Integral transport theory in various geometrics

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Integral Transport Theory in Various Geometries

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Abstract

The main equation of integral transport theory in multigroup version is shortly discussed. The calculation of the collision matrix in annular symmetric clusters by numerical integration in a modified CLUCOP scheme is shortly described. An approximate method for obtaining the same results is given in details and comparison between some results from this method and the original CLUCOP-programme is given. A short discussion of the construction of source terms and transport corrected cross sections is also given.

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1. Introduction

The method of integral transport theory as formulated with multi-region collision probability is excellently suited for cell calculations in particular when complicated geometrical configurations are considered.

The whole formalism may be expressed by the simple equation

$$\phi_i^g \Sigma_i^g V_i = \sum_j (\phi_j^g \Sigma_{js}^g + q_j^g) V_j P_{ij}^g \qquad (1.1)$$

where ϕ_i^g, Σ_i^g and Σ_{is}^g are respectively the average (flat) flux, total and scattering cross sections in energy group g and spatial region i of volume V_i.

q_i^g is the external source in energy group g and spatial region i, including up- and down-scattering from other groups.

The matrix element P_{ij}^g gives the probability that a neutron emitted in energy group g uniformly and isotropically over region j will make its first collision in region i.

When anisotropic scattering and fission occurs, as is usually the case, special conventions should be introduced for the construction of Σ_i^g, Σ_{is}^g and q_i^g.

This problem will be treated in a later section, but in the immediately following sections mainly concerned with finding the P_{ij}'s for various geometries (1.1) will be treated as a one-group problem, dropping the index g.

2. Annular Symmetry

Several methods have been proposed [1], [2] and [3] to find the collision matrix P_{ij} in systems of annular symmetry.

We have, however, adopted the so-called Flurig scheme from [3] in our CPM procedure since this solution is exact and at the same time comparable in speed with other methods.

In CPM white boundary conditions are used, but a greyness parameter can modify this through all shades of greyness to complete blackness.

A special version CPMB uses only black boundary conditions and calculates at the same time the sticking probabilities P_{is} that a neutron emitted

from the boundary according to a cosine law will collide in region i.

3. Clusters in Annular Symmetry

A solution of this type of problem, the so-called CLUCOP scheme, is described in [3]. Numerical integration in a network of lines in several directions is used inside the cluster proper whereas the Flurig system is used in the outside annular regions. The CLUCOP programme which is very general with options for very fine subdivisions of regions is an excellent reference, but is rather slow for multigroup application. It should be underlined that the reciprocity relation used on the white or grey boundary in order to transfer the black boundary P_{ij}'s to white or grey boundary is not exact for clusters as it is for purely annular symmetry, but gives a very good approximation as long as the cluster has a reasonable degree of symmetry.

A simplified version of CLUCOP has been adopted in which no annular subdivisions appear which may intersect with fuel rods. The subdivision of fuel rods is restricted to one canning zone and one fuel zone.

This version, called MICMAC, uses a linear network defined by only two directions. One direction is passing from the centre of the cell through the centre of a fuel pin and one is bisecting the angle between two neighbouring fuel pins. The mean value is taken from the results of the numerical integrations perpendicular to these two directions.

Gaussian integration is used defining a new integration interval whenever a line sweeping parallel to the direction considered makes or finishes contact with a new region.

4. The MAMIC Cluster Approximation

Several attempts have been made by us to construct an approximation based on a combination of CPM on homogenized regions with CPM on certain cylindricized sectors of annuli surrounding the individual fuel pins. In order to obtain a good approximation we have found that the following facts should be taken into consideration.

First of all a simple homogenization of an annular region will under-

estimate the transparency of such a region in the presence of very black fuel pins since it more or less ignores the possibility of neutrons passing through the space between the pins.

A device described by Bollacasa and Bonalumi in [5] copes very nicely with this problem.

Secondly, we have found it important that suitable weighted sums of the matrix elements pertaining to subregions of an annular macroregion should as closely as possible add up to the matrix elements of the macroregion. This requirement will to a certain extent be in conflict with the reciprocity theorem which we believe should be valid for any useful approximation.

Finally we have found less ambiguity in interpreting the approximation if the scattering matrix is first derived for black cell boundary condition.

Referring to fig. 1 the procedure is the following:

If an annular macroregion, i, contains fuel pins, it is divided into equally large sectors each containing one fuel pin. Analogue subregions in all sectors belonging to the same annulus are considered as belonging to one and the same subregion.

Conserving its volume the sector is transformed into a subcylinder, concentric with the fuel pin, which may consist of an arbitrary number of concentric subregions.

In this way the centre of the fuel pin will automatically be calculated as if situated roughly half way between inner and outer radius of the macroregion. Preferably the diameter of the fuel pin should be less than the difference between these two radii, and imperatively the area of the sector should be larger than the cross section area of the fuel pin.

The number of regions in the subcylinder will be the number of subregions in the pin plus one corresponding to the remaining region in the sector.

CPMB is applied to the subcylinder yielding the collision matrix $P^i_{p,q}$ and the sticking probabilities $P^i_{p,s}$, and the total sticking probability $G^i = \sum_p P^i_{p,s}$ is calculated.

According to [4] we now choose for the macroregion an effective cross section Σ_i, which would give the same sticking probability G^{hom} in a homogeneous cylinder with the same radius, r_{sub}, as the subcylinder.

A good approximation of G^{hom} is given by

$$G^{hom} = (l^2 + 2l)/(l^2 + 2l + 2) \; ; \; l = 2 \times r_{sub} \times \Sigma_i \qquad (4.1)$$

leading to the simple expression.

$$\Sigma_i = (\mathrm{sqrt}((1+G^1)/(1-G^1))-1)/l \qquad (4.2)$$

When a Σ_i value has been assigned to all macroregions, i, CPMB is applied to the annular symmetric system of macroregions.

In order to calculate the collision matrix element corresponding to two subregions within the same macroregion, we return to the CPMB results given for the subcylinder above.

Since the segments have boundaries in common and since neutrons leaving a segment through regions inside the corresponding annulus may return to another segment in the annulus, it is reasonable to assign a degree of greyness g to the houndary of the corresponding subcylinder.

The magnitude of g should be such that the total prohability of collission of neutrons emitted uniformly inside the cylinder should equal P_{ii}, when the greynes is taken into consideration.

If $P_c = \sum_{p,q} P^i_{p,q} \times V_q / \sum_q V_q$ is the collision probability of the subcylinder for black boundary condition, this equality may be expressed by

$$P_{ii} = P_c + (1-P_c) \times g \times G^i/(1-g \times (1-G^i)) \qquad (4.3)$$

leading to the expression

$$g = (P_{ii} - P_c)/(1 - P_c - (1 - G^i) \times (1 - P_{ij})) \qquad (4.4)$$

The final expression for the prohability $Pf^{i,j}_{p,g}$ that a neutron emitted uniformly in subregion q in macroregion i will collide in subregion p in the same macroregion becomes.

$$P^{j,i}_{p,q} = P^i_{p,q} + P^i_{S,p} \times P^1_{s,p} \times g \times r^i_{sub} \times \pi / (2 \times \Sigma^1_q \times V^i_q \times (1-g \times (1-G^i))) \qquad (4.5)$$

A consequence of this formulation is that

$$\sum_{p,q} P^{i,i}_{p,q} \times V^i_q = P_{i,i} \qquad (4.6)$$

as wanted and that the reciprocity relation

is valid $P^{i,i}_{p,q} \times V^i_q \times \Sigma^i_q = P^{ii}_{q,p} \times V^i_p \times \Sigma^i_p$ (4.7)

The probabillity, $P^{i,j}_{p,q}$ that a neutron emitted uniformly in subregion q in macroregion j will collide in subregion p in macroregion i is tentatively proposed as.

$$P^{i,j}_{p,q} = \text{norm}_j \times P^i_{ps} \times P^j_{qs} \times V_j/(\Sigma^j_q \times V^j_q) \quad (4.8)$$

$$\text{norm}_j = P_{i,j}/(G^i \times \sum_q (P^j_{qs}/V^j_q))$$

with the wanted property

$$\sum_{p,q} P^{i,j}_{p,q} \times V^j_q/V_j = P_{i,j} \quad (4.9)$$

The analogue expression for $P^{j,i}_{q,p}$ is

$$P^{j,i}_{q,p} = \text{norm}_i \times P^j_{qs} P^i_{ps} \times V_i /(\Sigma^i_j V^i_p) \quad (4.10)$$

$$\text{norm}_i = P_{j,i}/(G^j \times \sum_p (P^i_{ps}/V^i_p))$$

The reciprocity relation

$$P^{i,j}_{p,q} \times \Sigma^j_q \times V^j_q = P^{j,i}_{q,p} \times \Sigma^i_p \times V^i_p \quad (4.11)$$

used on (4.10) leads to a new expression

$$P^{i,j}_{p,q} = \text{norm}_i \times P^j_{qs} P^i_{ps} \times V_i /(\Sigma^j_g \times V^j_q)$$

Since both conditions (4.9) and (4.11) cannot generally be fullfilled at the same time the following compromise is chosen.

$$P^{i,j}_{p,q} = \tfrac{1}{2} \times(\text{norm}_j \times V_j + \text{norm}_i \times V_i) \times P^i_{ps} \times P^j_{qs} /(\Sigma^j_q V^j_q) \quad (4.12)$$

$$P^{j,i}_{q,p} = P_{ip,jg} \times \Sigma^{j}_{q} \times V^{j}_{g} / (\Sigma^{i}_{p} \times V^{i}_{p})$$

When macroregions i and j each consists of one single subregion, so that p and q can only assume the value 1 we have

$$P^{i,j}_{p,q} = P_{i,j}k \quad P^{j,i}_{q,p} = P_{j,i}$$

In this way a collision matrix $Pf_{i,j}$, so far with black cell boundary conditions, can be calculated, where i, and j, now runs over all individual subregions.

The transition to grey boundary conditions follows in the usual way.

First the prohability $Pf_{s,i}$ of a neutron from subregion i to cell surface is obtained by the summation.

$$Pf_{s,i} = 1 - \sum_{j} Pf_{j,i}$$

Then the prohability, $Pf_{i,s}$ of neutrons emitted from the cell boundary according to cosine law colliding in subregion i is calculated from the reciprocity relation with a white boundary condition

$$Pf_{i,s} = Pf_{s,i} \times \Sigma_{i} \times V_{i} / (r_{cell} \times \pi/2) \qquad (4.13)$$

This procedure is only strictly correct in case of complete annular symmetri since otherwise $Pf_{i,s}$ will vary along the cell boundary. (4.13) will however be a good approximation if the degree of symmetri of the cluster is high and/or the distance from the cluster to the cell boundary is large.

The collision matrix, $Pf^{gr}_{i,j}$ corresponding to a greynes parameter gr is the calculated as

$$Pf^{gr}_{i,j} = Pf_{ij} + Pf_{sj} \times gr/(1 - gr \times (1 - Gf)) \qquad (4.14)$$

Several comparisons have been made on the IBM 7094 of NEUCL between results obtained with the MAMIC written in Illinoyse Algol and the original CLUCOP program, written in FORTRAM IV, which we have received from the ENEA in Ispra.

Fig. 2 shows a relatively simple example with only 4 regions of which two are strongly absorbing and weakly moderating fuel regions and the two remaining regions are strongly moderating and weakly absorbing (heavy water).

In the scattering matrix deviations up to 10% from the exact matrix CLUOP) appears.

The distribution of the resulting flux between the two fuel regions is correct within 1%. However, since only 2 o/oo of the absorption takes place in the moderator regions, small errors in the fuel flux has to be compensated by larger errors in the moderator regions, in the present case 5.5% and 4%, in order to maintain neutron balance.

In fig. 3 is shown flux results from a calculation of a 31-rod Marviken fuel element, the details of which are given in [4]. The MAMIC results are compared with two sets of results calculated with CLUCOP. One set is calculated for the same subdivision as used in MAMIC and one set taken from [4] with a further subdivision of the three annular fuel regions.

It is seen from fig. 3 that the agreement between results from CLUCOP and MAMIC is remarkably good when the subdivision is identical. The maximum flux deviation, which appears in the central fuel pin, is 1.8%.

However, one weakness with the MAMIC approximation and also with the present version of MICMAC is that the fuel-bearing annuli considered as macroregions cannot be further divided. This in contrast to CLUCOP where further subdivision by circles concentric with the cell is possible.

A consequence of the more coarse annular subdivision is too high flux in the inner region and too low in the outer region.

If the subdivision used in the calculations from [4], shown as dotted lines, is considered fine enough, so that no significant change would result from further subdivision, the total error caused by the MAMIC approximation can be estimated to be 4% in the central fuel pins.

Calculation times are 4.5 minutes for CLUCOP and 4.2 seconds with MAMIC for the two identical 31-rod problems.

5. Cross sections

As mentioned in the introduction some conventions for calculating the quantities Σ_i^g Σ_{is}^g and q_i^g taking into account fission and anisotropy of scattering.

The data available for this calculation are microscopic group-cross sections produced by the SIGMA processing program.

The simplest standard output from SIGMA could for each nuclide and group g be σ_t^g total cross section, σ_a^g absorbtion cross section, σ_{fis}^g fission cross section, ν_g number of neutrons per fission; $\sigma_o^{g'g}$ transfer cross section from group g to group g' and $\sigma_1^{g'g}$ the first legendre moment of the transfer cross section from group g to group g'.

$\sigma_o^{g'g}$ and $\sigma_1^{g'g}$ could in principle include n, 2n-, n, 3n- and fission-processes. In this way it would be possible to make transport correction for the anisotropy of these processes. However, this would complicate the introduction of a suitable eigenvalue k_∞ into the complete system (1.1) taken for all g's.

In the output of the present version of SIGMA fission-, n, 2n- and n, 3n- processes are represented by a fission matrix $\sigma_f^{g'g}$ giving the number of neutrons appearing in group g' from fission-, n, 2n- and n, 3n-processes in group g per unit flux in this group.

Several ways have been proposed to make transport correction for anisotropy.

The simple transport correction consists as proposed in [6] of the transformation

$$\sigma_{tr}^g = \sigma_t^g - \sigma_1^{gg}$$

$$\sigma_{tr}^{g'g} = \sigma_o^{g'g} - \delta_{g'g}\,\sigma_1^{gg} \qquad (5.1)$$

This gives the right transport correction for the distribution of the neutrons inside group g but fails in correcting the anisotropy of the neutrons scattered to other groups.

An improved transport correction is obtained by

$$\sigma_{tr}^g = \sigma_t^g - \sum_{g'} \sigma_1^{g'g}$$

$$\sigma_{tr}^{g'g} = \sigma_o^{g'g} - \delta_{g'g} \sum_{g'} \sigma_1^{g'g} \qquad (5.2)$$

Both (5. 1) and (5. 2) fulfil the necessary condition that the use of σ_{tr}^{g} and $\sigma_{tr}^{gg'}$ instead of σ_{t}^{g} and σ_{o}^{gg} leads to the correct fluxes and reaction rates in an infinite homogeneous medium for a given volume source q^g as seen from

$$\phi^g = \frac{q_g}{\Sigma_t^g - \Sigma_o^{gg}} = \frac{q_g}{\Sigma_{tr}^g - \Sigma_{tr}^{gg}} \qquad (5.3)$$

The reaction rate, e. g. for absorption in group g, R_a^g or for scattering from group g to g', $R^{g'g}$ in both of the cases (5. 1) and (5. 2) becomes

$$R_a^g = \phi_g \sigma_a , \quad R^{g'g} = \phi_g \sigma_o^{g'g} = \phi_g \sigma_{tr}^{g'g} \qquad g \neq g' \qquad (5.4)$$

The reaction rate R^{gg} will of course be quite wrong, in the case of (5. 2) even negative for light nuclides.

As pointed out in [6] the consequence of this will be that the flux distribution in the groups for a calculation where the transport correction is made according to (5. 2) will be distorted, whereas the flux distribution in the lower groups, which is most important in thermal reactors, will be more correct compared with results obtained by (5. 1) or no correction at all.

This will, however, be the case if the major part of the neutrons in the lower groups has been scattered through several groups. In case of very light nuclides or inelastic scattering, where neutrons are scattered directly from high-energy groups to low-energy groups, the use of (5. 2) will lead to over-correction.

A way to get round this problem would in case of inelastic scattering be to put a suitable weight factor on the transport correction of the inelastic part of the scattering in the following way:

$$\sigma_{tr}^{g} = \sigma_a^g + \sigma_{fis}^g + \sum_{g'} (\sigma_{oel}^{g'g} + \sigma_{oinel}^{g'g} - \sigma_{lel}^{g'g} - a_g \sigma_{linel}^{g'g}) \qquad (5.5)$$

$$\sigma_{tr}^{g'g} = \sigma_{oel}^{g'g} + \sigma_{oinel}^{g'g} - \delta_{g'g} (\Sigma_{lel}^{g'g} - a_g \sigma_{linel}^{g'g})$$

a_g could be an empirical constant, $0 \leq a_g \leq 1$, dependent on the ratio

between the lower energy boundary of group g and the upper energy boundary of the first group, into which neutrons from group g is carried by inelastic scattering. In actual practice $a_g = 0$ is commonly used and is adopted in the present version of SIGMA.

For light nucleai a linear combination between (5.1) and (5.2)

$$\sigma_{tr}^{g} = \sigma_{t}^{g} - (1-a_g)\ \sigma_{l}^{gg} - a_g \sum_{g'} \sigma_{l}^{g'g}$$

$$\sigma_{tr}^{g'g} = \sigma_{o}^{g'g} - \delta_{g'g}\ (1-a_g)\ \sigma_{l}^{gg} - a_g \sum_{g'} \sigma_{l}^{g'g} \qquad (5.6)$$

might be a better approximation than either (5.1) and (5.2). However, the proper choice of a_g can hardly be made from simple physical considerations, but will have to be made empirical by comparison with more exact calculations.

From the microscopic cross sections and cross section matrices equivalent macroscopic quantities for each region are build up according to the density of the different nuclides.

For a given region i we get the following cross sections and source term:

$$\Sigma_{i}^{g} = \Sigma_{tr}^{g}$$

$$\Sigma_{is}^{g} = \Sigma_{tr}^{gg} \qquad (5.7)$$

$$q_i^g = \sum_{g' \neq g} \phi_i^{g'}\ \Sigma_{tr}^{gg'} + \sum_{g'} \phi_i^{g'}\ \Sigma_{f}^{gg'}$$

6. Future Developments

As pointed out in the introduction the method of integral transport theory is excellently suited for calulating flux distribution and spectrum in complicated geometry, however, provided suitable transport-corrected cross sections can be introduced.

One line of future development will therefore consist in a search for better transport corrections, maybe in the direction indicated by (5.5) and (5.6). At present an investigation is carried out comparing results obtained by use of (5.1) and (5.2) with more exact calculations (Sn. method).

A second line of development regards the extension of the method to systems of rectangular symmetry, in order to be able to use it on typical light-water systems.

Some development has been done in calculating the collision matrix of a system consisting of rectangular subcells. One further development could be to introduce circular fuel rods into the rectangular subcells and use the MAMIC principle to obtain the resulting matrix.

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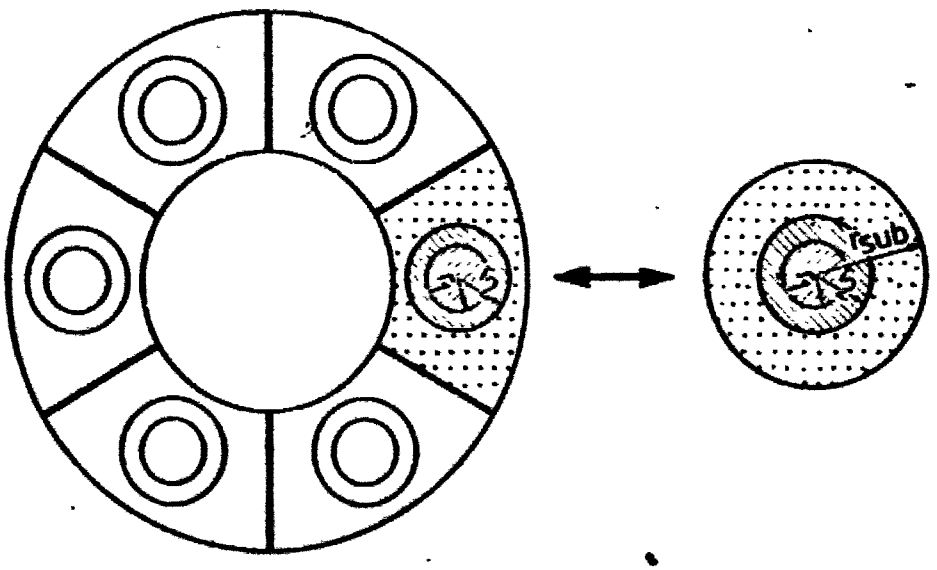
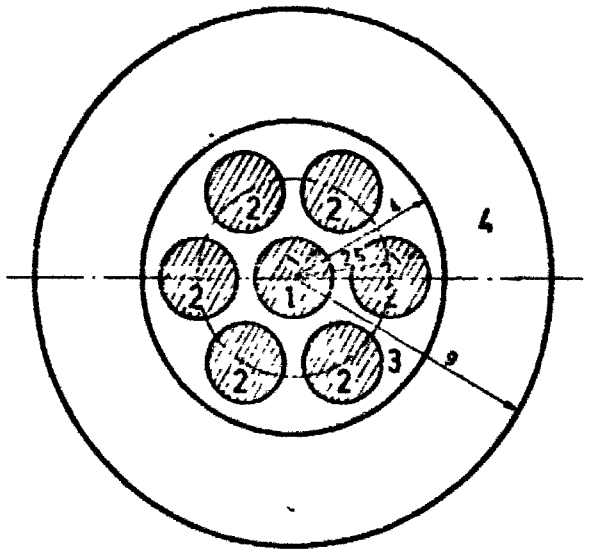


Fig. 1

TEST COMPARISON BETWEEN MAMIC AND CLUCOP



Region	Σtr	Σa	Source
1	0.79069	0.39500	0.00105
2	0.79069	0.39500	0.00105
3	0.39524	0.000033	0.05671
4	0.39524	0.000033	0.05671

Scattering Matrix

		from region 1	2	3	
to region	1	0.5265 (0.5276)	0.0304 (0.0325)	0.0490 (0.0474)	0.0022 (0,0020)
	2	0.1826 (0.1952)	0.5872 (0.6066)	0.2769 (0.2667)	0.0323 (0.0297)
	3	0.2203 (0.2132)	0.2076 (0.2000)	0.3929 (0.3872)	0.0389 (0.0414)
	4	0.0706 (0.0640)	0.1748 (0.1608)	0.2819 (0.2988)	0.9266 (0.9270)

Region	Volume	Flux	Volume x absorption
1	3.1416	1.214 (1.225)	1.5066 (1.5197)
2	18.850	15.682 (15.663)	11.676 (11.662)
3	28.274	21.322 (22.638)	0.002 (0.002)
4	204.20	33.789 (35.162)	0.023 (0.024)

Quantities in paranthesis are CLUCOP-results

Fig. 2

MARVIKEN 31-ROD CELL

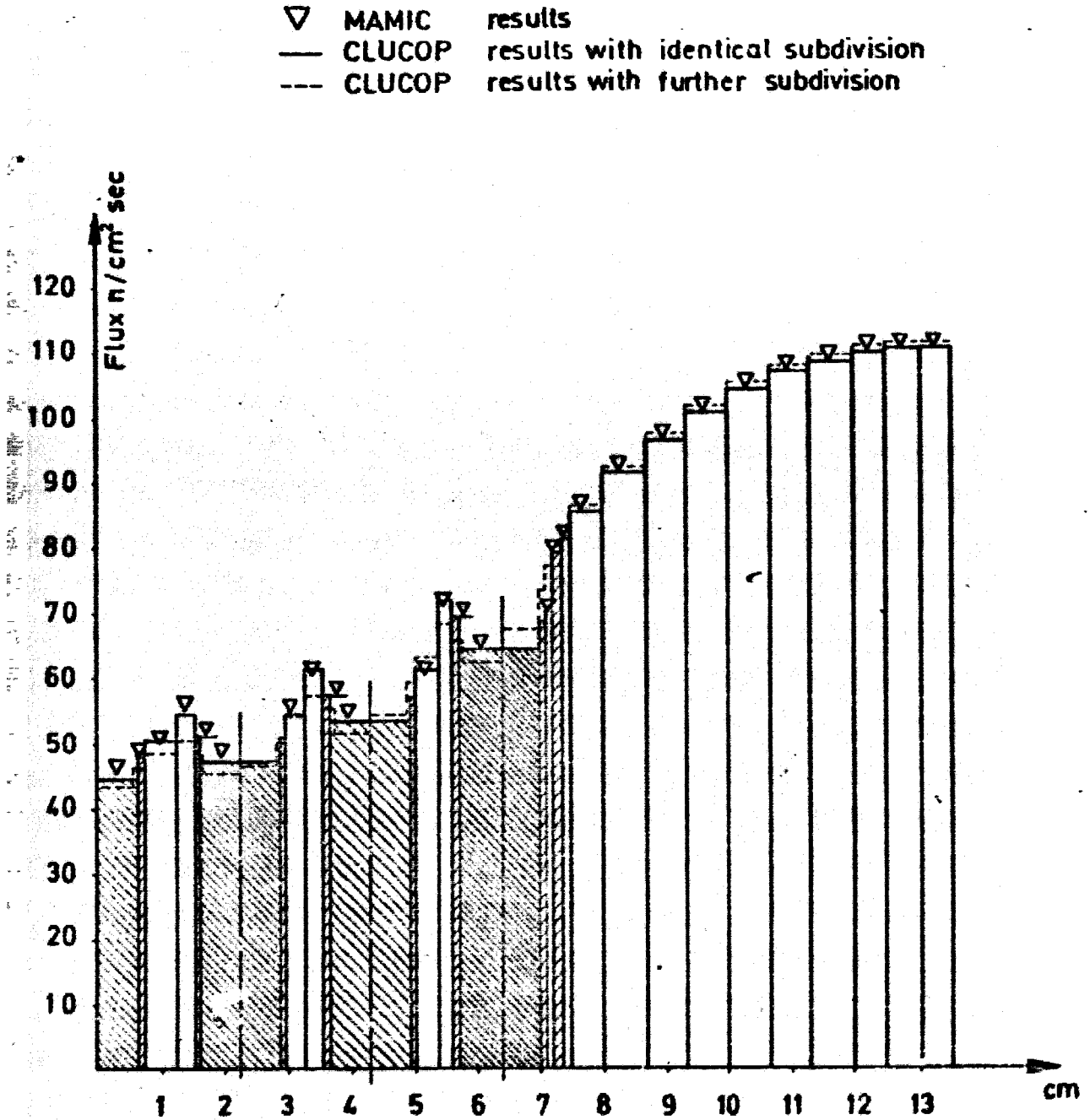


Fig. 3