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CALCULATION OF GAMMA-RAYS AND FAST NEUTRONS FLUXES WITH THE PROGRAM MERCURE-4

A. BAUR - C. DUPONT - B. TOTTH

COMMISSARIAT A L'ENERGIE ATOMIQUE
DRE/SERMA/LEP
B.P. N° 2
91190 - GIF SUR YVETTE -
FRANCE

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I - INTRODUCTION -

I.1. General presentation

The program MERCURE-4 evaluates gamma ray or fast neutron attenuation, through laminated or bulky three-dimensionnal shields. The method used is that of line of sight point attenuation kernel, the scattered rays being taken into account by means of build-up factors for γ and removal cross sections for fast neutrons. The integration of the point kernel over the range of sources distributed in space and energy, is performed by the Monte-Carlo method, with an automatic adjustment of the importance functions.

These main features greatly serve to make the program a very useful one for shielding designers, especially by its facility quickness and economy of use. In fact, since it is operationnal the program MERCURE-4 has been intensively used for many various problems, among the most current of which let us mention for example.

- the calculation of gamma heating in reactor cores, control rods and shielding screens, as well as in experimental devices and irradiation loops.

- the evaluation of fast neutron fluxes and corresponding damage in structural materials of reactors (vessel steels...)

- the estimation of gamma dose rates on nuclear instrumentation in the reactors, around the reactor circuits and around spent fuel shipping casks.

I.2. Brief history of the program

The fatherhood of the program belongs to C. DEVILLERS who entirely conceived and realised the initial version, called MERCURE-3, and in which the integration was analytically performed by means of a spatial mesh discretisation.

VII - NUCLEAR CONSTANT LIBRARY

VII.1. Gamma cross sections

VII.2. Build-up factors

VIII - EXAMPLE OF CALCULATION

- gamma dose rate around a spent fuel shipping cask

MERCURE-4 has benefited from several developments realised for the Monte Carlo program TRIPOLI, especially inasmuch as the geometrical treatment methods are concerned, the implantation of which in MERCURE-4 is mainly due to C. DUPONT as well as most of the others improvements. The maintenance of the code is presently assumed at the L.E.P.* (Saclay), by C. DUPONT for program improvements and by B. TOTTH for nuclear constants library updating.

This paper tries to describe the main features and performance of the last version, according to the following plan :

- Theoretical basis
  - line-of-sight point attenuation kernel
  - build-up factors
  - Monte Carlo method

- Detailed descriptions
  - geometrical description
  - source representation mode
  - integration technique

- Nuclear constants libraries
  - absorption coefficients
  - build-up factors

- Description of on actual calculation
  - gamma dose rate around a spent fuel shipping cask

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* Laboratoire d'Etudes de Protection

II - BRIEF THEORETICAL BASIS

II.1. The line of sight point attenuation kernel

In a material of total cross section $\Sigma_T(E)$ the uncollided flux at a distance ρ from a normalized, isotropic point source of particles of energy Eo, may be represented by the product of the geometrical effect times the probability of traveling the distance ρ whithout a collision. The fast neutron flux is calculated by replacing $\Sigma_T(E)$ with a removal cross-section

$$\Phi(\rho, E_o) = \frac{1}{4\pi\rho^2} \cdot \exp[-\Sigma_T(E_o)\cdot\rho] \qquad (2.1.)$$

For a distributed volume source of intensity $S(\vec{r}, E_o)$. One derives the expression of the flux at a point $\vec{r}_o$, by integrating each elementary source over the total volume of the source.

$$\Phi(\vec{r}_o, E_o) = \iiint_V \frac{S(\vec{r}, E_o)}{4\pi|\vec{r}_o - \vec{r}|^2} \cdot \exp[\Sigma_T(E_o)\cdot\rho]\cdot dv \qquad (2.2.)$$

This formula is extended for heterogeneous media by replacing the exponential argument with the sum of the relaxation lengths

$$\Phi(\vec{r}_o, E_o) = \iiint_V \frac{S(\vec{r}, E_o)}{4\pi|\vec{r}_o - \vec{r}|^2} \cdot \exp[-\tilde{\Sigma}_{o\text{-}4}]\cdot dv \qquad (2.3.)$$

where :

$$\tilde{\Sigma}_{o\text{-}4} = \sum_T \Sigma_{T,i}(E_o)\cdot\rho_i \qquad (2.4.)$$

Finally, for energy-dependent sources and in the multigroup approximation used in the program MERCURE-4, one obtains the integrated flux :

$$\Phi(\vec{r}_o) = \iiint_V \sum_{g=1}^{L} \frac{S(\vec{r}, E_g)}{4\pi|\vec{r}_o - \vec{r}|^2} \cdot \exp[-\tilde{\Sigma}_{g\text{-}4}]\cdot dv \qquad (2.5.)$$

II.2. Build-up factors

The actual flux is greater than the uncollided flux evaluated by the previous formula (2.5.), which does not take into account the multiple scatterings taking place in thick screens and with broad beams.

The allowance for this effect is classically made for gamma-rays by introduction of build-up factors, defined as the ratio at the point of interest, of the total gamma flux to the uncollided gamma flux.

Let us recall that the build-up factor determination depends on the following points :

- material through which the radiation is passing
- thickness of the material
- energy of the gamma radiation
- source geometry
- type of build-up (dose, flux, heating..)

The program automatically calculates the build-up factors from tabulated values available in one of the 2 associated libraries (see also : VII.2).

For multilayer media the user may :

- either use a single build-up factor ; for example, that of the last layer
- or use the modified Kitazume formula as used in the program SABINE :

$$B(t_1) = B_1(t_1)$$

$$B(t_N) = B_N(t_N) + [B(t_{N-1}) - B_N(t_{N-1})] \cdot Z_N \qquad (2.6.)$$

with

$$Z_N = (1-\beta_{N,N-1}) \cdot \exp(-\alpha_{N,N-1} \cdot \mu_x x_N) + \beta_{N,N-1}$$

II.3. General expression of results

Taking into account the previous remarks, one is led to calculate an integral of the general form :

$$j_R(\vec{r}_0) = \iiint_V \sum_g S(\vec{r},g) \cdot G(\vec{r},\vec{r}_0,g) \cdot dv \qquad (2.7.)$$

where the kernel $G_R(\vec{r},\vec{r}_0,g)$ is :

$$G_R(\vec{r},\vec{r}_0,g) = A_R(g) \cdot \frac{\exp[-\tilde{\Sigma}_g \cdot \delta]}{4\pi |\vec{r}_0 - \vec{r}|^2} \qquad (2.8.)$$

- for gamma rays, the function $A_R(g)$ is the product of the response fonction $R(g)$ times the corresponding build-up factor, $B_R(g)$ is a function of the group g and of relaxation lenghts in each medium.

$$A_R(g) = B_R(g) \cdot R(g) \qquad (2.9.)$$

- for neutrons, $A_R(g)$ is a constant depending on the type of spectrum.

II.4. Monte Carlo method

The numerical integration of the point kernel over the range of sources distributed in space and energy is performed in MERCURE-4 by the Monte Carlo method of which we recall now the main features.

II.4.1. Estimation of an integral

Let us consider the integral

$$j = \int_D f(x) \cdot dx \qquad (2.10)$$

where x is a spatial variable of one or more dimensions.

In addition, let $P(X)$ be a function of the variable defined, positive and normalised over the domain D :

$$\int_D p(x)\,dx = 1 \quad , \qquad p(x) > 0 \quad \forall x \in D \tag{2.11}$$

by introducing the notation

$$g(x) = \frac{f(x)}{p(x)} \tag{2.12}$$

the integral j may be written

$$j = \int_D g(x) \cdot p(x) \cdot dx \tag{2.13}$$

In probabilistic terminology, j is the mathematical expectation $E[g(X)]$ over the domain D, of the function g of the random variable X , with probability density $P(X)$

Then, let $\bar{J}_N$ be the mean of the values of the function g, corresponding to N choices x_i (i=1, 2,....,N) of the random variable X according to the probability density $p(x)$. The law of large numbers states that $\bar{J}_N$ converges towards j when N increases indifinitely and justifies the estimation of j by $\bar{J}_N$

$$\bar{J}_N = \frac{1}{N} \sum_{i=1}^{N} g(x_i) \xrightarrow[N \to \infty]{} j \tag{2 14}$$

The practical realisation of this estimation, constitutes the numerical method of calculation of an integral, called the Monte Carlo method, it consists of the three following operations :

- preparing a sample of N values selected at random from the distribution $p(x)$; this is the "game"
- attribution in function of the game, of numerical values $Y_i = g(x_i)$; this is the "score"

- calculation of the mean score :

$$\bar{J}_N = \frac{1}{N}\sum_{i=1}^{N} Y_i = \frac{1}{N}\sum_{i=1}^{N} g(x_i) \qquad (2.15.)$$

II.4.2. Variance of the estimation

$\bar{J}_N$ is also a random variable which converges in principal, according to the Central limit theorem, towards a normal (Gaussian) variable with a variance :

$$\sigma^2_{\bar{J}_N} = \frac{1}{N}\sigma^2_{Y_i} = \frac{1}{N}\int_D [g(x)-j]^2 \cdot p(x)\cdot dx \qquad (2.16.)$$

that one classically estimates by :

$$S^2_{\bar{J}_N} = \frac{1}{N}\sum_{1}[Y_i - \bar{J}_N]^2 = \frac{1}{N}\sum_{1}[g(x_i)-\bar{J}_N]^2 \qquad (2.17.)$$

a maximum of the variance $\sigma^2_{\bar{J}_N}$ may be obtained by replacing, the mean square $[g(x_i)-\bar{J}_N]^2$ in the relation (2.15) by its maximum over the range D.

$$\sigma^2_{\bar{J}_N} \leq \frac{1}{N}\text{Max}\,[g(x)-j]^2 \qquad (2.18.)$$

This inequality only translates the fact that the variance arises from fluctuation of the function $g(x)$ about its mean j (figure 2.1.)

II.4.3. Reducing the variance-importance sampling

Several games may be used for the resolution of one problem

- the direct (or natural) game is characterised by a probability density $p(x)$ constant over the domain D

$$p(x) = \frac{1}{V_D} \qquad (2.19.)$$

V_D being the volume of the source corresponding to the domain D.

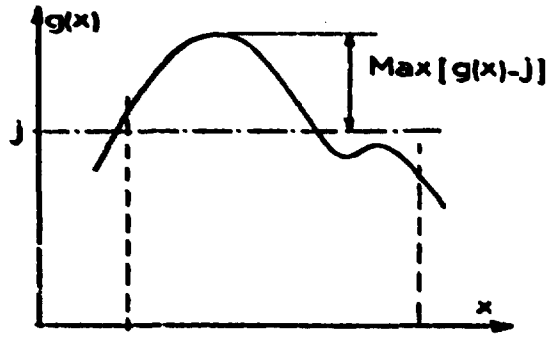


Fig : 2·1 - $\sigma_j^2 \leq \text{Max}\,[g(x)-j]^2$

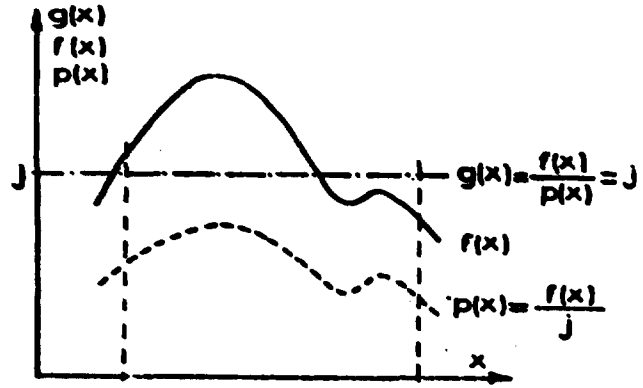


Fig : 2·2 - zero variance game

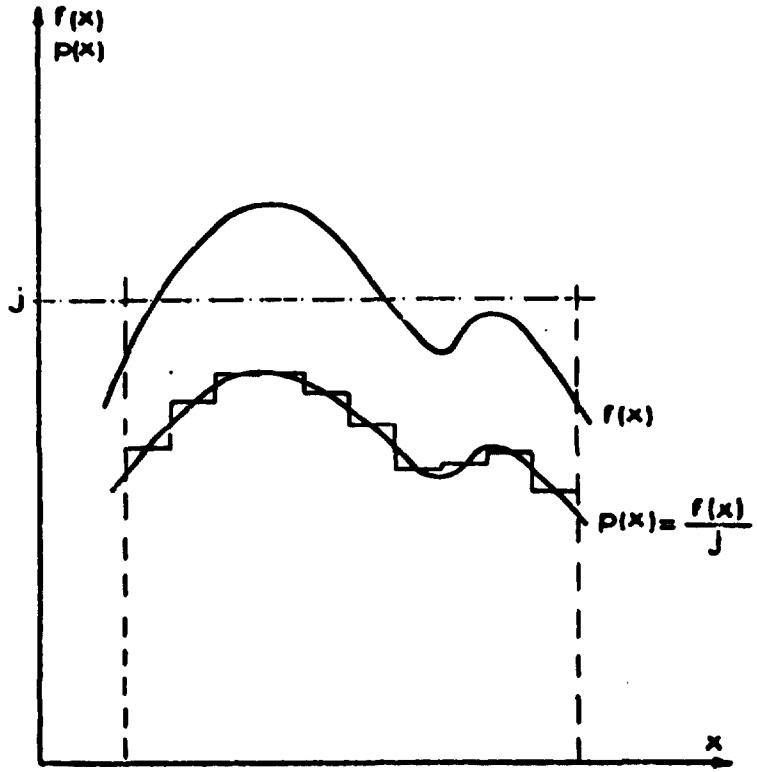


Fig : 2·3 - Approximation of the ideal density of probability by a step function

Then the score becomes

$$Y_i = g(x_i) = f(x_i) \cdot V_D \qquad (2.20.)$$

And the inequality (2.18)

$$\sigma^2_{\bar{j}_N} < \frac{1}{N} \text{Max} \left[f(x) \cdot V_D - \bar{j} \right]^2 \qquad (2.21.)$$

The variance is greater, especially as the function shows large variations over the domain D.

- the ideal game, with zero variance may be imagined as characterised by a density of probability proportional to the function which must be integrated

$$p(x) = C \cdot f(x) \qquad (2.22)$$

The constant C is determined by the normalisation condition :

$$C \cdot \int_D f(x) \cdot dx = 1 \longrightarrow C = \frac{1}{J} \qquad (2.23.)$$

and the score becomes :

$$Y_i = g(x) = \frac{1}{C} = j \qquad (2.24.)$$

its variance is evidently zero, as it is constant this game is a theoretical one as the determination of probability density needs a knowledge of j which is precisely the solution. Nevertheless any approximation, however rough, of the ideal probability density, is better than the unit scale which characterises the direct game.

- practically, in the program MERCURE-4, the ideal probability density is approximated by a step function (see figure 2.3.) The domain D is discretised in spatial meshes or "cases" and the function to be integrated is set equal in each case to its value $f(x_o^K)$ at the center of this case.

The probability of chosing one case k is then :

$$p(k) = \frac{f(x_K^o) \cdot V_{Dk}}{\sum_K f(x_k^o) \cdot V_{Dk}} \qquad (2.25)$$

The probability of choosing one point in the case k is set constant and equal to $1/V_{Dk}$ with :

$$V_{Dk} = \int_{Dk} dx \qquad (2.26.)$$

Finally the probability of choosing one point of the case k is :

$$p(x_k) = \frac{f(x_k^o)}{\sum_k f(x_k^o) \cdot V_{Dk}} \qquad (2.27.)$$

this method needs :

- a discretisation in cases such as the corresponding step function which gives a good representation of the ideal function
- a pre-calculation of the initial importances (or probabilities) which is an approximate estimation of the integral to be calculated, this estimation being refined by the Monte Carlo game. The practical application details of this method will be specified here after (see : integration technique paragraphe V.).

Let us notice now the compromise between the initial estimation and the Monte Carlo game, on which depends the efficiency of a calculation

- either a rough discretisation and an initial estimation : very quick but with a large variance which may only be reduced by an expensive Monte Carlo game.
- or a fine discretisation with expensive initial calculation but followed by a very quickly converging Monte Carlo game.

III - GEOMETRICAL DESCRIPTION OF A CONFIGURATION

The logic of the geometrical description, as well as the treatment of the intersections are strictly the same in MERCURE-4 and TRIPOLI. This identity simplifies for example the execution, for a given configuration, of photonic calculations with MERCURE-4 and neutronic calculations with TRIPOLI. It is used in present efforts of the L.E.P. for the consistency of the different shielding codes. The description of a configuration to be studied, is founded on a partition of the spatial domain in meshes (or volumes) satisfying the following characteristics.

III.1. Définition and characteristics of meshes (volumes)

A mesh (or volume) is a finite region :

- simply connected
- bounded by parts of surfaces of first or second degree
- chemically composed of only one homogeneous substance called "composition"

Any point must evidently belong to only one mesh and each point of the same mesh must in addition give a constant sign to each of the linear or quadratic forms corresponding to the surfaces bounding the mesh.

The figure 3.1. a shows the cross-section of a mesh improperly defined from this point a view. A possible description of the same configuration being formed of the two meshes of the figure 3.1.b.

The meshes are given in any order but numbered consecutively. Let us notice in addition that the energetic part of the importance function is constant in each mesh. It may be necessary for the user to subdivide some large meshes for a proper representation of this function.

III.2. Types of surfaces available

The surfaces bounding the meshes are defined by their equations in an initial, direct and orthogonal reference system OXYZ.

The various kinds of surfaces available are :

a) A plane perpendicular to one of the main axes defined by the value x_o , Y_o or Z_o of the corresponding equation :

plane	$\perp$	OX	$x+x_o=0$
plane	$\perp$	OY	$y+y_o=0$
plane	$\perp$	OZ	$z+z_o=0$

b) General plane defined by the four coefficients of the equation

$$Ax+By+Cz+D=0$$

c) Revolution cylinder whose axis is parallel to one of the main axes, and defined by the coordinates (Y_o,Z_o), (X_o,Z_o), (X_o,Y_o) of the intersection of the axis with the perpendicular plane of the reference system, and by the radius value

axis// to OX	$(y-y_o)^2+(z-z_o)^2-R_o^2=0$
axis //to OY	$(x-x_o)^2+(z-z_o)^2-R_o^2=0$
axis // to OZ	$(x-x_o)^2+(y-y_o)^2-R_o^2=0$

d) the general sphere defined by its center coordinates and its radius value

$$(x-x_o)^2+(y-y_o)^2+(z-z_o)^2-R_o^2=0$$

e) the general quadratic convex or not and defined by the ten coefficients of the equation

$$Ax^2+By^2+Cz^2+Dxy+Exz+Fyz+Gx+Hy+Iz+J=0$$

As for meshes, the surfaces are numbered consecutively.

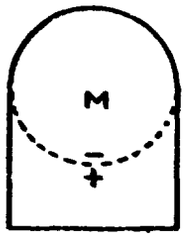


Fig: 3.1.a - wrong description of a configuration.

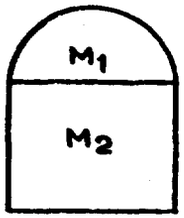
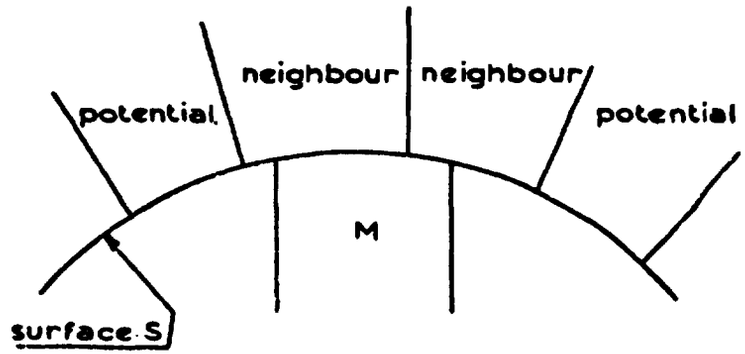


Fig: 3.1.b - correct description of the same configuration



III.3. Further information - Functional details

III.3.1. Potential and neighbouring meshes

The name "potential mesh" of a mesh M relative to a surface S is given to any mesh which is bounded by a part of the surface S and whose points give for the linear or quadratic form defining S an opposite sign to that given by the points of M.

The more restrictive notion of neighbour mesh needs in addition the possibility of direct travel from one mesh to the other through the surface S.

Each mesh may possess several potential or neighbour meshes relative to the same surface, the search for these potential or neighbour meshes being automatically done by geometrical programs.

Note :

Any one surface may be described by several identical equations with different numbers but the same number must be used for a surface separating two neighbour meshes.

III.3.2. Special leakage conditions

A special condition of leakage must be applied to every portion of surface bounding mesh M which does not possess a neighbour, this is particularly true for every surface bounding the geometry.

Let's notice also that this geometry must be a finite one.

IV - SOURCE REPRESENTATION -

IV.1. Source system notion

The fine and precise representation of sources distributed in space and energy is based in MERCURE 4 as in TRIPOLI on the notion of source system.

A source system is a function of spatial variation $S_s(\vec{r})$ defined by the user in a three-dimensional specification in meshes or "cases" containing the sources. It is superimposed on the mesh pattern used for the geometrical description of the physical system to be studied, and may be described in a cartesian, cylindrical or spherical system of coordinates, independently of the previous geometrical description. A source system is nevertheless associated with a set of geometrical meshes and the particles are emitted in the intersection of this collection of meshes and the range of definition of the function $S_s(\vec{r})$.

Several systems may coexist in one given problem, with or without overlap.

The index j will characterise here after the ordinal number of the system.

IV.2. General expression for the sources

Taking into account the previous definition, the density of particles to be emitted in the phase space S (r, E,Ω) is represented by using a linear combination of terms factorised in space, energy and direction, according to the general expression:

$$S(\vec{r},E_g,\vec{\Omega}) = \sum_j F'_j(m) \cdot S_{sj}(\vec{r}) \cdot \frac{S_{ej}(m,g)}{\|S_{ej}(m,g)\|} \cdot \frac{S_{aj}(\vec{\Omega})}{\|S_{aj}(\vec{\Omega})\|} \qquad (4.1.)$$

where :

$\vec{r}$ is a point of the mesh m

E_g is the energy of the g^{th} group of the multigroup structure and with :

$$F_j^*(m) = F_j(m) \sum_j S_{ej}(mg) \Delta E_g \iint_{2\pi} S_{aj}(\mu) d\mu \qquad (4.2.)$$

F_j (m) being a coefficient associated with each source mesh of each system, allowing the introduction of source discontinuities.

Several description modes may be used for each factor of the expression (4.1.), they allow representation of a density S ($\vec{r}$, E_g, $\vec{\Omega}$) equal or proportional at each point of the phase space, with the actual source density of the physical problem.

IV.3. The spatial factor (S_{sj} ($\vec{r}$)

The spatial variation function may be described in cartesian, cylindrical or spherical coordinates. It will be written :

$$S_{sj}(\vec{r}) = S_{sj}(U, V, W)$$

Where U, V, W represent the three coordinates of the chosen system according to the following list :

	U	V	W
Cartesian	X	Y	Z
Cylindrical	r	φ	Z
Spherical	r	θ	φ

With respect to the initial cartesian system OXYZ, used for the geometrical description, let us point out the following characteristics of the source systems :

- the cartesian system is identical to OXYZ
- three cylindrical systems may be used Fig. 4.1., with axis respectively parallel to OZ, OX and OY, the azimuthal angle

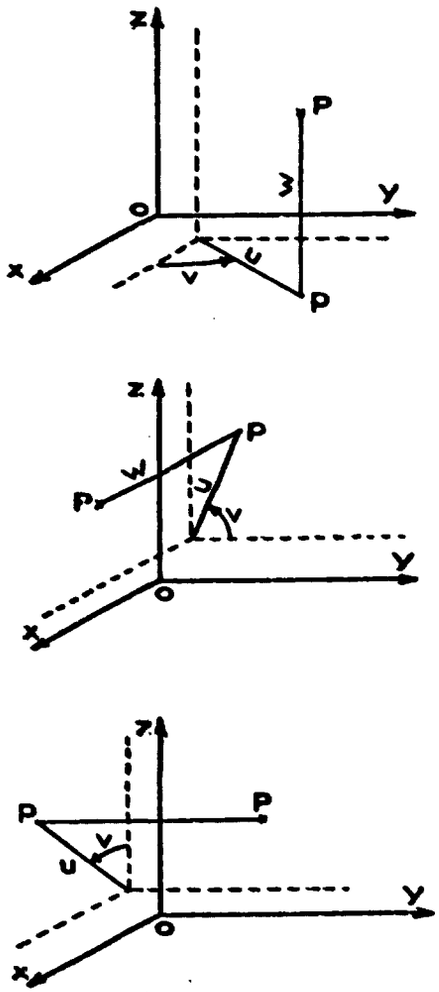


Fig: 4.1 - cylindrical systems

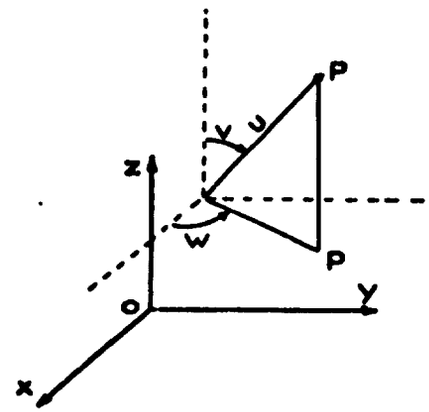


Fig: 4.2 - spherical system

is taken in the forward direction starting from an origin axis parallel to OX (resp. OY and OZ), and the Z dimension is counted along the axis of the cylindrical system starting from the coordinate plane which is perpendicular to it.

The spherical system (Fig.4.2.) has arbitrarily defined center, the azimuth angle φ is counted forward starting from an axis parallel to OX and the polarangle θ is taken starting from an axis parallel to OZ.

In the chosen system of coordinates, the spatial function $S_{sj}(r)$ may be factorised according to one of the forms :

$$S_{sj}(U,V,W) \quad \begin{cases} F_j^1(U).F_j^2(V).F_j^3(W) \\ F_j^1(U).G(V,W) \\ F_j^2(V).G(U,W) \\ F_j^3(W).G(U,V) \\ \text{constant in each case} \end{cases}$$

The functions of a single variable : F (T) - T being either U or V or W may be described :

- either analytically as constant, or varying in cosine or exponentially
- or numerically :
  - by point values at limits of the T network
  - by steps in each interval

The functions of 2 variables : G (T', T") may be described numerically :

- by point values at limits of the T', T" pattern
- by steps in each interval of this pattern.

Note :

1. the T network may be different than the cases network
2. the T' T" pattern must coïncide with the cases pattern

3. between two point values on the same coordinate of a pattern, one assumes that the spatial function is linearly varying, independently of the other set of coordinates.

IV.4. The energetic factor S_{ej} (m, g)

The spectrum of the source particles emitted in every mesh associated with a system j may be defined by the user :

- either in multigroup form and then in the same network as that used for the constitution of the multigroup library
- or in point form, the evaluation in the multigroup structure being then automatically made by the program
- the program normalises the spectra which are not already normalized and multiplies by the calculated integral of the corresponding spectrum, the discontinuity coefficient F_j (m) given by the user to each source mesh of each system (cf. relation 4.3. and paragraphe III.6.).

IV.5. The angular factor S_{aj} ( )

The angular distribution of the particles emitted in each system may be also described by the user, relative to a unit vector $\vec{N}$ and according to 3 different modes :

- isotropic distribution between two cones of axis $\vec{N}$
- cosine distribution, between two cones of axis $\vec{N}$
- point values definition, as a function of the cosine of the angle with the vector $\vec{N}$

The vector $\vec{N}$ may be :

- parallel to OX, OY or OZ if the system is cartesian
- the radius vector from the origin of coordinate to the emission point if the system is spherical
- a radius vector perpendicular to the Z -axis from a point on the axis to the emission point, or a vector parallel to the axis if the system is a cylindrical (fig. 4.3.).

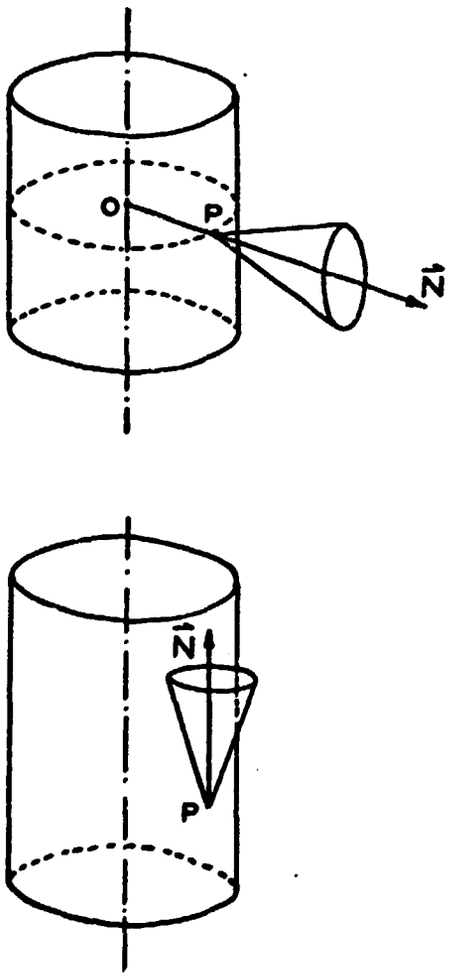


FIG: 4.3 - ANGULAR DISTRIBUTION OF SOURCES - CYLINDRICAL SYSTEM

Finally, as for the energy dependent factor, the program normalises the angular distributions which are not already normalised and multiplies the discontinuity coefficient of each mesh of the system by the calculated integral of the corresponding angular distribution.

IV.6. Discontinuity factors F_j (m)

In many cases the discontinuity factors give the user more choices for simplifying source data. These are multiplicative factors F_j (m) given by the user to any mesh m of every system j. Let us recall that the program MERCURE 4 modifies these factors, multiplying them by the calculated integrals of the corresponding energetic and angular distributions.

The coefficients actually used are then F'_j (m) :

$$F'_j(m) = F_j(m) \sum_g S_{ej}(mg) \Delta E_g \cdot \iint_{2\pi} S_{aj}(\mu) d\mu \qquad (4.3.)$$

These factors allow the user to describe some discontinuities of the source density at limits between emitting meshes. They may be used also as normalisation factors of spectra or conversion factors of nuclear constants.

For example, radiative capture gamma sources may be described by introducing for the values of thermal flux a spatial factor Ss, unnormalised gamma capture spectra as energy dependent factor Se, and discontinuity factors equal to the macroscopic capture cross-sections.

Another example is that of using mass attenuation coefficients ($cm^2.g^{-1}$) which the program will automatically convert to linear attenuation coefficients (cm^{-1}) by means of discontinuity factors set equal to the densities of corresponding materials ($cm^3.g^{-1}$).

V - PRACTICAL DETAILS OF THE INTEGRATION TECHNIQUE

V.1. Estimation of the integral

For each point of interest $\vec{r}_0$, the integral to be calculated has the general form :

$$j_R(\vec{r}_0) = \iiint_V \sum_g Ss_j(\vec{r}) \cdot Se_j(m,g) \cdot G_R(\vec{r},\vec{r}_0,g) \cdot dv \qquad (5.1.)$$

where :

- V is the spatial volume of the sources
- g the number of energy groups
- R the type of response function

As has been previously shown (cf. paragraphe II.4.3.), the ideal probability density for each point of interest assumes a knowledge of the results at that point :

$$p(\vec{r},g) = \frac{Ss_j(\vec{r}) \cdot Se_j(m,g) \cdot G_R(\vec{r},\vec{r}_0,g)}{j_R(\vec{r}_0)} \qquad (5.2.)$$

One approximates it by step functions "elements" network. The discrete probability of choosing one element k is pre-calculated as the product of the volume ΔV_k of this case times the intensity of the source and times an importance value in the element. For this calculation :

- the intensity of the source is set constant in the element and equal to its value at the center r_k^o of this element calculated according to the factorised representation previously described :

$$S_j(\vec{r}_k^o) = F_j(m) \cdot Ss_j(\vec{r}_k^o) \cdot \sum_g Se_j(m,g) \qquad (5.3.)$$

where m is the mesh containing the point r_k^o , the coordinates of which are the respective means of the bounding coordinates of the element.

The importance in the element evaluated by the program is also factorised in spatial importance constant in an element and energetic importance constant in a mesh m

$$I(k) = Is(k) \cdot Ie(m,g) \tag{5.4.}$$

Finally, the spatial probability of choosing an element k is :

$$Ps(k) = A \cdot F_j(m) \cdot Ss_j(\vec{r}_k^g) \cdot \Delta V_k \cdot Is(k) \cdot \sum_g Se_j(m,g) \cdot Ie_j(m,g) \tag{5.5.}$$

The coefficient A being defined by the normalisation condition :

$$\sum_k Ps(k) = 1 \tag{5.6.}$$

The game actually used may then be resumed as follows :

- first an element is chosen with the probability $P_s(k)$
- then a point $\vec{r}_k$ is chosen at random in the element with the probability

$$Qs(k) = \frac{1}{\Delta V_k} \tag{5.7.}$$

Figure 5.1. shows the possible results of the this choice :

1. the chosen point does not belong to any source mesh of the system, the corresponding score Y_i is set equal zero and another element is chosen.2 and 3, The chosen point belongs to a source mesh m' of the system , m' being either the mesh m containing the center of the element or another mesh. Then the energy group g is chosen with the discrete energetic probability of the mesh m' :

$$Pe_j(m',g) = \frac{Se_j(m',g) \cdot Ie_j(m',g)}{\sum_g Se_j(m',g) \cdot Ie_j(m',g)} \tag{5.8.}$$

and the corresponding score Y_i is calculated :

$$Y_i = \frac{1}{A} \frac{Ss_j(\vec{r})}{Ss_j(\vec{r}_k^g)} \frac{F_j(m')}{F_j(m)} \frac{\sum_g Se_j(m',g) \cdot Ie_j(m',g)}{\sum_g Se_j(m,g) \cdot Ie_j(m,g)} \cdot \frac{G(\vec{r},\vec{r}_c,g)}{Is(k) \cdot Ie(m,g)} \tag{5.9.}$$

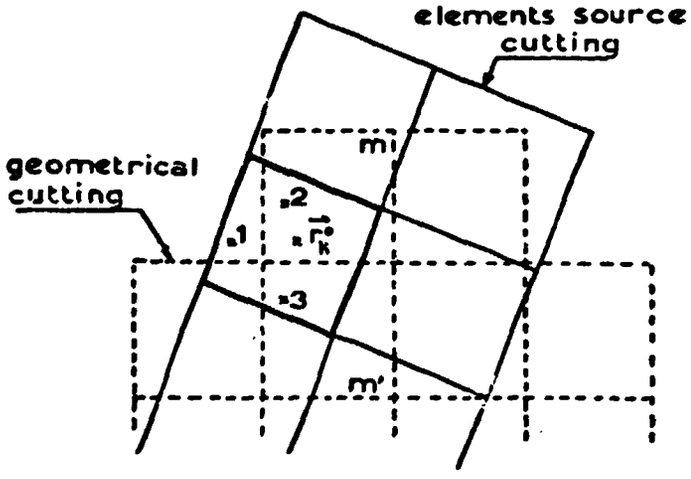


Fig : 5.1 - result of random selection of a point in the case k

the chosen point

1. does not belongs to any source mesh
2. belongs to the source mesh m which contains the center of the element k
3. belongs to a source mesh m' which does not contains the center of element k

The user specifies the number N of choices for each sample, the maximum number L_{max} of samples and the relative precision required for the results. The program treats a number of samples L less or equal to L_{max} if the precision is obtained, and limited to L_{max} if it is not. The mean value of the integral to be calculated is finally estimated by :

$$\bar{J} = \frac{1}{L} \sum_{l} \bar{J}_l \qquad (5.10.)$$

where : $\bar{J}_l$

is the estimate given by the l^{th} sample

$$\bar{J}_l = \frac{1}{N} \sum_{i} Y_i \qquad (5.11)$$

V.2. Precision of the estimate

The variance of the result is estimated at the same time according to two different methods the larger of the two estimates is used for the precision tests :

- First method

The L estimates $\bar{J}_l$ one corresponding to each sample, belong to a population of which the variance is estimated by :

$$[s^2_{\bar{J}_l}] = \frac{1}{L-1} \sum_{l} [\bar{J}_l - \bar{J}]^2 \qquad (5.12.)$$

then the variance of the estimated mean $\bar{J}$ is

$$[s^2_{\bar{J}}] = \frac{1}{L(L-1)} \sum_{l} [\bar{J}_l - \bar{J}]^2 \qquad (5.13)$$

- Second method

For each sample L , an estimate of the variance (s^2_Y) of the score is :

$$[s^2_Y] = \frac{1}{N} \sum_{i} [Y_i - \bar{Y}]^2 \qquad (5.14.)$$

from which the variance of the partial estimate $\bar{J}_l$ is :

$$[S^2_{J_i}] = \frac{1}{N^2} \sum_i [Y_i - \bar{Y}]^2 \qquad (5.15.)$$

and finally these estimates being independent, the variance of the estimated integral is :

$$[S^2_J] = \frac{1}{L^2} \sum [S^2_J] \qquad (5.16.)$$

VII - NEUTRONIC CALCULATIONS

Calculation of fast neutronic attenuation and corresponding responses (for example : damage) may be performed in three dimensional geometries, with the program MERCURE 4.

For this type of calculations the library is created by the user for each problem and introduced by means perforated cards.

Let's briefly describe the method presently used at the L.E.P.

A preliminary calculation is performed with the program ANISN in a cylindrical or spherical geometry similar to the configuration to be studied.

Some very quick MERCURE 4 calculations are after performed in the same geometry, allowing the fitting of removal cross-sections of the different materials.

These fitted removal cross-sections are finally used for a MERCURE 4 calculation in an actual three-dimensional geometry.

These calculations are generally performed with only one energy neutron group for each calculation. They also need the execution of one separate calculation for each response function (Ni, damage, dose) with removal cross sections depending on the response of interest.

calculated responses are in good agreement with experimental results.

VIII - NUCLEAR CONSTANT LIBRARY

For special cases such as neutronic or low energy gamma ray calculations (corrosion products, for example) the nuclear constants may be entered by the user by means of perforated cards.

For gamma rays calculations in the standard multigroup structure the program MERCURE 4 is presently coupled with 2 nuclear constants libraries stored on magnetic tapes.

VIII.1. Gamma cross-sections

The photonic library, called BIP-G1, has been created by the program GAMLEG/A ; it contains the multigroup cross sections in barns per atom and the gamma heating response functions in watts per gram for the 18 following elements :

Hydrogen	copper
beryllium	zirconium
carbon	silver
oxygen	antimony
sodium	barium
aluminum	tungsten
silicon	lead
calcium	uranium
iron	plutonium

These date are taken from (3) (LA.3753)

This library also contains the equivalent gamma dose rate response function in $mrem.h^{-1}/\ \gamma\ .cm^{-2}.s^{-1}$.

The multigroup structure given in table VII.1 consists of 17 groups between 8.53 MeV and 0.048 MeV.

TABLE VII.1. - MULTIGROUPE STRUCTURE, E_{max} = 8.53 MeV

Group	Lethargy	Lower energy
1	0.1287	7.4999
2	0.1430	6.5006
3	0.1670	5.5008
4	0.2007	4.5005
5	0.2517	3.4990
6	0.2412	2.7491
7	0.2007	2.2492
8	0.2517	1.7487
9	0.3365	1.2491
10	0.5108	7.4945
11	0.3925	0.50616
12	0.3925	0.34184
13	0.3925	0.23087
14	0.3925	0.15592
15	0.3925	0.10530
16	0.3925	0.071118
17	0.3925	0.048031

VIII.2. Build-up factor library

Presently this library contains the tabulated values of build-up factors for energy absorption, equivalent gamma dose rate and gamma heating, from 1 to 20 relaxation lengths, for the first 11 groups of the multigroup structure ; that is to say, from 8.53 to 0.5 MeV.

The library contains the 7 following elements :

Z = 7	water		
Z = 13	aluminium	Z = 74	tungsten
Z = 26	iron	Z = 82	lead
Z = 51	tin	Z = 92	uranium

For the elements or substances which do not exist in the library the values of corresponding build-up factors are automatically calculated by the program, by the method of "equivalent Z".

The library also contains the α and β coupling coefficients used in calculation of build-up factors of multilayer media by the Kitazume formula.

Present work for updating this library is directed particularly toward determination of build-up factors for relaxation length numbers greater than 20 and for energy ranges less than 0.5 MeV

IX - EXAMPLE OF APPLICATION

We shall conclude this presentation of the program MERCURE 4 with a brief description of the calculation of the equivalent gamma dose rate around a spent fuel shipping cask.

This cask (figure 8.1.) consists of 7 cylindrical alveoles with steel casing 1 cm in thickness. Each of these alveoles may contain one fuel element made of spin clusters cased with iron. The whole assembly is surrounded with a cylindrical gamma screen 18.5 cm thick, made of a uranium-iron eutectic, then with a neutronic shield made of a cylinder of water 14 cm thick

The fuel is homogenized in the cross-section of each alveole.

The gamma source is the same for each alveole with a cosine axial variation :

$$S(z) = 5.06.10^{12}.\cos(\pi z/135) \quad \gamma.cm^{3}.s^{-1}$$

4 cylindrical source systems are used for the description of the source :

- the first consists of central alveole (mesh 1)
- the second and third consist respectively of the meshes 5 and 7 corresponding to the alveoles nearest to the dose points
- the fourth one groups the four meshes 3, 9, 11, 13 together corresponding to the farthest alveoles.

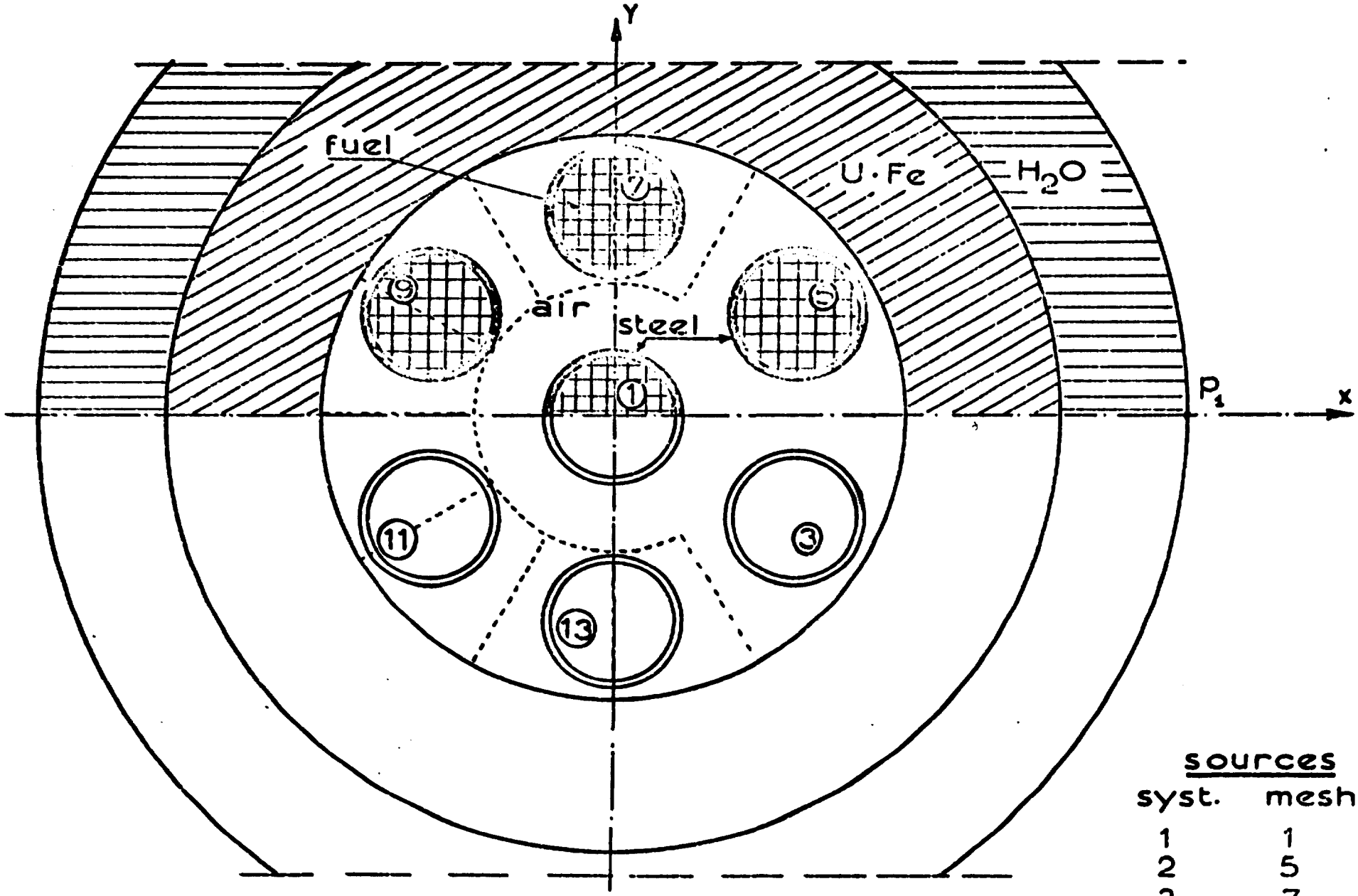


FIG: 8.1 - Spent fuel shipping cask

sources	
syst.	meshes
1	1
2	5
3	7
4	3,9,11,13

In each system, one alveole corresponds to only one element of the network. In spite of this voluntarily rough cutting, the results are obtained with a precision of 3 per cent in less than 30 seconds of IBM 360/91 central processor.

One finds :

26.2	$\pm$	0.7	mrem/h	near the caskwall
3.25	$\pm$	0.1	mrem/h	at a distance of 2 meters.

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* MERCURE 4 - TEST CASE DATA *

EQUATIONS

1	CYLZ	0.0	0.0	7.6238
2	CYLZ	0.0	0.0	8.6238
3	CYLZ	0.0	-24.52	7.6238
4	CYLZ	0.0	-24.52	8.6238
5	CYLZ	21.235	-12.26	7.6238
6	CYLZ	21.235	-12.26	8.6238
7	CYLZ	21.235	12.26	7.6238
8	CYLZ	21.235	12.26	8.6238
9	CYLZ	0.0	24.52	7.6238
10	CYLZ	0.0	24.52	8.6238
11	CYLZ	-21.235	12.26	7.6238
12	CYLZ	-21.235	12.26	8.6238
13	CYLZ	-21.235	-12.26	7.6238
14	CYLZ	-21.235	-12.26	8.6238
15	CYLZ	0.0	0.0	33.5000
16	CYLZ	0.0	0.0	52.0000
17	CYLZ	0.0	0.0	66.0000
18	CYLZ	0.0	0.0	400.0000
19	PLANZ	0.0		
20	PLANZ	-42.5		

MAILLES

1	3	PLUS	19								MOINS	1	20
2	4	PLUS	1	19							MOINS	2	20
3	3	PLUS	19								MOINS	3	20
4	4	PLUS	3	19							MOINS	4	20
5	3	PLUS	19								MOINS	5	20
6	4	PLUS	5	19							MOINS	6	20
7	3	PLUS	19								MOINS	7	20
8	4	PLUS	7	19							MOINS	8	20
9	3	PLUS	19								MOINS	9	20
10	4	PLUS	9	19							MOINS	10	20
11	3	PLUS	19								MOINS	11	20
12	4	PLUS	11	19							MOINS	12	20
13	3	PLUS	19								MOINS	13	20
14	4	PLUS	13	19							MOINS	14	20
15	10	PLUS	2	4	6	8	10	12	14	19	MOINS	15	20
16	4	PLUS	15	19							MOINS	16	20
17	4	PLUS	16	19							MOINS	17	20
18	4	PLUS	17	19							MOINS	18	20

SPECIAL

```
37
1  A  18  19   FUITC
1  A  18  20   FUITL
18  18         FUITS
FIN
```

```
8.53  11  11
0.1287 ! 0.1480 ! 0.1670 ! 0.2007 ! 0.2517 !
0.2412 ! 0.2007 ! 0.2517 ! 0.3305 ! 0.5106 ! 0.3925 !
```

```
6  11
1  1 4.24E9 2.09E10 7.15E9 4.43E11 1.50E12 3.08E12
4
     2  1          0.0         0.0
           1
              1  1            1.0
     2  1         21.23494 -12.26
           1
              5  1            1.0
     2  1         21.23494  12.26
           1
              7  1            1.0
     2  1            0.0         0.0
           4
              3  1            1.0
              9  1            1.0
             11  1            1.0
             13  1            1.0
 1  4  5
0.          7.6236
0.          1.570796 3.141592 4.712388 6.283184
0.0         8.5      17.0     25.5     34.0     42.5
0  1  1  2
 1.  2.  1.  135.  0.
 1  4  5
0.          7.6236
0.          1.570796 3.141592 4.712388 6.283184
0.0         8.5      17.0     25.5     34.0     42.5
0  1  1  2
 1.  2.  1.  135.  0.
 1  4  5
0.          7.6236
0.          1.570796 3.141592 4.712388 6.283184
0.0         8.5      17.0     25.5     34.0     42.5
0  1  1  2
 1.  2.  1.  135.  0.
 1  8  5
15.50     33.5
1.047197 1.570796 2.094395 2.617993 3.141592 3.66519  4.188789
4.712387 5.235985
0.0         8.5      17.0     25.5     34.0     42.5
0  1  1  2
 1.  2.  1.  135.  0.
1 1 -1. 1.    1 1 -1.  1.    1 1 -1.  1.    1 1 -1. 1.
0  0.    350    7
1  0  0.03  30
5
 1  3 80  8 0.017 200 26 0.022 920 92 0.00861 1
 2  1 260 20 0.0848 1
 3  1 80 8 1.E-15 1
 4  2 200 20 0.0103 920 92 0.0386 1
 5  2 10 1 0.060 80 8 0.033 1
 1  1  2  2  3  1  4  2  5  1  6  2  7  1  8  2  9  1
10  2 11  1 12  2 13  1 14  2 15  3 16  4 17  5 18  3
1  00.  0.  0.001  2000  2  1
2 266.  0.  0.  2000  2  1
0
```