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Heterogeneous Calculation of ε

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Summary:

A heterogeneous method of calculating the fast fission factor given by Naudet has been applied to the Carlvik - Pershagen definition of ϵ. An exact calculation of the collision probabilities is included in the programme developed for the Ferranti - Mercury computer by L. Persson.

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Heterogeneous calculation of ϵ.

1. Introduction.

R. Naudet (ref. 1) has given a method for the calculation of ϵ in fuel elements of cluster-type which explicitly takes into account the heterogeneous distribution of the fuel. This method leads to very comprehensive calculations and has therefore with slight modifications been adapted to machine calculation. The formulae given in section 4 have been programmed for the Ferranti-Mercury by Lennart Persson.

The programme assumes that the fuel is uranium or uranium oxide and that the coolant is heavy water. The number of individual rods is arbitrary. Their location must be such that an approximate value of ϵ can be obtained by the usual procedure of homogenizing within the rubber band surface. All the rods in the cluster must be equal with respect to composition and dimensions.

2. Naudet's method.

For a complete description of the method the reader is referred to Naudet's report (ref. 1). Here the main features only and the modifications introduced will be given.

The calculation of ϵ is done largely in the following way.

Neutrons which are born in the fuel or which have made their last collision against a fuel nucleus are distinguished from those who made their last collision against any other nucleus. The collision probabilities of the latter group is calculated homogeneously. The calculation of the probability that a neutron born (uniformly) in a certain rod shall make its first collision in a given rod is related to the corresponding probability in a geometry of concentric cylinders. Confer the figure on page 15. Naudet calculates this probability approximately. The exact calculation inserted in the programme results in somewhat higher collision probabilities and thus a larger heterogenity correction. The magnitude of this increase is illustrated by the results for the element G5 of ref. 2. Naudet gives for this element $\epsilon_{het} - \epsilon_{hom} = 200$ pcm. Using the exactly calculated collision probabilities this difference becomes 245 pcm. The formulae of Naudet are based on the definition of ϵ given by Spinrad. This definition of ϵ was used when testing the programme but in the final formulation the definition of Carlvik - Pershagen (ref. 3) was adopted. The generalisation of the formulae resulting from the introduction of this definition has been made as follows. The symbols used agree with those of Naudet.

ω = fraction of primary neutrons above the threshold for fast fission (group 2)

ω_1 = fraction of primary neutrons below the threshold (group 1)

f, c, e, i_{21}, i_{20}: cross-sections for fission, capture, elastic scattering and inelastic scattering averaged above the threshold and normalized so that their total = 1

c_1, e_1, i_1: the same definition below the threshold

ν' = number of neutrons from fast fission

$\underline{P}$ = collision probability of neutrons above the threshold

$\underline{P}_1$ = collision probability of neutrons below the threshold.

In the two-group formulation of Spinrad $\omega_1 = 1 - \omega$ and $i_{21} + i_{20} = i$ and $i_1 = 0$.

For a single rod we have:

$$\epsilon = U \cdot V$$

where U = total number of fission neutrons in the fuel per thermal fission neutron

$$U = \frac{1 - e\,\underline{P}}{1 - (e + \omega\,\nu' f)\,\underline{P}}$$

V_2 = probability of escape into the moderator (Spinrad's definition)

V_3 = probability of escape into the moderator + probability of slowing down to a lowest energy group

$$V_2 = \frac{\omega\,(1 - \underline{P})}{1 - e\,\underline{P}} + (1 - \gamma_2)\left[1 - \omega + \frac{\omega\, i\,\underline{P}}{1 - e\,\underline{P}}\right]$$

It is assumed that no inelastic collisions take place below the threshold, so that $1 - \gamma_2$, which is the escape probability of neutrons below the threshold can be written:

$$\gamma_2 = \frac{(1 - e_1)\,\underline{P}_1}{1 - e_1\,\underline{P}_1} \equiv \frac{c_1\,\underline{P}_1}{1 - (1 - c_1)\,\underline{P}_1}$$

It is also assumed that $1 - \gamma_2$ is the escape probability of neutrons which have been brought below the threshold as a result of inelastic scattering. This means that the spectrum of these neutrons is identical with the fission spectrum below the threshold. Using the Carlvik - Pershagen definition we have:

$$V_3 = \omega\,\frac{1 - \underline{P}}{1 - e\,\underline{P}} + (1 - \gamma_3)\left(\omega_1 + \frac{\omega\, i_{21}\,\underline{P}}{1 - e\,\underline{P}}\right) + (1 - \omega_1 - \omega) +$$

$$+ \frac{\omega\, i_{20}\,\underline{P}}{1 - e\,\underline{P}} + \frac{\omega_1\, i_{10}\,\underline{P}_1}{1 - e_1\,\underline{P}_1} + \frac{\omega\, i_{21}\,\underline{P}}{1 - e\,\underline{P}} \cdot \frac{i_{10}\,\underline{P}_1}{1 - e_1\,\underline{P}_1}$$

$$\gamma_3 = \frac{(1 - e_1)\,\underline{P}_1}{1 - e_1\,\underline{P}_1}$$

Here the first term gives the number of neutrons entering the moderator from group 2. The second term gives the corresponding number of group 1.

The last four terms represent the number of neutrons that directly or via groups 2 or 1 are slowed down to the lowest energy group. V_3 can be rewritten in the following way:

$$V_3 = \frac{\omega\,(1 - \underline{P})}{1 - e\,\underline{P}} + (1 - \gamma)\left(\omega_1 + \frac{\omega\, i_{21}\,\underline{P}}{1 - e\,\underline{P}}\right) + (1 - \omega_1 - \omega) + \frac{\omega\, i_{20}\,\underline{P}}{1 - e\,\underline{P}}$$

where

$$\gamma = \frac{c_1\,\underline{P}_1}{1 - e_1\,\underline{P}_1}$$

and this formula has been generalized to heterogeneous calculation in a manner analogous to the procedure in the two-group case (compare ref. 1 page 20).

As may be seen from the formulae above no difference is made between collision probabilities of different generations.

3. Comparison with homogeneous calculation.

The differences (apart from the calculation of collision probabilities) between this way of calculating ϵ and the homogeneous method as given for example in RFR-47 (ref. 4) will be given below together with some results.

Allowance for the non-uniform distribution of the sources in the cluster is made only when calculating the heterogeneous collision probability p, see formula 79 page 22. p, the probability that a neutron originating in the rods shall make its first collision against a uranium nucleus, is taken to be the same in all generations and is calculated for a source distributed as the thermal flux:

$$\phi = 1 + \frac{2\,(F - 1)}{2 - F} \cdot \left(\frac{r}{a}\right)^2$$

The source strength in the ith rod is $\phi(r_i)$, where r_i is the distance from the center of the cluster of that rod and a is the radius of the cluster defined by the rubber band contour. F is the ratio between thermal surface flux and average flux. The magnitude of the correction from an assumption of a flat source distribution is very small. In the case of a 19 rod cluster consisting of UO_2 rods with a diameter of 17 mm and a center to center distance of 22 mm ϵ (F = 1) - ϵ (F = 1.22) = 30 pcm.

The programme calculates the quantities p_{ij} which give the probability that a neutron born uniformly in the ith rod will make its first collision against the uranium of the jth rod. By using these quantities it is possible to obtain a picture of the source distribution of the second generation. This distribution is proportional to

$$Q_j = \phi(r_j)\, p_{jj} + \sum_i \phi(r_i)\, p_{ij}$$

For the 19-rod element mentioned above the result is as shown on graph 1.

In the homogeneous calculation the source distribution is assumed to be flat.

The table below shows the difference in absolute values of ϵ and size of the heterogeneity correction between this method and that given in ref. 4 where an intuitive heterogeneity correction is applied. Values according to the formula in ref. 4 are given within brackets.

TABLE 1.

Element nr	ϵ_{hom}	ϵ	F	$\epsilon - \epsilon_{hom}$ pcm
1	1, 03024	1, 03317	1, 33	293
	(1, 02884)	(1, 03489)	(1, 33)	(605)
2	1, 02574	1, 02685	1, 22	111
	(1, 02529)	(1, 02774)	(1, 22)	(245)

Element no 1 is the French 7-rod element G5 in ref. 2. It consist of uranium rods with a diameter of 16.55 mm contained in 1 mm aluminium and with a center to center distance of 24 mm. The coolant is D_2O at 20 ^{o}C between the rods. Element no 2 is a 19-rod cluster the fuel being uranium oxide contained in 0.7 mm zircalloy II and a mean center to center distance of 21.8 mm. The coolant is D_2O of density 0.9375 g/cm^3.

The heterogenity correction decreases when the mean free path in the cluster is increased with respect to the rod dimensions. The dependence on rod material, distance between rods and void formation is illustrated in Table 2 below.

TABLE 2.

Element nr	ϵ_{hom}	ϵ	$\epsilon - \epsilon_{hom}$ pcm	$(\Delta\epsilon)_{void}$ pcm
1	1,03024	1,03317	293	
2	1,02574	1,02685	111	+ 390
3	1,03008	1,03075	67	
4	1,02412	1,02543	131	+ 441
5	1,02910	1,02984	74	

Element 3 = element 2 but $\rho_{D_2O} = 0$

Element 4 = element 2 but with a mean distance betweem rods of 23.1 mm.

Element 5 = element 4 but $\rho_{D_2O} = 0$

Table 3 at last gives a comparison between ϵ as calculated with Spinrad´s definition (ϵ_2) and as calculated with the definition of Carlvik - Pershagen (ϵ_3).

TABLE 3.

Element nr	ϵ_2	ϵ_3
1	1,03039	1,03317
2	1,02460	1,02685
3	1,02886	1,03075
4	1,02325	1,02543
5	1,02808	1,02984

All the calculations shown in Tables 1 - 3 have been made with the group cross-sections of ref. 3 with the exception of those in the first column of Table 3, where the total cross-section of oxygen below the threshold was taken to be 3.00 barns instead of the 4.18 used in the other calculations. The correction to 4.18 barns is about - 30 pcm.

4. Description of the programme.

Input data

Cross-sections (3-group formulation).

$$\left.\begin{array}{ll}
\sigma_{2f}^{U} = 0.58 \cdot 10^{-24} & \sigma_{11}^{U} = 7.44 \\
\sigma_{22}^{U} = 4.56 & \sigma_{10}^{U} = 0.02 \\
\sigma_{21}^{U} = 2.30 & \sigma_{1c}^{U} = 0.13 \\
\sigma_{20}^{U} = 0.01 & \sigma_{1}^{U} = 7.59 \\
\sigma_{2c}^{U} = 0.03 & \\
\sigma_{2}^{U} = 7.48 &
\end{array}\right\} \quad \text{URANIUM}$$

$$\left.\begin{array}{ll}
\sigma_{22}^{D} = 0.89 & \sigma_{11}^{D} = 2.99 \\
\sigma_{21}^{D} = 1.29 & \sigma_{10}^{D} = 0.06 \\
\sigma_{20}^{D} = 0.00 & \sigma_{1c}^{D} = 0 \\
\sigma_{2c}^{D} = 0 & \sigma_{1}^{D} = 3.05 \\
\sigma_{2}^{D} = 2.18 &
\end{array}\right\} \quad \text{DEUTERIUM}$$

$$\left.\begin{array}{ll} \sigma^{O}_{22} = 1.64 & \sigma^{O}_{11} = 4.09 \\ \sigma^{O}_{21} = 0.28 & \sigma^{O}_{10} = 0.00 \\ \sigma^{O}_{20} = 0.00 & \sigma^{O}_{1c} = 0 \\ \sigma^{O}_{2c} = 0 & \sigma^{O}_{1} = 4.09 \\ \sigma^{O}_{2} = 1.92 & \end{array}\right\} \quad \text{OXYGEN}$$

$$\left.\begin{array}{ll} \sigma^{k}_{22} = 2.91 & \sigma^{k}_{11} = 7.05 \\ \sigma^{k}_{21} = 1.23 & \sigma^{k}_{11} = 0.00 \\ \sigma^{k}_{20} = 0.00 & \sigma^{k}_{1c} = 0 \\ \sigma^{k}_{2c} = 0 & \sigma^{k}_{1} = 7.05 \\ \sigma^{k}_{2} = 4.14 & \end{array}\right\} \quad \text{SHEATHING (Zr)}$$

ω = 0.528 = fraction of primary neutrons in group 2

ω_1 = 0.4697 = fraction of primary neutrons in group 1

ν' = 2.80 = number of neutrons from fast fission

ν = 2.43 = number of neutrons from thermal fission

The numerical values are those of ref. 5.

Rod coordinates

Rod nr.	Cartesian coordinates at 20 °C
1	$(x_1^{20},\ y_1^{20})$
⋮	⋮
M	$(x_M^{20},\ y_M^{20})$
M + 1	$(x_{M+1}^{20},\ y_{M+1}^{20})$
⋮	⋮
N	$(x_N^{20},\ y_N^{20})$

The M first rods must be the outer rods of the cluster arranged consecutively. It is assumed that the origin of the coordinate system does not lie outside the contour obtained when connecting the centers of these M rods with straight lines. If $F \neq 1$ (see below) the origin must lie on the central axis of the cluster.

Miscellaneous data

a_k	=	coefficient of linear expansion of sheathing
a_f	=	" " " " " fuel
a	=	" " " " " spacers
$\rho^{20}_{UO_2}$	=	density of UO_2 at 20 ^oC, g/cm^3
ρ^{20}_k	=	" " sheathing " "
ρ_u	=	density of uranium at prevailing temperature, g/cm^3
ρ_c	=	density of coolant at prevailing temperature, g/cm^3
A_k	=	chemical atomic weight of sheathing
r^{20}_f	=	radius of individual rod at 20 ^oC, cm
r^{20}_{ki}	=	inner radius of sheathing at 20 ^oC, cm
r^{20}_{ky}	=	outer radius of sheathing at 20 ^oC, cm
t_f	=	fuel temperature, ^oC
t_k	=	sheathing temperature, ^oC
t_c	=	coolant temperature, ^oC
F	=	ratio between thermal surface flux and average flux in cluster
N	=	number of rods
M	=	number of outer rods
q	=	$\begin{cases} 1 \text{ if fuel is } UO_2 \\ 2 \text{ if fuel is U} \end{cases}$

Index matrix

To keep the computing time within reasonable limits input should contain information of the collision probabilities p_{ij} which are necessary to calculate. This is done with the aid of an index matrix as follows. Let

i_k = index of a source rod in symmetry group k

a_k = corresponding number of symmetries

j_{kr} = index of a target rod in symmetry group kr

b_{kr} = corresponding number of symmetries

The index matrix is then written as given below

i		j
i_1	(a_1)	j_{11} (b_{11}) .... j_{1r} (b_{1r}) ....
⋮	⋮	....
		....
i_q	(a_q)	j_{q1} (b_{q1}) .... j_{qr} (b_{qr}) ....
⋮	⋮	....
i_k	(a_k)	j_{k1} (b_{k1}) .... j_{kr} (b_{kr}) ....

It should be pointed out that the way in which allowance is made for intermediate rods does not necessitate $p_{ij} = p_{ji}$.

Formulae

Functions

P (x) = Placzek's collision probability for a cylinder

$$\theta_1(R_1, R_2, D) = R_1^2 \left\{ \arccos \frac{D^2+R_1^2 - R_2^2}{2 R_1 D} - \frac{D^2+R_1^2 - R_2^2}{2 R_1 D} \sqrt{1 - \left(\frac{D^2+R_1^2 - R_2^2}{2 R_1 D} \right)^2} \right\}$$

$$+ R_2^2 \left\{ \arccos \frac{D^2+R_2^2 - R_1^2}{2 R_2 D} - \frac{D^2+R_2^2 - R_1^2}{2 R_2 D} \sqrt{1 - \left(\frac{D^2+R_2^2 - R_1^2}{2 R_2 D} \right)^2} \right\}$$

$$\theta_2(R_1, R_2, D) = R_2^2 \left\{ \arccos \frac{R_1^2 - R_2^2 - D^2}{2 R_2 D} - \frac{R_1^2 - R_2^2 - D^2}{2 R_2 D} \sqrt{1 - {\frac{R_1^2 - R_2^2 - D^2}{2 R_2 D}}^{2}} \right\} -$$

$$- R_1^2 \left\{ \arccos \frac{R_1^2 - R_2^2 + D^2}{2 R_1 D} - \frac{R_1^2 - R_2^2 + D^2}{2 R_1 D} \sqrt{1 - \left(\frac{R_1^2 - R_2^2 + D^2}{2 R_1 D} \right)^2} \right\}$$

$$\theta_3(r, \rho) = \begin{cases} r^2 \left\{ \arccos \frac{\rho}{r} - \frac{\rho}{r} \sqrt{1 - \left(\frac{\rho}{r} \right)^2} \right\} & \rho < r \\ 0 & \rho \geq r \end{cases}$$

Preliminary calculations

$$\rho_{UO_2} = \rho_{UO_2}^{20} \left[1 - 3\, a_f \,(t_f - 20) \right] (2 - q) \qquad (1)$$

$$\rho_k = \rho_k^{20} \left[1 - 3\, a_k (t_k - 20) \right] \tag{2}$$

$$x_i = x_i^{20} \left[1 + \alpha (t_c - 20) \right] \tag{3}$$

$$y_i = y_i^{20} \left[1 + \alpha (t_c - 20) \right] \tag{4}$$

$$r_f = r_f^{20} \left[1 + \alpha (t_f - 20) \right] \qquad (q = 1) \tag{5}$$

$$r_{ki} = r_{ki}^{20} \left[1 + \alpha (t_k - 20) \right] \tag{6}$$

$$r_{ky} = r_{ky}^{20} \left[1 + a_k (t_k - 20) \right] \tag{7}$$

<u>Volumes for homogeneous calculation</u>

$$V_{gb} = \pi\, r_f^2 + \frac{1}{2} \Big\{ \left| x_1 y_2 - x_2 y_1 \right| + \text{-----------} + \left| x_{M-1} y_M - x_M y_{M-1} \right| + \left| x_M y_1 - x_1 y_M \right| \Big\} + r_f \left\{ \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} + \text{-----} \sqrt{(x_1 - x_M)^2 + (y_1 - y_M)^2} \right\}; \tag{8}$$

$$V_f = N \pi\, r_f^2 ; \tag{9}$$

$$V_k = (N-1)\pi\, (r_{ky}^2 - r_{ki}^2) - M \left\{ r_{ky}^2 \arcsin \sqrt{1 - \left(\frac{r_f}{r_{ky}}\right)^2} - r_{ki}^2 \arcsin \sqrt{1 - \left(\frac{r_f}{r_{ki}}\right)^2} - r_f\, r_{ky} \sqrt{1 - \left(\frac{r_f}{r_{ky}}\right)^2} + r_f\, r_{ki} \sqrt{1 - \left(\frac{r_f}{r_{ki}}\right)^2} \right\}; \tag{10}$$

$$V_a = (N-1)\pi\,(r_{ki}^2 - r_f^2) - M\left\{r_{ki}^2 \arcsin\sqrt{1-\left(\frac{r_f}{r_{ki}}\right)^2} - r_f\, r_{ki}\sqrt{1-\left(\frac{r_f}{r_{ki}}\right)^2}\right\}; \quad (11)$$

$$V_c = V_{gb} - V_f - V_k - V_a \quad (12)$$

$$a = \sqrt{\frac{V_{gb}}{\pi}} \quad (13)$$

Volumes for heterogeneous calculation

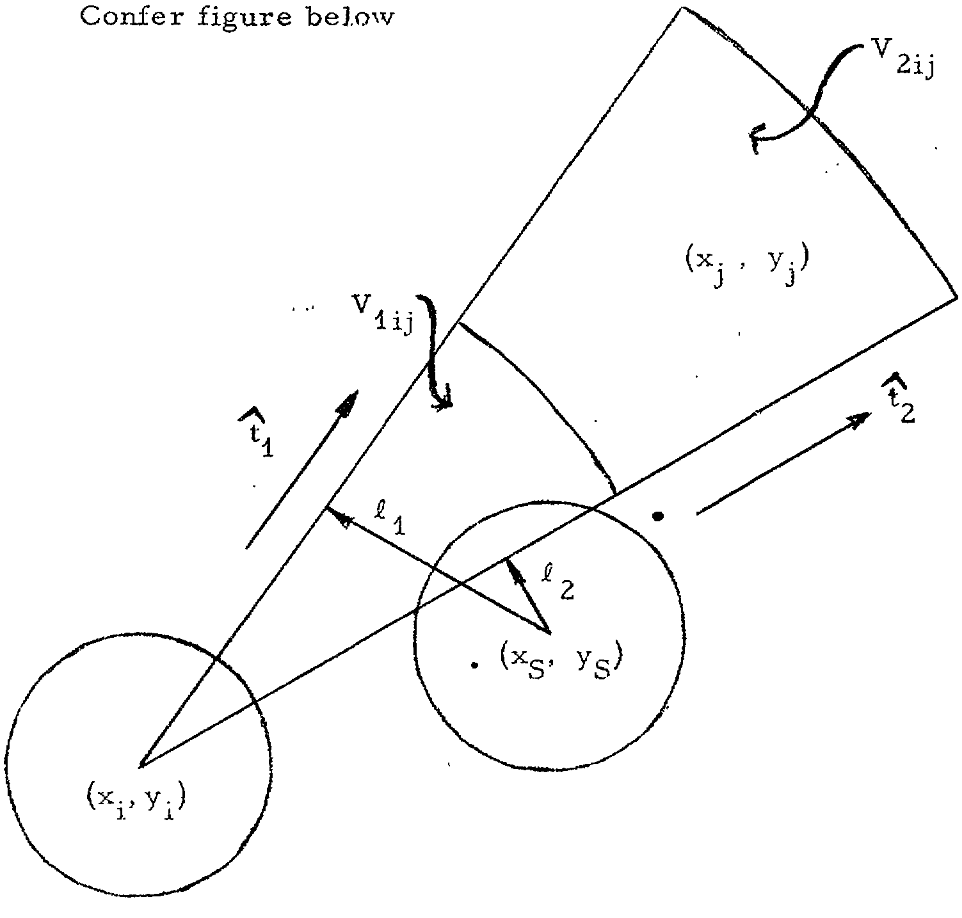
A pair of rods with the coordinates $(x_i,\ y_i)$ and $(x_j,\ y_j)$ are selected.

$$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \quad (14)$$

$$V_{1ij} = d_{ij}\,(d_{ij} - 2r_f)\arcsin\frac{r_f}{d_{ij}}; \quad (15)$$

$$V_{2ij} = 4\, r_f\, d_{ij} \arcsin\frac{r_f}{d_{ij}}; \quad (16)$$

Confer figure below



When calculating the collision probability p_{ij} the volumes of the intermediate materials are to be calculated. This is done as follows.

1) The tangent vectors are determined

$$\hat{t}_{1ij} = \frac{1}{d_{ij}^{2}} \left\{ (x_j - x_i)\sqrt{d_{ij}^2 - r_f^2} - r_f (y_j - y_i),\ (y_j - y_i)\sqrt{d_{ij}^2 - r_f^2} + r_f (x_j - x_i) \right\}$$

$$\hat{t}_{2ij} = \frac{1}{d_{ij}^{2}} \left\{ (x_j - x_i)\sqrt{d_{ij}^2 - r_f^2} + r_f (y_j - y_i),\ (y_j - y_i)\sqrt{d_{ij}^2 - r_f^2} - r_f (x_j - x_i) \right\} \qquad (17)$$

Then an intermediate rod is chosen (x_s, y_s)
(cf. fig. on page 12) $s \neq i$ and j

2) Calculate

$$\ell_{1sij} = \begin{vmatrix} x_s - x_i & y_s - y_i \\ (\hat{t}_{1ij})_x & (\hat{t}_{1ij})_y \end{vmatrix}$$

$$\ell_{2sij} = \begin{vmatrix} x_s - x_i, & y_s - y_i \\ (\hat{t}_{2ij})_x & (\hat{t}_{2ij})_y \end{vmatrix} \qquad (18)$$

3) If $(\bar{r}_s - \bar{r}_i) \cdot \hat{t}_{ij}$ and $(\bar{r}_s - \bar{r}_i) \cdot \hat{t}_{ij}$ are > 0 and $< \sqrt{d_{ij}^2 - r_f^2}$ proceed to 4). If not select a new value of s.

4) If $|\ell_{1s}| \leq r_{ky}$ or $|\ell_{2s}| \leq r_{ky}$ or both proceed to 5). If not select a new value of s.

5) If $\ell_{1s} \geq 0$ and $\ell_{2s} \geq 0$ calculate the volumes given by (19) - (21) and select a new value of s. If not proceed to 6)

$$V_{f1sij} = \theta_3 (r_f, \ell_{2sij}) - \theta_3 (r_f, \ell_{1sij}); \tag{19}$$

$$V_{a1sij} = \theta_3 (_{ki}, \ell_{2sij}) - \theta_3 (r_f, \ell_{2sij}) - \theta_3 (r_{ki}, \ell_{1sij}) + \theta_3 (r_f, \ell_{1sij}); \tag{20}$$

$$V_{k1sij} = \theta_3 (r_{ky}, \ell_{2sij}) - \theta_3 (r_{ki}, \ell_{2sij}) - \theta_3 (r_{ky}, \ell_{1sij}) + \theta_3 (r_{ki}, \ell_{1sij}); \tag{21}$$

6) If $\ell_{1s} \geq 0$ and $\ell_{2s} < 0$ calculate the volumes given by (22) - (24) and select a new value of s. If not proceed to 7).

$$V_{f1sij} = \pi\, r_f^2 - \theta_3 (r_f, \left| \ell_{2sij} \right|) - \theta_3 (r_f, \ell_{1sij}) ; \tag{22}$$

$$V_{a1sij} = \pi\, (r_{ki}^2 - r_f^2) - \theta_3 (r_{ki}, \left| \ell_{2sij} \right|) + \theta_3 (r_f, \left| \ell_{2sij} \right|) -$$

$$- \theta_3 (r_{ki}, \ell_{1sij}) + \theta_3 (r_f, \ell_{1sij}) ; \tag{23}$$

$$V_{k1sij} = \pi\, (r_{ky}^2 - r_{ki}^2) - \theta_3 (r_{ky}, \left| \ell_{2sij} \right|) + \theta_3 (r_{ki}, \left| \ell_{2sij} \right|) -$$

$$- \theta_3 (r_{ky}, \ell_{1sij}) + \theta_3 (r_{ki}, \ell_{1sij}) ; \tag{24}$$

7) Now $\ell_{1s} < 0$, $\ell_{2s} < 0$

Calculate the following volumes

$$V_{f1sij} = \theta_3 (r_f, |\ell_{1sij}|) - \theta_3 (r_f, |\ell_{2sij}|) \tag{25}$$

$$V_{a1sij} = \theta_3 (r_f, |\ell_{2sij}|) - \theta_3 (r_{ki}, |\ell_{2sij}|) + + \theta_3 (r_{ki}, |\ell_{1sij}|) - \theta_3 (r_f, |\ell_{1sij}|); \tag{26}$$

$$V_{k1sij} = \theta_3 (r_{ki}, |\ell_{2sij}|) - \theta_3 (r_{ky}, |\ell_{2sij}|) + + \theta_3 (r_{ky}, |\ell_{1sij}|) - \theta_3 (r_{ki}, |\ell_{1sij}|); \tag{27}$$

The procedure 2) - 7) is repeated with every value of s $\neq$ i and $\neq$ j. Then calculate

$$V_{f1ij} = \sum_s V_{f1sij} \tag{28}$$

$$V_{a1ij} = \sum_s V_{a1sij} + \theta_1 (r_{ki}, d_{ij} - r_f, d_{ij}) + (r_{ki}^2 - r_f^2) \arcsin \frac{r_f}{d_{ij}} \tag{29}$$

$$V_{k1ij} = \sum_s V_{k1sij} + \theta_1 (r_{ky}, d_{ij} - r_f, d_{ij}) - \theta_1 (r_{ki}, d_{ij} - r_f, d_{ij}) + + (r_{ky}^2 - r_{ki}^2) \arcsin \frac{r_f}{d_{ij}} \tag{30}$$

$$V_{c1ij} = V_{1ij} - V_{f1ij} - V_{a1ij} - V_{k1ij} \tag{31}$$

$$V_{f2ij} = \pi r_f^2 \tag{32}$$

$$V_{a2ij} = \pi \, (r_{ki}^2 - - r_f^2) - \theta_1 \, (r_{ki}, \; d_{ij} - r_f, \; d_{ij}) - 2 \, \theta_3 \, (r_{ki}, \; r_f) -$$

$$- \theta_2 \, (d_{ij} + r_f, \; r_{ki}, \; d_{ij}) \; ; \qquad (33)$$

$$V_{k2ij} = \pi \, (r_{ky}^2 - r_{ki}^2) - \theta_1 \, (r_{ky}, \; d_{ij} - r_f, \; d_{ij}) + \theta_1 \, (r_{ki}, \; d_{ij} - r_f, \; d_{ij}) -$$

$$- 2\theta_3 \, (r_{ky}, \; r_f) + 2\theta_3 \, (r_{ki}, \; r_f) - \theta_2 \, (d_{ij} + r_f, \; r_{ky}, \; d_{ij}) +$$

$$+ \theta_2 \, (d_{ij} + r_f, \; r_{ki}, \; d_{ij}) \; ; \qquad (34)$$

$$V_{c2ij} = V_{2ij} - V_{f2ij} - V_{a2ij} - V_{k2ij} \qquad (35)$$

Homogeneous calculation

$$N_f = 6,0232 \cdot 10^{23} \left[\frac{\rho_{UO_2}}{270,07} + (q - 1) \frac{\rho_U}{238,07} \right] \qquad (36)$$

$$N_c = 6,0232 \cdot 10^{23} \cdot \frac{\rho_c}{20,030} \qquad (37)$$

$$N_k = 6,0232 \cdot 10^{23} \cdot \frac{\rho_k}{A_k} \qquad (38)$$

$$\bar{\Sigma} = \frac{1}{V_{gb}} \left\{ \sigma_2^U \, N_f V_f + \sigma_2^O \cdot 2N_f V_f (2 - q) + \sigma_2^D \cdot 2 \cdot N_c V_c + \right.$$

$$\left. + \sigma_2^O \, N_c V_c + \sigma_2^k \, N_k V_k \right\} ; \qquad (39)$$

$$\bar{\Sigma}_1 = \frac{1}{V_{gb}} \left\{ \sigma_1^U \, N_f V_f + \sigma_1^O \, 2N_f V_f \, (2 - q) + \sigma_1^D \, 2N_c V_c + \right.$$

$$\left. + \sigma_1^O \, N_c V_c + \sigma_1^k \, N_k V_k \right\} ; \qquad (40)$$

$$\beta = \frac{\sigma_2^U \, N_f V_f}{V_{gb} \; \bar{\Sigma}} \qquad (41)$$

$$\beta_1 = \frac{\sigma_1^U N_f V_f}{V_{gb}\ \bar{\Sigma}_1} \tag{42}$$

$$\beta' = \frac{\sigma_{22}^O\ 2N_f V_f\,(2-q) + \sigma_{22}^D \cdot 2N_c V_c + \sigma_{22}^O\ N_c V_c + \sigma_{22}^k\ N_k V_k}{\sigma_2^U N_f V_f} \tag{43}$$

$$\beta_1' = \frac{\sigma_{11}^O\ 2N_f V_f\,(2-q) + \sigma_{11}^D\ 2N_c V_c + \sigma_{11}^O\ N_c V_c + \sigma_{11}^k\ N_k V_k}{\sigma_2^U N_f V_f} \tag{44}$$

$$\beta'' = \frac{\sigma_{21}^O\ 2N_f V_f\,(2-q) + \sigma_{21}^D\ 2N_c V_c + \sigma_{21}^O\ N_c V_c + \sigma_{21}^k\ N_k V_k}{\sigma_2^U N_f V_f} \tag{45}$$

$$\underline{P} = P\,(\bar{\Sigma}a) \tag{46}$$

$$\underline{P}_1 = P\,(\bar{\Sigma}_1 a) \tag{47}$$

$$f = \frac{\sigma_{2f}^U}{\sigma_2^U} \tag{48}$$

$$e = \frac{\sigma_{22}^U}{\sigma_2^U} \tag{49}$$

$$i_{21} = \frac{\sigma_{21}^U}{\sigma_2^U} \tag{50}$$

$$c = \frac{\sigma_{2c}^U}{\sigma_2^U} \tag{51}$$

$$e_1 = \frac{\sigma_{11}^U}{\sigma_1^U} \tag{52}$$

$$i_1 = \frac{\sigma_{10}^U}{\sigma_1^U} \tag{53}$$

$$\gamma_{hom} = \frac{c_1 \beta_1 \underline{P}_1}{1 - (e_1 + \beta_1') \beta_1 \underline{P}_1} \tag{55}$$

$$\epsilon_{hom} = 1 + \frac{\omega \left[(\nu' - 1) f - c \right] \beta \underline{P} - \gamma_{hom} \left[\omega_1 - \left\{ e \omega_1 - \omega i_{21} + \beta' \omega_1 - \omega p'' \right\} \beta \underline{P} \right]}{1 - \left[e + \omega \nu' f + \beta' \right] \beta \underline{P}} \tag{56}$$

$$R_{hom} = \frac{\omega \nu \beta \underline{P} f}{1 - \left[e + \omega \nu' f + \beta' \right] \beta \underline{P}} \tag{57}$$

Heterogeneous calculation

$$a_0 = r_f \tag{58}$$

$$a_{1ij} = d_{ij} - a_0 \tag{59}$$

$$a_{2ij} = d_{ij} + a_0 \tag{60}$$

$$\Sigma_f = (\sigma_2^U + 2\,(2-q)\,\sigma_2^O)\, N_f \tag{61}$$

$$\Sigma_c = (2\,\sigma_2^D + \sigma_2^O)\, N_c \tag{62}$$

$$\Sigma_k = \sigma_2^k \cdot N_k \tag{63}$$

$$\Sigma_{(0)} = \Sigma_f \tag{64}$$

$$\Sigma_{(1)ij} = \frac{\Sigma_f V_{f1ij} + \Sigma_c V_{c1ij} + \Sigma_k V_{k1ij}}{V_{1ij}} \; ; \tag{65}$$

$$\Sigma_{(2)ij} = \frac{\Sigma_f V_{f2ij} + \Sigma_m V_{m2ij} + \Sigma_k V_{k2ij}}{V_{2ij}} \; ; \tag{66}$$

$$\Sigma_U = \sigma_2^U \; N_f \tag{67}$$

$$p_0 = P\,(\Sigma_{(0)}\, a_0\,) \cdot \frac{\Sigma_U}{\Sigma_{(0)}} \tag{68}$$

$$\alpha = \frac{a_0}{a_2} \tag{69}$$

$$\beta = \frac{a_0}{a_1} \tag{70}$$

$$\xi_{ij} = a_2\, \Sigma_{(2)\, ij} \tag{71}$$

$$\eta_{ij} = a_0\, \Sigma_{(0)} \tag{72}$$

$$\zeta_{ij} = a_1 \Sigma_{(1)\, ij} \tag{73}$$

$$\begin{aligned} W_{ij} = {} & \frac{2\,\alpha}{\xi_{ij}\,\eta_{ij}\,\pi\,(1-\alpha^2)} \cdot \int_0^{\pi/2} d\,\varphi\,\cos\varphi \int_0^{\pi/2} d\,\theta\,\sin^2\theta \,\cdot \\ & \cdot \exp\left\{- \frac{\zeta_{ij}}{\sin\theta}\left(\sqrt{1-\beta^2\sin^2\varphi} - \beta\cos\varphi\right)\right\} \cdot \\ & \cdot \left[1 + \exp\left\{- \frac{1}{\sin\theta}\left(2\,\eta_{ij}\cos\varphi + \xi_{ij}\left[\sqrt{1-\alpha^2\sin^2\varphi} - \alpha\cos\varphi\right]\right)\right\} - \right. \\ & \left. - \exp\left(-\,2\,\eta_{ij}\,\frac{\cos\varphi}{\sin\theta}\right) - \exp\left(- \frac{\xi_{ij}}{\sin\theta}\left[\sqrt{1-\alpha^2\sin^2\varphi} - \alpha\cos\varphi\right]\right)\right]; \end{aligned} \tag{74}$$

$$p_{ij} = a_0\; \Sigma_U\, W_{ij} \tag{75}$$

$$r_i = \sqrt{x_i^2 + y_i^2} \tag{76}$$

$$\phi_i = 1 + \frac{2\,(F-1)}{a^2\,(2-F)} \quad r_i^2 \;; \tag{77}$$

$$\bar{\Phi} = \frac{1}{N} \sum_{i=1}^{N} \phi_i \tag{78}$$

$$p = p_0 + \frac{1}{N\,\bar{\Phi}} \sum_{q=1}^{k} a_q \;\; \phi_{i_q} \sum_{r=1}^{\ell} b_{qr}\, p_{i_q j_r} \tag{79}$$

$$p_1 = \beta_1 \underline{P}_1 + p - \beta\, \underline{P} \tag{80}$$

$$p_1^* = p_1 + \frac{p_1\, \underline{P}_1\, \beta_1}{1 - \underline{P}_1\, \beta_1\, \beta_1'} \tag{81}$$

$$p_1' = \frac{(\underline{P}_1 - p_1)\, \beta_1 \beta_1'}{1 - \beta_1} \tag{82}$$

$$\gamma^* = \frac{c_1\, p_1^*}{1 - e_1 p_1^*} \tag{83}$$

$$p' = \frac{(\underline{P} - p)\, \beta\, \beta'}{1 - \beta} \tag{84}$$

$$p^* = p + \frac{p'\, \underline{P}\, \beta}{1 - \underline{P}\, p\, p'} \tag{85}$$

$$\epsilon_{het} = 1 + \frac{\omega \left[(\nu' - 1) f - c \right] p^* - \gamma^* \left[\omega_1 - \left\{ e\, \omega_1 - i_{21} \omega \right\} p^* + \omega \dfrac{\beta''}{\beta'} \;\; \dfrac{p'}{1 - \beta\beta' \underline{P}} \right]}{1 - (e + \omega\, \nu' f)\, p^*} \tag{86}$$

$$R_{het} = \frac{\omega\, \nu\, p^*\, f}{1 - \left[e + \omega\, \nu' f \right] p^*} \;; \tag{87}$$

Output

The output will appear as follows.

INPUTDATA		α_k	α_f	α
$\rho^{20}_{UO_2}$	ρ^{20}_k	ρ_u	ρ_c	A_k
r^{20}_f	r^{20}_{ki}	r^{20}_{ky}	t_f	t_k
t_c	F	N	M	q

RESULTS

ρ_{UO_2}	ρ_k	r_f	r_{ki}	r_{ky}
V_{gb}	V_f	V_k	V_c	
N_f	N_c	N_k	β $\underline{P}$	
ϵ_{hom}	R_{hom}			
i =	j = 1	p_{ij}		
	-			
	-			
	-			
ϵ_{het}	R_{het}			

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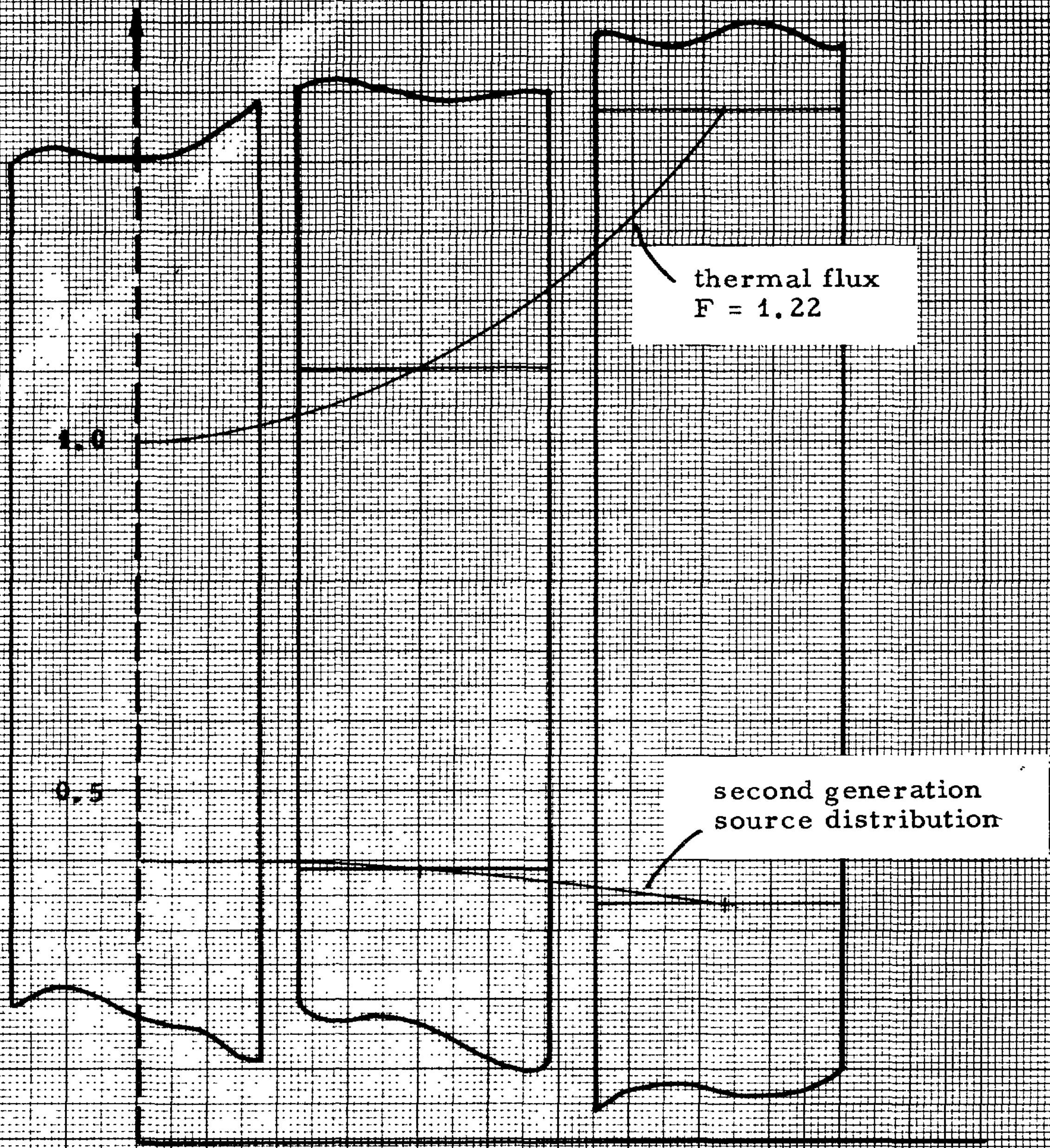
Graph 1

The source distribution of the second generation in a 19-rod cluster.



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