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ON THE APPLICATION OF MULTIGROUP DIFFUSION
THEORY TO FAST CRITICAL ASSEMBLIES

by

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ON THE APPLICATION OF MULTIGROUP DIFFUSION THEORY TO FAST CRITICAL ASSEMBLIES

by

David Okrent

SUMMARY

The experience at Argonne National Laboratory has been that multi-group diffusion theory does not accurately predict the existing, highly enriched, fast critical assemblies if the current "best" cross sections are employed. For example, a group of experimental assemblies has been calculated by diffusion theory using three different cross section sets, each prepared independently by a separate individual. In all cases the assemblies were computed to be less reactive than they were found to be experimentally. The deviations are greatest for the smallest cores where theoretical considerations and actual comparisons with higher approximations to transport theory show diffusion theory to be the least accurate. If one is designing a very dilute fast power reactor, however, such effects are not of paramount importance, since for the large systems the various methods of computation are found to converge fairly well. One can and does employ multigroup diffusion theory therefore, due to its relative simplicity and ready applicability to various geometries.

Nevertheless, the occasion does arise when highly enriched assemblies need to be predicted for safety and other considerations. It would be convenient if some adjustment could be made within the framework of diffusion theory such that the whole gamut of fast reactors would be predicted with reasonable accuracy within existing knowledge of cross sections. In this report there is described an attempt to achieve such a rapprochement, the technique employed being an adjustment to transport cross sections based on multigroup comparison of the Lady Godiva reactor by diffusion theory and the asymptotic solution to the Boltzmann equation. Under the guidance of such a prescription, diffusion theory is found to work well for the highly enriched critical assemblies and to deviate but little from the usual predictions made for very fast reactors. Diffusion theory using adjusted and unadjusted transport cross sections is compared with a transport theory solution for the Topsy reactor, and the adjusted cross section calculation compares more favorably.

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I. INTRODUCTION

In the course of establishing the theoretical aspects of the fast reactor program, Argonne has devoted a good deal of effort to reactor calculations using multigroup diffusion theory⁽¹⁾ with provision for inelastic scattering. The spherical geometry calculation was first programmed for the IBM CPC machine, and later both the spherical and the one-dimensional cylindrical geometry calculations were programmed for the UNIVAC, with the slab calculation a recent addition.

The reasons for this considerable emphasis on multigroup diffusion theory are manifold. It became obvious early in the work that one group, or even a few groups, would not be adequate to describe the variety of fast assemblies of interest. Of course, theoretical considerations, as well as actual comparisons, showed that unmodified diffusion theory could not be expected to work well for the small, very highly enriched fast criticals, such as have been performed at Los Alamos.⁽²⁾ Comparisons have been made for such assemblies at Argonne between diffusion theory and Serber-Wilson theory, both single⁽³⁾ and multigroup;⁽⁴⁾ these in turn have been compared with results obtained at Los Alamos using the integral theory method of Carlson.⁽⁵⁾ This work is on a continuing basis and is being expanded to include the S_n method of Carlson.⁽⁶⁾

The results to date indicate that diffusion theory errs in critical radius (~ 10 -15%) for the most enriched assemblies. However, as the assemblies become larger and more dilute in fissionable material, diffusion theory does approach closely the more accurate methods. Hence, for a reactor having a core volume of several hundred liters, diffusion theory should be adequate, at least in light of the inadequate status of basic cross section information. Furthermore, for purposes of design, where various means of flattening the power distribution are to be examined, or the distribution of plutonium production in the blanket is to be calculated, diffusion theory should be fairly accurate, even for reactors having an intermediate size core (50 liters). These facts, coupled with the relative simplicity of diffusion theory and its ready adaptability to various geometries, made multigroup diffusion theory, with direct provision for inelastic scattering, the "bread and butter" calculation at Argonne.

Once the multigroup diffusion theory calculation had been programmed for the UNIVAC, it was used to analyze existing experiments.* Although the experiments are of a nature such that they are not particularly well-suited to the method, one can at least observe the error of prediction and its trend with dilution. This is of considerable aid when one is faced with the problem, due to safety and other considerations, of predicting the critical mass of highly enriched configurations.

*It should be noted that the multigroup Serber-Wilson calculation is presently being programmed for the Argonne fast computer.

In general, the results have been quite consistent and relatively independent of the number of groups used and the energy breakdown used therein, or the specific assumptions on transport, capture and inelastic cross sections, so long as they are not widely at variance with existing data. Multigroup diffusion theory invariably predicts too high a critical mass for the small, highly enriched assemblies. In general, as the assemblies become larger and more dilute, calculation gets closer to experiment.

The question automatically arises: What should be done about these discrepancies between calculation and experiment? One reasonable procedure, in view of the known inadequacies of diffusion theory, is to ignore them. It would be convenient, however, if a single method of computation and set of cross sections could be developed which predicted existing experiments closely, yet was suitable for designing the larger, power reactors and would predict their critical masses as accurately as possible.

Assuming that a restriction to the use of multigroup diffusion theory exists, since that was the only currently programmed calculational setup at Argonne, not much freedom is left for "adjustment," whether it be on an empirical, intuitive, or rigorous basis. A variety of approaches are possible; one particular method which apparently yields appreciable success is described in the following sections.

II. PREDICTIONS OF MULTIGROUP DIFFUSION THEORY

Results are reported herein for criticality calculations made by multigroup diffusion theory using three different sets of cross sections, each prepared by a different individual at widely separated times.

The first cross section set, listed in Table I, was prepared by the author at Argonne early in 1953. This set uses six groups and reflects in some measure the knowledge available at that time. For example, the listed inelastic scattering cross sections and transfer coefficients are in agreement with the threshold detector measurements of Beyster and Carter.⁽⁷⁾ The inelastic scattering distributions, however, were not computed following a particular format, but represented intuitive guesses at what might be a reasonable first try in an attempt to fit the meagre spectral data available. In this and the next cross section set, any elastic moderation effect is lumped with the inelastic scattering into one cross section. Capture cross sections were mostly educated guesses, with some guidance from

$$\alpha = \frac{\sigma_c}{\sigma_f}$$

measurements in EBR.⁽⁸⁾ The transport cross sections used in the diffusion calculation were the sum of inelastic, fission, capture and elastic transport,

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Table I
CROSS SECTION SET NO..1
(In barns)

Group No.	Energy Band	Fraction of Fission Neutrons Born in Band					
1	$\infty - 1.6$ Mev	0.473					
2	1.6 - 0.7	0.305					
3	0.7 - 0.4	0.114					
4	0.4 - 0.2	0.065					
5	0.2 - 0.05	0.043					
6	0.05 - 0	0.0					
Group	Pu	U ²³⁵	U ²³⁸	Fe	Na	K	Al
σ_f							
1	1.92	1.25	0.58				
2	1.80	1.23	0.09				
3	1.67	1.25	0.0				
4	1.78	1.45	0.0				
5	2.07	1.97	0.0				
6	3.40	3.30	0.0				
σ_c							
1	0.07	0.075	0.05	0.003	0.00025	0.002	0.0003
2	0.09	0.12	0.09	0.010	0.0005	0.005	0.0006
3	0.10	0.17	0.14	0.016	0.0006	0.007	0.0009
4	0.18	0.26	0.18	0.030	0.0009	0.009	0.0015
5	0.34	0.43	0.25	0.060	0.002	0.013	0.0028
6	2.00	1.30	0.60	0.075	0.005	0.035	0.0050
σ_{in}							
1	0.8	1.4	2.3	0.85	0.31	0.31	0.44
2	0.2	0.5	1.3	0.30	0.44	0.12	0.22
3	0.1	0.1	0.7	0.20	0.63	0.15	0.45
4	0.09	0.09	0.2	0.13	0.41	0.11	0.31
5	0.07	0.07	0.07	0.08	0.23	0.06	0.2
σ_{tr}							
1	3.9	3.9	3.9	2.0	1.8	2.2	1.57
2	4.8	4.8	4.8	2.1	3.8	1.8	2.2
3	6.5	6.5	6.5	3.3	4.5	2.0	3.7
4	8.0	8.0	8.0	3.3	4.2	2.0	3.7
5	11.5	11.5	11.5	3.5	4.3	1.8	4.4
6	13.4	13.4	13.4	7.0	6.8	1.4	4.0

$$\sigma_{tr} = \sigma_f + \sigma_c + \sigma_{el\ tr} + \text{true } \sigma_{inelastic}$$

$$\nu \quad 2.9 \quad 2.5 \quad 2.5$$

Inelastic Scattering Distribution - $C_{i,j}$

$$\sigma_{in} (i \rightarrow j) = \sigma_{in, i} C_{i, j}$$

	Pu	U ²³⁵	U ²³⁸	Fe	Na	K	Al
C_{12}	0.4	0.4	0.4	0.4	1	1	0.7
C_{13}	0.3	0.3	0.3	0.3	0	0	0.3
C_{14}	0.2	0.2	0.2	0.2	0	0	0.0
C_{15}	0.1	0.1	0.1	0.1	0	0	0.0
C_{16}	0.0	0.0	0.0	0.0	0	0	0.0
C_{23}	0.5	0.5	0.5	0.7	1	1	1
C_{24}	0.5	0.3	0.3	0.2	0	0	0
C_{25}	0.0	0.15	0.15	0.1	0	0	0
C_{26}	0.0	0.05	0.05	0.0	0	0	0
C_{34}	1	1	0.7	1	1	1	1
C_{35}	0	0	0.2	0	0	0	0
C_{36}	0	0	0.1	0	0	0	0
C_{45}	1	1	0.7	1	1	1	1
C_{46}	0	0	0.3	0	0	0	0
C_{56}	1	1	1	1	1	1	1

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the latter based primarily on the Brookhaven compilation⁽⁹⁾ and some earlier measurements by Journey and Zabel,⁽¹⁰⁾ and Langsdorf.⁽¹¹⁾ It should be noted that

$$D = \frac{\lambda_{tr}}{3} = 1/3 \Sigma_{tr}$$

has been adopted in these diffusion theory calculations.

The second set of cross sections (Table II) is also a six-group set and was prepared recently by G. Hansen of LASL. It was intended as a first trial set for analysis of their fast criticals using the S_N method.⁽⁶⁾ The basis for this set of cross sections is similar to that of set No. 1 only in part. For example, the spectrum of neutrons inelastically scattered from an initial energy, E_0 , is taken to have the form $(E) \exp(-E/\sqrt{DE_0})$, with D chosen to be 1/9 mev in order to fit the Beyster-Carter data. Furthermore, the group energy breakdown is different, two groups being used above the U^{238} fission threshold as compared to one group in cross section set No. 1.

The third set of cross sections, listed in Table III, is a ten-group set prepared by R. Avery of Argonne in the summer of 1954. Here, still another basis for fixing the inelastic scattering energy distribution was used. Also, since this cross section set was prepared for use with a specific computing machine program, it was required to conform to limitations set up by the program, namely, only the next six lower energy groups can be scattered into inelastically from any group.

The results of the calculations made with the three cross section sets are presented in Table IV. In these calculations the actual geometry and composition of each critical were put into the machine and the solution iterated until the flux distribution converged. The column of numbers entitled k_{eff} gives the number of core fissions obtained in a succeeding neutron generation per core fission this generation.

It can be seen from Table IV that all the assemblies were computed to be subcritical. Furthermore, the smaller the core radius, the worse the agreement between calculation and experiment. The rather close agreement between the calculated results for the different cross section sets is surprising in view of the complete independence of their formulation.

The deviations between experiment and diffusion theory are rather similar to those found to exist between multigroup Serber-Wilson theory and diffusion theory. Some preliminary four-group comparisons, made by H. H. Hummel and the author, show diffusion theory to predict a k_{eff} which is 10 to 13% less for a reactor of the Topsy or EBR-I type.

Table II

CROSS SECTION SET NO. 2

Group No.	Energy Band, Mev	Fraction of Fission Neutrons Born in Band			
1	$\infty - 3$	0.212			
2	$3 - 1.4$	0.348			
3	$1.4 - 0.9$	0.166			
4	$0.9 - 0.4$	0.175			
5	$0.4 - 0.1$	0.085			
6	$0.1 - 0$	0.014			
	Group	Pu	Oy	Tu	
σ_f	1	1.95	1.287	0.621	
	2	1.94	1.219	0.484	
	3	1.94	1.176	0.047	
	4	1.94	1.123	0.009	
	5	1.87	1.47	0.011	
	6	1.95	2.26	0.017	
σ_c	1	0.02	0.05	0.015	
	2	0.05	0.10	0.049	
	3	0.10	0.15	0.097	
	4	0.15	0.20	0.135	
	5	0.25	0.3	0.193	
	6	0.50	0.5	0.360	
σ_{in}	1	1.5	2.0	2.8	
	2	1.3	1.8	2.4	
	3	0.9	1.3	1.7	
	4	0.4	0.7	0.9	
	5	0.1	0.1	0.1	
σ_{tr}	1	4.57	4.47	4.48	
	2	4.78	4.55	4.42	
	3	5.09	4.66	4.31	
	4	6.34	5.62	5.60	
	5	9.42	8.85	8.90	
	6	13.32	13.10	12.7	
$\sigma_{tr} = \sigma_f + \sigma_c + \sigma_{el\ tr} + \sigma_{inelastic}$					
ν		2.96	2.51	2.51	

Inelastic Scattering Distribution - $C_{i, j}$

(Same distribution for all materials)

From/to	1	2	3	4	5	6
1	0.05	0.33	0.23	0.27	0.11	0.01
2	0	0.15	0.25	0.38	0.20	0.02
3	0	0	0.14	0.49	0.33	0.04
4	0	0	0	0.38	0.54	0.08
5	0	0	0	0	0.80	0.20

NOTE: Oy = Oralloy = 93.7% U^{235} , 1.0% U^{234} , 5.3% U^{238}
 Tu = Tuballoy = 0.72% U^{235} , 99.28% U^{238}

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Table III
CROSS SECTION SET NO. 3

	Group No.	Energy Band, mev		Fraction of Fission Neutrons Born in Band			
	1	$\infty - 2.231$		0.346			
	2	2.231 - 1.353		0.229			
	3	1.353 - 0.4979		0.301			
	4	0.4979 - 0.1832		0.091			
	5	0.1832 - 0.0674		0.025			
	6	0.0674 - 0.0248		0.006			
	7	0.0248 - 0.00912		0.002			
	8	0.00912 - 0.00335		0			
	9	0.00335 - 0.001234		0			
	10	0.001234 - 0		0			
	Group	Pu	U ²³⁵	U ²³⁸	Fe	Na	K
σ_f	1	2.00	1.25	0.56			
	2	2.00	1.25	0.42			
	3	1.95	1.20	0.03			
	4	1.90	1.35	0			
	5	2.2	1.90	0			
	6	2.4	2.50	0			
	7	2.7	3.10	0			
	8	3	3.9	0			
	9	4	5.5	0			
	10	6	10	0			
σ_c	1	0.06	0.12	0.02	0.006	0.0002	0.02
	2	0.1	0.15	0.055	0.006	0.0005	0.02
	3	0.14	0.18	0.12	0.006	0.001	0.02
	4	0.23	0.27	0.175	0.006	0.001	0.02
	5	0.44	0.48	0.25	0.006	0.001	0.02
	6	0.72	0.75	0.35	0.006	0.001	0.02
	7	0.95	0.99	0.5	0.006	0.001	0.02
	8	1.2	1.37	0.7	0.006	0.001	0.02
	9	1.8	2.1	0.9	0.010	0.002	0.02
	10	3	4	1.0	0.015	0.003	0.02
true σ_{in}	1	1.2	2.0	2.7	1.0	0.1	0.3
	2	1.1	1.8	2.5	0.7	0.05	0.2
	3	0.7	1.0	1.0	0.3	0	0.1
	4	0.5	0.5	0.5	0	0	0
	5	0	0	0	0	0	0
	6	0	0	0	0	0	0
	7	0	0	0	0	0	0
	8	0	0	0	0	0	0
	9	0	0	0	0	0	0
	10	0	0	0	0	0	0
σ_{tr}	1	4.5	4.5	4.5	2	2	2.0
	2	5.0	5.0	4.8	2	2	2.0
	3	5.5	5.5	5.0	2	3	1.5
	4	7.0	7.0	6.5	3	3	1.5
	5	9.5	9.5	9.0	3	3	1.5
	6	12	12	12	3	5	2.0
	7	13	13	13	3	5	1.3
	8	16	18	13	7	15	1.5
	9	16	23	13.5	7	10	1.5
	10	16	28	13.5	10	4	1.5
$\sigma_{tr} = \sigma_f + \sigma_c + \sigma_{el\ tr} + \text{true } \sigma_{in}$							
ν		2.9	2.5	2.5			
$\sigma_{el\ mod}$	1	0.014	0.013	0.014	0.048	0.22	0.12
	2	0.028	0.028	0.028	0.085	0.31	0.17
	3	0.023	0.026	0.032	0.060	0.26	0.070
	4	0.037	0.041	0.049	0.11	0.26	0.075
	5	0.058	0.060	0.073	0.11	0.26	0.075
	6	0.075	0.073	0.098	0.11	0.43	0.10
	7	0.079	0.075	0.10	0.11	0.43	0.065
	8	0.099	0.11	0.10	0.25	1.28	0.075
	9	0.086	0.13	0.11	0.25	0.85	0.075

Inelastic Scattering Distribution - $C_{i,j}$

NOTE: $C_{i,j}$'s cover true inelastic scattering, are the same for all materials. Elastic moderation slows neutrons into next lower energy group.

From/to	2	3	4	5	6	7	8	9	10
1	0.3799	0.4402	0.1318	0.0366	0.0089	0.0026	0	0	0
2	--	0.7098	0.2126	0.0591	0.0143	0.0042	0	0	0
3	--	--	0.7324	0.2037	0.0493	0.0146	0	0	0
4	--	--	0	0.7612	0.1841	0.0547	0	0	0

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Table IV
PREDICTIONS OF MULTIGROUP DIFFUSION THEORY

No.	Description of Critical	Bibliography Reference	Core Radius cm	Core Composition atoms/cc x 10 ⁻²⁴	Blanket Thickness* cm	Blanket Composition atoms/cc x 10 ⁻²⁴	Calculated k _{eff}		
							Set No. 1	Set No. 2	Set No. 3
1	Popsy - a plutonium core with a natural U blanket	2	4.44	0.04 Pu	26.3	0.000346 U ²³⁵ 0.04765 U ²³⁸		0.8591	
2	Topsy - a fully enriched U ²³⁵ core with a natural uranium blanket	2	6.023	0.04503 U ²³⁵ 0.00293 U ²³⁸	25	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.8824	0.8946	0.8782
3	Topsy with a thin blanket	2	6.31	0.04503 U ²³⁵ 0.00293 U ²³⁸	12.1	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.8794		
4	80% enriched full density core	2	6.62	0.03864 U ²³⁵ 0.00936 U ²³⁸	24.4	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.9010		0.8936
5	85% density fully enriched core	2	6.79	0.03853 U ²³⁵ 0.00246 U ²³⁸	24.4	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.8963		0.8910
6	67.6% enriched full density core	2	7.31	0.03245 U ²³⁵ 0.01555 U ²³⁸	23.8	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.9106	0.9190	0.9014
7	70% density fully enriched core	2	7.88	0.03167 U ²³⁵ 0.00202 U ²³⁸	23.1	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.9093	0.9206	0.9028
8	47.3% enriched full density core	2	9.0	0.02270 U ²³⁵ 0.02530 U ²³⁸	21.9	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.9286	0.9327	
9	50% density fully enriched core	2	10.0	0.02256 U ²³⁵ 0.00144 U ²³⁸	20.6	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.9159	0.9258	0.9073
<u>Inner Blanket</u>									
10	EBR-I*** (second core loading)		10.655	0.02443 U ²³⁵ 0.00176 U ²³⁸ 0.0122 Fe 0.00315 K 0.00155 Na	12.1	0.00017 U ²³⁵ 0.0234 U ²³⁸ 0.0148 Fe 0.00346 K 0.00170 Na	0.9301		0.9308
<u>Outer Blanket</u>									
					16.4	0.00029 U ²³⁵ 0.0394 U ²³⁸ 0.0010 Fe			
11	LA Pilot Mockup***	12	19.31	0.00794 U ²³⁵ 0.00675 U ²³⁸ 0.0123 Fe 0.0323 Al	15.2	0.000346 U ²³⁵ 0.04765 U ²³⁸	0.9650		0.9341**

*Includes 2.1 cm extrapolation distance.

**No aluminum cross sections being available in this cross section set, the aluminum in the core was replaced by 0.022 atoms/cc of Na.

***This is really a cylindrical core. The core radius given is that for a sphere having the same volume.

An unpublished one-group comparison made at Argonne by R. Avery and S. Krasner gave similar results. It is interesting to note that when diffusion theory was modified so that the buckling, κ^2 , was computed as in Serber-Wilson theory,

$$\frac{1}{1+f} = \frac{\text{art} \frac{\kappa}{\Sigma}}{\frac{\kappa}{\Sigma}} \quad f > 0$$

$$\frac{1}{1+f} = \frac{\text{arth} \frac{\kappa}{\Sigma}}{\frac{\kappa}{\Sigma}} \quad f < 0$$

where

f = excess number of neutrons per collision

Σ = total macroscopic cross section

$$= \Sigma_f + \Sigma_c + \Sigma_{el\ tr}$$

the two were in appreciably closer agreement. There was still some difference however, as is shown in Figure 1, and it seems reasonable to assume that diffusion theory, modified or unmodified, will not be wholly adequate for reactors of the EBR-II type,⁽¹²⁾ having a core radius of about 23 cm.

Of course, there are bases for examination of diffusion theory which are better than Serber-Wilson. Comparisons have been made by Hummel between multigroup Serber-Wilson and some unpublished integral transport theory calculations made at LASL which presumably should be even more accurate. The results⁽¹³⁾ of this comparison show the Serber calculation to give a critical radius 2.8% too low for Topsy. This is in agreement with the results previously reported by Carlson.⁽⁴⁾

Further comparison calculations over a wider range of reactor sizes are in progress.

III. SUGGESTED MODIFICATION

An intuitive approach will now be presented to the problem of how to select one set of cross sections which should work well with multigroup diffusion theory for the entire range of fast reactors within the limit of existing cross section information.

The basic hypothesis is as follows: the major difficulty with diffusion theory is that it allows too much leakage from the core, the condition being aggravated as the core size in mean free paths decreases for higher

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FIG. 1
FRACTIONAL CHANGE IN CRITICAL MASS VS CORE RADIUS
BETWEEN SERBER-WILSON METHOD AND DIFFUSION THEORY

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neutron energies. There further exists the observation that upon comparison of diffusion theory with experiment, the theoretical fission rate falls off too slowly in the blanket. Now, both of these conditions would be altered in the proper direction by an increase in the transport cross sections used in diffusion theory. But what modification should be made so that leakage will be reduced for small reactors, yet left substantially unaffected for large reactors?

It was known that a fundamental mode analysis of the Lady Godiva reactor⁽¹⁴⁾ by multigroup diffusion theory predicted a buckling much less than experiment. It was also known that the same analysis by a multigroup form of the asymptotic solution to the transport equation* fit the experimental buckling rather well. The methods of calculation and some typical iterations are presented in Appendix A.

Examination of the two methods shows the numerators to be identical; the difference between the two theories appears in the denominators. Examination also indicates that diffusion theory can be made to give identical results with asymptotic transport theory by appropriate changes in the transport cross sections used in diffusion theory, holding all other cross sections constant. In other words, if in each group an appropriately larger elastic transport cross section, and hence a correspondingly larger transport cross section, is used in diffusion theory, than in asymptotic transport theory, the K for criticality and the neutron energy spectrum can be made identical. It is particularly interesting that the prescribed change is not the same in each group, but is large at the higher neutron energies, small at the lower ones. Thus, if cross sections were to be changed in this manner, the effect would be greatest on the small, highly-enriched reactors, where the neutron energy spectrum is the hardest and where leakage offers the most competition to fission.

The original transport cross sections for 94% enriched uranium and the revised values which would make diffusion theory identical with asymptotic transport theory for Godiva are listed in Table V for cross section sets No. 1 and No. 2. Rather arbitrarily, it was decided to change the transport cross sections of U^{235} , U^{238} and Pu all in the same fashion, and in such a fashion that diffusion theory fit Lady Godiva. The revised cross sections were then used to calculate the reflected reactors by multigroup diffusion theory to see if this approach would improve the situation.

For set No. 2, the transport cross sections of Oralloy, Tuballoy and plutonium were all adjusted to agree exactly with the prescription results given for Oralloy in Table V, thus making a new cross section set No. 2'. However, it was feared that the prescribed changes in the lower energy groups would result in deviations from reality in the larger, more dilute

* First used at Argonne by Hummel.

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reactors. Hence, for set No. 1, the prescribed results were only used as a guide. The prescription for the first three groups was generally accepted, that for the fourth group reduced, and that for the last two groups rejected, retaining original values. Again, the prescription is really for 94% enriched uranium but the changes were arbitrarily adopted for U^{235} , U^{238} and Pu, leaving all other materials untouched. It is noted that the deviations from the prescription would have little effect on an analysis of Godiva.

Table V
ORIGINAL AND ADJUSTED VALUES OF σ_{tr}
(In barns)

Group Number	Cross Section Set No. 1			Cross Section Set No. 2		
	Original	Prescribed	Used (1')	Original	Prescribed	Used (2')
1	3.9	5.60	5.7	4.47	6.07	6.07
2	4.8	6.30	6.5	4.55	6.13	6.13
3	6.5	7.73	7.6	4.66	6.22	6.22
4	8.0	9.04	8.7	5.62	7.00	7.00
5	11.5	12.26	11.5	8.85	9.83	9.83
6	13.4	14.07	13.4	13.10	13.80	13.80

IV. RESULTS

The critical assemblies listed in Table IV were recomputed using the adjusted cross section sets, No. 1' and No. 2'. Also, several "paper reactors," representative of the pilot plant, the full scale breeder, and other dilute assemblies, were computed using sets No. 1 and No. 2 and their adjusted forms, No. 1' and No. 2'.

The new results obtained for the critical assemblies are listed in Table VI, together with the corresponding values previously obtained with cross section sets No. 1 and No. 2. In general, the predictions made by the adjusted cross sections are in very good agreement with experiment. The small deviations from criticality are not random, however. There is a definite trend, namely, to make the smallest assemblies slightly subcritical and the larger ones slightly supercritical. The trend toward increasing reactivity with size is stronger for set No. 2' than for set No. 1'; this is reasonable, since in set No. 1' no adjustments were made in the lower energy transport cross sections which only become important in the more dilute assemblies.

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Table VI

EFFECT OF CROSS SECTION ADJUSTMENT ON PREDICTION OF k_{eff} FOR
EXPERIMENTAL ASSEMBLIES

No.	Description of Critical Assembly	Calculated k			
		Set No. 1	Set No. 1'	Set No. 2	Set No. 2'
1	Popsy	--	--	0.8591	0.9799
2	Topsy	0.8824	0.9883	0.8946	0.9958
3	Topsy with a thin blanket	0.8794	0.9967	--	--
4	80% enriched, full density core	0.9010	1.0032	--	--
5	85% density, fully enriched core	0.8963	0.9995	--	--
6	67.6% enriched, full density core	0.9106	1.0099	0.9190	1.0153
7	70% density, fully enriched core	0.9093	1.0097	0.9206	1.0171
8	47.3% enriched, full density core	0.9286	1.0194	0.9327	1.0224
9	50% density, fully enriched core	0.9159	1.0110	0.9258	1.0182
10	EBR-I (second core loading)	0.9301	1.0135	--	--
11	Los Alamos Pilot Mockup	0.9650	1.0278	--	--

The results obtained with the more dilute "paper reactors" are listed in Table VII. Only one comparison is available for sets No. 2 and No. 2', but it is adequate to establish the state of affairs. A 24-cm radius sphere of uranium, blanketed with natural uranium, was computed by both sets, allowing the enrichment of the uranium to vary for criticality. The enrichment computed for Set No. 2 was 13.09% and 11.80% for set No. 2', a reduction in critical mass of about 10%. These results confirm the trend observed in Table VI; thus, if one hopes to make a modification which leaves the dilute reactors essentially unaffected, the prescription cannot be followed rigorously.

For sets No. 1 and No. 1', a closer approach to the desired end result is obtained. For a very dilute reactor, e.g., the fast power breeder (PBR), only a 2.1% difference in k is obtained between the two cross sections sets. It is obvious that with some further minor adjustments, set No. 1' could be made to predict the critical assemblies more closely and to deviate less from set No. 1 in calculating the PBR.

A comment is perhaps desirable to the effect that the Los Alamos Pilot Mockup and the EBR are cylindrical assemblies, and hence, when they are computed as spheres of equal core volume, the calculation should give a somewhat supercritical result. Thus these two calculations by set No. 1' are better than is indicated at first glance.

V. DISCUSSION

It is emphasized that the procedure described is not recommended as a panacea, but rather is merely being reported as an interesting observation. It is not on any firm theoretical basis. Indeed, had Lady Godiva been of a somewhat different enrichment, a different set of changes in elastic transport cross section would have been prescribed. On the other hand, it is not being suggested that the rigid prescription be followed. Indeed, it has been shown to have difficulties and is intended only to suggest that modifications in elastic transport cross sections may make multigroup diffusion theory more applicable to a wide range of fast reactors.

Other methods come to mind, of course. The possibility of using the asymptotic transport formulation for computing buckling was considered; however, in the source-produced flux multigroup formulation, it effectively reduces reactivity if applied directly.

Of course, the asymptotic transport comparison used herein only on Godiva might somehow be applied to each problem separately, so that the transport cross sections were adjusted in accordance with the particular dimensions of the reactor core. Such a method was suggested by Hummel⁽¹⁵⁾ who later applied it to a few reflected cores, using the transcendental form

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Table VII

EFFECT OF CROSS SECTION ADJUSTMENT ON PREDICTION OF k_{eff} FOR "PAPER REACTORS"

No.	Description of Critical	Core Radius, cm	Core Composition atoms/ccx10 ⁻²⁴	Blanket Thickness, cm	Blanket Composition atoms/ccx10 ⁻²⁴	Calculated k or Critical Mass in kg of U ²³⁵			
						Set No. 1	Set No. 1'	Set No. 2	Set No. 2'
1	Dilute uranium core	16	0.01867 U ²³⁵ 0.02933 U ²³⁸	20	0.000346 U ²³⁵ 0.04765 U ²³⁸	k = 0.939	k = 1		
2	Dilute uranium core	24	0.048 U ²³⁵ + U ²³⁸	20	0.000346 U ²³⁵ 0.04765 U ²³⁸	k = 0.958 for loading of 130.2 kg	M _C = 130.2	M _C = 142.0	M _C = 128.0
3	PBR Pilot plant fueled with U ²³⁵	22.85	0.006312 U ²³⁵ 0.009048 U ²³⁸ 0.0119 Fe 0.0119 Na	45	0.000067 U ²³⁵ 0.0335 U ²³⁸ 0.00847 Fe 0.0044 Na	k = .9469	k = 1		
4	PBR (800-liter core)	57.59	0.001435 Pu 0.01364 U ²³⁸ 0.0119 Fe 0.0119 Na	45	0.000067 U ²³⁵ 0.0335 U ²³⁸ 0.00847 Fe 0.0044 Na	k = 0.979	k = 1		

for buckling in the blanket. Effectively, this raised transport cross sections in the core but lowered them in the blanket. The unpublished results are reported not to have been very good, too large a critical radius still being predicted for Topsy and EBR-I.

A comparison of the flux plots obtained by multigroup diffusion theory, with and without adjusted cross sections, and the flux plots obtained by G. Hansen and B. Carlson, using the S_4 method, is available for Topsy. The results are plotted in Figures 2, 3, 4 and 5. The reactor called Topsy in this report was computed to be critical by the S_4 method using cross section set No. 2 with a critical mass of 17.13 kg of uranium whereas the critical mass reported in the Reactor Handbook is 1% higher for a pseudo sphere. The flux plots presented for the two diffusion theory calculations are for this same 17.13 kg reactor with no change in enrichment or radius to achieve criticality.

In Figure 2 the six-group flux plots obtained by transport theory are compared with set No. 2 and with diffusion theory using set No. 2'. The relative normalization of the two sets of curves is such that the total flux at the core center is the same. It can be seen that the agreement is rather good throughout core and tamper. No significance should be attached to the deviations near the outer radius of 28 cm, since they are artificially induced, at least in part, by the two different approaches to an outer boundary condition. An enlarged view of the same curves for the core and inner portion of the blanket is given in Figure 3.

Figure 4 shows a comparison of the six-group flux plots obtained by transport theory and diffusion theory, both using the same cross sections, set No. 2. The transport theory normalization is as in Figure 2; the diffusion theory normalization is such that the total flux in the core is equal to that of the diffusion theory solution in Figure 2. Of course, the reactor is not critical by diffusion theory using set No. 2, so that the answer to the question of exactly what is being compared is not straightforward. However, it is rather clear that considerably greater deviations from the transport theory solution occur in Figure 4 than in Figure 2, and if the normalization is such as to have about the same core flux, those deviations appear in the blanket.

An enlarged view of the same curves for the core and inner portion of the blanket is given in Figure 5.

Perhaps a better indication of the effect of the different methods on the spectrum in the core is the comparison of computed threshold detector ratios at the core center. These are, of course, independent of the flux normalization. The values obtained for a few significant ratios are listed in Table VIII, together with the experimentally determined values.

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FIG. 3
COMPARISON OF 6-GROUP FLUX PLOTS FOR TOPSY BY
TRANSPORT THEORY AND BY DIFFUSION THEORY WITH
ADJUSTED TRANSPORT CROSS SECTIONS

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FIG. 5
COMPARISON OF 6-GROUP FLUX PLOTS FOR TOPSY BY
TRANSPORT THEORY AND BY DIFFUSION THEORY,
BOTH USING CROSS SECTION SET NO. 2

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Table VIII

RELATIVE FISSION RATES AT THE CENTER OF THE TOPSY REACTOR

Ratio	Transport Theory with set No. 2	Diffusion Theory with set No. 2	Diffusion Theory with set No. 2'	Experiment
$\frac{\sigma_f^{U^{235}}}{\sigma_f^{U^{238}}}$	7.0	7.4	7.2	6.9
$\frac{\sigma_f^{Np^{237}}}{\sigma_f^{U^{238}}}$	5.0	5.0	5.0	5.0
$\frac{\sigma_c^{Au}}{\sigma_f^{U^{238}}}$	1.05	1.1	1.1	0.85*

* Raised 5% from results reported in LA-1653⁽¹⁶⁾ in accordance with personal communication from H. Paxton.

It can be seen from Table VIII that the neutron energy spectrum is only slightly softer for diffusion theory than transport theory, and that the adjustment in transport cross sections produces little change between the two. Thus a large difference in reactivity between cross section sets No. 2 and No. 2' is accompanied by only a minor change in the predicted core spectrum, and the change is in the right direction.

A final comparison between the various methods can be obtained by plotting the relative fission rates throughout the reactor. In Figure 6, transport theory is compared with diffusion theory, both using cross section set No. 2. The experimental results⁽¹⁶⁾ are also presented here, all three sets of curves normalized so that the U^{238} fission rate is unity at the center. In Figure 7, transport theory is compared with diffusion theory, where the latter employs the adjusted transport cross sections, set No. 2'.

Close examination of Figures 6 and 7 shows the same trend as was indicated in Figures 2 and 4. If identical cross sections are used in transport theory and diffusion theory, the latter results in a somewhat flatter flux, so that if comparative curves are made equal at the core center, diffusion theory lies above transport theory in the blanket. On the other hand, when adjusted transport cross sections are used with diffusion theory, the agreement in the fluxes is rather good throughout the reactor.

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APPENDIX A

METHODS OF MULTIGROUP, FUNDAMENTAL MODE ANALYSIS AND TYPICAL ITERATIONS

A. Methods

1. Asymptotic transport theory:

$$\phi_j = \frac{S_j + \sum_{i=1}^{j-1} \Sigma_{in}(i \rightarrow j) \phi_i}{\left(\frac{\kappa}{\tan^{-1} \frac{\kappa}{\Sigma_{tr,j}}} \right) - \Sigma_{el\ tr, j}}$$

$$\sum_{j=1}^J \nu_j \Sigma_{f,j} \phi_j \stackrel{?}{=} \sum_{j=1}^J S_j$$

where

ϕ_j = flux in j'th group.

S_j = fission source in j'th group.

$\Sigma_{in}(i \rightarrow j)$ = macroscopic inelastic scattering cross section from group i to group j.

κ = square root of the buckling.

$\Sigma_{tr,j}$ = macroscopic transport cross section in j'th group.

$\Sigma_{el\ tr,j}$ = macroscopic elastic transport cross section in j'th group.

$\Sigma_{a,j}$ = macroscopic removal cross section from j'th group.

ν_j = neutrons produced per fission in j'th group.

$\Sigma_{f,j}$ = macroscopic fission cross section in j'th group.

For J groups, start at $j = 1$ and find successive ϕ_j , having guessed κ .

If second equation is not satisfied, further guesses on κ are made until it is.

$$\Sigma_{tr} = \Sigma_c + \Sigma_f + \text{true } \Sigma_{in} + \Sigma_{el\ tr}$$

$\Sigma_{in}(i \rightarrow j)$ includes true inelastic and elastic moderation, if any. S_j 's reflect fission neutron distribution.

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2. Diffusion theory:

$$\phi_j = \frac{S_j + \sum_{i=1}^{j-1} \Sigma_{in}(i \rightarrow j) \phi_i}{\frac{\kappa^2}{3\Sigma_{tr}} + \Sigma_{a,j}}$$

$$\sum_{j=1}^J \nu_j \Sigma_{f,j} \phi_j \stackrel{?}{=} \sum_{j=1}^J S_j$$

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B. Analysis of Godiva by multigroup asymptotic transport theory, using cross section set No. 1. Final iteration.

0.04498 x 10²⁴ atoms/cc U²³⁵
0.00302 x 10²⁴ atoms/cc U²³⁸

Try $\kappa = 0.285$

j	s_j	$\Sigma_1^{in} \rightarrow j \phi_1$	$\Sigma_2^{in} \rightarrow j \phi_2$	$\Sigma_3^{in} \rightarrow j \phi_3$	$\Sigma_4^{in} \rightarrow j \phi_4$	$\Sigma_5^{in} \rightarrow j \phi_5$	$s_j + \sum_{i=1}^{j-1} \Sigma_i^{in} \rightarrow j \phi_i$	$\Sigma_{tr, j}$	$\Sigma_{a, j}$	$\frac{\kappa}{\Sigma_{tr, j}}$	$\tan^{-1} \frac{\kappa}{\Sigma_{tr, j}}$	$\frac{\kappa}{\tan^{-1} \frac{\kappa}{\Sigma_{tr, j}}} - \Sigma_{tr, j}$	ϕ_j
1	1.1825	--	--	--	--	--	1.1825	0.0558	0.1872	1.5224	0.98963	0.2322	5.09259
2	0.7625	0.142429	--	--	--	--	0.904929	0.1427	0.2304	1.2370	0.89095	0.1772	5.10682
3	0.285	0.106822	0.067461	--	--	--	0.459283	0.2411	0.312	0.91346	0.74020	0.1439	3.19168
4	0.1625	0.071215	0.040477	0.021087	--	--	0.295289	0.3019	0.384	0.74219	0.63846	0.1445	2.04352
5	0.1075	0.035607	0.020238	0	0.009524	--	0.172847	0.4399	0.552	0.51630	0.47680	0.1581	1.09328
6	0.0	0	0.006746	0	0	0.0036734	0.010419	0.4345	0.6432	0.44310	0.41710	0.2488	0.04188

$$\sum_{j=1}^6 s_j = 2.5000; \quad \nu \sum_{j=1}^6 \phi_j \Sigma_{tr, j} = 2.4873, \text{ converges within } 1/2\%$$

C. Analysis of Godiva by multigroup diffusion theory using cross section set No. 1. Two iterations presented.
First iteration, try $\kappa = 0.285$

i	s_i	$\Sigma_1^{in} \rightarrow i \phi_1$	$\Sigma_2^{in} \rightarrow i \phi_2$	$\Sigma_3^{in} \rightarrow i \phi_3$	$\Sigma_4^{in} \rightarrow i \phi_4$	$\Sigma_5^{in} \rightarrow i \phi_5$	$s_i + \sum_{j=1}^{i-1} \Sigma_j^{in} \rightarrow i \phi_j$	$\Sigma_{tr, i}$	$\Sigma_{a, i}$	$\frac{\kappa^2}{\Sigma_{tr, i} + \Sigma_{a, i}}$	ϕ_i
1	1.1825	--	--	--	--	--	1.1825	0.5618	0.1314	0.2760	4.2844
2	0.7625	0.119626	--	--	--	--	0.882326	0.6912	0.08768	0.2052	4.2998
3	0.285	0.089870	0.056800	--	--	--	0.431670	0.936	0.07090	0.1577	2.7373
4	0.1625	0.059913	0.034080	0.018094	--	--	0.274587	1.152	0.08211	0.1526	1.7994
5	0.1075	0.029956	0.017040	0	0.0083672	--	0.162863	1.656	0.1121	0.1612	1.0103
6	0.0	0	0.005680	0	0	0.0033946	0.0090746	1.9296	0.2087	0.2508	0.036183

$$\nu \sum_{j=1}^6 \phi_j \Sigma_{tr, j} = 2.134, \text{ only converges to within } 15\%$$

A later iteration, try $\kappa = 0.25$

j	s_j	$\Sigma_1^{in} \rightarrow j \phi_1$	$\Sigma_2^{in} \rightarrow j \phi_2$	$\Sigma_3^{in} \rightarrow j \phi_3$	$\Sigma_4^{in} \rightarrow j \phi_4$	$\Sigma_5^{in} \rightarrow j \phi_5$	$s_j + \sum_{i=1}^{j-1} \Sigma_i^{in} \rightarrow j \phi_i$	$\Sigma_{tr, j}$	$\Sigma_{a, j}$	$\frac{\kappa^2}{\Sigma_{tr, j} + \Sigma_{a, j}}$	ϕ_j
1	1.1825	--	--	--	--	--	1.1825	0.5618	0.1314	0.2427	4.8723
2	0.7625	0.136268	--	--	--	--	0.898768	0.6912	0.08768	0.1781	5.0484
3	0.285	0.102201	0.066663	--	--	--	0.453864	0.936	0.07090	0.1377	3.2980
4	0.1625	0.068134	0.039998	0.021757	--	--	0.292419	1.152	0.08211	0.1364	2.1438
5	0.1075	0.034067	0.019999	0	0.0099487	--	0.171535	1.656	0.1121	0.1488	1.1451
6	0.0	0	0.006666	0	0	0.0038475	0.010514	1.9296	0.2087	0.2411	0.04361

$$\nu \sum_{j=1}^6 \phi_j \Sigma_{tr, j} = 2.49, \text{ converges to within } 1/2\%$$

D. Analysis of Godiva by multigroup asymptotic transport theory, using cross section set No. 2. Final iteration.

0.048 x 10²⁴ atoms/cc Orallloy

Try $\kappa = 0.2885$

j	s_j	$\Sigma_1^{in} \rightarrow j \phi_1$	$\Sigma_2^{in} \rightarrow j \phi_2$	$\Sigma_3^{in} \rightarrow j \phi_3$	$\Sigma_4^{in} \rightarrow j \phi_4$	$\Sigma_5^{in} \rightarrow j \phi_5$	$s_j + \sum_{i=1}^{j-1} \Sigma_i^{in} \rightarrow j \phi_i$	$\Sigma_{el\ tr, j}$	$\Sigma_{tr, j}$	$\frac{\kappa}{\Sigma_{tr, j}}$	$\tan^{-1} \frac{\kappa}{\Sigma_{tr, j}}$	$\frac{\kappa}{\tan^{-1} \frac{\kappa}{\Sigma_{tr, j}}} - \Sigma_{el\ tr, j}$	ϕ_j
1	0.53213	--	--	--	--	--	0.53213	0.05918	0.21456	1.3446	0.93133	0.25059	2.1235
2	0.87348	0.067272	--	--	--	--	0.940752	0.08165	0.21840	1.3210	0.92283	0.23098	4.0729
3	0.41666	0.046887	0.087975	--	--	--	0.551522	0.10637	0.22368	1.2898	0.91130	0.21021	2.6237
4	0.43925	0.055041	0.133721	0.080222	--	--	0.708234	0.18542	0.26976	1.0695	0.81895	0.16686	4.2445
5	0.21335	0.022424	0.070380	0.054027	0.077012	--	0.437193	0.33888	0.42480	0.67914	0.5966	0.14489	3.0216
6	0.03514	0.002039	0.007038	0.006549	0.011409	0.002901	0.065076	0.49632	0.62880	0.45881	0.43016	0.17436	0.3732

$$\sum_{j=1}^6 s_j = 2.5000; \quad \nu \sum_{j=1}^6 \phi_j \Sigma_{f, j} = 2.5003; \text{ converges.}$$

E. Analysis of Godiva by multigroup diffusion theory, using cross section set No. 2. Final iteration.

Try $\kappa = 0.255$

j	s_j	$\Sigma_1^{in} \rightarrow j \phi_1$	$\Sigma_2^{in} \rightarrow j \phi_2$	$\Sigma_3^{in} \rightarrow j \phi_3$	$\Sigma_4^{in} \rightarrow j \phi_4$	$\Sigma_5^{in} \rightarrow j \phi_5$	$s_j + \sum_{i=1}^{j-1} \Sigma_i^{in} \rightarrow j \phi_i$	$3\Sigma_{tr, j}$	$\Sigma_{a, j}$	$\frac{\kappa^2}{3\Sigma_{tr, j}} + \Sigma_{a, j}$	ϕ_j
1	0.53213	--	--	--	--	--	0.53213	0.64368	0.15538	0.25640	2.0754
2	0.87348	0.065748	--	--	--	--	0.939229	0.65520	0.13675	0.23599	3.9800
3	0.41666	0.045825	0.085968	--	--	--	0.548453	0.67104	0.11731	0.21421	2.5604
4	0.43925	0.053794	0.130671	0.078287	--	--	0.702002	0.80928	0.08434	0.16469	4.2626
5	0.21335	0.021916	0.068774	0.052724	0.077340	--	0.434104	1.27440	0.08592	0.13694	3.1700
6	0.03514	0.001992	0.006877	0.006391	0.011458	0.003043	0.064901	1.88640	0.13248	0.16695	0.3887

$$\nu \sum_{j=1}^6 \phi_j \Sigma_{f, j} = 2.503, \text{ converges.}$$

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