

CRITICALITY ANALYSIS FOR STORAGE AND SHIPPING  
OF NUCLEAR FUEL ELEMENTS OUTSIDE OF REACTORS

G. ERMUMCU - J. GONNORD - A. MONNIER - J.C. NIMAL

DRE/SERMA/SACLAY

## INTRODUCTION

Since two last years we have developed and tested a calculation method for criticality analysis of PWR elements in storage pool, shipping cask, reprocessing station or other enclosures. Safety requirements for these components are to ensure that their multiplication constant in nominal or accidental situations does not exceed 0.95.

This method is based on use of computer codes solving neutron propagation equation in transport theory. Its validity was checked by comparing with results of some criticality experiences and other Benchmarks obtained by computer Monte Carlo code TRIPOLI.

It was applied to obtain multiplication constant for some shipping cask, and several cases of storage pools were treated by this method in order to compute the sensitivity of the multiplication constant to water density, burn-up of fuel elements, nature of neutron absorbers, uncertainties on geometrical data.... Then it was necessary to optimize physical approximations for reducing computing time and decreasing cost of calculations. Additional tests were performed to ensure that these approximations did not bring any important loss of accuracy, or even implies over estimations of multiplication constant providing additional safety margin.

## DESCRIPTION OF THE METHOD

### Simplifying hypothesis

When criticality analysis is restricted to PWR fuel elements, where the mean free path of thermal neutrons is very short, it can be assumed infinite height for these elements. This hypothesis over-estimate slightly multiplication constant value and then, by neglecting leakage through the third dimension, two dimensional calculations are permitted.

In the same way, for storage pool problems if fuel elements are disposed in regular lattices, by assuming infinite lattice hypothesis, field of calculation can be restricted to the periodical pattern ; for shipping casks with larger shielding it can be restricted to a lower thickness : perfect reflection hypothesis at boundaries over estimates also the multiplication constant

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but reduces materially the geometry of computation.

Before continuing this discussion on retained hypothesis, let us consider besides their advantage, their necessity : they are also implied by use of the computer code DOT 3.5.

This code solves Boltzmann equation for neutrons in criticality research in two-dimensional geometries. It is based on :

- multigroup formation for the energy parameter
- $S_n$  formalism for the direction parameter
- discrete ordinates formalism for the space parameter.

A configuration must be composed by contiguous meshes defined in a rectangular or cylindrical or polar coordinates, each one of meshes must contain one homogeneous material ; and these meshes would have the same range of dimensions. DOT 3.5 fails if the ratio of sizes of any meshes is greater than 3 or 5, and also if dimensions of a mesh is less than 2 or 3 times the mean free path of thermal neutrons.

By its formalism, DOT 3.5 gives good results as well as the angular, spatial and energetical discretisation is sharper. We can note that a multigroup definition with closer bounds for lower energies causes stronger cross sections for materials and requires smaller meshes in geometrical description. But in reality, we must deal with 5 groups of energy, less than 2000 meshes and 12 angular directions, which gives a system of 120 000 equations to be solved.

These restraints implies two difficulties :

- to find a simple geometrical description of the real geometry of the problem : generally this geometry is very complex and presents two levels of heterogeneity : the first due to the disposition on square pitch lattice of cylindrical fins, the second due to the presence of neutrons absorber which have very small mean free path. We try to substitute to zones containing cylindrical pins one or more rectangular homogeneous zones and similarly replace strongly absorber zones and their neighbouring zones by homogeneous zones.

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- to build a 5 groups cross section library : such libraries can not be valid universally, even for a homogeneous material it can be needed to consider different sets of cross sections because of the alteration of spectra at interfaces between different materials. These libraries must be evaluated for each particular problem. Suggested method for this evaluation is to calculate at the neighbourhood of each interface, spectra variations by a one-dimensional transport code using a fine group library..

This library is then collapsed into 5 groups using the spectrum of the transport computation.

All this work is carried out using the code APOLLO. APOLLO solves the integral Boltzman equation in one dimensional geometry using the Collision Probability method. It uses a 99 groups library with 47 upscatter.

It calculates self shielded cross sections for principal isotops, provides neutron spectra at every point of calculation, reaction rates over each zone and furnishes a cross sections library weighted by the neutron spectra.

a) Cell calculations :

We define a one dimensional cylindrical geometry containing fuel element pin and its associated water, with reflection condition at the boundary (infinite lattice hypothesis).

Heterogeneity of lattices such as guide rods is taken into account by a special procedure called "MULTICELL" : we can define different types of cells and give probabilities of crossing surfaces between cells to ensure the coupling.

Self shielded cross sections are calculated for some isotopes, and by weighting cross sections of each material by its own neutron spectra, we obtain cross sections for a virtual, homogeneous material presenting same macroscopical properties that fuel element. (See figure 1).

We also run calculation for a homogeneous and infinite medium containing this material, and observe that reactivities of heterogeneous lattice and its homogeneous equivalent differs less than  $10^{-4}$ .

- b) Collapsing 99 groups cross sections library in five groups : this is the most difficult part of the method. We try to obtain mean values of cross sections in larger intervals of energy by weighting the 99 groups cross sections with convenient spectra. Unfortunately this spectra is strongly depending on space coordinates, and accurate calculations at each interfaces are necessary. (Figure 2 shows how the shape of spectra changes in a typical storage case which is treated in the Benchmark example explained further).

Then we run one-dimensional APOLLO calculations in slab geometries in which each zones contains materials encountered along some cut lines of the problem configuration. The choice of these cut lines is not arbitrary ; it must lead to nearest shapes of spectra with respect to the reality.

This method is sketched in figure 3.

For configurations presenting symmetry conditions, one calculation can be enough, but in other case several calculations are necessary.

In table n°1 we give variations of cross sections mean values for fuel element or water slab versus space point in the benchmark example.

We test validity of these cross sections by one dimensional 5-group APOLLO calculations in the same geometry ; when differentiating transitional zones for taking into account this change of mean values of cross sections these calculations are in good agreement with 99 group calculation.

In the case shown in figure 5a, respective multiplication constant values are :

- 99-group one dimensional slab geometry : 1.18693
- 5-group one dimensional slab geometry : 1.18525

(this difference is less than the accuracy required for these calculations :  $2.5 \times 10^{-3}$ ).

It ensures our collapsing method proper criticality calculation :

The particular five group cross section library obtained as above is translated in PO-P1 format for DOT 3.5 input. An example of geometry input is shown in figure 5b. Multiplication constant of the two dimensional model and partial reaction rates for different zones are obtained by DOT 3.5 which is run in  $S_4$  approximation ;  $S_6$  or  $S_8$  calculation in same cases do not bring sensitive accuracy.

Numerical precision of computation is less than  $10^{-3}$  and are neglectable with regard to uncertainties introduced by successive approximation of the method.

Block diagram of the method is shown in figure 6.

GLOBAL IMPROVEMENTS OF THE METHOD

Comparison with results of an exact Monte Carlo code : TRIPOLI

The example wich is sketched in figures 4 is treated by the Monte Carlo computer code TRIPOLI. This is a typical storage pool situation.

This code can solve critical Boltzman equation. It uses a real tridimensional geometry description ; no previous self shielding and collapsing of cross sections or geometrical homogeneizing procedures are necessary since it uses a ponctual cross section library (Defined actually by more than 40 000 values for each isotopes between 6 KeV-5 eV and a very sharp multigroup representation out of this interval).

Thermalisation phenomenas is processed with exact  $S(\alpha, \beta)$  formalism.

Precision of results is only related with the number of neutron stories simulated.

The storage example is processed in exact geometry, results are evaluated using :

- track lengh estimator
- collision estimator

In table 2 we summarize comparison of results between two methods and observes that APOLLO-DOT calculation stand very well with TRIPOLI output.

#### Experimental test

Interpretation of actual criticality approach experiences with PWR fuel elements are not convenient with two dimensional calculation methods. However some of them representing cylindrical symmetry was used to test validity of our method.

These experiences (see ANS-TRANSACTIONS 1978 Annual Meeting, p.302) consist to immerse progressively fuel pins in water and to count external radiative emission due to an internal source and emphasized as well as multiplication constant value approaches 1. By interpolating the curve of radiative intensity versus immersed height critical height is obtained.

These fuel pins are disposed in a regular hexagonal pitch lattices circumscribed approximately in a cylinder.

We applied our method to this critical configuration by :

- homogeneizing fuel element
- collapsing cross sections by three one-dimensional spectra calculation
- running a DOT 3.5 calculation in cylindrical coordinates.

Figure 7 gives a sketch of this work.

We obtain for such experimental configuration a multiplication constant changing from 1.01 to 1.015 we note that it is a limit case in which neutron spectra changes material and collapsed cross sections for emergent parts of pins are not evaluated very well : However it proves that the method over estimates the value of multiplication constant and this is conform to safety requirements.

#### ANOTHER ADVANCED WORKS ON CRITICALITY ANALYSIS

##### Multigroup Monte Carlo method

As we note, the APOLLO-DOT method gives good results in situations which can be represented by two dimensional models, however cross sections must be calculated in 5-group format and heterogeneities must be suppressed by substituting homogeneous zones.

In order to deal directly with the 99 group cross section library and process tridimensional geometries exactly, we developed a new computer code : TRIMARAN.

This code uses the 99-group cross section library and establishes reaction probabilities for each material. By sampling stories of neutrons it evaluates different reaction rates and furnishes the multiplication constant. Geometries are processed by the same method than TRIPOLI. Linear anisotropic scattering is assumed for collision processing.

Works for improvements are going on.



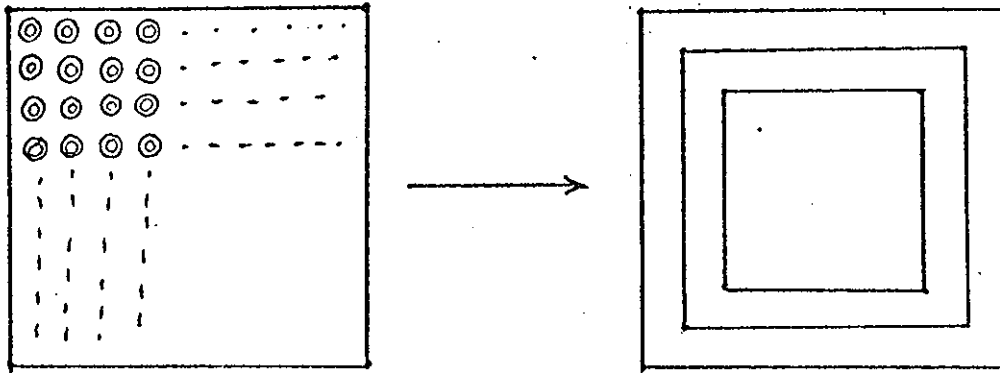
Group Zone	1 10MeV - 907KeV	2 907KeV - 5KeV	3 5KeV - 2.77eV	4 2.77eV-0.625eV	5 0.625eV-1.1E-4eV
1	2.60511 E-1	6.65562 E-1	1.07373	1.07696	1.94544
2	2.6026 E-1	6.61986 E-1	1.07374	1.07702	1.98576
3	2.59921 E-1	6.59682 E-1	1.07406	1.0771	2.02648
4	2.59400 E-1	6.61216 E-1	1.07494	1.07719	2.06847
5	7.87463	2.60696 E1	4.46145 E1	4.68012 E1	9.02656 E1
6	7.8112	2.6319 E1	4.4636 E1	4.68042 E1	9.11513 E1
7	7.73638	2.64437 E1	4.4657 E1	4.68078 E1	9.17506 E1
8	7.62569	2.6472 E1	4.46796 E1	4.68136 E1	9.22872 E1

Table 1 : Mean values of total cross sections for each energy interval and for different zones.

Zones 1 - 4 contain homogeneized fuel element

Zones 5 - 8 contain water.

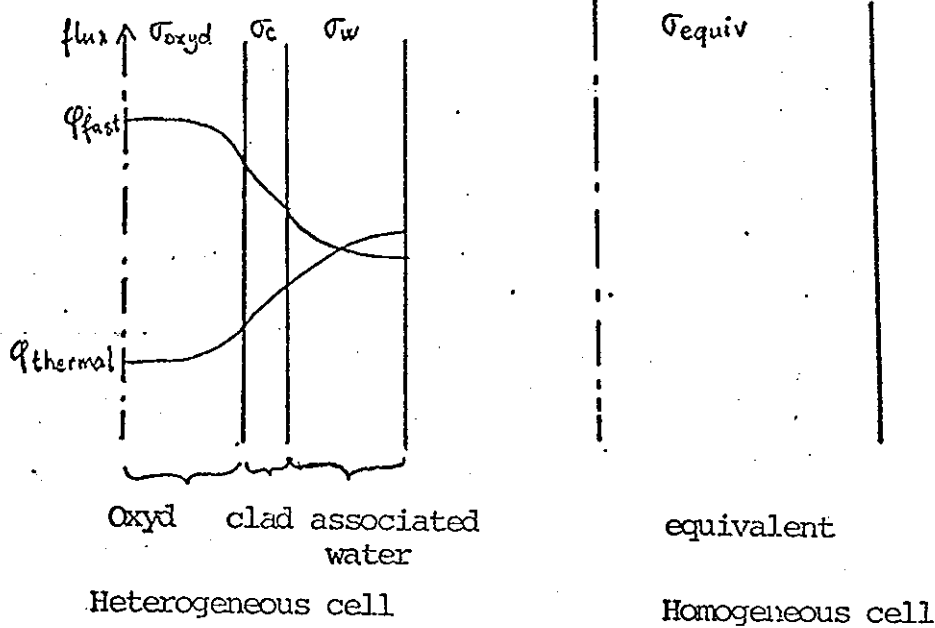
FIGURE 1 : Princip of homogenizing of fuel elements



Real geometry of a PWR fuel element

Equivalent geometry of a PWR fuel element

Cell calculations by APOLLO



Where :

$$\sigma_{\text{equiv}}^{\text{group}} = \frac{\int d^3r \sigma_{(r)}^{\text{group}} \varphi_{(r)}^{\text{group}}}{\int d^3r \varphi^{\text{group}}(r)}$$

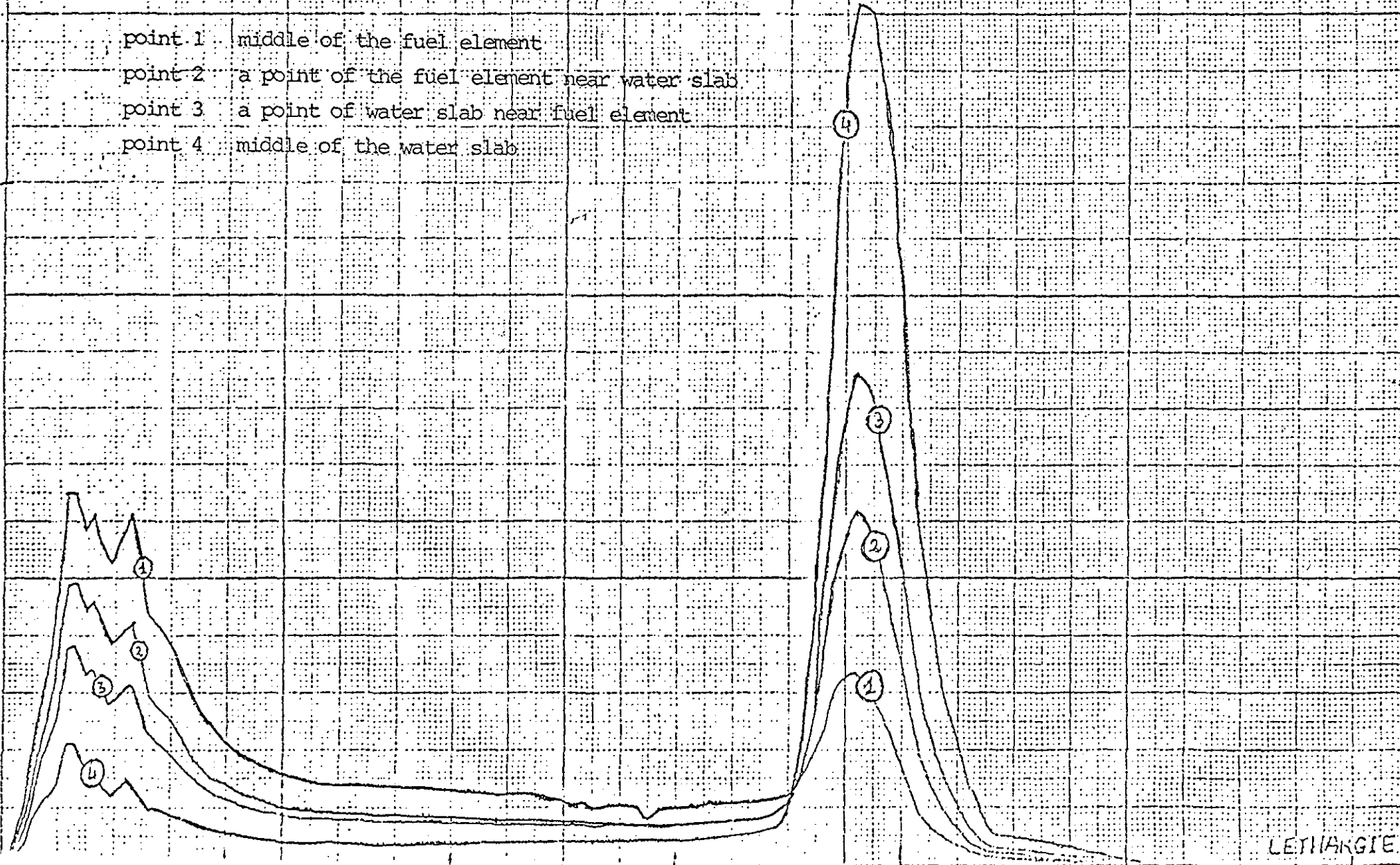
FIGURE 2 : Spectra variations across different zones of one dimensional and 99 groups APOLLO calculation  
 Each curve represents neutron spectrum versus lethargy at a given point of calculation

- point 1 middle of the fuel element
- point 2 a point of the fuel element near water slab
- point 3 a point of water slab near fuel element
- point 4 middle of the water slab

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TABLE 2 a : Comparison between multiplication constant value obtained by DOT 3.5 and different statistical estimations of TRIPOLI.

	DOT	0.95265		
Collision		0.9468	$\pm$	0.0086
Track length		0.9490	$\pm$	0.0116
Simulation		0.9463	$\pm$	0.0137

(Uncertainties are in three times standard deviation value).

TABLE 2 b : Comparison between results of TRIPOLI and APOLLO-DOT calculation for reaction rates

Group	Energy Boundary	Fuel element			Water	
		Flux	Production	Absorption	Flux	Absorption
5	1.1E-4 eV					
	DOT	4.8122	8.366E-1	5.0453E-1	1.9449E1	3.4037E-1
	TRIPOLI CHOC	4.517 ± 0.086	8.279E-1 ± 1.1E-2	5.028E-1 ± 6.8E-3	1.774E1 ± 0.42	3.39E-1 ± 8.E-3
	TRIPOLI CORDE	4.519 ± 0.092	8.312E-1 ± 1.6E-2	5.045E-1 ± 9.6E-3	1.773E1 ± 0.41	3.389E-1 ± 7.6E-3
4	0.625 eV					
	DOT	7.466E-1	1.4814E-2	1.1680E-2	5.5487E-1	1.7383E-3
	TRIPOLI CHOC	8.374E-1 ± 0.026	1.819E-2 ± 1.2E-3	1.411E-2 ± 7.2E-4	5.5996E-1 ± 0.012	2.01E-3 ± 4.2E-5
	TRIPOLI CORDE	8.354E-1 ± 0.022	1.826E-2 ± 8.9E-4	1.417E-2 ± 5.6E-4	5.974E-1 ± 0.014	2.001E-3 ± 4.8E-5
3	2.77 eV					
	DOT	4.0678	4.5731E-2	1.0322E-1	2.4691	1.3205E-3
	TRIPOLI CHOC	4.169 ± 0.064	4.672E-2 ± 1.9E-3	1.017E-1 ± 3.4E-3	2.500 ± 0.040	1.435E-3 ± 2.6E-5
	TRIPOLI CORDE	4.154 ± 0.054	4.608E-2 ± 1.3E-4	1.002E-1 ± 3.4E-3	2.494 ± 0.044	1.425E-3 ± 3.3E-5
2	5 KeV					
	DOT	6.7454	6.3521E-3	1.4625E-2	2.8205	2.83E-21
	TRIPOLI CHOC	6.992 ± 0.104	6.219E-3 ± 1.3E-4	1.601E-2 ± 4.E-4	2.809 ± 0.054	3.04E-5 ± 5.3E-7
	TRIPOLI CORDE	7.001 ± 0.116	6.273E-3 ± 9.6E-5	1.615E-2 ± 2.8E-4	2.832 ± 0.068	3.062E-5 ± 6.3E-7
	907 KeV					
	DOT	5.4130	4.9224E-2	2.2151E-2	2.3967	9.0479E-4
	TRIPOLI CHOC	5.598 ± 0.076	4.742E-2 ± 1.5E-3	2.154E-2 ± 6E-4	2.205 ± 0.070	7.615E-4 ± 5.5E-5
	TRIPOLI CORDE	5.568 ± 0.094	4.719E-2 ± 9.2E-4	2.141E-2 ± 4E-4	2.205 ± 0.068	7.581E-4 ± 4.6E-5
	14 MeV					

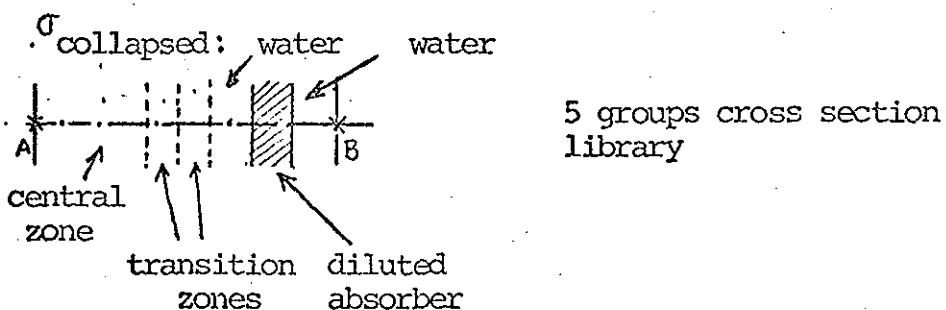
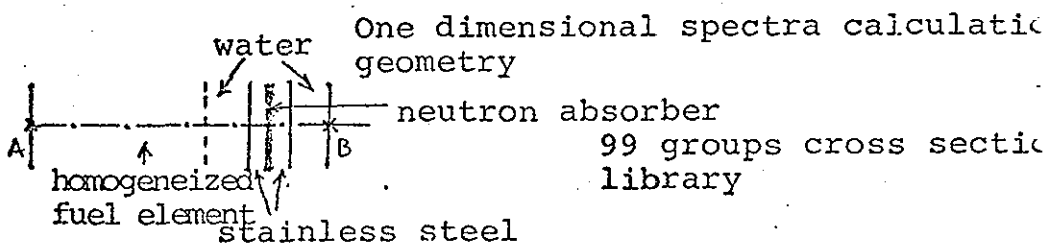
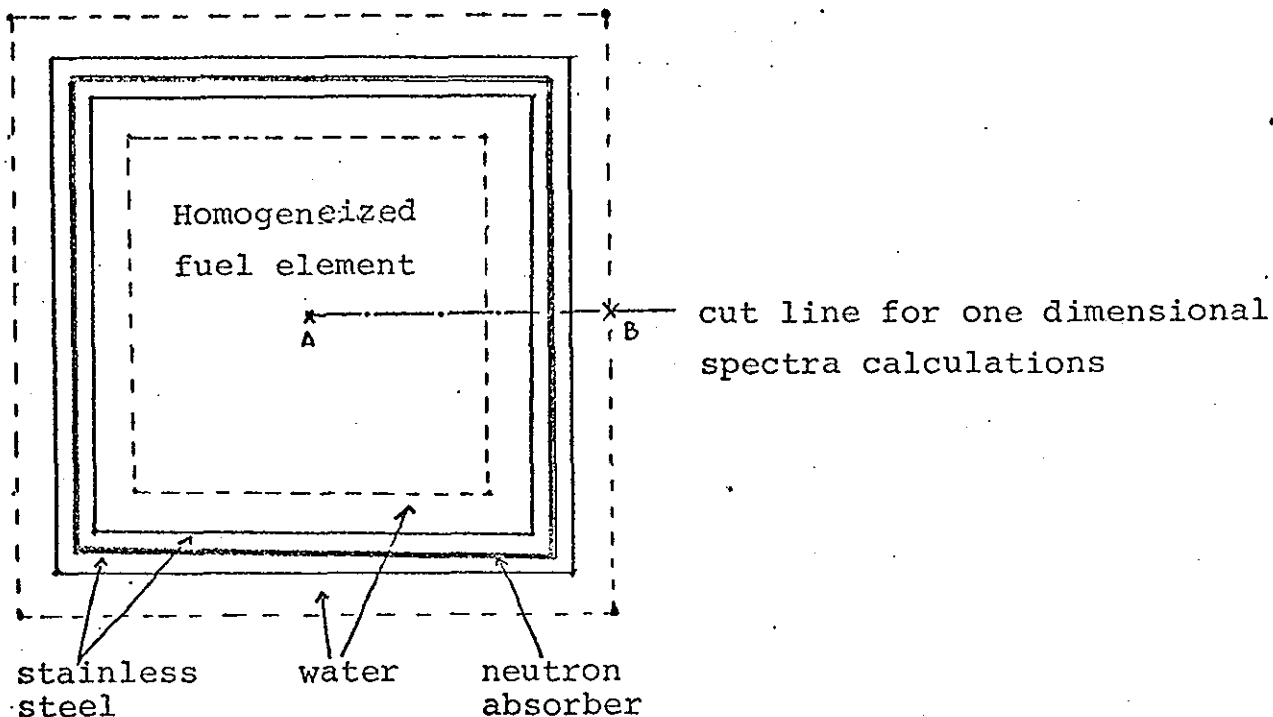
TRIPOLI CORDE : estimated by TRIPOLI by track lengths computation

TRIPOLI CHOC : estimated by TRIPOLI by probability of each reaction at each collision

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**FIGURE 3 :** Collapsing cross section library

Example : a storage pool configuration  
two dimensional model



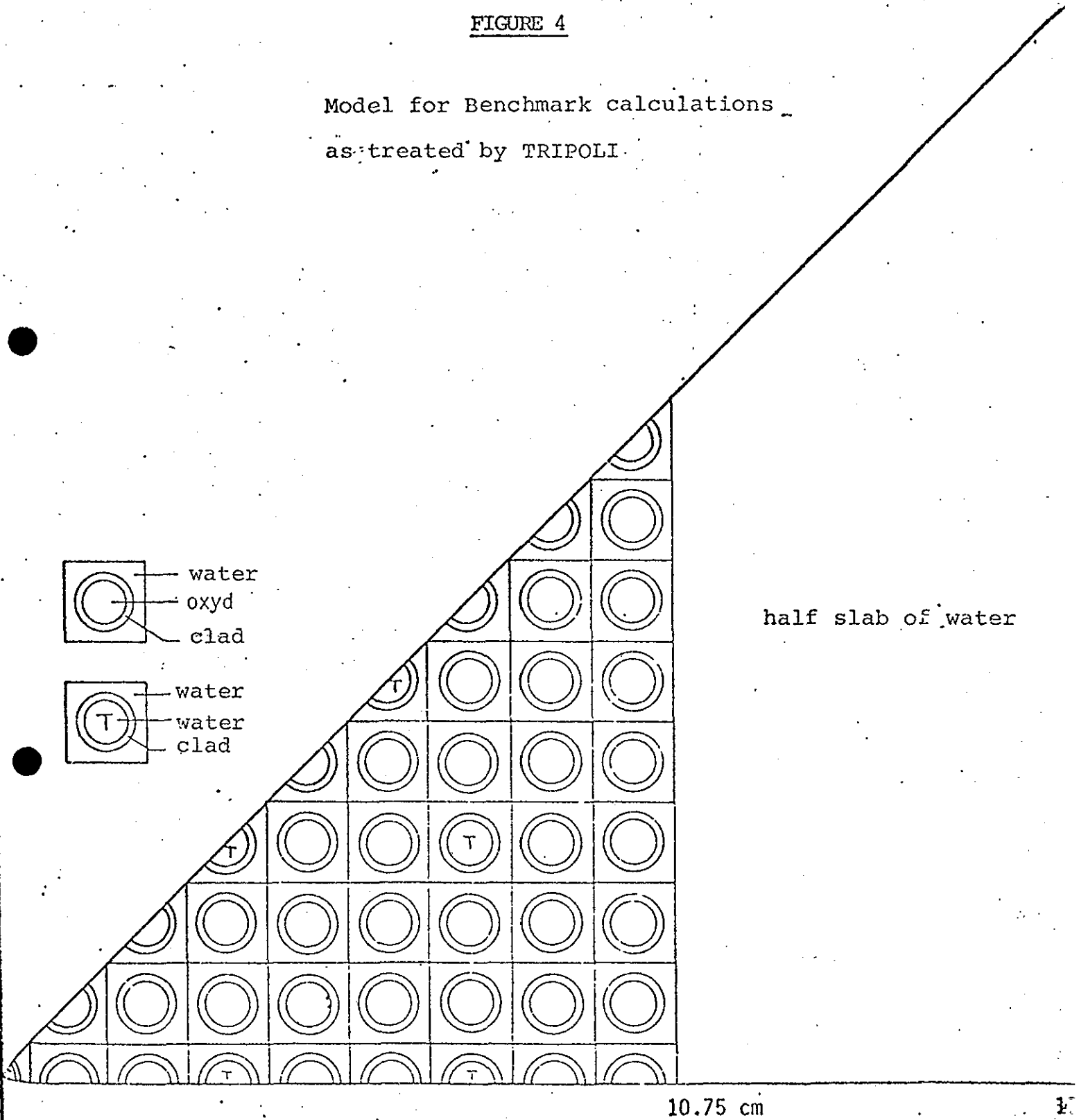
Spectra variations must be taken in consideration by transitional zones : each zone provides reduced cross sections weighted by its own spectra.

$$\sigma_{\text{collapsed}}^{\text{zone}} = \frac{\sum_{g_1}^{g_2} \int_{z_{mc}}^{z_{me}} d^3r \sigma_g^{\text{zone}}(r) \phi_g(r)}{\sum_{g_1}^{g_2} \int_{z_{mc}}^{z_{me}} d^3r \phi_g(r)}$$

$G = g_1 \text{ to } g_2$

FIGURE 4

Model for Benchmark calculations  
as treated by TRIPOLI.



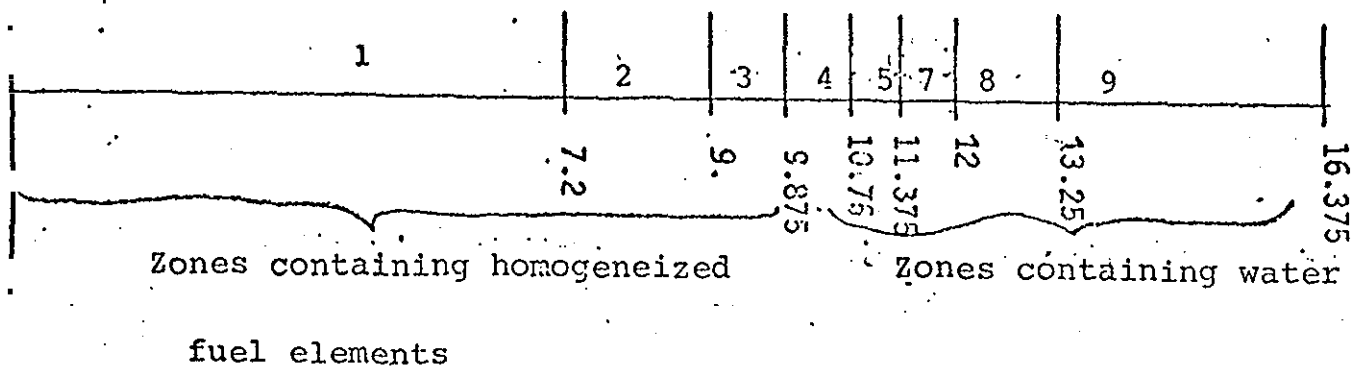


Figure 5 a :

Model for one dimensional APOLLO calculation which provides weighted

Mean values of cross section in 5 groups of energy

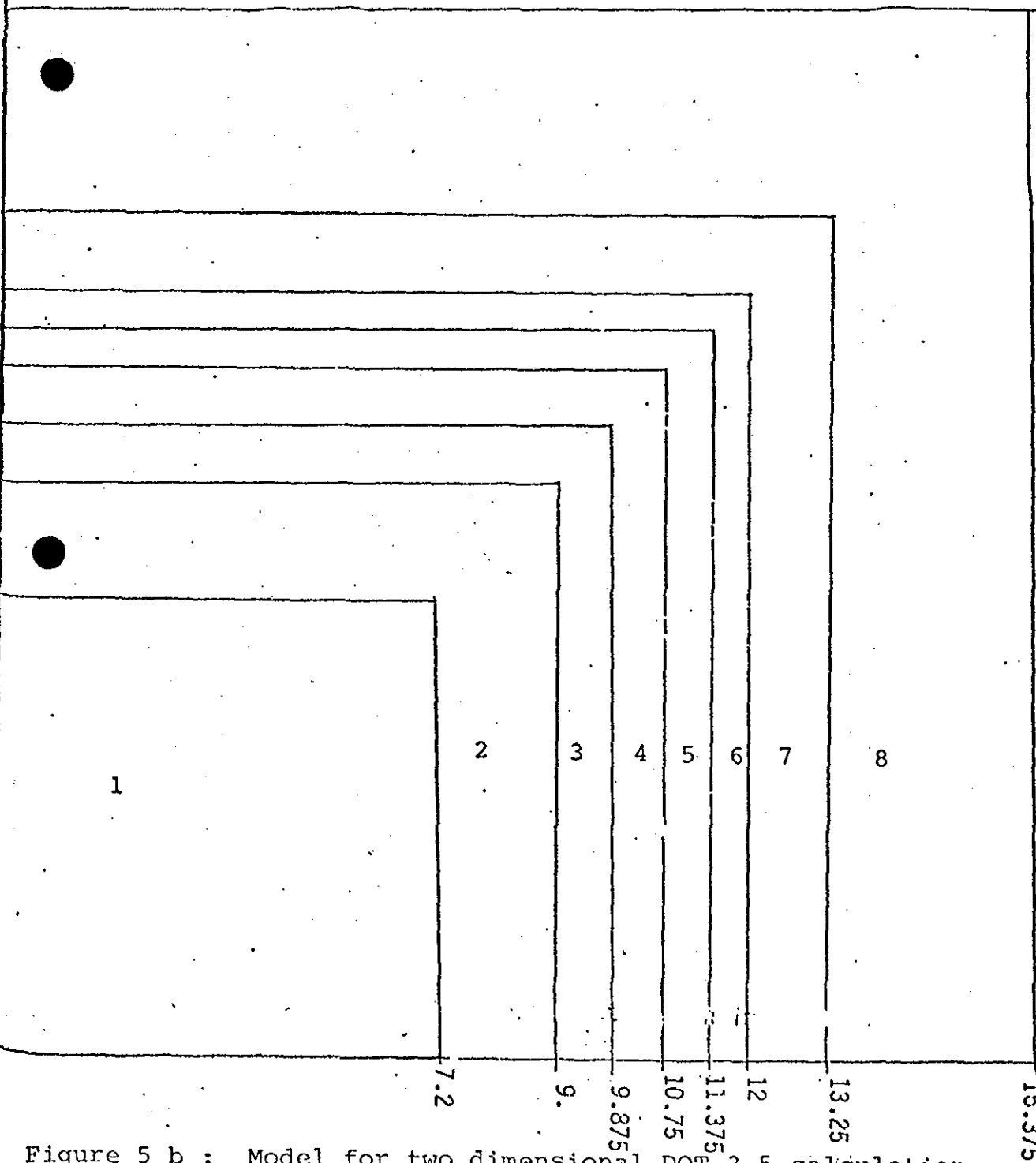


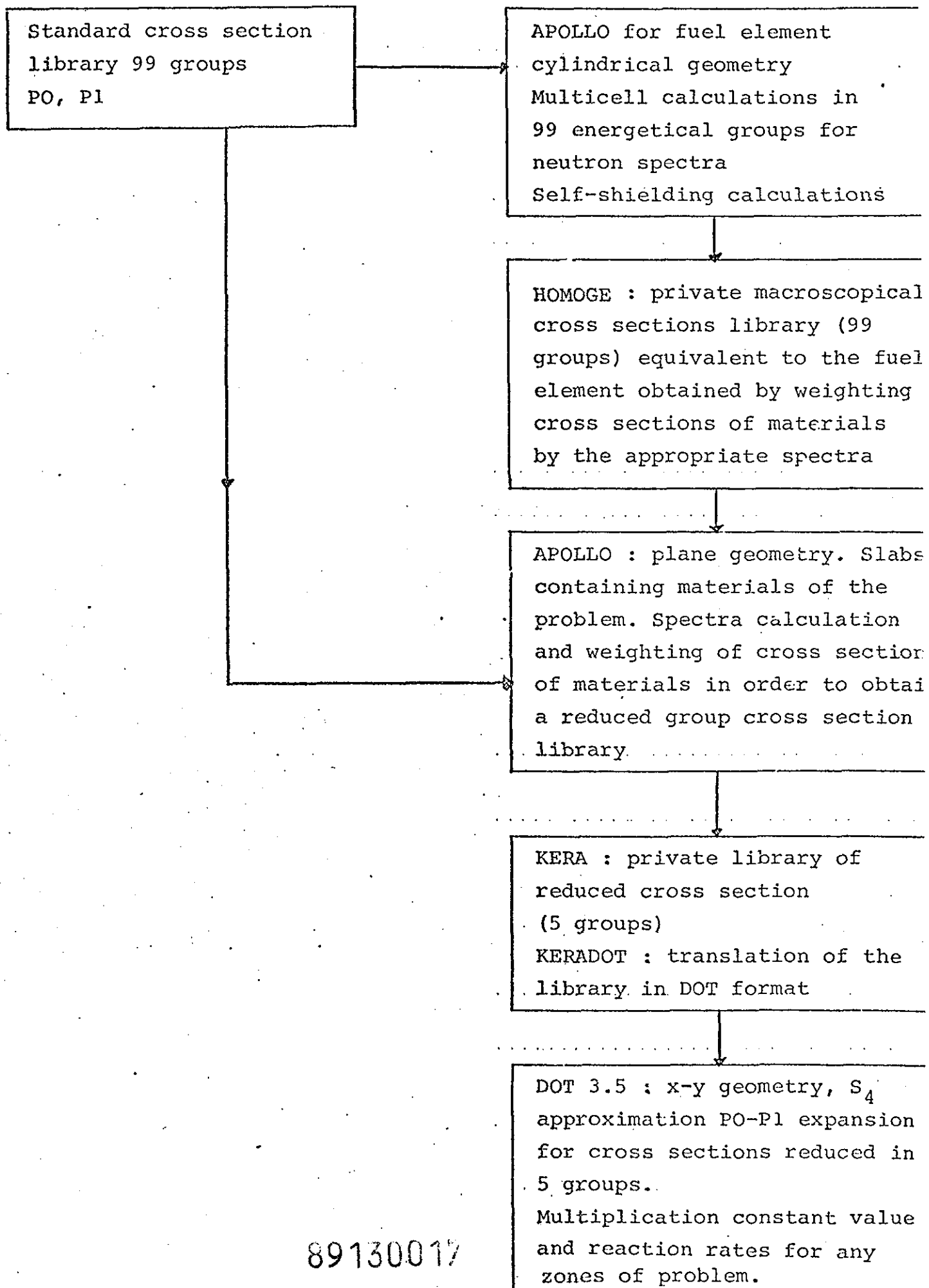
Figure 5 b : Model for two dimensional DOT 3.5 calculation

Marked zones contains reduced cross sections obtained as above

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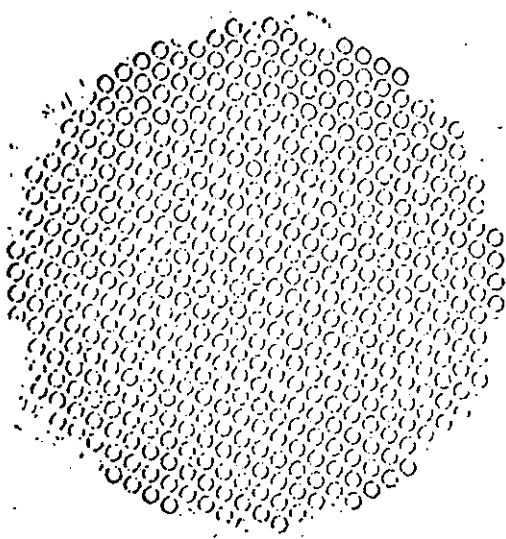


FIGURE 6 : BLOCK DIAGRAM OF THE ANALYTICAL SCHEME

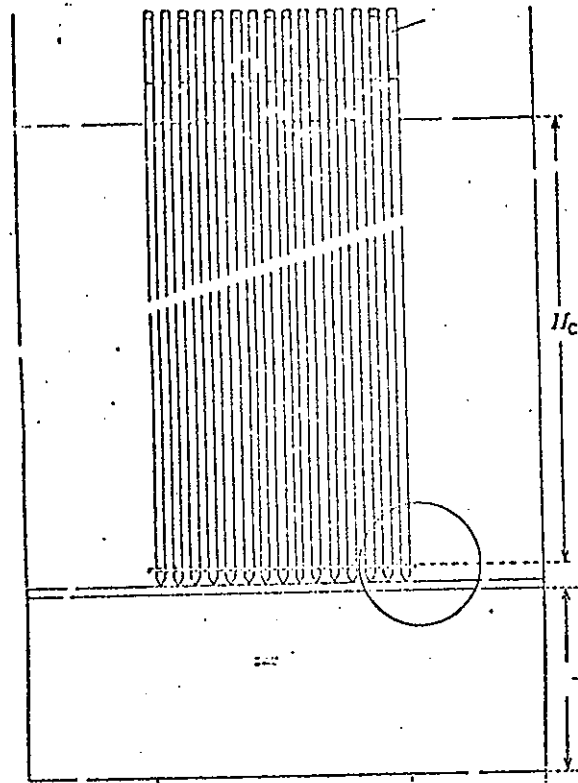


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7a Geometry of cell calculations

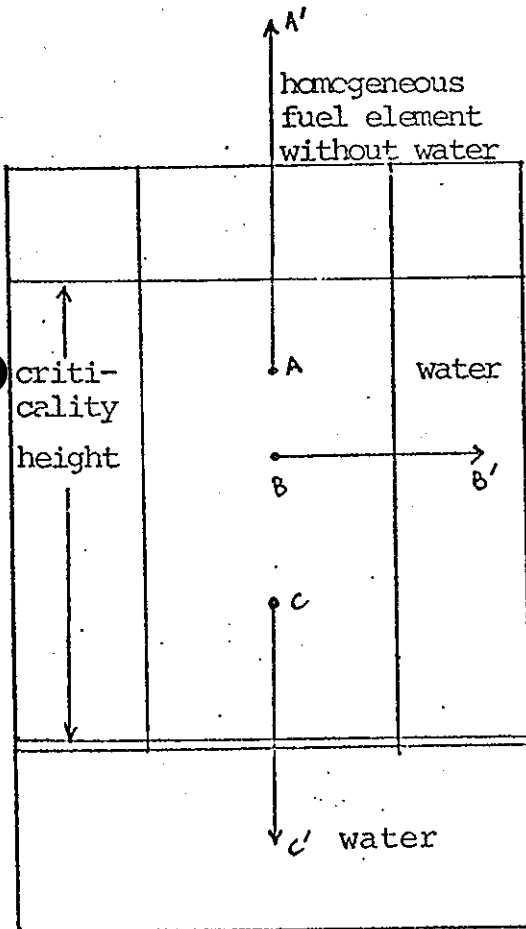


Heterogeneous fuel element  
hexagonal pitch lattice of PWR pins



Equivalent homogeneous fuel element (Either with  
and without water)

7b

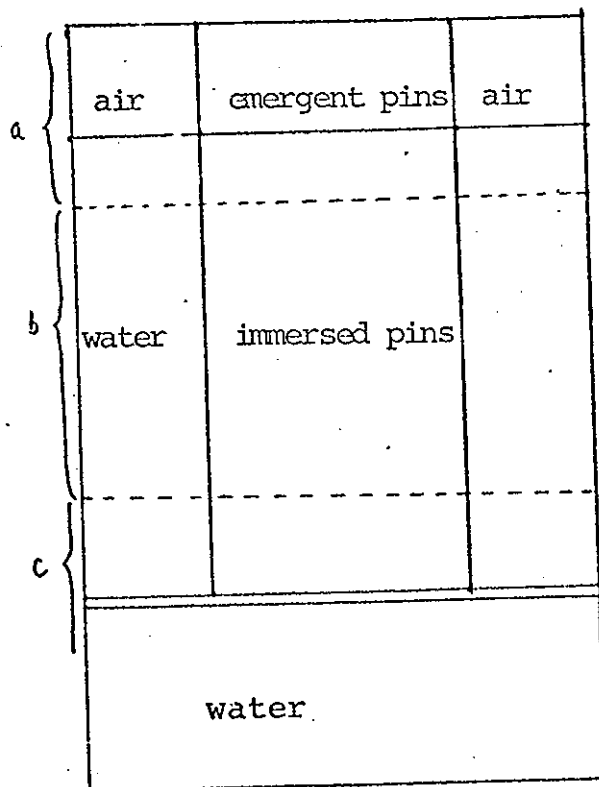


Homogeneous  
fuel element  
with water

Cut lines for APOLLO calculations

7c Model of R - Z geometry for DOT 3.5

Calculations



Cross sections of materials in a, b, c parts  
of geometry are provided by weighting those  
of 99 group standard library by spectras  
obtained in one dimensional APOLLO calculations  
across cut-lines AA', BB' and CC'.