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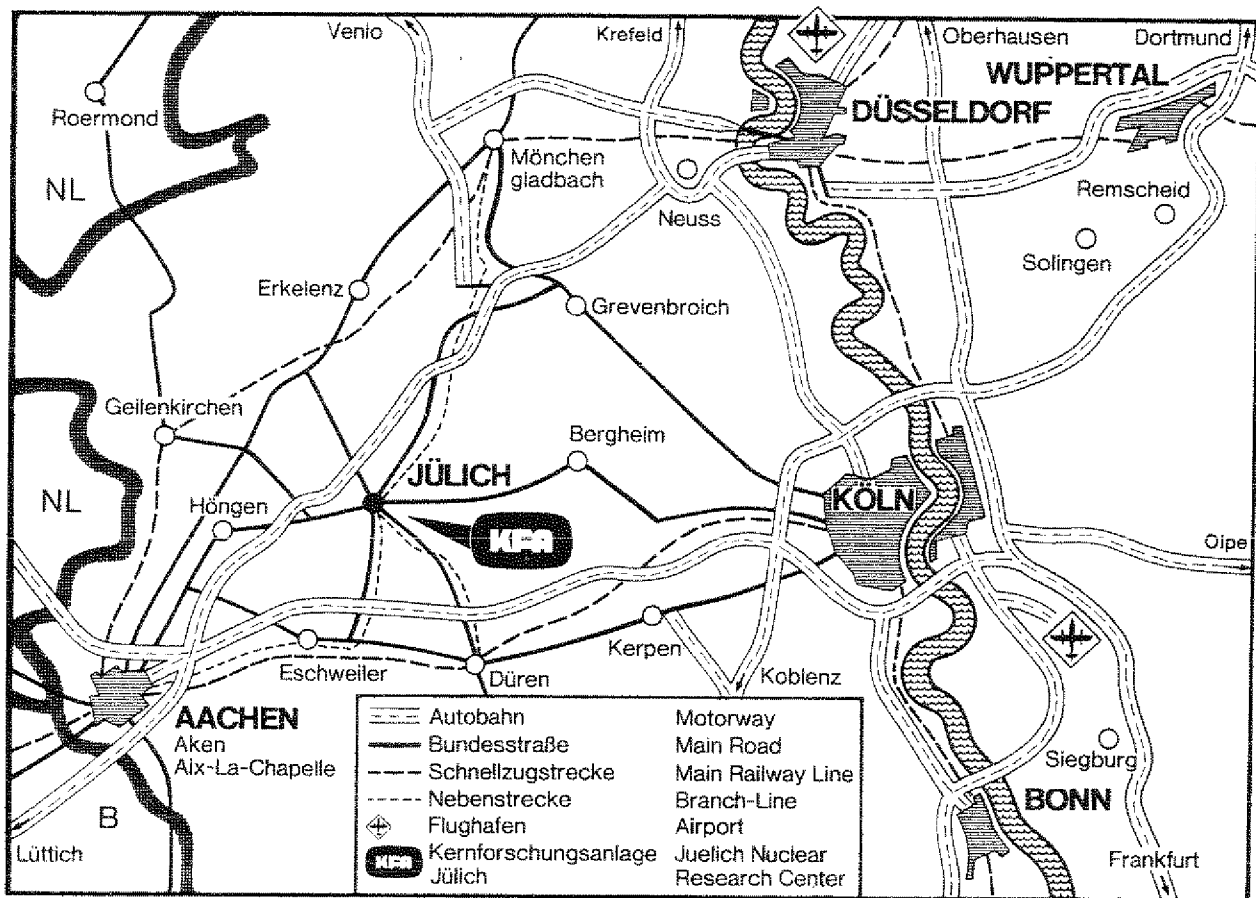
**Determination of Equivalent
Cross Sections for Representation
of Control Rod Regions in Diffusion
Calculations**

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W. Scherer and H.J. Neef

JÜI - 1311
Juli 1976

Als Manuskript gedruckt



Berichte der Kernforschungsanlage Jülich – Nr. 1311

Institut für Reaktorentwicklung Jül - 1311

Im Tausch zu beziehen durch: ZENTRALBIBLIOTHEK der Kernforschungsanlage Jülich GmbH,
Jülich, Bundesrepublik Deutschland

Determination of Equivalent Cross Sections for Representation of Control Rod Regions in Diffusion Calculations

by

W. Scherer and H.J. Neef

BESTIMMUNG ÄQUIVALENTER WIRKUNGSQUERSCHNITTE ZUR DARSTELLUNG VON ABSORBERSTÄBEN IN DIFFUSIONSRECHNUNGEN

von

W. Scherer
H.J. Neef

KURZFASSUNG

Die Darstellung von Absorberstabgebieten in Reaktorberechnungen erfordert eine Kombination von Diffusions- und Transporttheorie. Es wird eine Methode beschrieben, mit der äquivalente Wirkungsquerschnitte für ein Stabgebiet bestimmt werden können. Mit diesen Querschnitten erhält man diesselbe Stabwirksamkeit und diesselben Reaktionsratenverteilungen sowohl in der Diffusionsrechnung als auch in der Transportrechnung für den heterogenen Kontrollstab. Die Beschreibung der Methode wird durch Beispiele vervollständigt.

DETERMINATION OF EQUIVALENT CROSS SECTIONS FOR REPRESENTATION
OF CONTROL ROD REGIONS IN DIFFUSION CALCULATIONS

by

W. Scherer
H.J. Neef⁺)

ABSTRACT

The representation of control rod regions in reactor calculations requires a combination of transport and diffusion theory calculations. A method is described which produces equivalent cross sections for a rodded region. These cross sections used in a diffusion theory calculation yield the same rod efficiency and reaction rate distribution as the transport theory calculation for the explicit heterogeneous control rod. The description of the method is complemented by sample problems.

⁺) PNP-Projektleitung

CONTENT

	Page
1. Introduction and Basic Description of Methods	1
2. Determination of Equivalent Cross Sections	2
2.1 Central Rod	5
2.2 Excentric Rod in R- θ -Z-Geometry	6
2.3 Rod in Triangular Geometry	8
3. Computer Codes for the Evaluation of Equivalent Cross Sections	9
4. Sample Problems	10
4.1 1. Sample Problem (XSDRN-XRRR-CITATION)	10
4.2 2. Sample Problem (ANISN-RCS-CITATION)	13
References	15

List of Tables

	Page
1 Results of 1. Sample Problem (XSDRN-XRRR-CITATION)	16
2 Results of 2. Sample Problem (ANISN-RCS-CITATION)	17

List of Figures

	Page
1 Supercell with control rod	18
2 Rodded region in R- θ -Z geometry	19
3 Layout of meshgrid in triangular geometry	20
4 Calculation scheme for a rodded reactor, using XSDRN, XRRR, and CITATION	21
5 GA1160 MWE: Layout of patch-cell and single control rod for 1. sample problem	22
6 Flux profile in a supercell with control rod for 1. sample problem	23
7 Supercell configuration for 2. sample problem	24

1. INTRODUCTION AND BASIC DESCRIPTION OF METHODS

The calculation of the neutronic behaviour of a nuclear reactor in design studies is based on 1- or 2-dimensional diffusion theory codes. Partly or fully inserted control rods require a more detailed treatment; firstly the assumptions of the diffusion theory are not valid in the surrounding of a control rod and secondly the problem requires a 3-dimensional treatment. A 3-dimensional transport code is not yet available; therefore one has to use a 3-dimensional diffusion code and to find ways of representing the rods accordingly.

Two ways have been discussed up to now: The representation by boundary conditions at the surface of rodded regions and the use of equivalent cross sections in those regions. Both representations are based on the calculation of the heterogeneous control rod in a 1-dimensional supercell with a transport theory code.

The use of boundary conditions ^{1,2} has some basic and practical disadvantages. The coupling of transport and diffusion theory via boundary conditions only achieves identical leakage through the surface of the rodded region in both theories, whereas the use of equivalent cross sections results in identical reaction rate distributions, as will be shown later. One practical disadvantage occurs when the 3-dimensional code CITATION ³ is used. In this code fluxes are determined at the midpoint of a mesh, which will cause a strong dependence of the calculated rod efficiency on the meshpoint distribution when using boundary conditions. A further disadvantage results from a restriction in the input scheme of CITATION; it is only possible to provide one set of boundary conditions for all rodded regions.

The representation of control rod regions by equivalent cross sections has the advantage of being theoretically more lucid and enables a higher degree of flexibility in practical applications. Equivalent cross sections can be determined from a transport theory calculation in different ways.

The simplest method ⁴ is to add a certain amount of neutron absorber

(e.g. Boron) to the rodded region. The concentration of the neutron absorber is adjusted to give the same rod effectiveness in the diffusion calculation as in the transport code. The method results in agreement of the rod effectiveness, but flux distribution and reaction rates from the diffusion calculation are not the exact ones.

Another method to derive equivalent cross sections from the transport calculation consists of flux weighting the actual cross sections in the rodded region ². In this case one has to relate the cross sections to the boundary flux of the rodded region and not to the average flux in this region, as it is done in unit cell calculations. Used in a diffusion calculation these cross sections lead to good agreement of reactivity and reaction rates compared with the transport theory results.

In the method described in this report all reaction rates in the rodded region and outside are made equal in transport and diffusion theory. The equivalent cross sections to calculate the reaction rates in the diffusion theory depend on geometry and meshpoint distribution inside and outside the rodded region. In the case of only one meshpoint in a central rodded region the diffusion flux is easily defined. In the case of an excentric region one has to make additional assumptions. Consequently the cross section set derived by this method includes the information of the meshpoint distribution in the diffusion calculation. The method discussed here is similar to the approach used in the WIMS Code System ⁵, and has been adopted for the use with the KFA computer-codes and the Dragon computer codes ¹⁰.

The sample problems for rodded 1-dimensional supercells show a very good agreement of reactivity and reaction rates in both theories.

2. DETERMINATION OF EQUIVALENT CROSS SECTIONS

Let us define the effectiveness of a control rod (CR) or an array of CRs by:

$$\rho = \frac{k_0 - k_1}{k_0 \cdot k_1}$$

where k_0 is the multiplication factor of the reactor without rods, and k_1 the multiplication factor with rods inserted. Under the assumption that diffusion theory is valid everywhere in the unrodded reactor, one can conclude that k_0^D from a diffusion calculation is equal to k_0^T from a transport calculation. In a rodded reactor the rodded regions require a special treatment with the aim that k_1^D from the diffusion calculation is equal k_1^T from a transport calculation. The proof is of course possible only for simple geometries and will be made in the sample calculations in chapter 4 of this report.

For a real 3-dimensional reactor one has to make the assumption that perturbations which are far apart from a CR, for example other CRs, material boundaries etc., do not influence the neutron behaviour in the neighbourhood of the CR. This assumption makes it possible to define a rodded cell, normally called supercell, for the transport calculation. With the assumption that the supercell concept is valid, the aim is to get as a result that ρ^D is equal ρ^T .

Starting point for the method discussed in the following is the data for the homogeneous reactor and the heterogeneous CR. These data contain homogenised densities in core zones and the heterogeneous layout of the CR according to Fig. 1.

Condensed cross sections for the homogeneous core zones are derived from unit cell calculations.

A rodded supercell contains consequently the heterogeneous control rod surrounded by one or more homogeneous reactor regions. The result of the transport calculation for such a cell is the flux distribution $\phi(r)$, from which reaction rate distributions, currents, etc., can be determined. The flux $\phi(r)$ is the correct one (or best available one) as it is calculated by transport theory. Only in the vicinity of the rod this flux differs from the flux solution $\varphi(r)$, obtained with diffusion theory methods. Therefore it is possible to write:

$$\phi(r) = \varphi(r) + \gamma(r) \quad (1)$$

with the transient flux $\psi(r) \rightarrow 0$ for $r \rightarrow R$, the outer radius of the cell. One divides the cell into two regions (Fig. 1), and makes the assumption:

$$\phi(r) = \begin{cases} \varphi(r) & r > r_1 \\ \varphi(r) + \psi(r) & r \leq r_1 \end{cases} \quad (1a)$$

r_1 divides the cell in a rodded region ($r \leq r_1$) and an unrodded region ($r > r_1$). The rodded region may contain parts of the homogeneous surrounding of the CR. The unrodded region needs no correction if it is calculated with diffusion theory methods, but for the rodded region one has to look for an appropriate way of representation in the diffusion theory.

The aim is to equalise reaction rates in both calculations in the rodded region. If this is achieved, the reaction rates as well as the neutron balance are correct everywhere. This results in the correct multiplication factor k_1^D in the diffusion theory.

The radius r_1 obviously determines the size of the rodded region in the subsequent diffusion calculation. For this region a set of macroscopic cross sections for all reactions will be determined, so that reaction rates in both theories are equal, at least on supercell level. This cross section set is called the equivalent cross section set.

The reaction rate A for any reaction inside r_1 is known from the transport calculation. The equivalent reaction rate a inside r_1 calculated by diffusion theory is:

$$a = A = \Sigma \cdot \bar{\varphi} \cdot V. \quad (2)$$

Σ is the macroscopic cross section and just the value to be determined. V is the volume of the rodded region, and $\bar{\varphi}$ is the average diffusion flux inside r_1 . If one chooses only one mesh point inside r_1 in the diffusion code, say at r_1' (Fig. 1), then

$$\bar{\varphi} = \varphi(r_2') \quad (3)$$

The determination of $\bar{\varphi}$ and hence Σ depends on the special geometric representation of the rodded region. Three of the most common situations are now discussed in detail.

2.1 Central Rod

The leakage for the rodded region in transport theory $L(r_1)$ is set equal to the leakage as calculated in the diffusion theory $l(r_1)$. Using the notation in the code CITATION we get:

$$L(r_1) = l(r_1) = 2\pi r_1 \cdot \frac{\varphi(r_2') - \varphi(r_1')}{\frac{r_2' - r_1}{D_2} + \frac{r_1 - r_1'}{D_1}} \quad (4)$$

where r_2' is the first meshpoint in the diffusion theory calculation outside the rodded region (Fig. 1).

According to the assumption (1a) it is $\varphi(r_2') = \phi(r_2)$, which is known. Choosing $D_1 = D_2$ (which is always possible) for the diffusion coefficient we find:

$$\bar{\varphi} = \phi(r_2') - \frac{(r_2' - r_1') \cdot L(r_1)}{2\pi r_1 \cdot D_2} \quad (5)$$

In case the transport leakage $L(r_1)$ is not known explicitly from the transport calculation, it can be determined by the neutron balance of that calculation as follows:

$$L(r_1) = (\text{inscatter rate} + \text{fission rate} - \text{absorption rate} - \text{outscatter rate})^T \quad (6)$$

These reaction rates are known (A in (2)) and the combination of (5) and (2) will give the equivalent cross sections:

$$\Sigma = \frac{A}{\bar{\psi} \cdot V} \quad (7)$$

Formula (4) is valid for the CITATION code in cylindrical geometry. Using other codes and/or different geometries may change this formula, but it should always be possible to calculate $\bar{\psi}$ from $L = 1$. It is now possible to calculate from (2) all Σ , namely Σ_a , $\nu\Sigma_f$ and the scatter matrix $\Sigma_{gg'}$. For the rodded region the same diffusion coefficient has to be applied as for the surrounding unrodded region, which means that Σ_{tr} remains unchanged.

The method described even takes into account the mesh point distribution in the diffusion code; provided that only one mesh point is in the rodded region. This case is, however, very important as one normally wants to reduce the number of mesh points in the final reactor calculation.

2.2 Excentric Rod in R- θ -Z Geometry

For exact calculations of rod efficiencies in pebble bed reactors 3-D-diffusion calculations in R- θ -Z-geometry have to be performed. In this case the rodded region is represented in the diffusion calculation by a segment of a cylindrical annulus (Fig. 2).

In the transport calculation r_1 is the radius of the rodded region. The

rodded region in the diffusion theory has the same volume. Therefore and because of symmetry conditions the mesh size of the rodded region in the diffusion calculation is:

$$\Delta_1 = r_1 \sqrt{\pi} \quad (8)$$

$$\Theta_1 = \Delta_1 / R_c \quad (9)$$

with R_c the average position radius of the rodded region.

For the adjacent mesh in R- or θ -direction Δ_2 or Θ_2 can be chosen. The relation to be fulfilled is

$$\Theta_2 = \Delta_2 / R_c \quad (10)$$

The flux $\phi(r_2')$ from the transport calculation, necessary to solve (5) has to be determined at transport meshpoint

$$r_2' = (\Delta_1 + \Delta_2) / \sqrt{\pi} \quad (11)$$

because the affected volumes in both representations have to be equal. Of course it is also possible to define r_2' and to calculate Δ_2 and Θ_2 from (11) and (10).

In CITATION the position of the flux point inside a mesh is determined by equalizing the volumes of the four quadrants of the mesh. Therefore the fluxpoint in the rodded region is not at R_c but at R_1' . The leakage in the diffusion calculation as evaluated by CITATION and using $D_1 = D_2$ is:

$$l = \alpha \cdot D_2 \cdot (\varphi(R_1') - \varphi_s) \quad (12)$$

with

$$\alpha = 2 \cdot \frac{R_1 - R_0}{R_1 + R_0} \cdot \left(\frac{R_1}{R_2' - R_1'} + \frac{R_0}{R_1' - R_0'} \right) + 2 \cdot \frac{R_1^2 - R_0^2}{R_1' \cdot (\Delta_1 + \Delta_2)} \quad (13)$$

In most practical cases

$$\alpha \approx 8 \cdot \frac{\Delta_1}{\Delta_1 + \Delta_2} \quad \text{because } R_2' - R_1' \approx R_1' - R_0' \approx \frac{1}{2} (\Delta_1 + \Delta_2)$$

(13a) and $R_1' \approx \frac{1}{2} (R_1 + R_0).$

ψ_s is the average flux of the four adjacent flux points. With the assumption

$$\psi_s = \phi(r_0') \quad (1a')$$

in analogy to (1a) the calculation can be continued as before.

2.3 Rod in Triangular Geometry

Triangular geometry is often used for the calculation of reactors with hexagonal block-type fuel elements. The layout of the meshgrid in this geometry can be seen from Fig. 3. There are 6 meshpoints in the rodded region. If the rod is in central position these six meshpoints represent the radius r_1 whereas the meshpoints in the six triangles which have their base towards the inner hexagon represent r_2 . The volume of this hexagon

is the same as the volume of the rodded region in the cylindrical transport calculation.

As in the case of the excentric rod in R- θ -Z geometry, one has to make the assumption that the average flux over the outer mesh points is equal to the transport flux $\phi(r_2')$. In addition to this, it is assumed that the average over the six mesh points in the inner hexagon is representative for $\bar{\phi}$.

Under these assumptions, the formulas in 2.1 can be used for the cases with triangular geometry in CITATION.

3. COMPUTER CODES FOR THE CALCULATION OF EQUIVALENT CROSS SECTIONS

As mentioned before the diffusion code used for the representation of rodded regions is the 3-dimensional program CITATION. For the determination of the equivalent cross sections for CITATION two S_N -codes have been used: XSDRN⁶ and ANISN⁷. Both codes have been modified and auxiliary programs (XRRR for XSDRN and RCS for ANISN) have been written to calculate the equivalent cross section sets. The XSDRN route is described in⁸, whereas the ANISN route can be found in⁹. A calculation scheme for the XSDRN route, starting with a unit cell calculation, is given in Fig. 4. With respect to triangular geometry problems it is convenient to include the spectral influence of the rod on the surrounding regions inside the supercell as shown in Fig. 4. (Set B data). For practical reasons one may neglect this influence in large pebble bed calculations in (R- θ -Z) geometry. As the corresponding example in the next chapter shows, this approximation can be justified.

The cross section set calculated from case-4-data is dependent on the mesh spacing in the diffusion calculation, which should have only one mesh point inside the inner region. This point has been chosen to $r_1' = 13.364$ cm, whereas the first mesh point outside the inner region is at $r_2' = 23.141$ cm. Both radii are input values to XRRR.

There are six further mesh points between r_2' and $R = 50$ cm in the CITATION calculation. The result from the diffusion calculation with case-4-data is listed as Case 5. The k-value is in agreement with the transport calculation by 110 mN, the effectiveness differs only by 1% if one compares transport and diffusion calculation.

Cases 6 to 12 in Table 1 are basically the same as Case 5, but with some variations in mesh point distribution and cross section data:

- Case 6 Same as Case 5, but two mesh points in the inner zone.
- Case 7 Same as Case 5, but ten mesh points in the inner zone.
- Case 8 Same as Case 5, but twelve instead of six mesh points in the outer zone. r_2' remains at 23.14 cm.

The larger disagreement between Case 6, 7 and 5 compared to Case 8 and Case 5 shows the importance of having only 1 mesh point in the inner zone. The mesh point distribution in the outer zone does not influence the multiplication factor very much.

- Case 9 Same mesh point distribution as in Case 5, scattering in rod material not taken into account.
- Case 10 As Case 5, scattering cross sections not processed by XRRR. The scatter matrix of the outer zone is used in the inner zone as well.

These cases show that the multiplication factor is not only affected by the absorption events, but that all events including scattering in the inner zone are important especially if the rodded region contains much core material.

Compared to the scatter events in the outer block, the scatter events in the rod materials are negligible.

Cases 11, 12 The first mesh point outside the inner zone is changed from 23.14 cm to 20.31 and 28.76. Cross sections for the inner zone are re-calculated by XRRR according to the new mesh point distribution.

These cases are in very good agreement with Case 5 and show the insensitivity of the calculation method to the choice of the outer mesh point distribution. A variation of the only inner mesh point at r_1' is not possible in CITATION, but discrepancies are not expected for this case.

Case 13 is of special importance: Here the inner zone is reduced to $r_1 = 5.08$ cm, the outer radius of the rod channel. The mesh points used for the cross section calculation are $r_1' = 3.59$ cm and $r_2' = 6.25$ cm. For this case the multiplication factor is in very good agreement with the transport theory multiplication factor for the explicit rod.

An advantage of having a small inner zone can be seen from Fig. 6. Here the flux profile is shown in energy group 7, the group with the highest thermal absorption in the rod. The fluxes from Case 4 (S_4 -explicit rod), Case 5 (large rodded region), and Case 13 (small rodded region) are compared here. The flux profile of Case 13 is everywhere in very good agreement with the transport theory flux, whereas Case 5 gives only the average flux value for the inner block. The correct flux is, however, of importance when one is assessing the burn-up of a rodded core or the interaction of burnable poison with a CR.

The 7-block patch of the GA reactor can be represented in its actual triangular geometry in the CITATION code. The layout of the patch is shown in Fig. 3. With an across flats value of 36 cm one gets $r_1' = 12$ cm and $r_2' = 24$ cm. The region surrounding the patch has the property of reflecting neutrons.

Case 3 is the homogeneous case without rod and the k-value is naturally the same as in the cylindrical Case 2.

The use of XRRR-cross-sections in this geometry (Case 14) gave a very good result, as can be seen from the k values in Table 1.

4.2 2. Sample problem (ANISN-RCS-CITATION)

In this chapter the results of supercell calculations in 18 energy groups with ANISN are compared with 4 group calculations with CITATION. In both codes 1-dimensional cylindrical geometry has been used. In the supercell a control rod filled with B_4C and with an aluminium canning has been inserted into a surrounding, which is equivalent to a pebble bed reactor, similar to the KAHTER-core III².

The supercell configuration is given in Fig. 7. The rodDED region is defined by the outer boundary of the Al-guide tube ($r_1 = 5,0$ cm). The outer supercell boundary was arbitrarily chosen to be $R=35$ cm.

The comparison has been carried out for a fictitious very strong rod by increasing the boron concentration of a realistic design by a factor of 100 so that diffusion theory is extremely inaccurate in the rodDED region. In addition to the test of the method of equivalent cross-sections other methods have been investigated such as boundary conditions and region weighted cross-sections using the average flux or the boundary flux of the rodDED region.

The results of the comparison are listed in table 2. Case 1 refers to the ANISN supercell calculation without rod (including the Al-guide tube). Case 2 represents CITATION results for that configuration using all of the mentioned methods to describe the 'rodDED region' without rod but including the Al-guide tube. The difference between the methods is not significant and the k_{eff} -values are in very good agreement with the transport calculation result.

Case 3 gives the ANISN result for the rodged configuration and indicates the very large effectiveness of the rod.

The following cases 4 to 12 refer to the rodged configuration calculated with CITATION using different methods. The average flux weighted cross sections overestimate the rod worth by approx. 12%. On the contrary using the boundary flux for weighting, one underestimates the rod effectiveness by 5%. The new method of equivalent cross-sections gives excellent results for radii r_2' not too far from the rod boundary. Nevertheless this method is very insensitive against variation of the meshgrid outside the rodged region. (Case 6 - 9).

The boundary condition method gives a very good result in this example (case 11). Here the mesh spacing immediately adjacent to the rodged region is the same as in the transport calculation. Changing this mesh spacing (case 12) leads to major discrepancies, although the mesh has been refined in this special case.

Finally case 10 shows the influence of neglecting the spectral effect of the rod on the neighbourhood of the rodged region. In this special example the calculated effectiveness is too low by about 3%. It can be concluded, however, that for realistic rod designs in large pebble bed cores this effect will be even less significant.

The given examples show that the method of equivalent cross sections is very useful for the description of rodged regions in diffusion theory calculations. In addition this method gives better results than other methods, without any trouble of choosing a well adapted mesh grid.

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Table 1
Results of 1. Sample Problem
(XSDRN-XRRR-CITATION)

Case Number m	Code	k_m	Compared With Case n	$k_n - k_m$	Remarks
1	XSDRN-S ₄	1.0574	-	-	No rod
2	CITATION	1.0578	1	0.0004	No rod
3	"	1.0578	1	0.0004	No rod, triangular geometry, as in Fig. 3
4	XSDRN-S ₄	0.9160	1	0.1414	Explicit rod
5	CITATION	0.9149	2	0.1429	r_1 at 18.9 cm
			4	0.0011	
6	"	0.9137	2	0.1441	r_1 at 18.9 cm, 2 MP in rodded region
			5	0.0012	
			4	0.0023	
7	"	0.9133	2	0.1445	r_1 at 18.9 cm, 10 MP in rodded region
8	"	0.9147	5	0.0002	r_1 at 18.9 cm, 12 MP in unrodded region
9	"	0.9148	5	0.0001	r_1 at 18.9 cm, no scatter for explicit rod
10	"	0.9180	5	-0.0031	r_1 at 18.9 cm, scatter data for unrodded region used everywhere
11	"	0.9151	5	0.0002	r_1 at 18.9 cm, r_2 at 20.31 cm
12	"	0.9151	5	0.0002	r_1 at 18.9 cm, r_2 at 28.76 cm
13	"	0.9155	2	0.1423	r_1 at 5.08 cm
			5	-0.0006	
			4	0.0005	
14	"	0.9162	3	0.1416	Triangular geometry with rodded region, as in Fig. 3.
			4	-0.0002	

Table 2
Results of 2. Sample Problem
(ANISN-RCS-CITATION)

Case Number m	Code	k_m	Compared With Case n	$k_n - k_m$	ρ (rod)	Remarks
1	ANISN-S ₈	1.6114	-	-	-	No rod (but Al-tube)
2	CITATION	1.6116+0.0002	1	0.0002+0.0002	-	No rod, all methods used
3	ANISN-S ₈	1.0972	1	0.5142	29.1%	explicit rod
4	CITATION	1.0553	2	0.5563	32.7%	region weighted cross-sections using average flux
			3	0.0419		
5	"	1.1129	2	0.4987	27.8%	region weighted cross-sections using boundary flux
			3	-0.0157		equiv. cross-sections
6		1.0980	2	0.5136	29.0%	$r_2^i = 6.15$ cm
			3	-0.0008		
7	"	1.0920	2	0.5196	29.5%	$r_2^i = 10.77$ cm
			3	+0.0052		
8	"	1.0942	2	0.5174	29.3%	$r_2^i = 15.38$ cm
			3	+0.0030		
9	"	1.1032	2	0.5084	28.6%	$r_2^i = 22.30$ cm
			3	-0.0060		
10	"	1.1074	2	0.5042	28.2%	$r_2^i = 6.15$ cm
			3	-0.0102		rod spectral effect on unrodded region of supercell neglected
			6	-0.0094		
11	"	1.0997	2	0.5119	28.9%	D/ λ -boundary conditions
			3	-0.0025		next mesh $r^i = 6.15$ cm (like in transport calculation)
12	"	1.1137	2	0.4979	27.7%	D/ λ -boundary conditions
			3	-0.0165		next mesh $r^i = 5.10$ cm

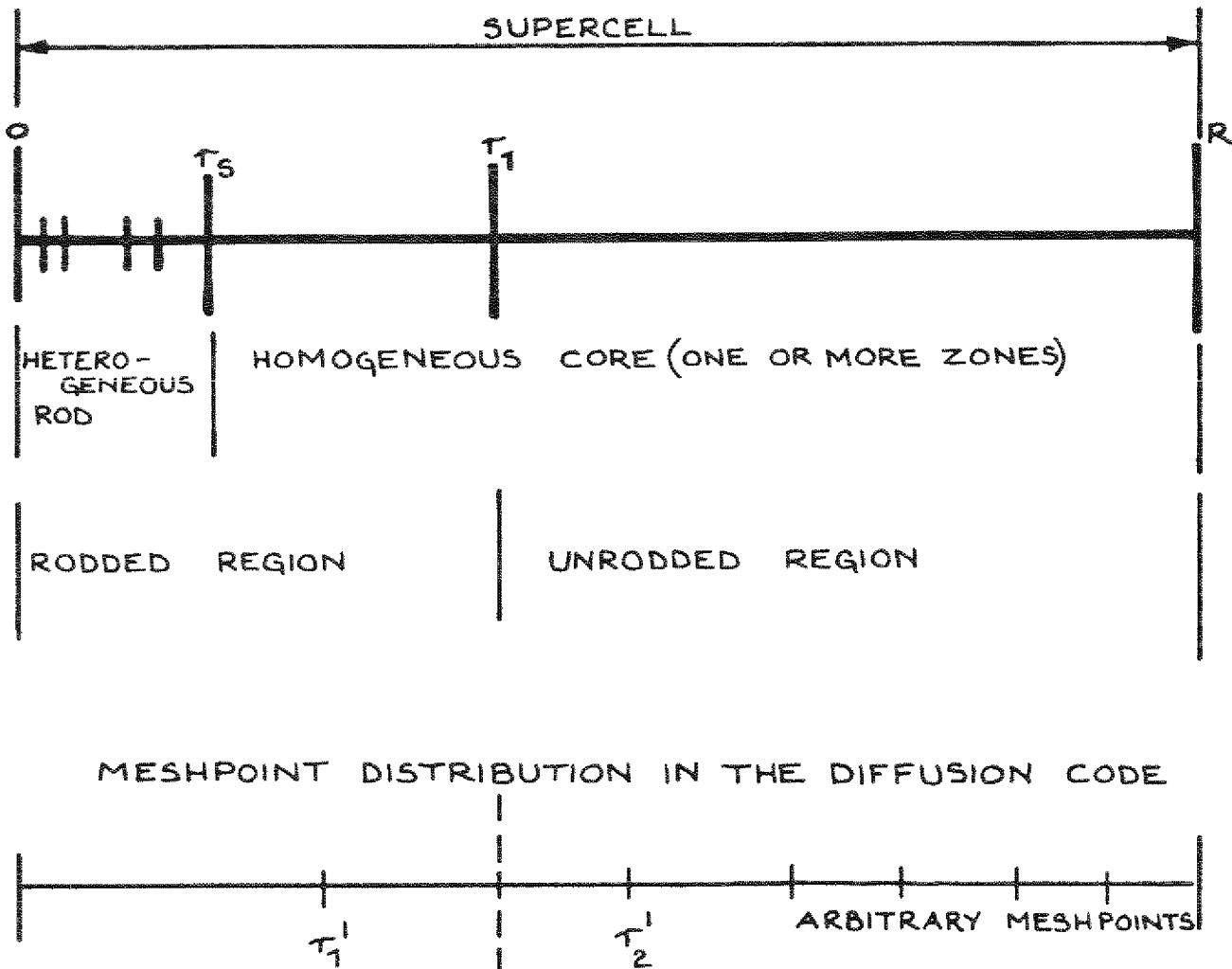


Fig. 1: Supercell with control rod

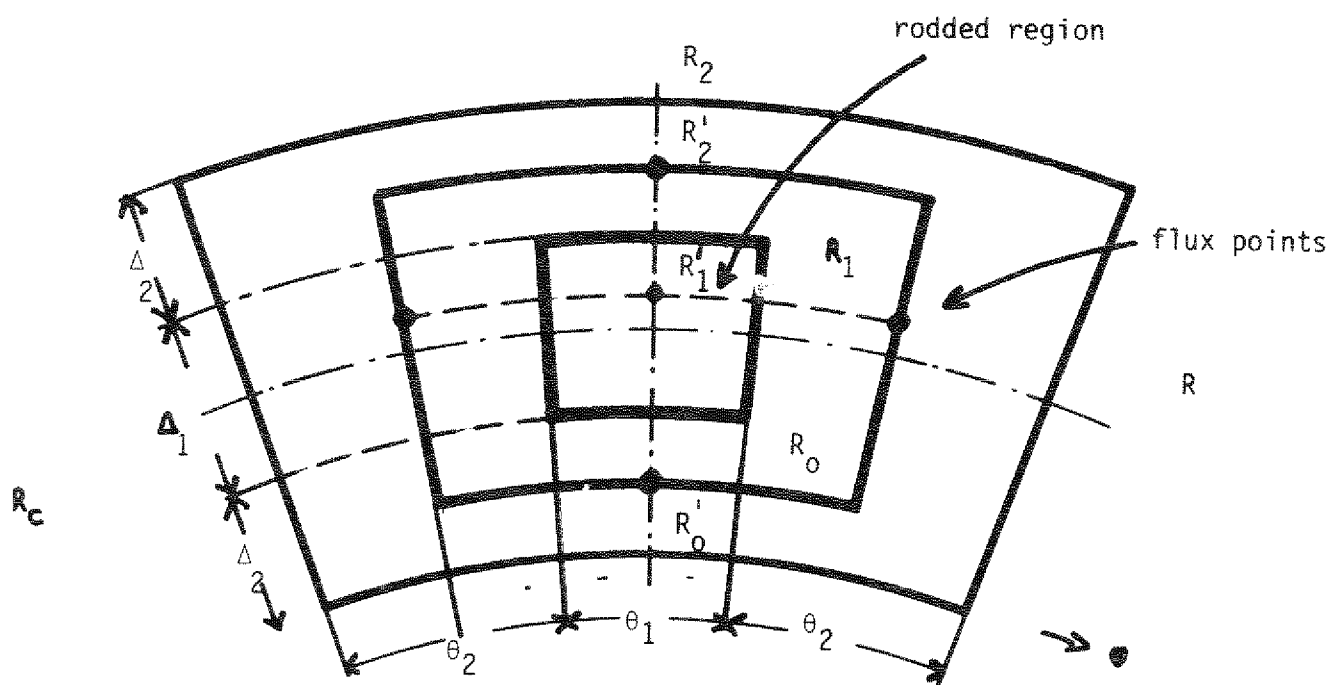


Fig. 2: Rodded region in R-θ-Z-geometry

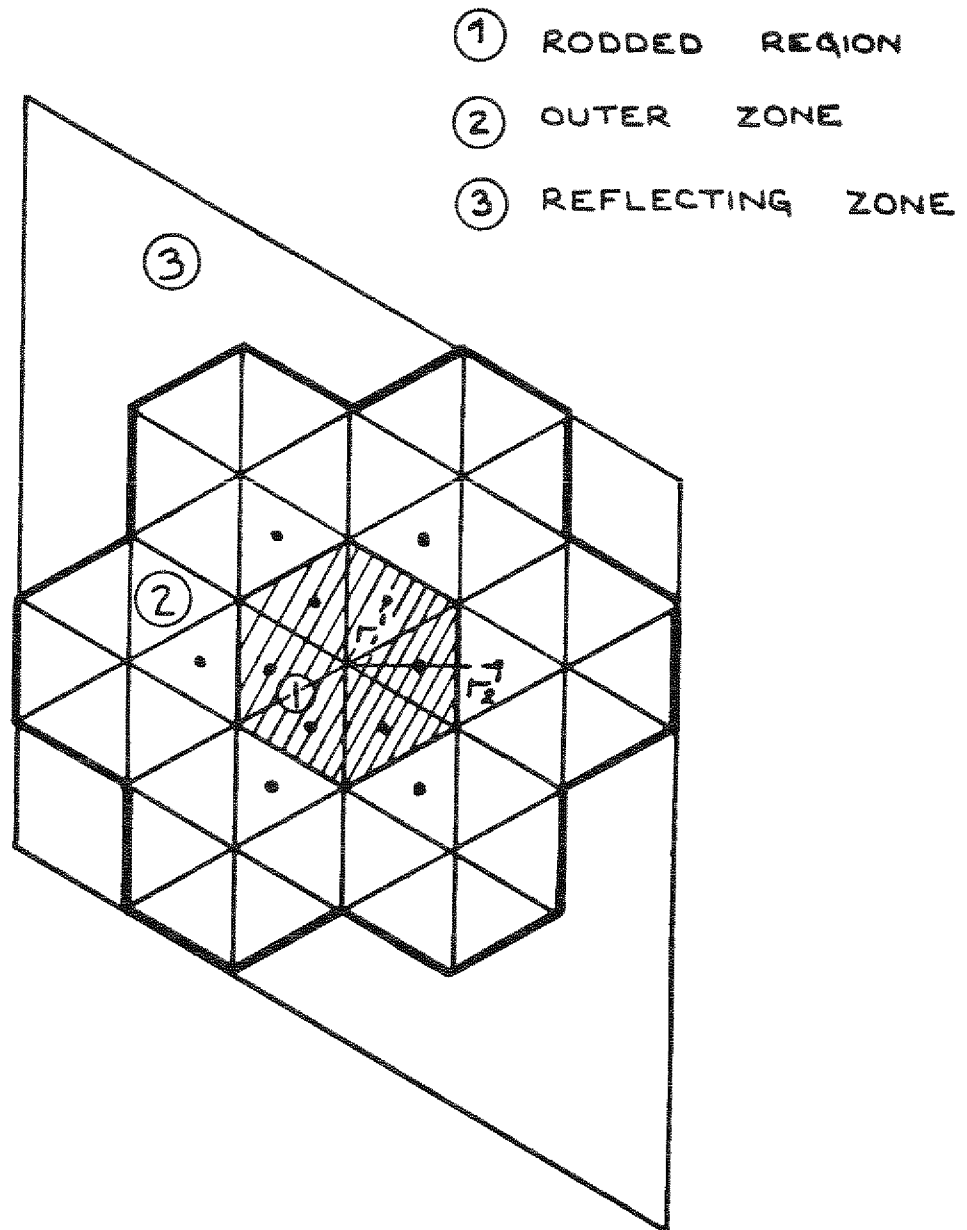


Fig. 3: Layout of meshgrid in triangular geometry

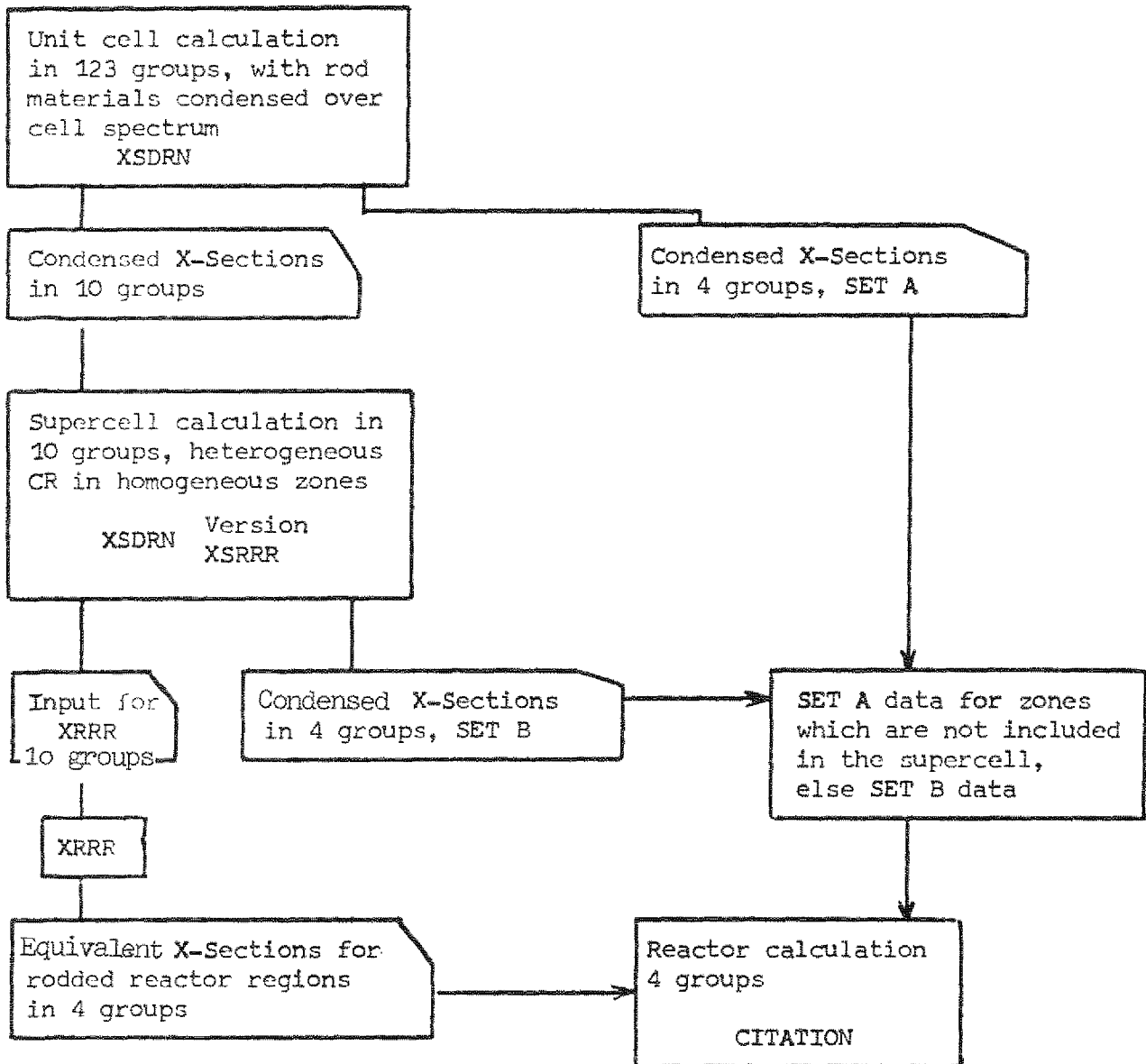


Fig. 4: Calculation scheme for a rodded reactor, using XSDRN, XRRR and CITATION

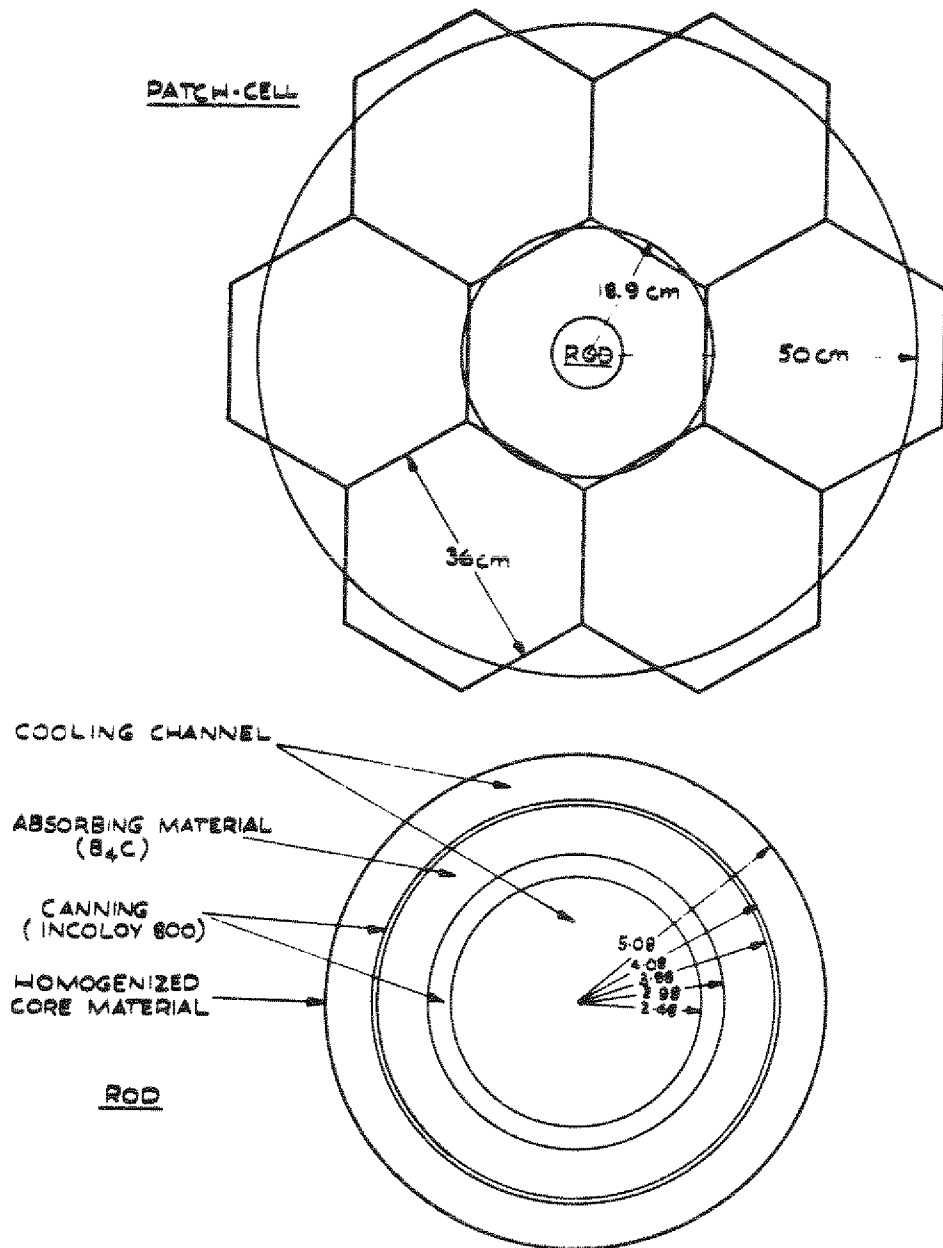


Fig. 5: GA-1160 MWe: Layout of patch-cell and single control rod for 1. sample problem

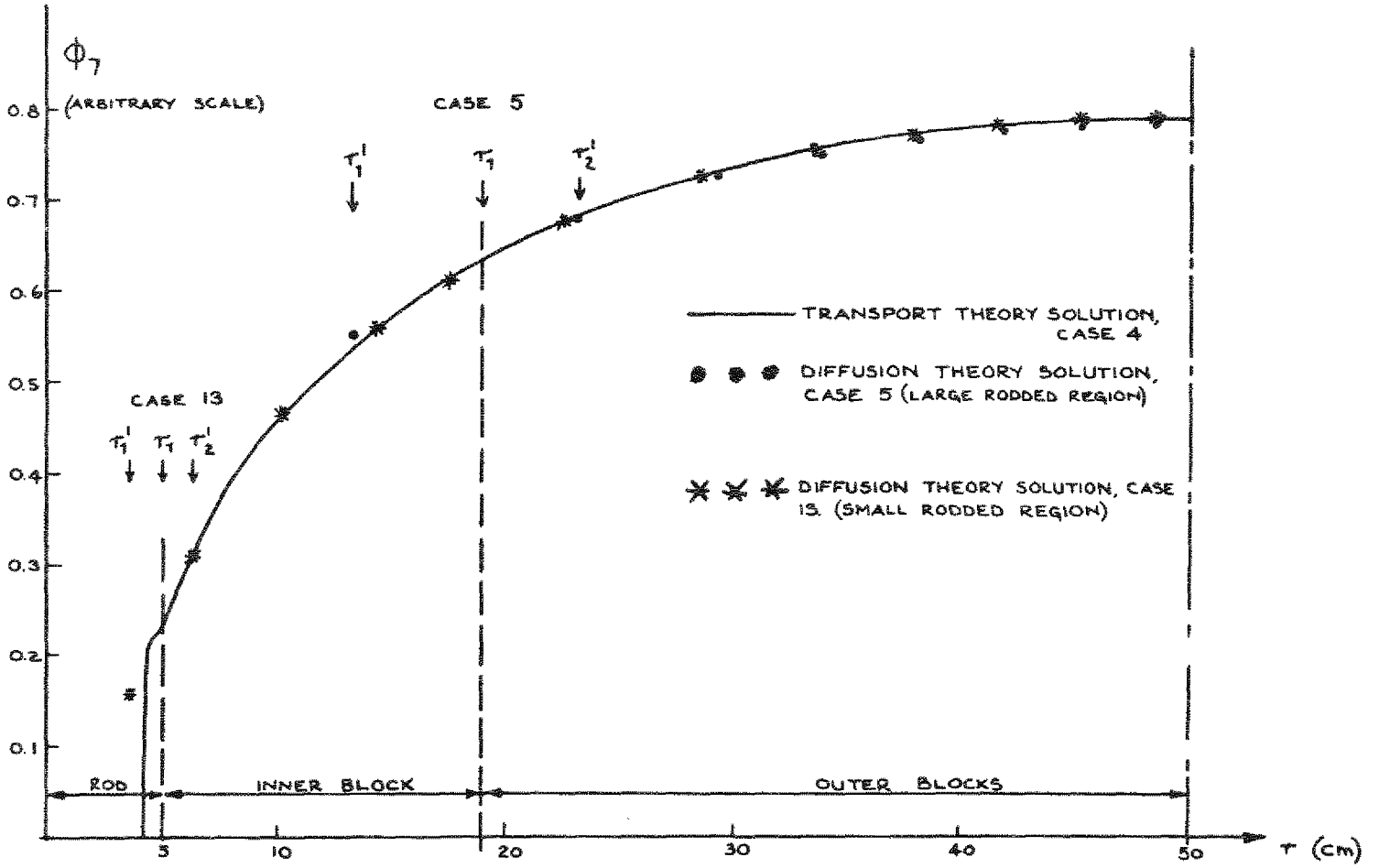
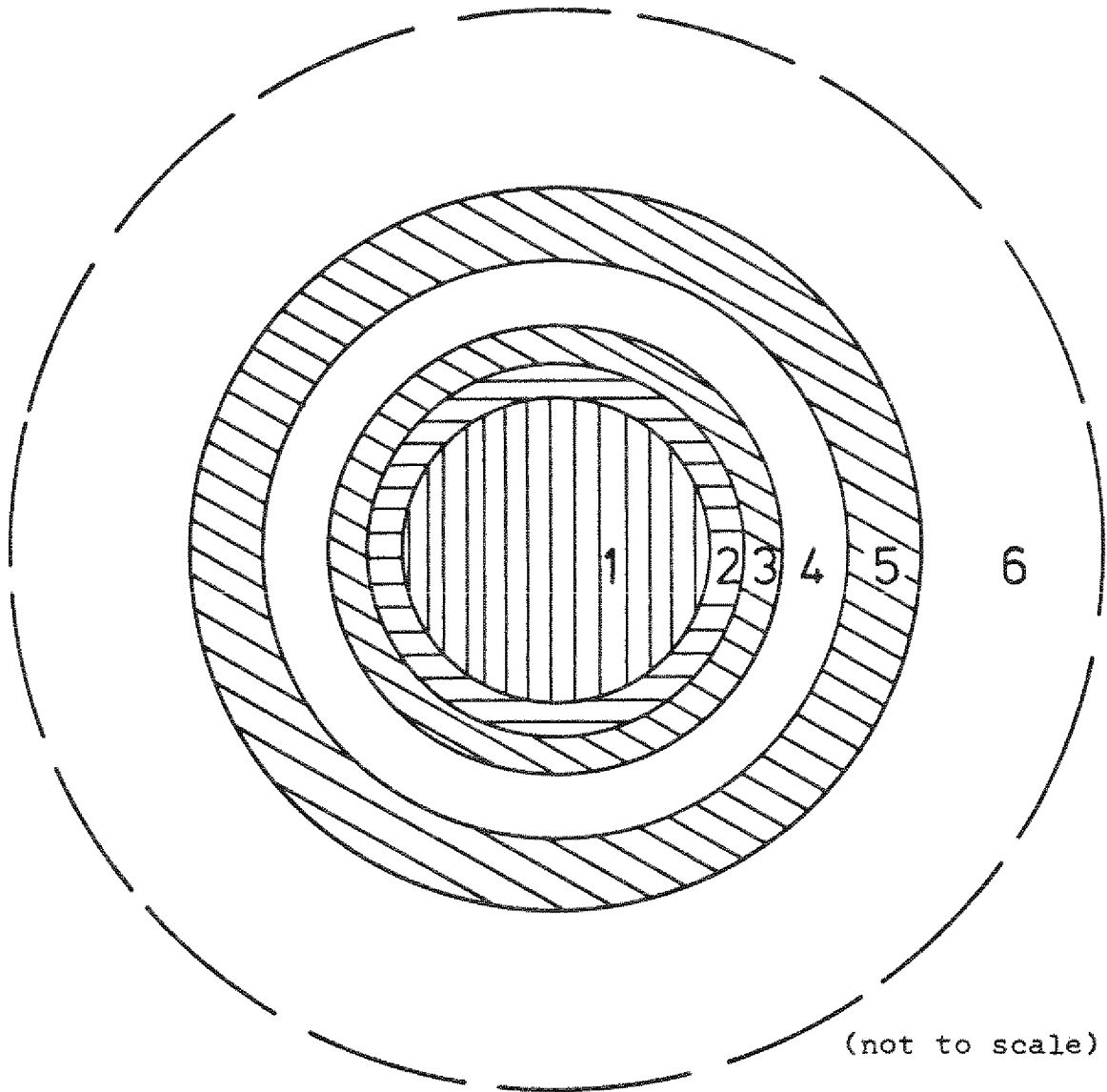


Fig. 6: Flux profile in a supercell with control rod for 1. sample problem



Region 1:	B_4C	$R1 = 2.2$ cm	} rodded region
2:	C	$R2 = 2.7$ cm	
3:	Al canning	$R3 = 3.15$ cm	
4:	Air	$R4 = 4.00$ cm	
5:	Al tube	$R5 = 5.00$ cm	
6:	Core	$R6 = 35.0$ cm	

Fig. 7: Supercell configuration for 2. sample problem



