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REACTOR PHYSICS PROGRAM AT EURATOM CCR-ISPRA

by

V. RAIEVSKI

1964

Joint Nuclear Research Center
Ispra Establishment - Italy
Reactor Physics Department

Paper presented at the IAEA Study Group Meeting
on Research Reactor Utilization
Athens (Greece), September 9-13, 1963

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It is divided into two parts :

The first one describes general reactor physics work including such topics as shielding, burn-up, fast reactor physics, and Monte-Carlo codes.

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The second part is connected with work required by the development of the Orgel program and deals with Orgel recipe, thermal neutron spectrum, resonance escape probability and fast neutron multiplication factor.

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C O N T E N T S

REACTOR PHYSICS PROGRAM AT EURATOM CCR-ISPRA

INTRODUCTION

It is a very interesting but not easy task, to report in the short time allowed for an oral presentation, on the reactor physics work in progress in a center. Each group is doing a good job, but a somewhat arbitrary selection has to be made, in order to stay within the imposed time limits.

I hope that the topics presented here will sufficiently illustrate our activity without tiring the audience and without deceiving too large a number of groups.

I have divided this presentation into two parts :

part A deals with work not directly connected with the ORGEL program; however, some of this work is or will be helpful for this program.

Part B deals with work required by the development of the ORGEL program.

PART A - GENERAL REACTOR PHYSICS

I. SHIELDING PHYSICS

In the field of shielding nuclear energy plants, certain problems of outstanding importance still require satisfactory solutions. Among these, particular importance is assumed by that of determining removal cross sections for fission neutrons and that of calculating the propagation of neutrons and gamma rays in ducts. Theoretical and experimental research has been undertaken in this direction.

a) Removal cross sections :

It is an useful integral parameter to describe the attenuation of neutrons through shielding. After some distance, an asymptotic distribution characterized by an exponential behaviour is achieved, which can be properly described in terms of a single cross section, the removal cross section. For many materials this parameter has been measured for a fission spectrum. As neutron spectrums impinging on a shielding are often different from fission spectrum, need for measurements with monoenergetic sources is obvious.

These measurements have been performed with water using the 5,5 Mev Van de Graaff of the Padova university. A source of neutrons with energy varying in the range 0-8 Mev and 15-20 Mev was obtained in the center of a water tank 300 x 300 x 270 cm using Li, D_2O and H^3 targets. Detectors used were indium, indium under cadmium, sulphur in cadmium, other measurements with Ni, Fe, Al and boron and fission chambers are in preparation.

(1) A. Kind, R. Nicks - EUR 233.i (1963)

The first results obtained for the water removal cross sections :

E	Σ_R
Mev	cm^{-1}
4,8	0,15
6,8	0,12

are in reasonable agreement with the previous one. (2)

A Monte Carlo program to deal with the problem has been prepared, other materials as iron and lead are now measured.

b) Propagation of neutrons through ducts : (1)

The facility used for this experiment is the 1 MW SORIN swimming pool reactor (Saluggia, Italy). A cubical water tank (3 m edge) was put in front of the shielding facility, a fission spectrum is obtained by using an uranium converter plate, the diameter of which may vary between 5 and 45 cm. The neutrons propagating through a tube extending from the uranium converter plate, were measured with different thermal, resonance and threshold detectors and fission chambers (U, Th, Np). Two different diameter tubes were used in these experiments (5 and 15 cm.)

Theoretical results obtained with a Monte Carlo program were found in good agreement with the experimental ones.

(2) J. Bourgeois and Al. - Rapport CEA n°1307

II. MONTE CARLO CODE

A general Monte-Carlo code for fast effect calculations, named MOCA-II [3] was written by Rief for the IBM 7090. It is an extension and an improvement of an early work initiated at BNL.[4] MOCA-II allows the solution of the general two or three dimensional energy dependent transport equations under the assumption of the following scattering kernels :

a) elastic scattering, isotropic or anisotropic in the c.m. system.

b) inelastic scattering either by the level excitation or by the statistical model.

c) fast fission for energy dependent ν value

The primary neutron source can be spatially distributed, monoenergetic or as a fission spectrum, and anisotropic.

The present geometry routines allow the calculation of slab, cylindrical and spherical lattices, a geometry of arbitrary rod bundles is also provided.
The code allows the calculation of the following quantities :

1) The classical fast fission factor.

2) The slowing down probability of neutrons below a certain energy limit.

3) The ratio of secondary to primary neutrons.

4) Absorption per geometrical region and energy group.

In addition to these results, the following quantities can be calculated :

5) The fast fission ratio (δ)

6) The neutron flux averaged for each geometrical region as a function of energy.

7) The Fermi age τ and its x, y and z components.

8) The energy deposition due to elastic neutron scattering.

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(3) H. Rief - MOCA-II, a multipurpose Monte Carlo code for fast-effect calculations / Transactions of the American Nuclear Society, Vol. 6 n°1, June, 1963.

(4) H. Rief - BNL 647 (T-206), 1961

A lot of applications of this general code have been made or are under way. For example, energy deposition in the different media of a heavy water moderated, organic cooled reactor has been calculated as a function of the deposited energy. This quantity is of interest for the fouling process; of course, material damage rate cannot be directly inferred from these calculations, but very likely some relation can be found between radiation damage rate and energy deposition.

These calculations were carried out for the energy range 10 Mev to .5 Kev, which was subdivided into 26 energy groups with group averaged cross sections. Including a detailed flux calculation for each of the 12 geometrical regions, reasonable variance can be achieved with 5.000 histories, which need approximately 7 minutes of IBM 7090 computer time.

A full description of the code and all these results will be shortly issued as an external Euratom report.

III. BURN-UP PHYSICS

There are two steps in burn-up physics :

a) to determine the isotopic composition of a sample as a function of the irradiation in a given spectrum ;

b) the isotopic composition being known, to find the effect on the reactivity.

This second step can be more easily solved by measuring in a given reactor the reactivity effect of synthetic fuel elements made by homogeneous mixture of depleted uranium and Pu of different isotopic composition.

As synthetic fuel elements are very expensive materials, one way to perform the measurements, is the substitution technique, [5] the results of which are generally interpreted in terms of two group theory, dealing with the substituted and reference lattices as two homogeneous zones. Though more economic than a complete critical loading, this method is still expensive. Heterogeneous theory [6] is a good way to interpret the result of substitution experiments with a few elements. From measurements of critical level for different lattice pitches and using the kernel heterogeneous theory, the γ , η parameters of the substituted elements can be obtained in terms of the corresponding parameters of the reference elements These parameters describe the absorption and production of neutrons when the fuel element is immersed in the unperturbed flux at a lattice position. In principle, measurement with a single fuel element can be meaningful in this theory. In such a case, difficulty will arise from the weak reactivity effect due to the substitution of an element.

The great sensitivity of the oscillation technique will allow us to perform the measurement in this case [7].

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(5) Y. Girard and Al. - II. Geneva Conference 15/8/336

(6) G. Blässer - Symposium on Exponential and Critical Experiments, Amsterdam (2-6/9/63)

(7) G. Blässer - EUR 221. e (1963)

The central part of a fuel element, being long enough to minimize end effects, is substituted by a sample of the same geometry, but made of a different material, simulating the isotopic composition after a given burn-up. A normal fuel element is attached to this composite one, and the whole assembly is oscillated in the central thimble of a critical facility. The ECO reactor will allow such measurements thanks to a central thimble extending well below the bottom face of the tank.

The reactor signal measured with a detector placed at a point $\vec{r}$ is given for a thermal reactor and non moderating sample by the relation :

$$s_\rho = G_f(\vec{r}, \vec{ro}, \rho)\, P(\vec{ro}) - G_a(\vec{r}, \vec{ro}, \rho)\, A(\vec{ro})$$

where ro, are the sample position and the oscillation frequency.

where $A(\vec{r}_o) = V \iint dE\, d\vec{\omega}\, \sigma_a(E)\, \upsilon N(\vec{r}_o, E, \vec{\omega})$

and $P(\vec{r}_o) = V \iint dE\, d\vec{\omega}\, \nu(E)\, \sigma_f(E)\, \upsilon N(\vec{r}_o, E, \vec{\omega})$

are the total absorption and production rate of neutrons in the sample in the $vN(r_o, E, \vec{\omega})$flux. G_a and G_f are absorption and production response function which are characteristic of the reactor and detector used. These functions can be calculated by a standard approximation method as multigroup diffusion theory, Monte-Carlo or S_N from the general expression given in the report[7], or can be better deduced by calibrating the reactor with boron and U-235 samples.

Oscillating first a standard boron sample, one obtains (the index "O" referring to the standard sample) :

$$s^\circ_\rho = -G_a(\vec{r}, \vec{r_o}, \rho)\, A_o(\vec{r_o})$$

If a second standard containing U-235 is now oscillated, since the absorption cross section of U-235 is an almost pure 1/v behaviour, the ratio :

$$Z = A\,25/Ao$$

will be independent of the position in the reactor and can be obtained by a simple calculation.

The U-235 signal can be written :

$$s_f^{25} = s_f^\circ Z + G_f(\vec{r}, \vec{r}_o)\, P_{25}$$

For an arbitrary sample containing fissionable material, we can now write:

$$s_f = s_f^\circ \frac{A}{A_o} + (s_f^{25} - s_f^\circ Z)\frac{P}{P_{25}}$$

or :

$$s_f = a(\vec{r}, \vec{r}_o, f)\frac{A}{A_o} + b(\vec{r}, \vec{r}_o, f)\frac{P}{P_{25}}$$

where a and b are now experimentally known functions from the standards.

By performing the experiments for two detector positions one can vary the ratio b/a and measure separately the absorption and the production of neutrons.

Question may now arise as to the neutron spectrum at the oscillation position. To answer this question, Diana [8] has investigated the influence of Pu on the spectrum in the fuel and in the moderator using the Thermos code (see ref. part B). As expected, this influence is very important within the fuel while calculation has shown that in the moderator the effect is negligible at a distance of about 2 cm from the fuel surface. From these results, the following conclusion can be drawn :
The moderator spectrum far from the fuel element is not sensitive to the details of thermal absorption. Therefore, the absorption integral, as measured by the oscillation technique, is already a sufficient characteristic for the thermal spectrum in the moderator far from the elements. This facilitates the interpretation of the behaviour of Pu-containing samples in a reactor containing only natural U-fuel.

Additional calculations have been made on the non uniform distribution of Pu in the fuel. Calculation has shown that the η fuel parameter is relatively insensitive to the Pu distribution, the effect on γ is bigger but as this parameter is less important for the reactivity, one can be confident that using theoretical Pu distribution, small errors will be made, in predicting reactivity change in a reactor, from uniform Pu distribution measurements.

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(8) E. Diana - Euratom - Internal Report ISPRA-471 (1963)

IV. FAST REACTOR PHYSICS

The Ispra center is not directly involved in the Euratom fast reactor program. This work is pursued in different national laboratories under association contracts with Euratom. However, as some knowledge in fast reactor physics may be of interest in the future, a limited theoretical program has recently started in Ispra. Some efforts were devoted to Doppler effect and neutron spectrum in fast assemblies.

a) Doppler effect :

The influence of non uniform temperature distribution within the fuel was investigated. This problem is of interest for power reactors with high power densities and fueled with poor thermal conductors as for instance UO_2.

A Monte-Carlo approach of this problem was made [9] by Matthes, who investigated the Doppler effect in the energy region where resonances are well separated but not measured, so statistical distribution of resonance spacing and reaction widths must be used. The necessary parameters for these distributions were taken from Nicholson's report [10].
The multiplication factor is defined by :

$$K = \frac{1}{N} \sum Ni$$

where N is the number of fission neutrons starting in the reactor.
Ni the number of fission neutrons produced in the energy interval ΔE_i,
the summation is extended over the whole reactor spectrum.

If the temperature is changed, a new value of the multiplication factor K' is obtained :

$$K' = \frac{1}{N} \sum N'i$$

The change of reactivity due to this change of temperature or the Doppler effect, is then given by :

$$\Delta K = K' - K = \frac{1}{N} \sum \Delta Ni.$$

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(9) W. Matthes - Euratom Ispra 380 (1963)

(10) R. B. Nicholson - APDA 139

If interests are paid only to those neutrons which are absorbed below a given energy E_o, the relation can be written :

$$\Delta K = \frac{N_o}{N} \quad \frac{1}{N_o} \quad \sum_{E_i \leq E_o} \Delta N_i$$

Matthes has performed these calculations for the energy range 1 Kev-10 Kev where resonances are not experimentally resolved but overlapping can be neglected.

The calculation of the quantity $\frac{N_o}{N}$ is straight forward and is not given in the report.

A basic difficulty to evaluate a differential effect in the Monte-Carlo method arises from the inherent statistical fluctuations. To avoid this, the method described by Goertzl and Kalos [11] was used. The same set of random path is selected to calculate K and K' , the differences of collision points density in the two cases, due to the difference in cross sections are taken into account by properly modifying the weight of the neutron during its flight. Application of this program was made for the following situation [12] :

- Diameter of the fuel elements 0,317 cm
- Distance of the fuel elements 0,368 cm (square lattice)
- Composition of the fuel elements 10% U-235, 90% U-238
- Temperatures T center (° C) 700-1000-1300-1500
  T surface (°C) 500

If a mean temperature can be defined, such that $K(T_c, T_s) = K(T_m)$ where T_m can be calculated out of T_c and T_s by a procedure which is independent of T_s and T_c, the following condition must be verified :

$$\frac{\partial K}{\partial T_c} = \text{const} \frac{\partial K}{\partial T_s}$$

Calculation has shown that presently this is not the case. For the type of reactor considered, one has to employ two Doppler coefficients, $\partial K / \partial T_s$ and $\partial K / \partial T_c$ which can be calculated by the Monte-Carlo program described here.

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(11) G. Goertzl, M. H. Kalos - Progress in Nuclear Energy, Vol. 2 (1958)

(12) G. Blässer, W. Matthes - X. Congresso Nucleare, Roma, (June 1963)

An analytical approach of the problem was also made by Elässer (13) for a single resonance in the narrow resonance approximation anda parabolic distribution of the temperature in the fuel plates. A slab geometry consisting of fuel elements and moderator was used. As for the previous Monte Carlo program, this analytical program was written for the IBM-7090. Application was made to the following configuration. (12)

- Fuel element thickness	.3 cm
- Moderator thickness	10 cm
- Resonance parameters	E_r = 1000 ev
	r = 1950 b
	Γ_γ = 0,03 ev

Calculation has shown that for the given resonance a mean temperature defined by $T_m = T_s + \frac{2}{3}(T_s - T_c)$ can be used.

This result is in some contradiction with KEANE calculations (10), which were made in the Infinite Absorber Mass approximation; it seems possible that this difference comes from the smoothing of absorption due to the slowing down of neutrons within the fuel.

Further calculations will be made with this programme to study the range of applicability of the effective temperature concept.

b) Neutron Spectrum in Fast Assemblies :

A tentative was made to find a simplerrepresentation of the spectrum in a fast assembly than the multigroup one. A superposition of a virgin fission spectrum and an unknown spectrum was tried. (14)

$$\phi = A(\alpha X + \rho)$$

where ϕ, X and ρ are normalized spectrum

ϕ the neutron spectrum in the assembly

X the fission spectrum

ρ the unknown spectrum.

α is a proportionality constant, and $A = 1/1+\alpha$ as required by the normalization.

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(13) G. Blässer - Euratom Ispra 205 R (1962)

(14) G. Blässer, E. Diana - VIII Congr. Nucl. Roma (1963)

Furthermore, the constant α can be determined by the condition that $\rho(E) = o$ for high values of E. By instance $E > E_o$
$\phi(E) = A \alpha X(E)$ for all $E > E_o$.

This way, the unknown spectrum can be studied by subtracting the fission spectrum from the reactor spectrum

$$\rho(E) = \frac{\phi}{A} - \alpha X$$

The reactor spectrum was calculated in the center of the assembly by a multigroup code (ZOOM 7090 version) using 16 groups and YOM cross sections [15], and the properties of the unknown spectrum ρ were studied following the PEARSON [16] method. In this method, extensively used in statistical problems, it is shown that distribution curves can be classified in eight types according to the values of their moments up to the fourth. This calculation was repeated for a lot of core assemblies including U metal, oxide and carbide with different enrichment and proportions of sodium and stainless steel. It turned out that all spectra could be fitted by type I curves of the Pearson system, the expression of which is :

$$\rho = \text{const} \left(1+\frac{x}{a_1}\right)^{m_1} \left(1-\frac{x}{a_2}\right)^{m_2}$$

where x is the lethargy, the origin of lethargies being taken at the point where the distribution reaches its maximum value.

Furthermore, a linearity was found between the parameter α and the enrichment down to 15% and the first and second moment of the distribution appears quite independent of core composition.

The results of these calculations seem to indicate the feasibility of two group calculations for fast reactors, using two overlapping groups. The cross sections being properly averaged on these two groups. One can write :

$$O_x X + \Sigma_{\rho \to x} = S_x$$
$$\Sigma_{x \to \rho} X + O_\rho \rho = S_\rho$$

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(15) S. Yiftah, O. Okrent, P. A. Moldauer - Pergamon Press, Oxford (1960)

(16) E. S. Pearson, H. O. Hartley - Cambridge University Press (1958)

where O_x, O_ρ are transport operators with cross sections averaged on these distributions.

The transfer cross section $\Sigma_{x \to \rho}$ from the fission group can be taken as the average on the fission spectrum of the scattering cross section (elastic and inelastic) and $\Sigma_{\rho \to x}$ is simply the $\nu\Sigma_f$ production cross section averaged over the ρ spectrum. Another way to define the transfer cross section $\Sigma_{x \to \rho}$ is by the requirement that the ratio of the two fluxes far from boundaries be equal to α

The averaged cross sections over the ρ spectrum can be obtained from a table as a function of the core composition. Or the ρ spectrum can be first computed for the given core composition using a multigroup theory in a one dimensional geometry from which average cross sections can be obtained. This reduction of the number of groups permits the use of more elaborated methods such as two dimensional S_N calculations. Marchuk [17] has shown that one group transport (P_3) theory using averaged cross sections (which are obtained from 25 group P_1 calculations) give almost the same results as direct 25 groups P_3 calculations.

The effect of the reflector was also investigated by using multigroup, one dimensional and two regions calculations. The spatial variation of average cross sections is important only for the threshold fission cross section of U-238 near the boundary.

From this one can expect that two group calculations according to the here defined model can be made for reflected assemblies.
Boundary conditions in this case are a delicate point which can be solved by using properly integral boundary conditions.

Another interest of the procedure described, is the interpretation of critical experiments, by reducing the number of parameters to be determined to 5 (α, a_1, a_2, m_1, m_2) integral quantities can be easily and accurately obtained with a reduced set of detectors.

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(17) G. I. Marchuk - Proceedings of the Vienna Conference (1962) on the Physics of fast and Intermediate Reactors - Vol. II - p. 19 ff

PART B - ORGEL REACTOR PHYSICS

Reactor design calculation from first principles, is still doubtful for a natural uranium fueled reactor, due to the poor reactivity of this system which must be calculated with a high accuracy, in order that criticality may be achieved during the whole life of the fuel element.

For this reason, calculations must rely on integral experiments which cover a range being wide enough for the designer's needs. This does not mean that refined theories are unnecessary. On the contrary, needs for such theories are continuously increasing, as they furnish a better insight in the physics of the system. Furthermore, they may decrease the number of high cost experiments needed, thus allowing the designer to use safely the codes in a range where no or few experimental results exist, and enable one to obtain quantities of interest for the designer, which are not directly given by the experiments.

Our basic philosophy for predicting the performances of a natural uranium fueled reactor, lies in refined theory based on high accuracy experiments. For reactor design calculations, some simplified models may be used which give as accurate results as the general theory, but in a more limited range.

I. THE ORGEL RECIPE :

Up to now, ORGEL calculations use a recipe called CAROLINE-I.
The ambition of a reactor physicist is of course to do good physics. However, the reactor physicist has also to provide the reactor designer with means of calculation. As reactor physics is an applied science, mainly justified by the construction of reactors, this means that priority has to be given to this second task. Calculations which do not take into account all the phenomena, which use some oversimplified models, are called by reactor physicists "a recipe". This term is by no means pejorative. A recipe is good if it is based on experiments and it generally gives better results in the range covered by the experiments than more refined theories based on first principles only. A recipe is not a simple calculation. Even the simplified model on which it is based leads to rather lengthy calculations which require the use of digital computers. Furthermore, up to now, all reactor design calculations were based on the use of more or less sophisticated recipes.

Caroline-I :

Caroline-I was developed from the beginning for this purpose. Caroline I [1], is based on the French correlation for heavy water lattices. In this correlation, three parameters : η , A, B are deduced from buckling measurements. η is the classical natural uranium thermal fission factor, A and B are the constants of the effective resonance integral. In order to make allowance for the characteristics for which the studied lattices differ from those on which the French correlation was based, particularly the presence of organic liquid instead of heavy water in the fuel elements, appropriate modifications to Naudet's [2] calculation method have been introduced.
The presence of organic moflifies the slowing down properties of the lattice, thus affecting the ε , p factors and the slowing down area. It modifies also the thermal neutron spectrum; however, this effect is not directly dealt with by Caroline, but by another code called Thermidor[3] which provides averaged

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(1) Caroline-I, -G. Casini, W. de Haan, E. Diana, C. Foggi, A. Kind, G. Rossi EUR-134 e. (1962)
(2) Réseaux à eau lourde - R. Na_u det / Génie Atomique B XV
(3) A simplified model for the determination of the thermal neutron spectrum in a fuel element - A. Kind, G. Rossi - Energia Nucleare 9-11 (Nbv. 62)

thermal cross sections as input data for Caroline.

Furthermore, as uranium carbide seems a very promising material for ORGEL reactors, the correlated values for the resonance integral were obtained from the correlated values for U metal and U oxide following the method given by Vernon [4].

A set of buckling experiments was performed with the French critical facility Aquilon-II, in order to check the recipe. During the experiments, three types of fuel elements were used: [5]

a) cluster of 19 magnesium-clad uranium oxide rods - 12mm diameter, immersed in monoisopropyl diphenyl contained in a hexagonal aluminum tube; the distance between the boundaries of two adjacent rods was 1 mm.

b) the same fuel element, but with adjacent rods in contact

c) cluster of 19 uranium oxide rods 16,2 mm in diameter, with a distance of 1 mm between rods, arranged as in the previous cases.

The Caroline-I code is programmed on the IBM-7090 in Fortran language. It gives the following results : ε ,p,f, L^2, L_s^2, k_∞ , B_m^2, and the thermal flux in each region.

Times of calculation are of the order of 1'.

When compared to the experiments, Caroline I gives buckling in agreement within $\pm$ .1 m^{-2}.

Thermal neutron spectrum and resonance escape probability are receiving more and more consideration since a few years. Improved solutions of the energy dependent Boltzman equation were given, it is also a field where usually some quantum mechanics and nuclear physics are welcome and this explains their great attraction for some runaway from these disciplines to reactor physics.

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(4) Effective resonance integral for uranium carbide - R. Vernon - Nuclear Science and Engineering - 6(2),163 (1959)

(5) Critical experiments on natural uranium oxide, organic cooled, heavy water moderated lattices - G. Casini, C. Foggi, F. Toselli - Energia Nucleare, Vol. 9 N. 8(1962)

II. THERMAL NEUTRON SPECTRUM :

These effects are important, both for investigating neutron economy when Plutonium isotopes are present in the fuel elements and for dynamic through the temperature coefficient. In ORGEL lattices these effects are still complicated by the presence of two moderators at different temperatures.

A first approach of these effects[6] was made in connection with reactor design calculation. As the problems dealt with are by no means classical, this first approach can hardly be considered as a recipe. It is based on the assumption that rethermalization effect due to heating up of neutrons by the hot organic coolant and hardening effect due to selective absorption of neutrons by fuel material can be separated.

The rethermalization effect is dealt with by the two overlapping thermal group approximations proposed by Selengut [7]. These two groups are Maxwellian distribution at the physical temperatures of the coolant and moderator. The fundamental parameter is the transfer cross sections from one group to the other. For the deuteron bound in the heavy water molecule, the model proposed by Brown and St. John [8] can be regarded as sufficiently accurate. For the proton, the phenomenological model of Drozdov et al. [9] is used.

The hardening into the fuel is dealt with by assuming a maxwellian distribution entering the fuel element. Inside the fuel, a multigroup diffusion equation is used without energy transfer. Boundary conditions between moderator and fuel element are continuity of incoming current for each group, for the outgoing current only an integral continuity condition over the whole energy range is imposed.

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(6) A simplified model for the determination of the thermal neutron spectrum in a fuel element - A. Kind, G. Rossi - EUR 260 e.
(7) D. S. Selengut - Nuclear Science and Engineering, 9, 94 (1961)
(8) Handbuch der Physik, XXXVIII/2 page 465 - E. Amaldi
(9) S. I. Drozdov et al. - Geneva Conference 1958, P/2033

These perturbations of the main moderator spectrum due to the rethermalization and hardening effects are summed up independently to find the fuel spectrum.

This procedure is supported by the hot loop experiments made in Chalk River,[10] where a "neutron temperature" in the fuel was measured as a function of coolant temperature, the test event in these experiments is the fission reaction rate ratio Pu^{239}/U^{235}.

The Thermidor code based on this theory is already used for Orgel design calculations in connection with RLT2 [11], a code for burn up evaluation, and Caroline I.

For the more refined theory, new approaches proposed by different authors are now investigated. Among these, the most promising seems to be the Horowitz and Tretiakoff [12] theory and the first flight collision probability used by Honeck[13] in his Thermos code. Which one is the most suitable for our purpose depends on several conditions. A decision will be made later on this year, and work will be pursued on the selected one.

A great attention is paid to the energy transfer of neutrons colliding with protons bound in organic molecules. A preliminary analysis was made by Ardente[14] on the scattering by the proton bounded in the benzene molecule, which is taken as the fundamental dynamic unit. Different models were tried and new ones proposed. The criterium for selection is the comparison of the total scattering cross section as a function of neutron incident energy computed from the model, with the experimental values.

(14 bis)

The first and simplest model is the "gas model" introduced by Sachs and Teller. By means of one parameter, the effective mass, it takes into account the translational and rotational motions.

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(10) C. B. Bigham, B. G. Chidley, R. B. Turner - AECL 1350 (1961)
(11) G. Blässer, G. Casini, J. Pillon - EUR/C/IS/784/61 f
(12) Effective cross section for thermal reactors - EANDC(E)14 (1960)
(13) H. C. Honeck - Thermalization transport theory code for reactor lattice calculations - BNL 5826
(14) V. Ardente - Colloque International de diffusion et de diffraction des neutrons - Grenoble, 3-5 Sept. 1963
(14 bis) R. G. Sachs, E. Teller - Physics Review 60 18 (1941)

Comparison with experimental values, shows that it fails in the energy range .02-.3 ev. A more elaborated model due to Krieger and Nelkin (14 ter), the "free molecular gas" using two parameters : the effective mass and a vibrational constant taking into account the elastic vibrational transitions from the ground state, gives - as expected - a better result, but is still in disagreement with the experimental curve in the energy range above .1 ev.

Improved models with an increased number of parameters would evidently give a better agreement. Ardente has investigated two of these models for the benzene molecule. As the proposed parameters are not correlated directly with the total scattering cross section, in which case agreement will be trivial, but with some known dynamical properties, as the vibrational frequency distribution deduced from optical measurements, good confidence in the validity of the model can be gained and extension to more complicated organic molecules can be made.

The first of these models is the "two vibrational model". It takes into account the translational motion with the real mass of the benzene molecule (78).

The rotational motion is replaced by a torsional isotropic oscillation with a single frequency W_r and mass M_r. For the vibrational states, the frequency distribution of the benzene molecule shows concentration of the vibrational states around .12 ev and .38 ev. Thus, the simplified model retains only two vibrational states at these energies.
The comparison with experiment shows a very good agreement.

The second of these models is the "polycrystalline model", which takes into account only the vibrational states, in complete opposition to the "free gas model". Agreement with experiment is also very good. A further advantage of this approach is the formal equivalence with a crystalline model, for which extensively developed mathematical methods are available.

(14 ter) T.J.Krieger, M.S.Nelkin - Phys.Review 106, 290 (1957)

These studies lead to the conclusion that the proposed models can be used for other polyphenyls. The refinement of the model would likely require a check with more sensitive quantities than the total cross section, as the differential scattering cross section or the scattering law.

Experimental effort is not absent. Experiments will be carried out this year on the total cross section of different organic liquids as a function of the temperature, using the time of flight technique. Measurements of neutron spectrum in poisoned organic and at the interface of two different temperature organics are also in preparation, in order to support Ardente's calculations.

A measurement of the fine structure of the thermal flux in simple geometry ORGEL type lattices , also related to neutron spectrum, has been performed [15] in the French critical facility Aquilon II, by activation of dysprosium detectors. Two organic compounds, i.e. monoisopropyldiphenyl (Monsanto) and diphyl (Bayer) have been investigated. Good accuracy was achieved in these experiments, $\pm$ 1% on the disadvantage factors leading to about $\pm$ .1% in the thermal utilization factor. These different factors were computed by Sturm [16] using the Thermos code and two different models for the scattering kernel of the proton bound in the organic: the Brown and St. John model and the Nelkin one [17]. Generally, the predicted disadvantage factors are slightly higher than the experimental ones, leading to overestimate f by .1 to .3%. As these different models are not satisfactory for the organic molecule, calculation will be repeated using the more elaborated Ardente model.

These experiments, too, will be systematically performed with the ECO facility, with more complicated geometries including clusters and possibly at different coolant temperatures.

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(15) A. Boeuf, S. Tassan - EUR 206.e (1963)
(16) A. Sturm - private communication, Euratom
(17) Nelkin - Phys. Review 119 (1960) 741

III. RESONANCE ESCAPE PROBABILITY :

This is another problem which requires a good deal of efforts. In the Caroline-I code, resonance escape probability is given by the well known relation :

$$p = e^{-\frac{N_f V_f I_{eff}}{\xi \Sigma_s V_m}}$$

where $I_{eff} = A + B \sqrt{S/M}$

A and B together with η are parameters correlated with buckling experiments, in this case, accurate prediction of buckling can be made but wrong values of the resonance escape probability are obtained. This situation is rather unsatisfactory and better formulations are now under investigation.

Calculation of resonance escape probability for complicated fuel geometries as clusters for a power reactor, is a very difficult task. In fact, only Monte Carlo calculations can deal with the problem without oversimplifying assumptions. But these calculations, due to their inherently statistical errors need long machine-time, even with the best available computers, to give the required accuracy; for this reason it is excluded that these calculations will be used for reactor design work. More likely, a combination of the Monte-Carlo and the analytical method will be used. All these new theories are based on the multigroup technique. The first thing to be done is to check the validity of the already available codes. GAM-I, a code [18] developed by GA, allows the calculation of averaged group constants, it uses the resonance parameters in the resolved region and statistical distribution of these in the unresolved one. The best thing to be done is to compare the prediction of GAM-I with the Hellstrand experimental results [19]. For this purpose, Sturm[20] has done the comparison for cylindrical fuel elements of U metal, oxide and carbide small enough so that the assumption of a flat flux and 1/E spectrum may be reasonably made. This comparison has shown that the resonance integral calculated by GAM-I is systematically lower by about 14% than the Hellstrand's values. After a detailed analysis it can be shown that these discrepancies can be attributed to the neglect of high angular momentum resonances and absorption of neutrons at energies above 30 Kev.

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(18) G. O. Ionon and I. S. Dudek - GA-1850 / (1961)
(19) E. Hellstrand - Journal of Appl. Physics. 28 (1957) 1493
(20) B. Sturm - Euratom internal report ISPRA-476

The importance of these effects had already been demonstrated by Adler[21] who found a value of 1,4 b for U metal and U oxide in a range $\sqrt{S/M} > 0,2$. Adler's calculations are coherent with Hellstrand's results except for UO_2 where they are in excess of .5 b over the extrapolated experimental results for $\sqrt{S/M} = 0,2$.

Vernon[22] pointed out that about 0,8 b must be attributed for absorption at energies above 30 Kev, which are geometry independent.
A value of 1,4 b was also found by Nordheim [23]. For UC, a difference of the same order was found by comparing GAM-I calculations with the value deduced by Vernon from the Hellstrand's experiments, using the equivalence theorem, which is also coherent with Müller's [24] theoretical calculations.

Another effect of importance for the large pitches (20-25 cm) encountered in power reactors is the spatial dependence of the flux within the cell and deviations from 1/E law due to absorption at higher resonance. These effects were investigated by De Haan[25], who derived an IBM-7090 multigroup code, named SKÅL for resonance escape probability in heterogeneous lattices.

NDA has already developed a code[26] using the age theory to take these effects into account, but this method fails in case of a cell containing more than one moderator and for large fuel sections of the order of 25 cm^2.

The code developed by De Haan is a multigroup, multiregion code based on the solution of the transport equation by the collision probability technique. Effective cross sections by energy groups are calculated by GAM-I modified to take into account the higher angular momentum resonances and absorption above 30 Kev, and the neutron distribution within the cell is calculated by SKÅL, which gives also the advantage-disadvantage factors and the resonance escape probability. Theory is going along these lines and an experimental program to support it is now in progress. The effective resonance integral of an ECO cluster was made by Tassan [27].

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(21) Adler et al. - PIGG 16 (1958) - 155
(22) A.R. Vernon - Nuclear Science by 6 (1959) 163
(23) Nordheim - Lecture given in the Techn. Hochschule München, July 1963
(24) A. Müller - Nukleonik 3 (7) (1961) 303
(25) W. De Haan - Ispra Internal Report DPR-305 (1963)
(26) NDA-2131.38 (May 62) - W.L. Brooks, H. Soodak
(27) S. Tassan - unpublished results - Ispra (July 1963)

The ECO element consists of 19 Al clad natural uranium metal rods, 12 mm in diameter, arranged in an Al tube filled with organic. Measurements have been performed by the activation technique, using the central thimble of ISPRA-I, a 5 MW D_2O moderated and cooled reactor at the Ispra Center. Depleted uranium (300 ppm) detectors, 0,1 mm thick and 12mm in diameter were used and the induced Pu-239 activity of the detectors was counted by a coincidence technique, actually one γ and one X ray from de-excitation of Pu-239. In order to avoid corrections for deviation from the $^1/E$ law in the few ev regions, as mentioned by the Swedes for the RI reactor, the RI of the cluster was referred to the RI of a single U rod, using the Hellstrand measured value, a check was made by measuring the RI of the reference rod by comparison with the infinite dilution resonance integral of gold. The agreement obtained with the Hellstrand original results (uncorrected for the departure of the flux from the 1/E law); indicates that the above correction term is, as expected, very similar for the Swedish RI and the Ispra I reactors.

Results obtained are given in the following table :

Organic	Formula	Spacing rod mm.	RI measured barns	RI calculated Hellstrand Carl vik Peshagen barns	RI calcul ated Hellstrand rubber band barns
Monoisopropyl dyphenil	$H_{16}\ C_{15}$	1	11,25	11,66	9,07
"	"	0	11,24	11,35	8,83
Dyphil	$H_{10}\ C_{12}$	1	11,49	11,23	9,07
"	"	0	10,85	10,9	8,83

The last column gives the RI integral calculated by neglecting the slowing down of neutrons due to the organic.

Accuracy which may be achieved in these experiments is $\mp$ 4% .

This is not actually the case for these experiments, which are preliminary and for these reasons, the experimental errors are not quoted.
The measurement will be extended to a rather general investigation of the coolant and geometry effects, and successively to the determination of the effective resonance integral of UC cluster elements.

IV. FAST NEUTRON MULTIPLICATION FACTOR :

Another quantity of importance in reactor calculation, and which requires some efforts, is the fast neutron multiplication factor. This quantity was investigated by L. Amyot [28], who performed a calculation on an Orgel cluster fuel element, using a DSN code, and eighteen groups of energy between 10 Mev and .1 Mev. The average group cross sections were obtained with GAM. The DSN obtained spectrum exhibits a fission spectrum behaviour above threshold, and is softer than the uncollided fission spectrum below threshold. As a matter of interest, the subthreshold spectrum resulting from inelastic scattering in U-238 according to the evaporation model and the $E\, e^{-E}$ law suggested by Spinrad was compared to the uncollided fission spectrum and shows a striking resemblance which justifies two groups assumption of Naudet [29]. According to these calculations, the DSN eighteen groups were collapsed into two groups (10 Mev - 1,4 Mev and 1,4 Mev - 0,1 Mev), the cross sections averaged on these two groups and the ε factor calculated. Comparison with Naudet's and Spinrad's calculation show an agreement within 1‰ in ε. Such a difference is comparable with errors resulting in σ_{c8} uncertainties, which is the important parameter. Due to elastic collision with the coolant nucleus, the ε factor in Orgel fuel element is less sensitive to U_8 inelastic cross section uncertainties.

The second step in Amyot's calculation [31] was a general formulation taking into account : the cluster geometry, the non uniform distribution of fission sources within the fuel, moderator backscattering, cell to cell interaction, (γ, n) and (n, 2 n) contributions.
The ε factor is defined according to Carlvik and Pershagen [32] definition, as the number of neutrons slowing past a given energy anywhere in the lattice per primary fission neutron. The boundary energy is taken at .1 Mev.

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(28) L. Amyot - EUR 305. e (1963)
(29) R. Naudet - SPM n°401 (1958)
(30) B. Spinrad - Nucl. Science and Eng. - 1,455 (1956)
(31) L. Amyot - Internal report DPR - ISPRA (July 1963)
(32) I. Carlvik, B. Pershagen, AE-21 (AEF 70) 1956

The ε factor is given by the following formula :

$$\varepsilon = f_o + (1-f_o) \int_{\vec{r}} \int_{.1\ \mathrm{Mev}} g_o(\vec{r}, E)\ C(\vec{r}, E)\ dE\ d\vec{r}$$

where f_o is the fraction of fission neutrons born below .1 Mev; $g_o(\vec{r}, E)$ is the probability for a neutron of energy E suffering a collision in $\vec{r}$ to be transferred below .1 Mev ; $C(\vec{r}, E)$ is the collision density of neutrons of energy E at point $\vec{r}$ by primary fission neutrons.

Using a division in 3 regions :

fuel	F
diluent	D
moderator	M

and in energy group i, this relation can be rewritten, with obvious notations :

$$\varepsilon = f_o + (1-f_o) \sum_i (a_{io}\ C_{iF} + b_{io}\ C_{io} + n_{io}\ C_{im})$$

a, b, n are transfert cross sections independent of geometry.

The C'_s are obtained from a system of balance equations similar to the Almgren's [33].

The balance equations depend on collision probabilities; in this report, the general expression of ε is given for a cluster geometry. The number of groups is taken equal to two according to the study [28] previously made.

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(33) B. Almgren - AE-27 (1960)

CONCLUSION :

Caution must be taken before introducing improved reactor physics theories in Orgel design calculations. One must be sure that the improvements thus introduced will not decrease the accuracy of predictions. An extensive experimental program is necessary to check and adjust the theory.
A few of these experiments have already been mentioned in this report.
The main program will start early in 1964 with ECO [34], a critical facility now under completion in Ispra. Fuel elements made of 19 (Ø 12) Al clad, uranium metal, assembled in cluster, inside a pressure tube filled with mono-isopropyldiphenyl, and UC (Ø 25,2 and 30,9) assembled in clusters of 7 and 4 rods would be investigated in 64. Buckling, k_∞, cell fine structure parameters will be measured using the ECO critical facility, the EXPO, an exponential facility, and the RB1 reactor of Montecuccolino (Bologna, Italy), a PCTR type facility.

Some of these experiments will be repeated with hot organic using loop type special fuel elements, and neutron spectrum measured both by activation and time of flight techniques. The effect of burn-up on reactivity will be measured by oscillating in the central thimble of the ECO reactor, samples of synthetic fuel elements made by mixture of depleted uranium and plutonium with two different isotopic compositions, 6% and 15% in Pu-240.

Such an experimental and theoretical program must lead to a good understanding of the physics of heavy water reactors, especially of the organic cooled type, and enables the reactor designers to make accurate predictions of the performance which can be expected for a power reactor.

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(34) G. Blässer, P. Bonnaure, G. Casini, R. Cenerini, V. Raievski, F. Toselli - EUR 130.f