ON THE SENSITIVITY OF HCPWR MICROCELL CALCULATIONS TO GEOMETRICAL TREATMENT

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ABSTRACT

Nuclear reactor microcell calculations are, normally, carried out using simplified geometrical models which do not include the total number of homogeneous zones actually present.

Regarding the particular case of High Conversion Pressurized Water Reactors (HCPWR), the revision of this approximation has been done to determine the sensitivity of its neutronic parameters to the use of these models.

The study was performed comparing multiplication factors, reaction rates and neutron spectra, obtained using different geometrical treatments for a HCPWR typical microcell.

From the results it can be asserted that, if only two zones should be used in the calculation, the model which dilutes the clad into the moderator gives best results for the neutron fluxes, but the model that mix it with the fuel is better for k-infinite and reaction rate values.

Considering the significance of these parameters on the physical behaviour of the reactor, the last one is recommended for cell calculations.

Even if there is a slight difference between the cells considered, some results of this work were also compared with those of the NEACRP HCLWR benchmark with good agreement, so it can be concluded that the methodology here used for data processing and calculations is applicable to HCR's cell studies.

I. INTRODUCTION

Sometimes, due to code restrictions or to reduce or to simplify the problem, microcell calculations do not consider explicitly a complete geometrical representation, with all the homogeneous zones which are present, i.e. fuel, gap, clad and moderator.

Instead, geometrical models which include mixing or homogenization are used to diminish the number of zones to be treated, and consequently the many-groups nuclear data libraries.

A question arises on which is the error introduced in this way in multiplication factors, reaction rates, and neutron spectra, which will be used for final condensation and/or homogenization.

The aim of this work is to evaluate the so generated differences, specially for the case of a HCPWR cell defined in studies related with high conversion reactors (HCR) design as the one reported by Oldekop et al.(1982).

It is a part of the research program under development in the High Conversion Reactors Group of the Neutrons and Reactors Division of the Centro Atómico Bariloche (CAB).

II. CONSIDERED CASES

The typical microcell considered was the one defined by Oldekop et al.(1982) for their design's studies. It was

previously calculated by collision probabilities method in two zones: one containing the fuel and the other a mix of clad, structural material and moderator, Zeggel et al.(1988).

Then, to study the mentioned sensitivity, the following cases were defined:

a.Three zones representation (TUBCAB1).

The microcell is described by three homogeneous zones in cylindrical geometry: a central one with fuel, which takes also into account gaps, dishing volumes and oxygen atomic mass; a second one with clad and structural material and a third and peripherical one, with moderator. This representation is the closest picture of the real cell, so this case was taken as reference.

b.Two zones with clad in fuel (TUBCAB2).

In this case, the central zone has its radius equal to the outer radius of the clad and contains a volume mix of 79.7% of fuel and 20.3% of clad (zones 1 and 2 of the previous representation). The second zone is filled with moderator.

c.Two zones with clad in moderator (TUBCAB3).

The central zone is equal to the zone 1 in case a., while clad and structural material are included in the second zone mixed with the moderator, 27.1% and 72.9% respectively. This case is equivalent to the one calculated by Zeggel et al.(1988).

All the cases were calculated with a moderator to fuel ratio (Vm/Vf) of 0.6865, which corresponds to a pitch to diameter ratio (p/d) of 1.1845.

III. CALCULATIONAL METHODS AND DATA

a. Cell data

The corresponding general data, Oldekop (1988), can be seen in Tables I and II.

b. Nuclear data

The basic nuclear data were taken from the ENDF/B-IV library and were locally processed with the AMPX-II system, Greene et al.(1978), to create the working libraries.

In order to obtain fine details on the flux, 110 energy groups were used, 47 of them being thermal. It includes most of the limits of the 69 groups WIMS mesh, to facilitate any possible comparison (through condensation).

The weighting spectrum was composed by three parts: fission of Pu239, 1/E and maxwellian spectrum. This kind of spectrum has previously proved to be a good one for this type of microcells, Patino (1988).

Self-shielding of U238 resonances was treated with Nordheim integral method in cylindrical geometry, while the other isotopes's main resonances were represented using a fine energy mesh.

The temperatures used were 900 K for the fuel and 585 K for clad and moderator.

c. Calculational method

All the calculations were made using the DOT3.5-CAB code, Sbaffoni and Abbate (1985), in its transport - Sn option, with the following conditions:

- -cylindrical geometry
- -r , z calculation
- -P_0 cross sections
- -S_6 (30 angles) approximation

Different tests were made concerning the spatial mesh. It was proved that to use only one point per zone, with reflecting boundary conditions, is enough for this case.

The error in k-infinite is always smaller than 500 pcm (1 pcm = (k - k') * 1.E+05), there are no noticeable differences with average neutron fluxes from more refined meshes, and the calculation time for each outer iteration is greatly reduced (by a factor bigger than four), an important fact in a case like the present one, with almost fifty thermal groups.

A study on the convergence was also done, in order to test the accuracy of the results.

It was proved that, as the authors of the code mentioned, Rhoades (1977), for a case with fission source the pointwise convergence criterion for inner iterations gives the best results, and a convergence in outer iterations to a degree better than 0.1% is very difficult to reach; anyhow, this value is good enough for the present work because it could mean a dispersion of 100 pcm in k-infinite.

From the results, it was also concluded that in 25 to 30 outer iterations the k-infinite is approximately converged; to run the code in batches of less than this number of iterations is useless because k will never converge to its real value.

Of course if one is interested in neutron fluxes, much more than 30 outer iterations are needed for it to converge, and the integral degree of convergence of all of them should be better than 0.5%.

IV. CALCULATIONS AND ANALYSIS OF RESULTS

As central results of this work, k-infinite, neutron spectra and reaction rates were obtained.

In figure 1 and Table III, calculated k-infinite for the different cases are presented. All of them were obtained as mean values of a number of runs; as it can be seen in the figure, they are all well defined and correctly converged. It should be also noted that their standard deviation is always less than 300 pcm, and the maximum dispersion only in a few points is of the order of 800 pcm.

As it can be seen there, mixing the clad with the fuel underestimates the k-infinite in 0.98 % (1000 pcm), while diluting the clad into the moderator produces an underestimation of 1.35 % (1350 pcm).

The mean value of the multiplication factors calculated by the participants of the NEACRP HCLWR benchmark, Akie (1986), was also included in Table III. It corresponds to the

zero percent of voidage and burnup case. Even if the cell there defined is somehow different from the one reported here, (Vm/Vf = 0.6), the comparison with the values of this work showed that they are included into the present dispersion of the benchmark, so having a good check-point for the calculational system here used.

Typical zonewise neutron spectra for TUBCAB1 case can be seen in figure 2, and a comparison of the fuel neutron fluxes for the three geometrical representations is included in figure 3.

No noticeable differences can be seen between TUBCAB1 and TUBCAB3 cases. The effect is opposite to the one seen in k values, mainly because the dilution of the fuel with the clad increases the importance of its resonances.

Referring to the reaction rates, the calculations were carried out in three energy groups: thermal from 1.0E-05 eV to 4.0 eV; epithermal from 4.0 eV to 9.118 KeV and fast from this energy to 10 MeV.

At first, total (integrated over the three energy goups) absorption and production for the whole cells were calculated. No differences larger than 0.2% were found among the cases in both rates. See Table IV.

If we make a zonewise analysis of the results, we can see that, regarding total absorption, clad absorption increases when it is mixed with the moderator (6.6%) and decreases when mixed into the fuel (13%); anyhow, its overall

effect is lower than 2.0% . In the fuel zone there are no noticeable differences, and in the moderator it is 8% lower. The total value increases in both cases.

A groupwise description showed that, as it was expected, the most important energetic zone for these compact cells is the resonance region, where 57% of the absorptions occurs, then the thermal region with 25% , and finally the fast one, with 18% .

Concerning total production, it is smaller in approximately 1% when the calculation is performed in two zones, increasing 2% in the epithermal group and decreasing 5% and 7.6% in the thermal group in TUBCAB2 and TUBCAB3 cases, respectively. The total value decreases in both cases.

In order to complete the analysis and comparison with the benchmark, total production and absorption rates for some individual isotopes were calculated (Pu239, Pu240, Pu241, Pu242, U235 and U238), and also the same but groupwise for Pu240, Pu241 and Pu242. The values can be seen in tables V and VI, and the agreement is quite good.

Looking at the importance of each isotope, 62 % of the neutron production come from the Pu239, 21 % from the Pu241 and 11 % from the U238. Regarding the absorptions, 37% occur in the Pu239, 34 % in the U238, 13 % in the Pu240 and 9.7 % in the Pu241.

About the reaction rates of the individual isotopes, there are not big differences among the values for the three

cases integrated over the whole energy range, and the difference observed in the total production, and consequently in k-infinite, is mainly due to the lower production in the Pu239.

V. CONCLUSIONS

As it was said, the aim of this work was to evaluate the error introduced in some of the main neutronic parameters of High Conversion Reactor Cells by homogenization.

From the point of view of the calculation of multiplication factors, which could mean performance or viability of the reactor, mixing the clad with the fuel instead of mixing it with the moderator as it is usual, produces a lower underestimation and better result. The k - infinite obtained is approximately 1000 pcm lower than the one obtained in the three regions case.

For the fluxes, which we may want to use in condensation, the effect is opposite, mainly because the inclusion of clad in fuel dilutes the fuel, increasing the importance of its resonances.

Regarding the results of the reaction rates, of great importance on conversion ratios and fuel utilization, again the best agreement is found with the case TUBCAB2.

This work was also used as a first check-point of the quality of the results of the local system for data

processing and cell calculations for this special kind of cells, comparing with the NEACRP benchmark preliminary results.

The agreement was satisfactory, so it can be said that the methodology here applied is adequate for other HCR cell calculations.

As general conclusion, and considering that in this kind of cases, with small pitch or low moderator to fuel ratio, the most important energetic region is the epithermal one, with more than fifty percent of the absorptions and productions, it is recommended to calculate the cells, if possible, treating explicitly at least fuel, clad and moderator zones. If this three zones treatment is not possible, to dilute the clad in the fuel is suggested for k - infinite or reaction rate calculations.

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REFERENCES

Akie H. et al. (1986), "Preliminary report of HCLWR cell burnup benchmark calculation", Tokai, Japan Atomic Research Institute.

Greene N.M. et al.(1978), "AMPX-II Modular code system for generating multigroup neutron-gamma-ray cross-section libraries from data in ENDF format", PSR-63, RSIC, ORNL.

Oldekop W. et al.(1982), Nucl.Technol. 59, 212.

Oldekop W. (1988), Private communication.

Patino N.E.(1988), "Validación de un sistema de generación de secciones eficaces multigrupo y su aplicación al cálculo de reactores de alta conversión", Trabajo Especial, Instituto Balseiro, Bariloche.

Rhoades W.A.(1977), "DOT 3.5 - Two dimensional discrete ordinates radiation transport code", CCC-276, RSIC, ORNL.

Sbaffoni M.M. and Abbate M.J.(1985), "DOT 3.5 CAB - A new version of DOT 3.5 code", CNEA-NT 18/85.

Zeggel W. et al.(1988), Nucl.Technol. 80(2), 292.

TABLE I

General data

Hexagonal lattice ; cylindrized cell	
Fuel radius	0.38500 cm
Outer clad radius	0.43130 cm
Cell radius	0.53645 cm
Vm/Vf (moderator to fuel volume ratio)	0.6865
p/d (pitch to diameter ratio)	1.1845

TABLE II

Number densities (atom/barn cm)

Moderator: Light water
Density 0.7 g/cm^3

H	4.68257 E-02
O	2.34128 E-02

Clad: Stainless steel (316)
Density 7.92 g/cm^3

Fe	5.72195 E-02
Cr	1.37591 E-02
Ni	1.21877 E-02
Mn	1.30223 E-03
Mo	0.74569 E-04

Fuel: Depleted Uranium,
8% enriched in fissile Pu
Apparent density 9.673 g/cm^3

U235	3.79876 E-05
U238	1.89558 E-02
Pu238	5.05390 E-05
Pu239	1.42612 E-03
Pu240	6.33148 E-04
Pu241	2.98661 E-04
Pu242	1.57005 E-04
O	4.31185 E-02

TABLE III

K-infinite values for the calculated cases

Case	k-infinite	Standard deviation
TUBCAB1 (f/c/m)	1.09538	0.00356
TUBCAB2 (f+c/m)	1.08576	0.00285
TUBCAB3 (f/c+m)	1.08172	0.00172
NEACRP benchmark	1.09250	0.00240

TABLE IV

Total cell's rates

Case	Absorption			
	Zone 1	Zone 2	Zone 3	Total
TUBCAB1	0.97594	0.02288	0.00303	1.00185
TUBCAB2	0.97969	0.02018	0.00287	1.00274
TUBCAB3	0.97632	0.02438	0.00281	1.00351
	Production			
TUBCAB1	1.08394	--	--	1.08394
TUBCAB2	1.07460	--	--	1.07460
TUBCAB3	1.07260	--	--	1.07260

TABLE V

Comparison of reaction rates

Reaction	Case: TUBCAB1	TUBCAB2	TUBCAB3	NEACRP
Production:				
Pu239	0.679	0.675	0.669	0.685
Pu240	0.0296	0.0291	0.0294	0.030
Pu241	0.227	0.226	0.225	0.220
Pu242	0.0058	0.0057	0.0058	< 0.01
U235	0.0126	0.0126	0.0126	0.020
U238	0.125	0.121	0.125	0.125
Absorption:				
Pu239	0.366	0.365	0.362	0.370
Pu240	0.131	0.132	0.132	0.125
Pu241	0.0955	0.0952	0.0948	0.090
Pu242	0.0310	0.0317	0.0314	0.035
U235	0.0073	0.0073	0.0073	0.012
U238	0.336	0.340	0.341	0.335

TABLE VI

Groupwise reaction rates

Reaction	Group	Case TUBCAB1	NEACRP
Absorption:			
Pu240	1	0.0114	0.012
	2	0.0341	0.034 to 0.040
	3	0.084	0.073 to 0.080
Pu242	1	0.0023	0.0030
	2	0.0050	0.006 to 0.010
	3	0.023	0.016 to 0.032
Production:			
Pu241	1	0.031	0.024 to 0.030
	2	0.150	0.144 to 0.160
	3	0.040	0.030 to 0.040

FIGURE CAPTIONS

Figure 1: Convergence of k-infinite for the three cases.

Figure 2: TUBCAB1 case, zonewise neutron spectra.

Figure 3: Neutron fluxes in the fuel zone.
Comparison of the three cases.

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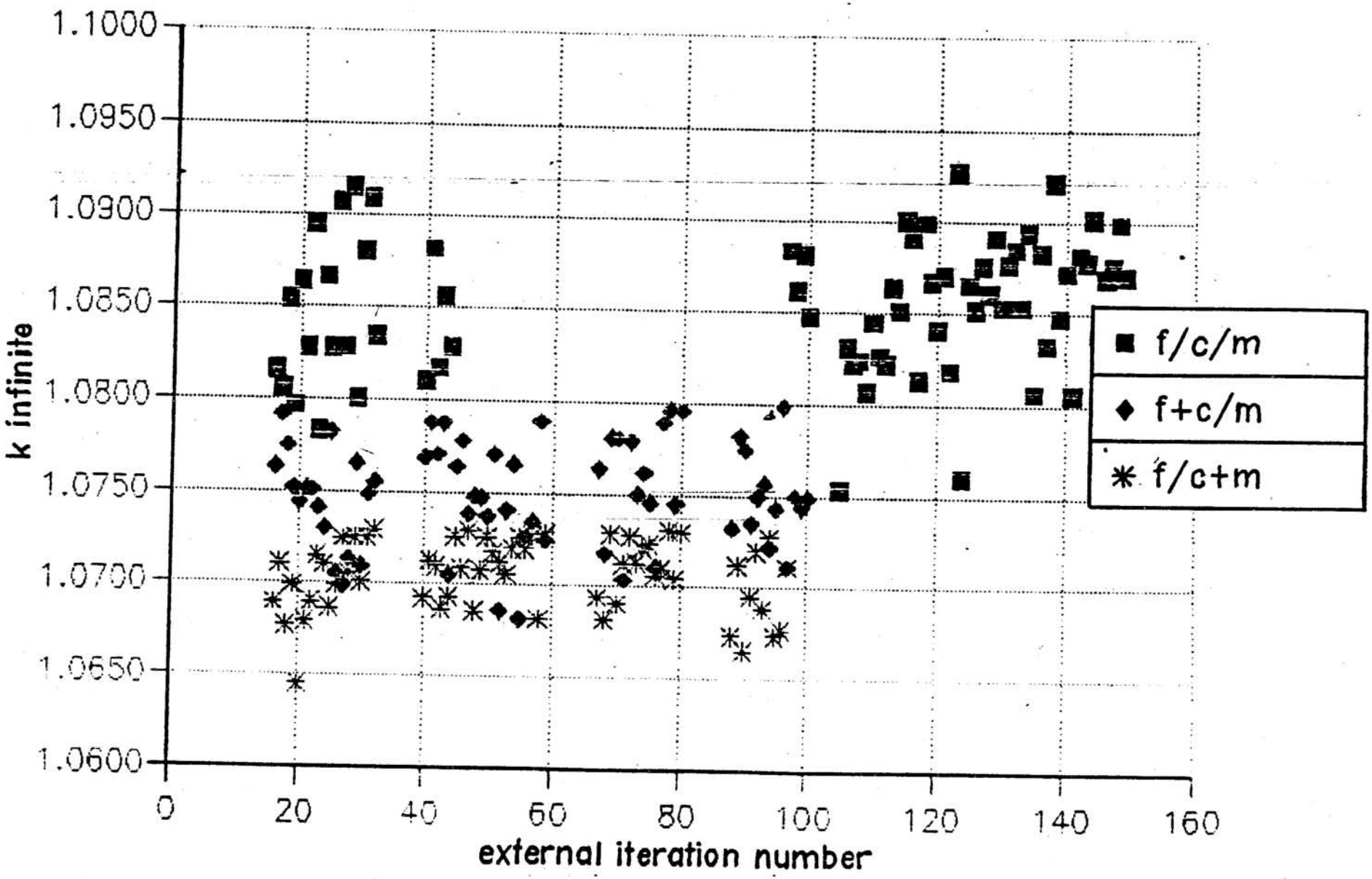
k infinite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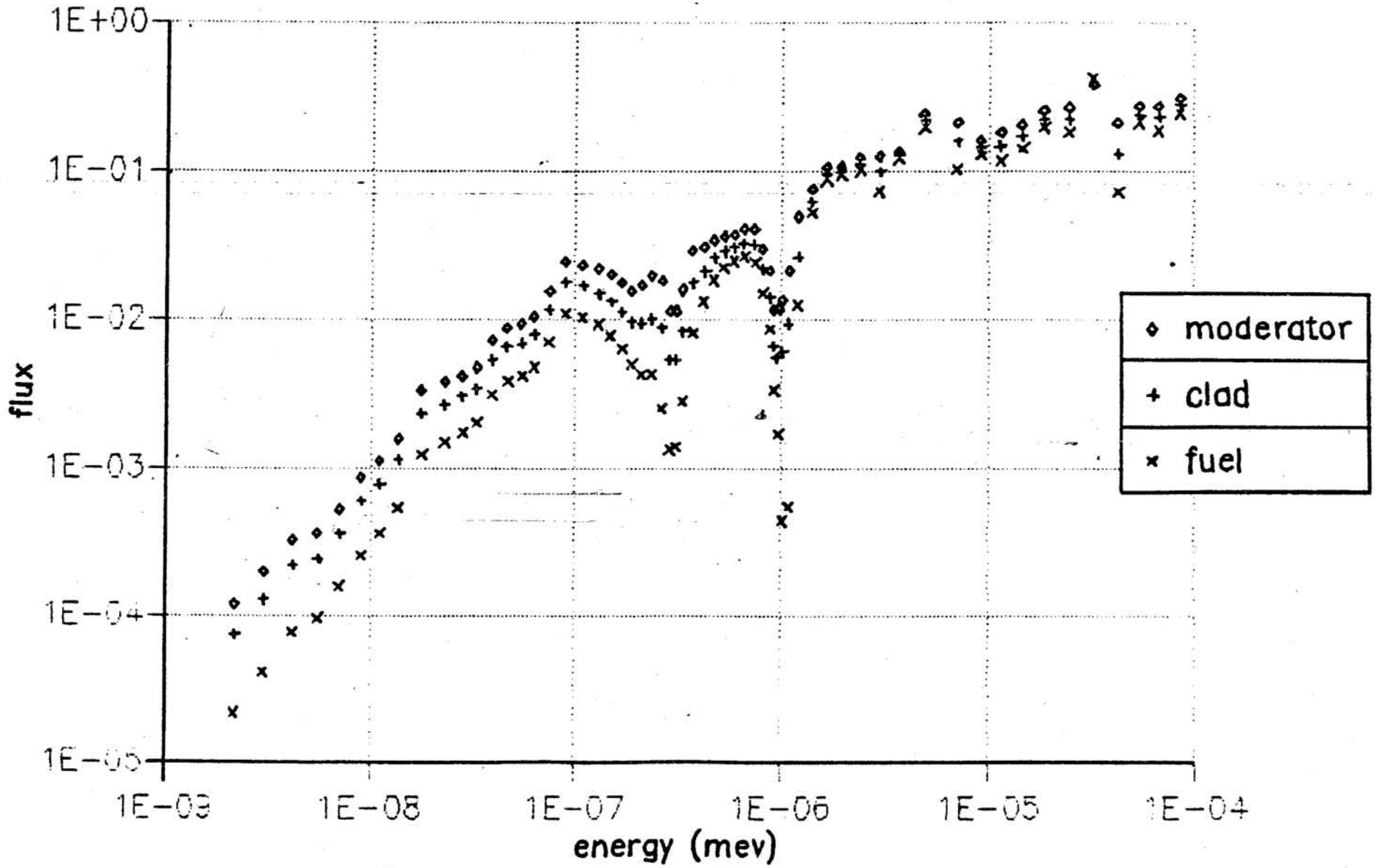
3 zones flux
fuel / clad / moderator



FIGURES (SCATTERING, ABSORPTION) COMPARISON OF THE THREE CASES