 296 and 3000°K were considered.

For most important isotopes, including heavy materials, the free gas neutron scattering distributions were calculated. Also calculated were scattering distributions for incolherent and coherent scattering using $S(\alpha,\beta)$ matrices available on the ENDF/B-III files.

6.0 LOTUS FUSION-FISSION HYBRID BLANKET EXPERIMENT

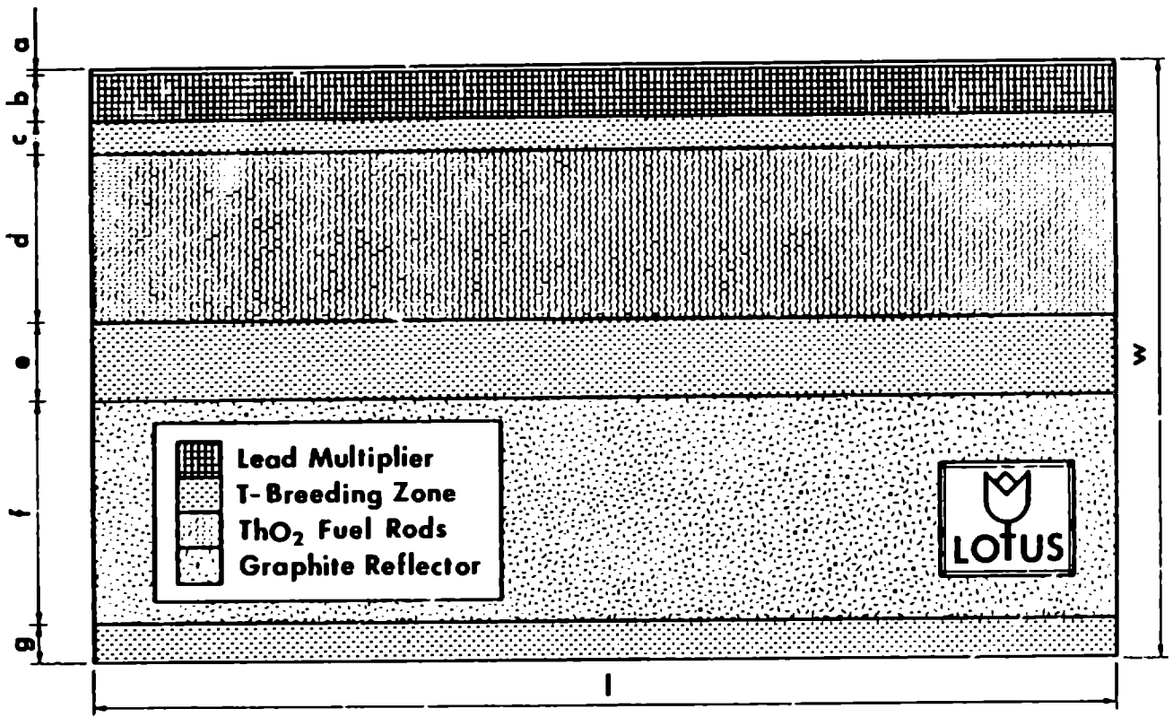
The preparations for the fusion-fission hybrid blanket experiment LOTUS at the "Institut de Genie Atomique" of the Federal Institute of Technology, Lausanne, are progressing well. The Haefely neutron generator with a source strength of 5.10^{12} n/s is being installed in the test cavity and the various components of the blanket, which has the form of an 85-cm thick, 100-cm high and 100-cm wide parallelepiped, are currently being fabricated. The first experiments were performed in early 1984.

Starting at the source end, the reference blanket is composed of a 1 to 3-cm thick stainless steel sheet to simulate the first wall of a fusion reactor, a 100-mm thick neutron multiplier zone made of lead plate, a 35-mm thick spectrum adjustment zone of lithium carbonate, a 277-mm thick ^{233}U breeding zone of thorium oxide, a 150-mm thick tritium breeding zone of lithium carbonate, a 250-mm thick graphite reflector and, finally, a 35-mm thick lithium carbonate absorber zone. The purpose of the spectrum adjustment zone is to harden the neutron spectrum in the ThO_2 breeding zone and thereby maximize the net rate of ^{233}U production. The absorber zone behind the reflector captures thermal leakage neutrons which would otherwise be lost.

The ThO_2 in the form of rods is obtained on a loan basis from the Bhabha Atomic Research Centre, India. The lithium carbonate is encased in rectangular boxes made from extruded aluminium channel. Although lithium carbonate is not a viable material for fusion power reactor applications, it is an adequate substitute for the purpose of the LOTUS experiments, which are primarily intended as a neutron physics benchmark. Compared to lithium oxide it has the advantage that high purity material can be purchased at an acceptable price.

Particular emphasis is being put on adequate diagnostic techniques. These include neutron spectroscopy (NE-213 scintillators and proton recoil telescopes) and integral reaction rate measurement techniques, the latter being developed and adapted in collaboration with EIR. For Th(n,γ), Th(n,f) and Th(n,2n) measurements, methods will be applied which had been developed earlier in connection with a zero-power reactor physics program on thorium-bearing fast reactor lattices at the PROTEUS reactor. To measure tritium production rates two independent techniques utilizing a liquid scintillator method and the self-irradiation of TLD's are being tested at EIR.

The present status of the LOTUS experiments is described in Ref. 28. A detailed account of the diagnostic techniques and other complementary information is presented in a NEACRP-A paper (1983).



Schematic Diagram of the Basic Thorium Fast-Fission Blanket Assembly to Tested in the LOTUS Test Facility (Dimensions and Material Compositions are given in the next Table)

DESIGN PARAMETERS FOR THE ThO_2/Li_2CO_3 LOTUS BLANKET

ZONE	Description	Composition (vol %)	Thickness (mm)	"Active" volume* (dm^3)	Total weight (kg)
First wall	Sheet	100% SS-316	2.0	2.8	22.3
Neutron Multiplier	Plate	90% Pb; 10% Void	100.0	140.0	1428.8
Spectrum Adjustment	Al-clad Blocks	35.5% Li_2CO_3; 17.4% Al; 47.1% Void***	35.0	49.0	62.5
Fissile Breeding	Al-clad Rods	34.9% ThO_2; 12.6% Al; 52.5% Void	277.2	388.1	1397.0**
Tritium Breeding	Al-clad Blocks	35.5% Li_2CO_3; 17.4% Al; 47.1% Void***	150.0	210.0	259.0
Reflector	Blocks	100% C	250.0	350.0	787.5
Scavenging Zone	Al-clad Blocks	35.5% Li_2CO_3; 17.4% Al; 47.1% Void***	35.0	49.0	62.5

* Based on an active height of 100 cm and width of 140 cm

** Accounts for the fact that the total cladding length is 120cm while the active blanket height is only 100cm.

*** Li_2CO_3 powder encased in Al boxes is assumed to be at 43% of the maximum theoretical density

For theoretical purposes an accurate computational scheme will be developed to consider correctly the effects of resonances caused by the hybrid system.

Starting from the ENDF basic library and from the produced PENDF files a 39-group neutron library for fusion applications (especially for hybrid systems) in connection with the LOTUS experiment is being created. The library will contain most important ENDF reactions, including prompt and delayed fission data, and is aimed toward transport computations. These are given in Table 1. Room temperature, P_3 anisotropy and self shielding treatment of resonance absorption have been considered: the Bondarenko model will be applied to 4 tabulated dilutions (i.e. ∞ ,10^4, 10^2, 1 b) for non fissionable isotopes and to 5 background cross-sections (∞, 10^4, 10^2, 10, 1 b) for strong resonance absorbers such as fissionable isotopes. The group structure of the library is depicted in table 2 and is similar to the standard 30-group LANL library. More care is given to the specific presence of Th-232 and to the resonances in the structural materials.

The generation of the cross-section library happens following this model: first a GENDF file is produced with GROUPR, containing the desired isotopes starting from the ENDF and PENDF files. Second the MATXS library is created applying to the GENDF file the NMATXS code. The result is an optimised file with regard to its length, since only the significant part of cross-sections (i.e. those which are not equal to zero) is stored. Finally the geometry of the blanket is considered in the TRANSX-CTR module to generate specific cross-sections for usual transport codes.

In order to guarantee best accuracy the library is based on both ENDFB/IV and ENDFB/V. A conversion module from the ENDFB/V format into the ENDFB/IV format was necessary to mix into the GENDF file both data sources. At the present stage the GENDF file contains the isotopes included in Table 3.

Table 1: NJOY Group Structure for LOTUS Fusion Blanket Calculations

Group	E_U (eV)	E_L (eV)	Comments
1	1.49182 + 7	1.41907 + 7	Source Groups
2	1.41907 + 7	1.34986 + 7	
3	1.34986 + 7	1.22140 + 7	
4	1.22140 + 7	1.00000 + 6	Room Return Structure
5	1.00000 + 7	7.40818 + 6	
6	7.40818 + 6	6.70320 + 6	
7	6.70320 + 6	6.06531 + 6	Thorium 2nd Chance
8	6.06531 + 6	5.48812 + 6	Fission Structure
9	5.48812 + 6	4.49329 + 6	Oxygen
10	4.49329 + 6	4.06570 + 6	Scattering
11	4.06570 + 6	3.67879 + 6	Minimum
12	3.67879 + 6	3.32871 + 6	
13	3.32871 + 6	3.01194 + 6	Carbon
14	3.01194 + 6	2.72532 + 6	Window
15	2.72532 + 6	2.46597 + 6	
16	2.46597 + 6	2.01897 + 6	Inelastic
17	2.01897 + 6	1.65299 + 6	Scattering
18	1.65299 + 6	1.10803 + 6	(Unresolved)
19	1.10803 + 6	8.20850 + 5	
20	8.20850 + 5	4.97871 + 5	
21	4.97871 + 5	3.01970 + 5	Lithium
22	3.01970 + 5	2.73237 + 5	Resonance
23	2.73237 + 5	2.23708 + 5	
24	2.23708 + 5	1.83156 + 5	
25	1.83156 + 5	1.11090 + 5	
26	1.11090 + 5	4.08677 + 4	
27	4.08677 + 4	1.50344 + 4	Resolved
28	1.50344 + 4	5.53084 + 3	Resonance
29	5.53084 + 3	2.03468 + 3	Range
30	2.03468 + 3	7.48518 + 2	
31	7.48518 + 2	2.75364 + 2	
32	2.75364 + 2	1.01301 + 2	
33	1.01301 + 2	3.72665 + 1	
34	3.72667 + 1	1.37096 + 1	Thorium
35	1.37096 + 1	5.04348 + 0	Absorption
36	5.04348 + 0	1.85539 + 0	Resonances
37	1.85539 + 0	6.82560 - 1	
38	6.82560 - 1	4.13994 - 1	
39	4.13994 - 1	1.0 - 5	Thermal Group

Table 2: ENDF/B Reaction numbers used in the GROUPR module

Process at 296°K and at the dilutions $\sigma_o = 10^{10}$, 10^4, 10^2, 1 barns

```
3      1 *TOTAL*/
3      2 *ELASTIC*/
3      4 *INELASTIC*/
3     16 *(N,2N)*/
3     17 *(N,3N)*/
3     18 *(N,TOTAL FISSION)*/
3     19 *(N,FISSION)*/
3     20 *(N,N FISSION)*/
3     21 *(N,2N FISSION)*/
3     38 *(N,3N FISSION)*/
3     22 *(N,NPRIME ALFA)*/
3     24 *(N,2N ALFA)*/
3     28 *(N,NPRIME P)*/
3     51 *DISCRETE INELASTIC FIRST LEVEL*/
3    -90 *DISCRETE INELASTIC HIGHER LEVELS*/
3     90 *CONTINUUM INELASTIC*/
3    102 *CAPTURE*/
3    103 *CAPUTRE*/
3    104 *(N,D)*/
3    105 *(N,T)*/
3    106 *(N,3HE)*/
3    107 *(N,ALFA)*/
3    221 *FREE GAS*/
3    452 *TOTAL NUBAR*/
3    455 *DELAYED NUBAR*/
5    452 *TOTAL NU*/
5    455 *DELAYED NU*/

6      2 *ELASTIC*/
6     16 *(N,2N)*/
6     17 *(N.3N)*/
6     18 *(N,TOTAL FISSION)*/
6     19 *(N,FISSION)*/
6     20 *(N,N FISSION)*/
6     21 *(N,2N FISSION)*/
6     38 *(N,3N FISSION)*/
6     22 *(N,NPRIME ALFA)*/
6     24 *(N,2N ALFA)*/
6     28 *(N,NPRIME P)*/
6     51 *DISCRETE INELASTIC FIRST LEVEL*/
6    -90 *DISCRETE INELASTIC HIGHER LEVELS*/
6     91 *CONTINUUM INELASTIC*/
6    221 *FREE GAS*/
```

* For ENDFB/4: MT=201 instead of 221.

Table 3: Isotopes on the GENDF file

90-U-235*
5-B-11
5-B-10
40-Zr
1-H-2
4-Be-9
14-S
79-Au-197*
8-O-16
92-U-233
22-Ti
29-Cu
1-H-1
27-Cu
6-C-12
26-Fe
28-Ni
24-Cr
25-Mn-55
13-Al-27
82-Pb
3-Li-7
3-Li-6
41-Nb**
92-U-238
94-Pu-239
90-Th-232
42-Mo

* : without upscatter
** : from ENDFB/5

7.0 FUSION BLANKET STUDIES AT EIR

Over the past two years EIR has developed methods and tested nuclear data needed for the physics analysis of the blankets of fusion and fusion-fission hybrid reactors with magnetic confinement. Although for the blanket physics the computational approaches are basically the same as those used for fission reactors, difficulties arise due to the presence of additional nuclides, new reaction types, different neutron spectra, and novel geometric configurations. A particular problem is the adequate prediction of tritium breeding, which is not only affected by the lithium cross-sections but also by the (n,xn) cross-sections of various multiplying materials.

In cooperation with General Atomic Company, cross-section sensitivity and uncertainty analysis studies were made for the European INTOR and the U.S. FED design of a fusion reactor (Refs. 30 and 31). An extension of this work included a comparison of the performance of the data libraries DLC-37, VITAMIN-C/DLC-41, VITAMIN-C/MACKLIB-IV and the Los Alamos NJOY fusion library (Ref. 19). Furthermore, three of the before mentioned libraries, together with various transport theory approximations for the blanket calculation, were tested for the hybrid design of a Tandem Mirror Reactor originating from the Lawrence Livermore Laboratory and General Atomic Company.

The methods also have been applied for the neutronic analysis of a fusion-fission hybrid reactor based on the UK design of the Reversed Field Pinch Reactor. The EIR concept of this reactor is characterized by either an aluminium or copper first wall/shell, which has a secondary function as a neutron multiplier, and a He-cooled hybrid blanket consisting of a Th metal multiplier and breeder, a Li_2O tritium breeder and a stainless steel reflector zone. Helium is used as a coolant to minimize the non-fertile neutron captures. The study (reported in Ref. 15) showed that from the neutronics point of view the concept is feasible. In addition to being self-sufficient in the tritium fuel, the reactor breeds 0.7 kg of ^{233}U per MW(th)-year. However, an assessment of the radiation damage indicated that the lifetime of the first wall is not adequate. The possibility of using a thinner first wall is therefore being investigated.

In view of possible future design studies at EIR and planned hybrid blanket experiments at the Swiss Federal Institute of Technology at Lausanne, the EIR computational methods are being further refined. With the support of the Los Alamos National Laboratory and General Atomic Company a cross-section generation and calculational scheme including NJOY/TRANSX-EIR/MIXTROX, the three-dimensional Monte Carlo codes MCNP and NMTC and the two-dimensional finite-element discrete-ordinates code TRIDENT-CTR for toroidal blanket geometry are being developed and tested.

8.0 LWHCR-PROTEUS EXPERIMENTS

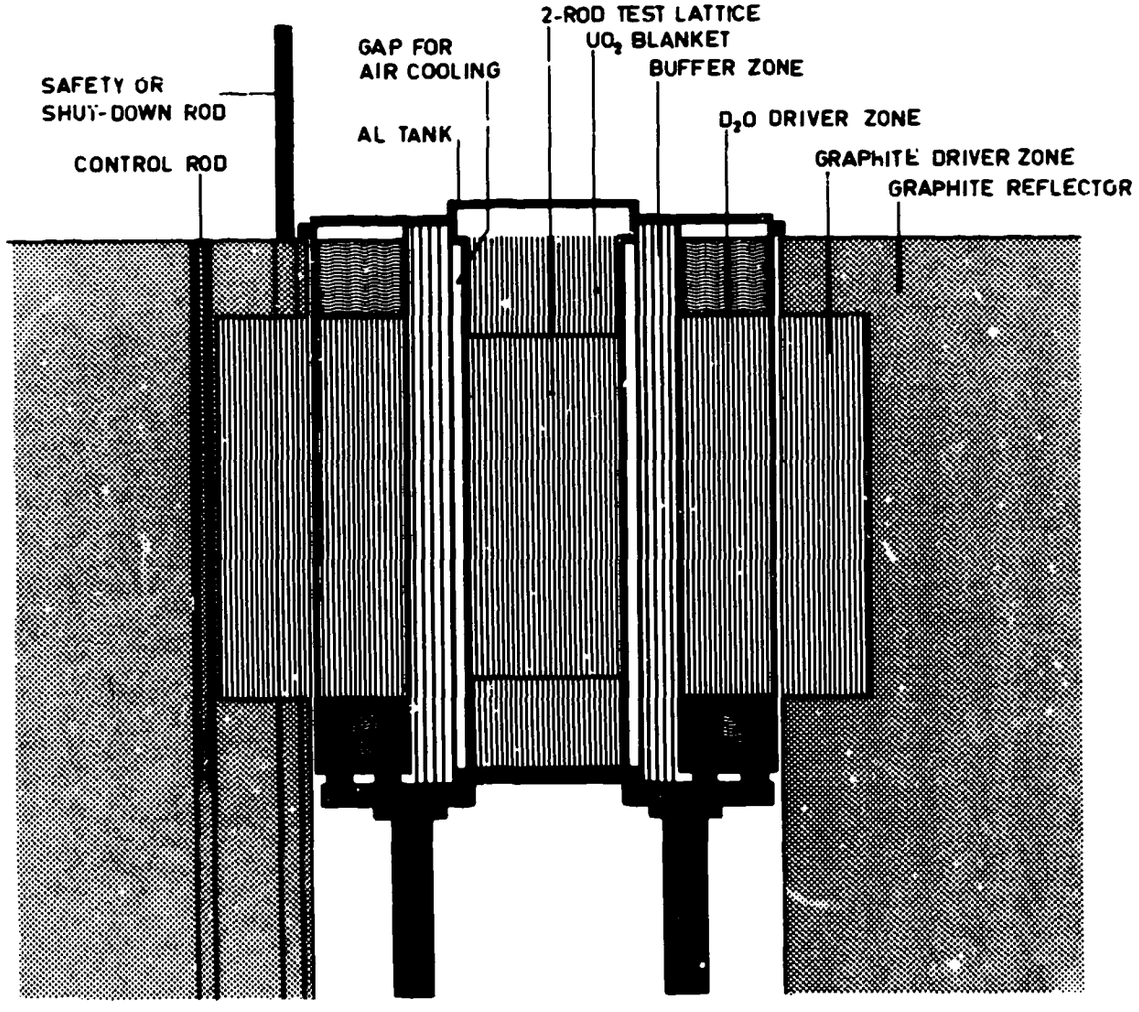
A program of experiments on LWHCR (Light Water High Converter Reactor) lattices was initiated at the PROTEUS reactor facility at EIR in August 1981. Investigation of the effects of moderator voidage on the physics of an LWHCR core is an important aim of these experiments. Since, as such, a range of neutron spectra (intermediate to fast) is covered, the integral data obtained could also be used for testing cross-sections important to fusion blanket design. Analysis of the experimental lattices investigated in the LWHCR-PROTEUS program was therefore considered as a possible topic to be embedded into the EIR/Los Alamos agreement on co-operation in the fusion field.

As a first step it was decided that the LWHCR-PROTEUS Core 1 test lattice be proposed as a CSEWG (Cross-Section Evaluation Working Group) benchmark, and this was done in June 1983. In November 1983 the suggestion was made that the test lattices of LWHCR-PROTEUS Cores 2 and 3 (with air and Dowtherm, respectively, as moderator instead of the H_2O used in Core 1) also be considered as part of the CSEWG benchmark specifications. Since it is only U.S. laboratories that participate in co-ordinating CSEWG activities, it was agreed that the proposal of the benchmark would be formally made by Los Alamos. In effect, of course, it would be both EIR and Los Alamos that would be jointly responsible for conducting the comparisons of measured and calculated results.

The figure below gives a vertical sectional view of the PROTEUS facility, which consists essentially of a central LWHCR test region driven critical by surrounding thermal driver zones. As indicated, the D_2O- and graphite-moderated driver zones are separated from the test lattice by an annular buffer zone consisting of natural-uranium metal rods. The net influence of the outer reactor regions on the neutron spectrum is minimal, the principal reaction rate ratios being effected by typically $\leq$ 2 %.

The test zone in LWHCR-PROTEUS Cores 1-3 was made up of over 2000 fuel rods of two different types - 15 % PuO_2/UO_2 and depleted UO_2. These were arranged in a hexagonal 1:1 arrangement, corresponding to a mean fissile-Pu enrichment of about 6 %. The fuel/moderator (F/M) volumetric ratio for the lattice was 2.0. Measurements carried out included various central reaction rate ratios and k_∞.

Although there have not yet been any U.S. calculations carried out for the PROTEUS experiments under the EIR/Los Alamos agreement, it is hoped that their detailed documentation and recently made availability in the open literature (39) will lead to useful comparisons of the alternative calculational methodologies being developed.



VERTICAL SECTIONAL VIEW OF THE PROTEUS REACTOR

10.0 CONCLUSIONS

Although the cooperation officially started actively only at the beginning of 1983, a good exchange of information and understanding has been reached already. EIR adapted or started to adapt, in different fields of common interest, computer codes which are in use at LANL. This should later enable a closer and more concrete cooperation in the solving of different problems, enable common studies and also enable an efficient personnel exchange. Although the cooperation has existed for only a brief period, there were already some direct fruits of this cooperation, such as the following common publications:

1. D.J. Dudziak, J. Stepanek, W.T. Urban and G. Friedrich: "Comparison of Los Alamos MATXS, VITAMIN-C and DLC-37 Multigroup Libraries for a Reference Fusion Hybrid Blanket", Data for Science and Technology, Antwerp (1982)

2. S. Pelloni, J. Stepanek and D.J. Dudziak, "Intercomparison of Nuclear Data Library Sources, Group Structures, and Collapsing Spectra for INTOR-ED", Fifth Topical Meeting on the Technology of Fusion Energy, Knoxville, Tennessee, (1983) (see also LA-UR-83-910)

3. S. Pelloni, J. Stepanek and D.J. Dudziak, "Comparison of Different Fusion Nuclear Data Libraries Using the European INTOR Blanket Design", EIR-Report No. 479 (1982)

4. R.D. O'Dell, J. Stepanek and M.R. Wagner, "Intercomparison of the Finite Difference and Nodal Discrete Ordinates and Surface Flux Transport Methods for a LWR Pool Reactor Benchmark Problem in X-Y Geometry", ANS Topical Meeting on Advances in Reactor Computations, Salt Lake City (1983)

5. D.J. Dudziak, J. Stepanek "Applicability of Finite Element to transport theory (The code TRIDENT)" Proc. Workshop Seminar on Finite Element Multidimensional Diffusion CODES, NEA Newsletter No. 30 (Dec. 1983)

We hope that in spite of the unequal size of the two laboratories, this cooperation will lead step after step to equal benefits on both sides in the future. In the past stronger U.S. contributions in a general U.S./other-partners exchange could be observed. One of the main aims of our cooperation is to contribute to a better balance of the exchange, at least in this bilateral way.

Whereas the technical aspects of the cooperation were readily clarified, there were initially some ambiguities of an administrative and financial character. These were clarified during a visit to LANL by EIR's Director, Prof.Gränicher, in November 1983. As a result of

his visit a policy was proposed to share expenses of personnel exchanges according to the following general guideline: Each inititution would pay expenses for its own personnel while visiting the other institution under the auspices of the agreement,except for airline transportation where in both cases LANL would pay air fare within the US (Boston or New York to Los Alamos) and EIR would pay air fare from Boston or New York to and from Zürich.

Several exchanges have occured in the past under the agreement, mainly for preparing status reports, planning future cooperation, exchange of technical information on developments at the respective institutions, and to draft joint technical papers. Several possible future exchanges are now under consideration for specific technical tasks such as development of a common TRIDENT-CTR source code for EIR and LANL computers, participation in the TRIDENT-CTR workshop, and implementation of an unresolved resonance treatment in MCNP.

From the LANL side D.J. Dudziak worked at EIR in July 83 and July 84 both about 3 weeks, D. Muir consulted with EIR personnel 2 days in December 82, R. MacFarlane visited EIR for 3 days in April 84 and worked on MICROR and consulted with EIR personnel. Beginning October 84 D. Muir will start to work at EIR for 4 months as an EIR guest scientist to debug different open problems in NJOY found during the pointwise cross-section generation and to consult with EIR personel in the production of the photon groupwise library and Monte Carlo ACE library. His salary will be paid by EIR.

From the EIR side J. Stepanek visited LANL for 4 days consulting about different open questions of the common programm. Starting end September 84 J. Arkuszewski will work at LANL and help to develope a formalism for shielding of the unresolved resonance range in the MCNP code in cooperation with the Monte Carlo group and R. MacFarlane. He will stay about 5 1/2 weeks. It is foreseen to send C. Higgs to LANL group S-4 in January 85 for about 2 months to cooperate with J.W. Davison and D.J. Dudziak in TRIDENT-CTR developments.

In summary, the agreement has led to an active cooperation that clearly benefits both parties as anticipated. Under the agreement several major LANL codes have been implemented successfully at EIR (viz., NJOY, TRANSX, ONEDANT, TRIDENT-CTR and MCNP), and major improvements have been made to some of these codes during their assimilation. Major examples of code enhancements by EIR of value to LANL are the MICROR module of NJOY, the iteration acceleration of TRIDENT-CTR, and additional graphics capability in MCNP. In addition, most of these codes are now available for distribution by code centers in a CDC Cyber form. The above accomplishments have occurred with little addition, if any, to the total resources applied by both institutions to the field of reactor physics and transport theory. Rather, they have occurred as a result of synergism and coordination of effort without duplication, as well as a commitment to long-term compability of formats, interfaces and coding standards. Planning for the 1985 implementation program is now proceeding within the same general policy.

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