AE-257
UDC 621.039.512.26:
681.3

AE-257

Dancoff Correction in Square and Hexagonal Lattices

I. Carlvik

AKTIEBOLAGET ATOMENERGI

STOCKHOLM, SWEDEN 1967

THE DANCOFF CORRECTION IN SQUARE AND HEXAGONAL LATTICES

I Carlvik

SUMMARY

This report presents the results of a series of calculations of Dancoff corrections for square and hexagonal rod lattices. The tables cover a wide range of volume ratios and moderator cross sections.

The results were utilized for checking the approximative formula of Sauer and also the modification of Bonalumi to Sauer's formula. The modified formula calculates the Dancoff correction with an accuracy of 0.01 - 0.02 in cases of practical interest.

Calculations have also been performed on square lattices with an empty gap surrounding the rods. The results demonstrate the error involved in treating this kind of geometry by means of homogenizing the gap and the moderator.

The calculations were made on the Ferranti Mercury computer of AB Atomenergi before it was closed down. Since then FORTRAN routines for Dancoff corrections have been written, and a subroutine DASQHE is included in the report.

Printed and distributed in November 1966

LIST OF CONTENTS

1. INTRODUCTION

The calculation of resonance absorption in thermal nuclear reactors is an important problem. It is difficult even for homogeneous cores, but is still more troublesome for heterogeneous lattices. It is possible to make calculations based on first principles by means of the Monte Carlo method, but because of the long computing times needed by this method it is mainly used for providing check points, and in practical reactor calculations one has to rely on simpler schemes.

The first method used for calculating resonance absorption in heterogeneous lattices separated the absorption into a volume term and a surface term (1). The volume term gives the absorption of neutrons scattered into the resonance in the fuel, and the surface term gives the absorption of neutrons scattered into the resonance in the moderator and then entering the fuel. It was pointed out by Dancoff and Ginsburg (2) that in a closely packed lattice the in-current of resonance neutrons into the fuel is reduced as compared to the in-current into a single fuel rod in an infinite moderator because of the shadowing effect of adjacent rods. The relative reduction is called the Dancoff correction.

In this physical model the Dancoff effect can be interpreted as a reduction in the effective surface of the fuel so that

$$S_{eff} = (1 - C)\, S \qquad (1)$$

where S_{eff} is the effective surface, S is the real surface and C is the Dancoff correction.

The notation varies with different authors. In this paper C will be used for the Dancoff correction and D for the Dancoff factor with $D = 1 - C$.

Subsequent methods for calculating resonance absorption are usually based on the concept of collision probabilities (3,4,5,6,7), and the heterogeneous problem is often transformed to a homogeneous one by means of equivalence theorems. The Dancoff effect is still taken into account, but the interpretation now is that D is the probability of collision in the moderator for neutrons entering the moderator through the fuel moderator interface with a $\cos\theta$ distribution. The two definitions are equivalent.

The problem studied in this paper is the calculation of the Dancoff correction in an infinite array of circular rods placed in a square or hexagonal lattice in a moderator. In a real reactor lattice the fuel is generally contained in a can. The effect of the can will be considered only insofar as the effect of an empty gap around the rod is studied.

There are several methods for calculating Dancoff corrections in lattices, some based on correct formulae and others using approximation schemes. When choosing a method, one should make clear what it should be used for. When critical experiments are analysed, one can very well spend a minute of computer time on a correct calculation. On the other hand a routine to be included in a standard cell reactivity programme for project calculations must be fast. In the latter case one knows beforehand the possible variation of the important parameters. It is then possible to calculate a suitable table and to derive, e.g., polynomial approximations to the table or to make interpolations in the table if the parameter variation is not too large. Or one could check an approximate method against accurate values in the allowed parameter region. In both cases a good table is needed.

The strongest shadowing in a lattice comes from the nearest neighbours. Therefore Dancoff and Ginsburg in their original paper studied the shadowing effect in the case of two equal parallel rods. They derived a formula for C and also gave some numerical results. Later Carlvik and Pershagen (8) arrived at a somewhat simpler formula by means of transformations, and they also produced tables (9).

Two-rod results can be used for nearest neighbours in an ordinary lattice, often also for next nearest neighbours, but the effect of more distant rods is reduced in most cases because of rods between. This reduction can even take place for nearest neighbours in the case of an hexagonal lattice. Carlvik and Pershagen discussed how intermediate rods can be accounted for in their formula, and this method was used by Almgren and Pörn (10) in combination with an integration by means of random numbers. Rothenstein and Helholtz (11) developed the method further to the case with an empty gap around the rods.

The method used by Fukai (12) for calculating two-region collision probabilities in a lattice has the integrations over a pair of rods arranged in a similar way. Naturally a large series of pairs of rods must be taken into consideration. By using a very large fuel cross section it is possible to obtain the Dancoff correction.

The methods discussed up till now are exact inasmuch as the formulae they use are correct, and the errors are of a mathematical nature, that is errors involved when carrying out integrations numerically. They are, however, not very fast. Various approximations have been suggested in order to achieve faster methods.

Fukai (13) has proposed an approximate method to reduce the effect of partly shadowed rods to get a quick method based on two-rod values.

Several authors have utilized equivalent circular cells (14, 15). Such methods can often give good results provided the cell boundary is assumed to be "white". They do not, however, distinguish between square and hexagonal lattices.

Another approach has been taken by Sauer (16). He tries to characterize the chord distribution of the moderator by means of a small number of parameters. It is found that the Dancoff correction is not very sensitive to the detailed form of the chord distribution function as long as certain moments of the distribution function are correct. It is then possible to use an approximate distribution function and make integrations analytically. The result is a simple formula which gives good results, particularly when one parameter has been correlated to Monte Carlo results.

Now, considering again exact methods, it seems that a sophisticated formula like the one of reference (8) is of value for simple geometries like two parallel rods. But for complicated geometries such as rod lattices - and also rod clusters - it is more attractive to use a straight-forward "chopper" method instead of considering a series of pairs of rods.

A computer programme of this kind, DANCOFF-5, was written in 1963 in Autocode for the Ferranti Mercury computer of AB Atomenergi. This programme has now been utilized for producing

extensive tables of Dancoff corrections for square and hexagonal lattices. It may be mentioned that the total computing time for all calculations reported here was about 14 hours including some unusable runs with input blunders.

An important incentive for the calculations was the fact that the computer was closed down in July 1966. However, since then a corresponding Fortran IV routine has been written. A Fortran listing of the DASQHE routine is shown in appendix 2. It may also be of interest that the values of table 5, comparison with Monte Carlo results, were recalculated by means of DASQHE together with a simple main routine on an IBM 7044 computer. The total computing time for the 48 cases of table 5 was 2.4 minutes.

The present paper contains the tables of Dancoff corrections, a discussion of the accuracy, and an investigation of the error related to the homogenization of a gap surrounding the rods. Among the various approximate methods, we have selected that of Sauer (16) and checked it against the tables. A modification of Sauer's formula, proposed by Bonalumi (17), has also been studied.

2. METHOD OF CALCULATION

Only a very brief account of the method will be given as its principles have been described elsewhere (18). The Dancoff correction is expressed as a double integral over a linear coordinate y along the rod diameter and over an angular coordinate α.

$$C = \frac{1}{\alpha_o} \int_o^{\alpha_o} d\alpha \, \frac{1}{2r} \int_{-r}^{+r} dy \, \frac{Ki_3(\tau)}{Ki_3(o)} \qquad (2)$$

The notations are given in figure 1. τ is the optical length of t, and $Ki_3(\tau)$ is a Bickley function (19). Due to the symmetry of the lattice the angular integration is carried out only over the angle α_o, which is 45^o for a square lattice and 30^o for a hexagonal lattice.

The trapezoidal rule is used for the integration. The accuracy is characterized by two numbers L and V (NRAD and NALF in the

Fortran routine DASQHE), so defined that the linear step length is $\frac{r}{L}$, and the angular step is $\frac{\alpha_o}{V}$. The total number of points in the two-dimensional mesh is consequently 2LV. Equation 2 is approximated by

$$C = \frac{4}{\pi} \frac{1}{2L \cdot V} \sum_{\ell=1}^{2L} \sum_{v=1}^{V} Ki_3(\tau_{\ell, v}) \tag{3}$$

An essential point of the method is to determine for a given neutron path starting at a given point of the rod surface in a given direction where it is cut off by another rod. Should the reader be interested in how this trivial problem is solved in DANCOFF-5, he is referred to Carlvik (20).

The neutron path is followed through 100 rows of rods if no intersection is found, that is the Dancoff correction is calculated for the central rod in an array of 201x201 rods. Even for the smallest moderator cross section used in the calculations (moderator cross section times pitch = 0.1) the distance to the nearest disregarded rod is 10 mean free paths.

3. PARAMETER VARIATION

In a pure two-region system (fuel-moderator) the Dancoff correction is a function of two variables. We use the following two dimensionless variables

$$\left.\begin{aligned} x &= \Sigma\, d \\ y &= \frac{r}{d} \end{aligned}\right\} \tag{4}$$

where Σ = moderator macroscopic cross section

d = lattice pitch

r = rod radius

The volume ratio moderator to fuel is, using these variables,

square lattice $$\frac{V_m}{V_f} = \frac{1}{\pi y^2} - 1 \tag{5}$$

hexagonal lattice $$\frac{V_m}{V_f} = \frac{\frac{\sqrt{3}}{2}}{\pi y^2} - 1 \qquad (5)$$

Another important parameter is the mean chord length of the moderator $\bar{\ell}$ defined as

$$\bar{\ell} = \frac{4V_m}{S} \qquad (6)$$

where V_m is the moderator volume per cell and S is the surface area of a fuel rod, both counted per unit length. With our notation we obtain

$$\left.\begin{aligned} &\text{square lattice} \quad \Sigma\bar{\ell} = \frac{2x}{\pi y}(1 - \pi y^2) \\ &\text{hexagonal lattice} \quad \Sigma\bar{\ell} = \frac{2x}{\pi y}\left(\frac{\sqrt{3}}{2} - \pi y^2\right) \end{aligned}\right\} \qquad (7)$$

The region we have chosen for calculations is as follows

$$\left.\begin{aligned} &0.1 \leq \Sigma d \leq 6 \\ &0.1 \leq \frac{r}{d} \leq 0.5 \end{aligned}\right\} \qquad (8)$$

$\frac{r}{d} = 0.5$ gives a lattice with the rods in contact. The variation of $\frac{r}{d}$ corresponds to the following volume ratios

$$\left.\begin{aligned} &\text{square lattice} \quad 0.2732 \leq \frac{V_m}{V_f} \leq 30.83 \\ &\text{hexagonal lattice} \quad 0.1027 \leq \frac{V_m}{V_f} \leq 26.566 \end{aligned}\right\} \qquad (9)$$

The region covered by calculations is illustrated in figure 2, which also shows typical regions for light water lattices and for so called homogenized heavy water lattices. We hope that the calculations will cover most cases occurring in practice and also cases not yet conceived.

4. ACCURACY

The effect of varying the two accuracy parameters L and V is illustrated by calculations on two square lattices with $\Sigma d = 0.8$, $\frac{r}{d} = 0.3$ and $\Sigma d = 0.5$, $\frac{r}{d} = 0.4$. L and V were given the values 16, 32, 64, and 128. The calculated Dancoff corrections are given in tables 1 and 2 to five decimal places together with the errors defined as C(L,V) - - C(128,128). The values L = V = 32 were first chosen as a standard for the main calculations.

Tables 1 and 2 do not, however, give enough information about the accuracy. Therefore the calculations using L = V = 32 were checked over the whole region by means of calculations using L = V = 64 for a reduced set of x- and y-values. The differences between the two calculations, that is C(32,32) - C(64,64) are given in table 3.

The largest absolute "error" in table 3 is 0.0005 except in regions of small x- and y-values, that is in the region of small radius to pitch and small moderator cross section. For these open lattices it was thought that the accuracy would improve more for an increase of the number of angular steps than for an increase of the number of linear steps. This was verified in two new calculations using L = 32, V = 64 and L = 64, V = 128 for the region $x \leq 1.0$, $y \leq 0.2$. The results are given in table 4. The maximum absolute "error" here is 0.0004.

In accordance with this investigation the calculations for the main tables were made with L = 32, V = 64 for the region $x \leq 1.0$, $y \leq 0.2$ and with L = V = 32 for the rest of the tables, as indicated in figure 2.

Another factor which influences the accuracy is the approximation used for the Bickley function Ki_3. The routine used by DANCOFF-5 was developed by Tollander (21), and its maximum absolute error is 0.00003. Since C is calculated from equation 3, the maximum absolute error arising from this source is less than 0.00004.

From these considerations we draw the conclusion that the absolute error in the main tables is less than 0.0005 for most entries.

The DANCOFF-5 programme was of course also checked against available data in the literature. The Monte Carlo values re-

ported by Fukai (13) have been used as check points by several authors. The twelve lattices were also calculated with DANCOFF-5. Three accuracies were used, L = V = 16, L = V = 32, and L = V = 64. It is not clear from Fukai's paper which moderator cross section was used. According to Kiesewetter and Marbach (14) it was $\Sigma_m = 1.49$, but in the papers of Sauer (16) and of Bonalumi (17) the value $\Sigma_m = 1.492$ is used. We made the calculation for both cross sections with L = V = 32, and the difference in C is very small.

Table 5 shows the results of our calculation together with the Monte Carlo results. In three cases the difference between our result and the Monte Carlo result exceeds the quoted error of the Monte Carlo calculation. Since our three values of different accuracy agree so well, we believe that they are correct. As a matter of fact differences of this magnitude are to be expected, provided the quoted errors of the Monte Carlo calculation are standard errors.

Another comparison was made with values calculated by Rothenstein and Helholtz (11) for gap geometry in a hexagonal lattice. Here only L = V = 32 was used. 100 values were compared. In two cases the difference was 0.0031, in two others it was 0.0014, and in the other 96 cases the difference was 0.0010 at most. Also in this comparison we believe that our values have smaller errors than these differences.

5. RESULTS

Dancoff corrections were calculated for square and hexagonal lattices without gap using the values of L and V given above. The variation of the parameters was

$$x = \Sigma d = 0.1(0.1)2.0(0.5)6.0$$

$$y = \frac{r}{d} = 0.1(0.02)0.5$$

thus in total 616 values for each of the two lattice types.

As shown in paragraph 4 the accuracy is about 0.0005.

The tables for both lattice types are given in appendix 1.

The results could be presented graphically in various ways. In particular, curves giving C as a function of $\Sigma\bar{\ell}$ almost coincide for small values of $\Sigma\bar{\ell}$, irrespective of which volume ratio they correspond to. This is shown in figure 3 for the square lattice. Curves for $\frac{r}{d}$ between 0.1 and 0.42 (not shown in the figure) are all quite close to the curves for $\frac{r}{d} = 0.44$ and $\frac{r}{d} = 0.46$, although they intersect in a somewhat irregular manner. We think, however, that there is no point in trying to find an approximate formula by a detailed analysis of such curves. It will be shown in paragraph 7 that a formula of the Sauer type reproduces the results very well.

6. THE EFFECT OF A GAP

In a real reactor lattice the fuel is contained in a can. In gas-cooled reactors there is also a gas channel around the fuel, with the gas having a relatively low macroscopic cross section. The simplest way to account for complications of this kind is to homogenize all material outside the proper fuel.

The DANCOFF-5 programme allows an empty circular channel around the fuel, and this option was used in order to investigate the effect of homogenization.

For a certain value of $\frac{r}{d}$ and Σd, the Dancoff correction with a gap, C_{gap}, was calculated. The Dancoff correction without gap, C_w, was known before. It should be noticed that $\frac{r}{d}$ was kept constant, so the two C-values do not correspond to the same volume ratio moderator to fuel. The Dancoff correction for the equivalent lattice, where the moderator and the gap are mixed, C_{hom}, was then calculated.

The calculations were done for a square lattice only, but for a series of values Σd and $\frac{r}{d}$ and for two gap thicknesses, 10% and 20% of the rod radius. The accuracy parameters were L = V = 32.

The results are given in table 6. For each case three values are given, $\Delta_{gap} = C_{gap} - C_w$, $\Delta_{hom} = C_{hom} - C_w$, and $\Delta = \Delta_{hom} - \Delta_{gap}$. The last of the three is the error obtained when the calculation is made for the homogenized system instead of the correct system with gap.

When the gap is introduced in the system, C increases. This

is quite clear, because the moderator region must become more transparent when some moderator is removed. Thus Δ_{gap} is always positive. If the gap and the remaining moderator are homogenized, C decreases again, which can also be understood from a physical point of view. Thus Δ_{hom} is less than Δ_{gap}, and the error Δ is always negative.

As would be expected, the homogenization works well with small Σd and small $\frac{r}{d}$ and less well for large values of these parameters. The worst cases, however, are not very realistic because the volume ratio moderator to fuel is very small.

7. DISCUSSION OF SAUER'S FORMULA AND BONALUMI'S MODIFICATION

The requirements for a simple approximation method seem to be best fulfilled by the formula of Sauer (16). It accounts for the particular properties of the lattice geometry in an attractive way, and in contrast to methods that employ equivalent circular cells it can distinguish between square and hexagonal lattices. Furthermore the formula is very simple.

Using our variables, x and y, Sauer's formula can be written

$$C_S = \frac{e^{-\tau \cdot \Sigma\bar{\ell}}}{1 + (1 - \tau)\Sigma\bar{\ell}} \tag{10}$$

where $\Sigma\bar{\ell}$ is given by equations 7 and the correlated geometrical index τ is

$$\left.\begin{aligned} &\text{square lattice} \quad \tau = \frac{\pi}{2}\, y\, \frac{1 - 2y}{1 - \pi y^2} - 0.08 \\ &\text{hexagonal lattice} \quad \tau = \frac{\pi}{2}\, y\, \frac{1 - 2y}{\sqrt{\frac{3}{2}} - \pi y^2} - 0.12 \end{aligned}\right\} \tag{11}$$

Dancoff corrections calculated by means of Sauer's formula, C_S, are compared with our values, C, in tables 7 and 8 for a set of x- and y-values.

A relative maximum in the absolute error of C_S occurs for the largest volume ratio investigated, when the pitch is about one mean free path. The maximum absolute errors in the table in this region are 0.025 for the square lattice and 0.039 for the hexagonal lattice. There is also a relative maximum for the smallest volume ratio in the case of the square lattice, when the cross section is large.

These errors are, however, tolerable in most practical calculations. The errors are also in general smaller in the region of normal light water lattices.

Bonalumi (17) has pointed out that Sauer's Dancoff correction, C_S, shows a pathological behaviour for very large moderator cross sections in the two cases of very large and very small volume ratios, that is $y = \frac{r}{d}$ near 0 and near 0.5. The first term on the right hand side of equations 11 is $T/\bar{\ell}$ where T is the shortest distance between two rods, so these equations can be written

$$\left.\begin{array}{ll} \text{square lattice} & \tau = \frac{T}{\bar{\ell}} - 0.08 \\ \text{hexagonal lattice} & \tau = \frac{T}{\bar{\ell}} - 0.12 \end{array}\right\} \quad (12)$$

The terms 0.08 and 0.12 were obtained by Sauer by correlation with the logarithmic moment of the chord distribution. When $\frac{T}{\bar{\ell}}$ is very small, τ becomes negative so that the argument of the exponential function in equation 10 becomes positive, and for large $\Sigma\bar{\ell}$ the expression for C_S tends to infinity instead of zero.

As shown by the numerical comparison above, this effect does not cause any large errors in the region covered by the present calculations. One should, however, be cautious when Sauer's formula is used for lattices with very high volume ratio. At the other end, touching rods, the effect is probably not important until the cross section is so large that the pitch is of the order of tens of mean free paths.

Although Sauer's formula still seems to work well for all practical lattices, it is unsatisfactory that it does not behave properly in the limit. Therefore Bonalumi suggested a modification as follows

$$C_B = \frac{e^{-\tau \Sigma \bar{\ell}}}{1 + (1 - \tau_1)\Sigma \bar{\ell}}$$

with $\tau_1 = \tau + \delta\tau$

$$\tau = \frac{T}{\bar{\ell}}$$

$$\delta\tau = \frac{\Sigma \bar{\ell}}{7 + \beta \Sigma \bar{\ell}}$$

(13)

$$\beta = \begin{cases} 5.67 & \text{square lattice} \\ 2.125 & \text{hexagonal lattice} \end{cases} \quad (14)$$

The numerical constants were obtained by correlation.

This formula gives the correct variation in the limit $\tau = 0$.

We studied Bonalumi's formula by putting $C_B = C$ as obtained by DANCOFF-5 and solving for $\delta\tau$. Figure 4 shows $\frac{\Sigma \bar{\ell}}{\delta\tau}$ as a function of $\Sigma \bar{\ell}$ for various values of $\frac{r}{d}$ for a square lattice. According to equation 13 the curves should all coincide with the straight line $7 + 5.67\, \Sigma \bar{\ell}$. Actually they deviate considerably from the line. This does not necessarily mean that Bonalumi's formula gives bad results. C_B is in fact not very sensitive to $\delta\tau$.

A comparison was also made between C_B and our Dancoff corrections, tables 9 and 10. In spite of the somewhat depressing appearance of figure 4, the agreement is rather good, the maximum absolute error being 0.04. If one looks only at what is thought to be regions of practical interest, the Bonalumi modification implies a considerable improvement.

8. CONCLUSIONS

Dancoff corrections have been calculated for a series of square and hexagonal lattices with an accuracy of about $\pm$ 0.0005. The parameter variation should cover all cases occurring in practice.

The effect of a gap surrounding the rods was investigated. It was found that the error in the Dancoff correction caused by treating

the gap by homogenization is at most about 0.02 for a gap less than 20% of the rod radius and for volume ratios larger than about 3. For smaller volume ratios one should use a better method than homogenization.

The accuracy of the method of Sauer was investigated. It was found that it works well in the region studied with a maximum absolute error of about 0.04 and smaller errors in regions of practical interest. The modification proposed by Bonalumi gives a considerable improvement in most of the region of practical interest. Since the increased complexity of the formula is insignificant, the use of Bonalumi's modification in the formula of Sauer is to be recommended.

9. REFERENCES

1. WIGNER, E P, CREUTZ, E, JUPNIK, H, SNYDER, T,
Resonance absorption of neutrons by spheres
J. Appl. Phys. 26 (1955) 260

2. DANCOFF, S M, GINSBURG, M,
Surface resonance absorption in a close-packed lattice
1944 (CP-2157)

3. CHERNICK, J, VERNON, R,
Some refinements in the calculation of resonance integrals
Nuclear Sci. and Eng. 4 (1958) 649

4. ADLER, F T, HINMAN, G W, NORDHEIM, L W,
The quantititative evaluation of resonance integrals
U.N. Int. Conf. on the Peaceful Uses of Atomic Energy,
Geneva, 2. 1958. Vol. 16. Geneva 1958, p. 155

5. DRESNER, L,
Resonance absorption of neutrons in nuclear reactors.
Diss. 1959. (ORNL-2659)

6. ROTHENSTEIN, W,
Collision probabilities and resonance integrals for lattices
Nucl. Sci. and Eng. 7 (1960) 162

7. NORDHEIM, L W,
A program of research and calculations of resonance absorption
Final report. 1961 (GA-2527)

8. CARLVIK, I, PERSHAGEN, B,
The Dancoff correction in various geometries. 1959.
(AE-16)

9. CARLVIK, I, PERSHAGEN, B, 1959. AB Atomenergi, Sweden
(Internal report RFR-20)
(The tables are also included in ANL-5800, 2 ed., 1963, p. 283)

10. ALMGREN, B, PÖRN, K, 1963. AB Atomenergi, Sweden
(Internal report RFR-222)

11. ROTHENSTEIN, W, HELHOLTZ, J,
The Dancoff correction in gap geometry
Nucl. Sci. and Eng. 14 (1962) 239

12. FUKAI, Y,
First-flight collision probability in moderator-cylindrical fuel system
Reactor Sci. and Tech. 17 (1963) 115

13. FUKAI, Y,
New analytical formula for Dancoff correction for cylindrical fuel lattices
Nucl. Sci. and Eng. 9 (1961) 370

14. KIESEWETTER, H, MARBACH, H,
Tabellen für die Dancoff-Korrektion in regulären Stabgittern
Kernenergie 6 (1963) 608

15. LESLIE, D C, HILL, J G, JONSSON, A,
Improvements to the theory of resonance escape in heterogeneous fuel
Nucl. Sci. and Eng. 22 (1965) 78

16. SAUER, A,
Approximate escape probabilities
Nucl. Sci. and Eng. 16 (1963) 329

17. BONALUMI, R,
Systematic approximations of neutron first-collision probabilities
Energia Nucleare 12 (1965) 1

18. CARLVIK, I,
A method for calculating collision probabilities in general cylindrical geometry and applications to flux distributions and Dancoff factors
U.N. Int. Conf. on the Peaceful Uses of Atomic Energy, Geneva, 3. 1964. Vol. 2. Geneva 1965, p. 225

19. BICKLEY, W G, NAYLER, J,
A short table of the functions $Ki_n(X)$, from N = 1 to N = 16.
Phil. Mag. 20 (1935) 343

20. CARLVIK, I, 1964, AB Atomenergi, Sweden
(Internal report RFR-282)

21. TOLLANDER, B,
Private communication

APPENDIX 1. TABLES OVER DANCOFF CORRECTIONS

DANCOFF CORRECTION FOR SQUARE LATTICE

VM/VF	30.8310	21.1049	15.2403	11.4340	8.8244	6.9577	5.5766	4.5262
R/D	0.10	0.12	0.14	0.16	0.18	0.20	0.22	0.24
SIG*D								
0.10	0.6150	0.6625	0.7010	0.7331	0.7602	0.7835	0.8036	0.8228
0.20	0.4256	0.4796	0.5264	0.5676	0.6039	0.6363	0.6654	0.6939
0.30	0.3146	0.3652	0.4114	0.4539	0.4925	0.5282	0.5611	0.5941
0.40	0.2432	0.2882	0.3309	0.3714	0.4094	0.4455	0.4797	0.5145
0.50	0.1942	0.2335	0.2720	0.3095	0.3456	0.3806	0.4145	0.4496
0.60	0.1589	0.1932	0.2275	0.2616	0.2953	0.3286	0.3614	0.3959
0.70	0.1325	0.1623	0.1928	0.2238	0.2548	0.2861	0.3175	0.3508
0.80	0.1120	0.1382	0.1653	0.1932	0.2218	0.2510	0.2806	0.3126
0.90	0.0958	0.1188	0.1430	0.1682	0.1944	0.2215	0.2495	0.2798
1.00	0.0826	0.1030	0.1246	0.1474	0.1714	0.1965	0.2228	0.2515
1.10	0.0716	0.0898	0.1091	0.1302	0.1516	0.1753	0.1998	0.2269
1.20	0.0626	0.0788	0.0962	0.1153	0.1350	0.1569	0.1798	0.2054
1.30	0.0550	0.0695	0.0851	0.1026	0.1206	0.1409	0.1623	0.1864
1.40	0.0485	0.0615	0.0757	0.0915	0.1081	0.1270	0.1470	0.1696
1.50	0.0429	0.0547	0.0675	0.0819	0.0972	0.1147	0.1334	0.1547
1.60	0.0380	0.0487	0.0603	0.0736	0.0876	0.1038	0.1213	0.1413
1.70	0.0339	0.0435	0.0541	0.0662	0.0792	0.0942	0.1106	0.1294
1.80	0.0302	0.0389	0.0486	0.0597	0.0717	0.0857	0.1010	0.1187
1.90	0.0270	0.0349	0.0437	0.0539	0.0650	0.0780	0.0924	0.1090
2.00	0.0241	0.0313	0.0394	0.0488	0.0591	0.0712	0.0846	0.1003
2.50	0.0141	0.0187	0.0239	0.0302	0.0373	0.0458	0.0555	0.0672
3.00	0.0085	0.0114	0.0149	0.0191	0.0241	0.0301	0.0373	0.0460
3.50	0.0052	0.0071	0.0094	0.0123	0.0158	0.0201	0.0254	0.0319
4.00	0.0032	0.0044	0.0060	0.0080	0.0105	0.0136	0.0175	0.0224
4.50	0.0020	0.0028	0.0039	0.0053	0.0070	0.0093	0.0122	0.0159
5.00	0.0012	0.0018	0.0025	0.0035	0.0047	0.0064	0.0085	0.0114
5.50	0.0008	0.0012	0.0016	0.0023	0.0032	0.0044	0.0060	0.0082
6.00	0.0005	0.0007	0.0011	0.0016	0.0022	0.0031	0.0042	0.0059

DANCOFF CORRECTION FOR SQUARE LATTICE,CONTINUED

VM/VF	3.7087	3.0601	2.5368	2.1085	1.7535	1.4561	1.2044	0.9894
R/D	0.26	0.28	0.30	0.32	0.34	0.36	0.38	0.40
SIG*D								
0.10	0.8391	0.8548	0.8688	0.8817	0.8945	0.9057	0.9170	0.9268
0.20	0.7189	0.7429	0.7651	0.7862	0.8072	0.8262	0.8458	0.8631
0.30	0.6238	0.6526	0.6799	0.7062	0.7329	0.7576	0.7834	0.8065
0.40	0.5465	0.5780	0.6084	0.6382	0.6687	0.6975	0.7279	0.7557
0.50	0.4825	0.5153	0.5475	0.5795	0.6126	0.6444	0.6783	0.7097
0.60	0.4288	0.4619	0.4950	0.5283	0.5632	0.5971	0.6336	0.6680
0.70	0.3831	0.4161	0.4494	0.4834	0.5193	0.5547	0.5931	0.6298
0.80	0.3440	0.3763	0.4095	0.4436	0.4801	0.5165	0.5563	0.5948
0.90	0.3101	0.3416	0.3743	0.4083	0.4450	0.4819	0.5227	0.5626
1.00	0.2805	0.3110	0.3431	0.3763	0.4133	0.4505	0.4919	0.5329
1.10	0.2546	0.2841	0.3153	0.3484	0.3846	0.4218	0.4635	0.5054
1.20	0.2318	0.2601	0.2904	0.3228	0.3585	0.3956	0.4374	0.4798
1.30	0.2115	0.2387	0.2680	0.2996	0.3348	0.3715	0.4133	0.4561
1.40	0.1935	0.2195	0.2479	0.2786	0.3130	0.3494	0.3909	0.4339
1.50	0.1773	0.2022	0.2296	0.2595	0.2931	0.3290	0.3701	0.4132
1.60	0.1628	0.1867	0.2130	0.2420	0.2748	0.3101	0.5508	0.3939
1.70	0.1498	0.1726	0.1979	0.2260	0.2580	0.2926	0.3328	0.3757
1.80	0.1380	0.1597	0.1841	0.2113	0.2424	0.2764	0.3160	0.3587
1.90	0.1274	0.1481	0.1715	0.1978	0.2281	0.2613	0.3003	0.3427
2.00	0.1177	0.1374	0.1599	0.1853	0.2147	0.2473	0.2856	0.3277
2.50	0.0805	0.0961	0.1144	0.1356	0.1607	0.1897	0.2245	0.2642
3.00	0.0562	0.0686	0.0833	0.1010	0.1225	0.1478	0.1790	0.2158
3.50	0.0399	0.0496	0.0616	0.0762	0.0944	0.1165	0.1443	0.1782
4.00	0.0286	0.0363	0.0460	0.0581	0.0736	0.0927	0.1174	0.1483
4.50	0.0207	0.0268	0.0346	0.0447	0.0577	0.0744	0.0962	0.1244
5.00	0.0151	0.0199	0.0262	0.0346	0.0456	0.0600	0.0794	0.1049
5.50	0.0110	0.0149	0.0200	0.0269	0.0362	0.0487	0.0658	0.0890
6.00	0.0081	0.0112	0.0153	0.0210	0.0289	0.0397	0.0548	0.0758

DANCOFF CORRECTION FOR SQUARE LATTICE,CONTINUED

VM/VF	0.8045	0.6442	0.5043	0.3816	0.3257	0.2732
R/D	0.42	0.44	0.46	0.48	0.49	0.50
SIG*D						
0.10	0.9368	0.9465	0.9557	0.9648	0.9691	0.9735
0.20	0.8809	0.8983	0.9152	0.9321	0.9402	0.9486
0.30	0.8305	0.8543	0.8777	0.9014	0.9130	0.9251
0.40	0.7847	0.8139	0.8430	0.8726	0.8874	0.9028
0.50	0.7429	0.7766	0.8106	0.8456	0.8632	0.8818
0.60	0.7045	0.7420	0.7802	0.8201	0.8404	0.8618
0.70	0.6691	0.7098	0.7518	0.7960	0.8187	0.8429
0.80	0.6364	0.6798	0.7251	0.7731	0.7981	0.8248
0.90	0.6060	0.6517	0.7000	0.7515	0.7786	0.8077
1.00	0.5777	0.6254	0.6762	0.7310	0.7600	0.7914
1.10	0.5514	0.6007	0.6538	0.7115	0.7424	0.7759
1.20	0.5268	0.5775	0.6326	0.6930	0.7255	0.7611
1.30	0.5037	0.5556	0.6125	0.6753	0.7095	0.7469
1.40	0.4821	0.5350	0.5934	0.6585	0.6941	0.7334
1.50	0.4618	0.5155	0.5753	0.6424	0.6795	0.7205
1.60	0.4426	0.4970	0.5581	0.6271	0.6655	0.7082
1.70	0.4246	0.4796	0.5417	0.6125	0.6521	0.6963
1.80	0.4076	0.4630	0.5261	0.5984	0.6392	0.6850
1.90	0.3916	0.4472	0.5112	0.5850	0.6269	0.6742
2.00	0.3764	0.4323	0.4969	0.5722	0.6151	0.6638
2.50	0.3114	0.3674	0.4344	0.5152	0.5627	0.6176
3.00	0.2608	0.3158	0.3836	0.4682	0.5193	0.5795
3.50	0.2206	0.2738	0.3416	0.4288	0.4828	0.5476
4.00	0.1880	0.2393	0.3064	0.3952	0.4517	0.5206
4.50	0.1614	0.2104	0.2764	0.3664	0.4248	0.4974
5.00	0.1394	0.1861	0.2506	0.3412	0.4013	0.4773
5.50	0.1209	0.1653	0.2281	0.3189	0.3805	0.4596
6.00	0.1053	0.1474	0.2085	0.2992	0.3620	0.4440

DANCOFF CORRECTION FOR HEXAGONAL LATTICE

VM/VF	26.5664	18.1434	13.0645	9.7681	7.5082	5.8916	4.6955	3.7858
R/D	0.10	0.12	0.14	0.16	0.18	0.20	0.22	0.24
SIG*D								
0.10	0.6518	0.6971	0.7332	0.7635	0.7892	0.8108	0.8302	0.8476
0.20	0.4672	0.5217	0.5679	0.6085	0.6446	0.6760	0.7049	0.7315
0.30	0.3536	0.4069	0.4543	0.4976	0.5377	0.5733	0.6070	0.6387
0.40	0.2780	0.3269	0.3721	0.4148	0.4554	0.4924	0.5283	0.5627
0.50	0.2249	0.2686	0.3104	0.3510	0.3905	0.4273	0.4637	0.4992
0.60	0.1858	0.2246	0.2627	0.3005	0.3382	0.3739	0.4099	0.4456
0.70	0.1562	0.1905	0.2250	0.2599	0.2953	0.3295	0.3646	0.3998
0.80	0.1330	0.1634	0.1946	0.2267	0.2596	0.2922	0.3259	0.3602
0.90	0.1145	0.1415	0.1697	0.1990	0.2297	0.2604	0.2926	0.3258
1.00	0.0993	0.1235	0.1485	0.1758	0.2042	0.2331	0.2637	0.2957
1.10	0.0865	0.1083	0.1315	0.1562	0.1820	0.2097	0.2386	0.2692
1.20	0.0760	0.0960	0.1167	0.1393	0.1632	0.1891	0.2164	0.2457
1.30	0.0671	0.0848	0.1039	0.1247	0.1469	0.1711	0.1969	0.2248
1.40	0.0595	0.0754	0.0929	0.1120	0.1325	0.1552	0.1795	0.2061
1.50	0.0529	0.0674	0.0833	0.1009	0.1199	0.1411	0.1640	0.1893
1.60	0.0472	0.0603	0.0749	0.0911	0.1087	0.1285	0.1502	0.1742
1.70	0.0422	0.0541	0.0675	0.0824	0.0988	0.1173	0.1378	0.1606
1.80	0.0378	0.0487	0.0609	0.0747	0.0900	0.1073	0.1265	0.1482
1.90	0.0340	0.0439	0.0551	0.0678	0.0820	0.0982	0.1164	0.1369
2.00	0.0305	0.0396	0.0499	0.0617	0.0749	0.0901	0.1072	0.1267
2.50	0.0183	0.0242	0.0310	0.0391	0.0484	0.0594	0.0722	0.0871
3.00	0.0112	0.0151	0.0197	0.0253	0.0319	0.0399	0.0495	0.0609
3.50	0.0070	0.0095	0.0127	0.0166	0.0213	0.0272	0.0344	0.0432
4.00	0.0044	0.0061	0.0082	0.0110	0.0144	0.0187	0.0241	0.0309
4.50	0.0028	0.0039	0.0054	0.0073	0.0098	0.0129	0.0170	0.0222
5.00	0.0018	0.0025	0.0036	0.0049	0.0067	0.0090	0.0120	0.0160
5.50	0.0011	0.0016	0.0024	0.0033	0.0046	0.0063	0.0086	0.0116
6.00	0.0007	0.0011	0.0016	0.0022	0.0032	0.0044	0.0061	0.0085

CANCOFF CORRECTION FOR HEXAGONAL LATTICE,CONTINUED

VM/VF	3.0779	2.5161	2.0629	1.6920	1.3846	1.1270	0.9090	0.7229
R/D	0.26	0.28	0.30	0.32	0.34	0.36	0.38	0.40
SIG*D								
0.10	0.8632	0.8772	0.8904	0.9029	0.9142	0.9250	0.9353	0.9452
0.20	0.7562	0.7790	0.8007	0.8215	0.8407	0.8595	0.8777	0.8955
0.30	0.6689	0.6974	0.7247	0.7513	0.7764	0.8014	0.8258	0.8500
0.40	0.5961	0.6282	0.6593	0.6900	0.7194	0.7491	0.7785	0.8081
0.50	0.5344	0.5686	0.6022	0.6359	0.6686	0.7019	0.7353	0.7694
0.60	0.4814	0.5169	0.5521	0.5877	0.6228	0.6590	0.6956	0.7334
0.70	0.4356	0.4716	0.5077	0.5446	0.5814	0.6198	0.6590	0.6999
0.80	0.3956	0.4316	0.4681	0.5058	0.5438	0.5838	0.6251	0.6686
0.90	0.3605	0.3961	0.4326	0.4706	0.5095	0.5507	0.5937	0.6393
1.00	0.3294	0.3644	0.4007	0.4388	0.4781	0.5202	0.5644	0.6119
1.10	0.3018	0.3360	0.3718	0.4097	0.4492	0.4919	0.5371	0.5860
1.20	0.2771	0.3104	0.3456	0.3831	0.4227	0.4657	0.5116	0.5618
1.30	0.2550	0.2873	0.3217	0.3588	0.3982	0.4413	0.4878	0.5388
1.40	0.2351	0.2664	0.2999	0.3364	0.3755	0.4186	0.4654	0.5172
1.50	0.2171	0.2473	0.2800	0.3158	0.3544	0.3974	0.4444	0.4967
1.60	0.2008	0.2299	0.2617	0.2967	0.3349	0.3775	0.4246	0.4774
1.70	0.1859	0.2140	0.2448	0.2791	0.3167	0.3589	0.4059	0.4590
1.80	0.1724	0.1994	0.2293	0.2627	0.2997	0.3415	0.3883	0.4415
1.90	0.1600	0.1860	0.2150	0.2475	0.2838	0.3251	0.3717	0.4249
2.00	0.1488	0.1737	0.2017	0.2334	0.2690	0.3097	0.3559	0.4091
2.50	0.1045	0.1248	0.1483	0.1757	0.2075	0.2449	0.2887	0.3405
3.00	0.0746	0.0910	0.1106	0.1340	0.1620	0.1957	0.2363	0.2857
3.50	0.0540	0.0672	0.0833	0.1032	0.1275	0.1576	0.1948	0.2412
4.00	0.0393	0.0500	0.0633	0.0800	0.1011	0.1277	0.1614	0.2046
4.50	0.0288	0.0374	0.0483	0.0624	0.0805	0.1040	0.1344	0.1742
5.00	0.0213	0.0281	0.0371	0.0489	0.0644	0.0850	0.1123	0.1489
5.50	0.0157	0.0212	0.0286	0.0385	0.0518	0.0697	0.0941	0.1276
6.00	0.0117	0.0161	0.0221	0.0303	0.0417	0.0574	0.0791	0.1096

DANCOFF CORRECTION FOR HEXAGONAL LATTICE,CONTINUED

VM/VF	0.5627	0.4239	0.3028	0.1965	0.1481	0.1027
R/D	0.42	0.44	0.46	0.48	0.49	0.50
SIG*D						
0.10	0.9546	0.9639	0.9729	0.9815	0.9858	0.9899
0.20	0.9127	0.9301	0.9472	0.9636	0.9720	0.9800
0.30	0.8738	0.8983	0.9226	0.9464	0.9586	0.9704
0.40	0.8376	0.8683	0.8991	0.9298	0.9456	0.9610
0.50	0.8037	0.8399	0.8767	0.9136	0.9329	0.9518
0.60	0.7719	0.8129	0.8552	0.8980	0.9206	0.9428
0.70	0.7420	0.7873	0.8345	0.8829	0.9086	0.9340
0.80	0.7139	0.7630	0.8146	0.8682	0.8968	0.9255
0.90	0.6873	0.7398	0.7956	0.8540	0.8854	0.9171
1.00	0.6622	0.7177	0.7772	0.8402	0.8742	0.9089
1.10	0.6384	0.6966	0.7594	0.8267	0.8634	0.9009
1.20	0.6158	0.6763	0.7424	0.8137	0.8527	0.8930
1.30	0.5944	0.6570	0.7258	0.8010	0.8423	0.8853
1.40	0.5740	0.6384	0.7099	0.7886	0.8322	0.8778
1.50	0.5546	0.6206	0.6945	0.7765	0.8223	0.8704
1.60	0.5361	0.6035	0.6796	0.7648	0.8126	0.8632
1.70	0.5184	0.5871	0.6651	0.7533	0.8031	0.8561
1.80	0.5015	0.5713	0.6512	0.7421	0.7938	0.8492
1.90	0.4854	0.5561	0.6376	0.7312	0.7847	0.8424
2.00	0.4699	0.5414	0.6245	0.7206	0.7758	0.8357
2.50	0.4016	0.4755	0.5643	0.6710	0.7340	0.8042
3.00	0.3455	0.4199	0.5120	0.6267	0.6962	0.7755
3.50	0.2989	0.3724	0.4661	0.5868	0.6617	0.7492
4.00	0.2596	0.3314	0.4256	0.5507	0.6302	0.7251
4.50	0.2263	0.2959	0.3896	0.5179	0.6013	0.7029
5.00	0.1979	0.2649	0.3575	0.4879	0.5746	0.6824
5.50	0.1734	0.2377	0.3286	0.4605	0.5500	0.6634
6.00	0.1524	0.2137	0.3027	0.4352	0.5272	0.6457

APPENDIX 2

The subroutine DASQHE

DASQHE, written in FORTRAN IV, calculates the Dancoff correction for a square or hexagonal lattice. The calculation is done for one geometrical configuration but for a series of moderator cross sections if desired. The subroutine is called by

```
CALL DASQHE(NLAT,PITCH,RADIUS,GAPWID,NSIGMA,SIGMA,
            NALF,NRAD,DC)
```

The variables in the call statement have the following meaning.

NLAT defines the type of lattice. NLAT = 4 means a square lattice, and NLAT = 6 means a hexagonal lattice. For other values the routine assumes a square lattice.

PITCH = lattice pitch

RADIUS = rod radius

GAPWID = width of an empty gap surrounding the rods

NSIGMA = number of moderator cross sections

SIGMA = Σ_{mod}, moderator cross section. Vector of order NSIGMA.

NALF, NRAD are accuracy parameters defined in paragraph 4.

DC = the calculated Dancoff corrections. Vector of order NSIGMA.

DASQHE needs the Bickley function Ki_3. This function is called BIC3(X).

```
  0 $IBFTC DASQHE
  1       SUBROUTINE DASQHE(NLAT,PITCH,RADIUS,GAPWID,
       1                    NSIGMA,SIGMA,NALF,NRAD,DC)
  2       DIMENSION SIGMA(1),DC(1),SIG(100)
  3       PI=3.14159
  4       IF(NLAT.NE.6)NLAT=4
  7       GAM=0.0
 10       IF(NLAT.EQ.6) GAM=PI/6.0
 13       R=RADIUS/PITCH
 14       E=(RADIUS+GAPWID)/PITCH
 15       E2=E**2
 16       CONST=2.0/(PI*FLOAT(NALF)*FLOAT(NRAD))
 17       SIGMIN=SIGMA(1)*PITCH
 20       DO 5 NS=1,NSIGMA
 21       SIG(NS)=SIGMA(NS)*PITCH
 22       SIGMIN=AMIN1(SIGMIN,SIG(NS))
 23     5 DC(NS)=0.0
 25     8 NROW=MIN0(100,INT(10.0/SIGMIN+1.0))
 26       I1=2*NRAD
 27       DZ=R/FLOAT(NRAD)
 30       DALF=PI/FLOAT(NLAT*NALF)
 31       ALF=-0.5*DALF
 32       DO 60 N=1,NALF
 33       ALF=ALF+DALF
 34       CAG=COS(ALF+GAM)
 35       DX=COS(GAM)/CAG
 36       DY=SIN(ALF)/CAG
 37       T=SIN(ALF+GAM)/CAG
 40       Z=-R-0.5*DZ
 41       DO 50 I=1,I1
 42       Z=Z+DZ
 43       X=Z*T-SQRT(E2-Z**2)
 44       F=CAG-Z
 45       IF(F.GE.E) GO TO 10
 50       IF(F.LE.R) GO TO 40
 53       X=X-2.0*SQRT(E2-F**2)
 54    10 Y=Z/CAG+1.0
 55       DO 30 J=1,NROW
 56       Y=Y+DY-FLOAT(INT(Y+DY))
 57       X=X+DX
 60       F=-CAG*Y
 61       IF(F.LE.(-E)) GO TO 12
 64       IF(F.GE.(-R)) GO TO 40
 67       X=X-2.0*SQRT(E2-F**2)
 70    12 F=CAG+F
 71       IF(F.GE.E) GO TO 30
 74       IF(F.LE.R) GO TO 40
 77       X=X-2.0*SQRT(E2-F**2)
100    30 CONTINUE
102       GO TO 50
103    40 X=X+F*T-SQRT(E2-F**2)
104       DO 45 NS=1,NSIGMA
105    45 DC(NS)=DC(NS)+BIC3(SIG(NS)*X)
107    50 CONTINUE
111    60 CONTINUE
113       DO 65 NS=1,NSIGMA
114    65 DC(NS)=CONST*DC(NS)
116       RETURN
117       END
```

TABLE 1

Convergence with L and V

Square lattice $\Sigma d = 0.8$, $\frac{r}{d} = 0.3$

Entries: C (L, V)
C (L, V) - C (128, 128) = "error"

V \ L	16	32	64	128
16	0.40809 -144	0.41038 +85	0.40956 +3	0.40955 +2
32	0.40952 -1	0.40952 -1	0.40962 +9	0.40950 -3
64	0.40964 +11	0.40941 -12	0.40950 -3	0.40954 +1
128	0.40978 +25	0.40956 +3	0.40953 0	0.40953

TABLE 2

Convergence with L and V

Square lattice $\Sigma d = 0.5$, $\frac{r}{d} = 0.4$

Entries: C (L, V)
C (L, V) - C (128, 128) = "error"

V \ L	16	32	64	128
16	0.70960 -46	0.70992 -14	0.70973 -33	0.71003 -3
32	0.71205 +199	0.70974 -32	0.70993 -13	0.71012 +6
64	0.71028 +22	0.71074 +68	0.70995 -11	0.71008 +2
128	0.70989 -17	0.71025 +19	0.71030 +24	0.71006

TABLE 3

$\left[C(32,32) - C(64,64)\right] \times 10^4$

Σd \ $\frac{r}{d}$	Square lattice					Hexagonal lattice				
	0.1	0.2	0.3	0.4	0.5	0.1	0.2	0.3	0.4	0.5
0.1	-23	-1	0	-2	0	-11	+1	-2	+1	0
0.2	-23	0	-1	-1	0	-11	+1	-2	+2	0
0.5	-11	0	0	-2	-1	-7	+1	-4	+4	0
1.0	-3	+1	0	-2	-2	-3	+1	-2	+5	+1
2.0	-1	0	0	0	-2	-1	0	-1	+4	+1
4.0	0	0	0	0	-1	0	0	0	+2	+1
6.0	0	0	0	0	-1	0	0	0	+1	+2

TABLE 4

High volume ratios, small cross sections

$\left[C(32,64) - C(64,128)\right] \times 10^4$

Σd \ $\frac{r}{d}$	Square lattice			Hexagonal lattice		
	0.1	0.14	0.20	0.1	0.14	0.20
0.1	-3	-3	-2	-1	-1	-2
0.2	-4	-3	-3	-2	-1	-2
0.5	+3	-1	-2	-1	-1	-3
1.0	-2	0	-2	-1	-1	-2

TABLE 5

Comparison with Monte Carlo values reported by Fukai

Type of lattice	Rod radius cm	$\frac{V_1}{V_0}$	Monte Carlo values	C(16,16)	C(32,32)		C(64,64)
				Σ_m=1.492	Σ_m=1.49	Σ_m=1.492	Σ_m=1.492
Hexagonal	0.3175	1	0.474±0.002	0.4719	0.4733	0.4729	0.4726
	"	3	0.179±0.006	0.1748	0.1752	0.1749	0.1751
	0.762	1	0.217±0.005	0.2119	0.2127	0.2123	0.2121
	"	3	0.040±0.011	0.0330	0.0332	0.0330	0.0331
Square	0.3175	0.2732	0.7995±0.0005	0.8001	0.8001	0.7999	0.8000
	"	0.6	0.628±0.001	0.6257	0.6257	0.6253	0.6251
	"	1	0.479±0.002	0.4808	0.4810	0.4806	0.4807
	"	3	0.174±0.006	0.1789	0.1785	0.1782	0.1782
	0.762	0.2732	0.638±0.001	0.6377	0.6376	0.6374	0.6375
	"	0.6	0.391±0.003	0.3814	0.3811	0.3807	0.3806
	"	1	0.222±0.005	0.2270	0.2272	0.2268	0.2269
	"	3	0.024±0.009	0.0368	0.0366	0.0365	0.0366

TABLE 6

The effect of a gap around the rod

Square lattice

Σd \ $\frac{r}{d}$		0.1			0.2			0.3			0.4		
	gap thickness % of r	Δ_{gap}	Δ_{hom}	Δ	Δ_{gap}	Δ_{hom}	Δ	Δ_{gap}	Δ_{hom}	Δ	Δ_{gap}	Δ_{hom}	Δ
0.1	10	0.0022	0.0017	-0.0005	0.0059	0.0052	-0.0007	0.0102	0.0097	-0.0005	0.0151	0.0147	-0.0004
	20	44	37	-7	122	111	-11	213	205	-8	317	312	-5
0.2	10	28	19	-9	91	76	-15	174	157	-17	274	249	-25
	20	57	41	-16	187	160	-27	362	335	-27	581	563	-18
0.5	10	31	14	-17	128	89	-39	292	241	-51	542	489	-53
	20	52	30	-22	256	190	-66	607	523	-84	1167	1089	-78
1.0	10	25	8	-17	125	71	-54	350	256	-94	787	661	-126
	20	48	17	-31	251	153	-98	730	566	-164	1744	1533	-211
2.0	10	15	4	-6	111	41	-70	318	197	-121	954	709	-245
	20	29	8	-21	181	88	-93	679	449	-230	2232	1749	-483
3.0	10	8	2	-6	57	24	-33	249	140	-109	954	640	-314
	20	15	4	-11	119	51	-68	553	326	-227	2369	1660	-709
4.0	10	4	1	-3	34	14	-20	185	97	-88	897	552	-345
	20	8	2	-6	74	30	-44	430	232	-198	2367	1490	-877

$\Delta_{gap} = C_{gap} - C_w$, $\Delta_{hom} = C_{hom} - C_w$, $\Delta = \Delta_{hom} - \Delta_{gap}$

TABLE 7

Accuracy of Sauer's approximation

Square lattice

$(C_{Sauer} - C_{Carlvik}) \cdot 10^4$

$\frac{V_m}{V_f}$	30.831	15.240	6.958	2.537	0.9894	0.3816	0.3257	0.2732
$\frac{r}{d}$	0.10	0.14	0.20	0.30	0.40	0.48	0.49	0.50
$\Sigma\overline{d}$								
0.1	-35	-77	-73	-38	-10	-2	0	0
0.2	+74	-49	-102	-77	-27	-5	-2	-2
0.4	+213	+54	-73	-110	-54	-9	-4	-5
0.6	+253	+115	-23	-104	-66	-12	-7	-10
1.0	+247	+155	+48	-57	-58	-12	-10	-22
1.5	+216	+154	+85	+3	-22	-6	-15	-42
2.0	+185	+140	+97	+45	+17	-2	-21	-68
3.0	+129	+105	+91	+84	+80	+4	-43	-131
4.0	+88	+73	+72	+90	+116	+3	-70	-201
5.0	+59	+49	+52	+83	+132	0	-95	-267
6.0	+39	+31	+36	+70	+135	+1	-114	-325

TABLE 8

Accuracy of Sauer's approximation

Hexagonal lattice

$(C_{Sauer} - C_{Carlvik}) \cdot 10^4$

$\frac{V_m}{V_f}$	26.5664	13.0645	5.8916	2.0629	0.7229	0.1965	0.1481	0.1027
$\frac{r}{d}$	0.10	0.14	0.20	0.30	0.40	0.48	0.49	0.50
$\Sigma\bar{d}$								
0.1	-24	-63	-61	-28	-5	0	-1	0
0.2	+96	-37	-94	-64	-13	-1	-2	-1
0.4	+282	+81	-73	-108	-32	-4	-5	-2
0.6	+360	+165	-21	-119	-46	-6	-8	-4
1.0	+389	+236	+65	-92	-57	-11	-12	-9
1.5	+369	+249	+120	-34	-49	-13	-17	-16
2.0	+334	+236	+143	+17	-28	-11	-17	-24
3.0	+261	+190	+143	+82	+27	+4	-12	-40
4.0	+198	+142	+120	+107	+79	+3	+1	-55
5.0	+148	+101	+93	+108	+12	+6	+17	-71
6.0	+111	+71	+69	+99	+14	+9	+35	-85

TABLE 9

Accuracy of Sauer's approximation with Bonalumi's modification

Square lattice

$(C_{Bonalumi} - C_{Carlvik}) \cdot 10^4$

$\frac{V_m}{V_f}$	30.831	15.240	6.958	2.537	0.9894	0.3816	0.3257	0.2732
$\frac{r}{d}$	0.10	0.14	0.20	0.30	0.40	0.48	0.49	0.50
$\Sigma\bar{d}$								
0.1	+2	-42	-47	-26	-6	-1	0	0
0.2	+82	-10	-55	-46	-15	-2	+1	0
0.4	+110	+32	-36	-55	-23	0	+3	-1
0.6	+70	+24	-27	-48	-20	+4	+5	-1
1.0	-3	-18	-35	-35	-2	+16	+12	-6
1.5	-33	-43	-50	-30	+19	+28	+14	-20
2.0	-34	-45	-52	-29	+31	+31	+8	-46
3.0	-20	-29	-37	-26	+38	+17	-30	-120
4.0	-10	-15	-22	-21	+33	-16	-84	-212
5.0	-4	-7	-12	-14	+25	-54	-142	-308
6.0	-2	-4	-7	-9	+17	-89	-169	-399

TABLE 10

Accuracy of Sauer's approximation with Bonalumi's modification

Hexagonal lattice

$(C_{Bonalumi} - C_{Carlvik}) \cdot 10^4$

$\frac{V_m}{V_f}$	26.5664	13.0645	5.8916	2.0629	0.7229	0.1965	0.1481	0.1027
$\frac{r}{d}$	0.10	0.14	0.20	0.30	0.40	0.48	0.49	0.50
$\Sigma\bar{d}$								
0.1	-2	-43	-47	-22	-3	0	-1	0
0.2	+113	-1	-59	-45	-8	0	-2	-1
0.4	+229	+98	-20	-61	-13	-2	-4	-2
0.6	+225	+136	+24	-52	-13	-2	-6	-3
1.0	+139	+116	+61	-14	+2	-2	-8	-8
1.5	+60	+62	+55	+26	+30	+3	-9	-14
2.0	+20	+27	+38	+48	+59	+12	-5	-21
3.0	-3	0	+14	+58	+104	+38	+6	-36
4.0	-5	-3	+4	+51	+131	+69	+22	-53
5.0	-3	-3	+1	+41	+142	+100	+39	-71
6.0	-1	-2	0	+31	+142	+129	+54	-89

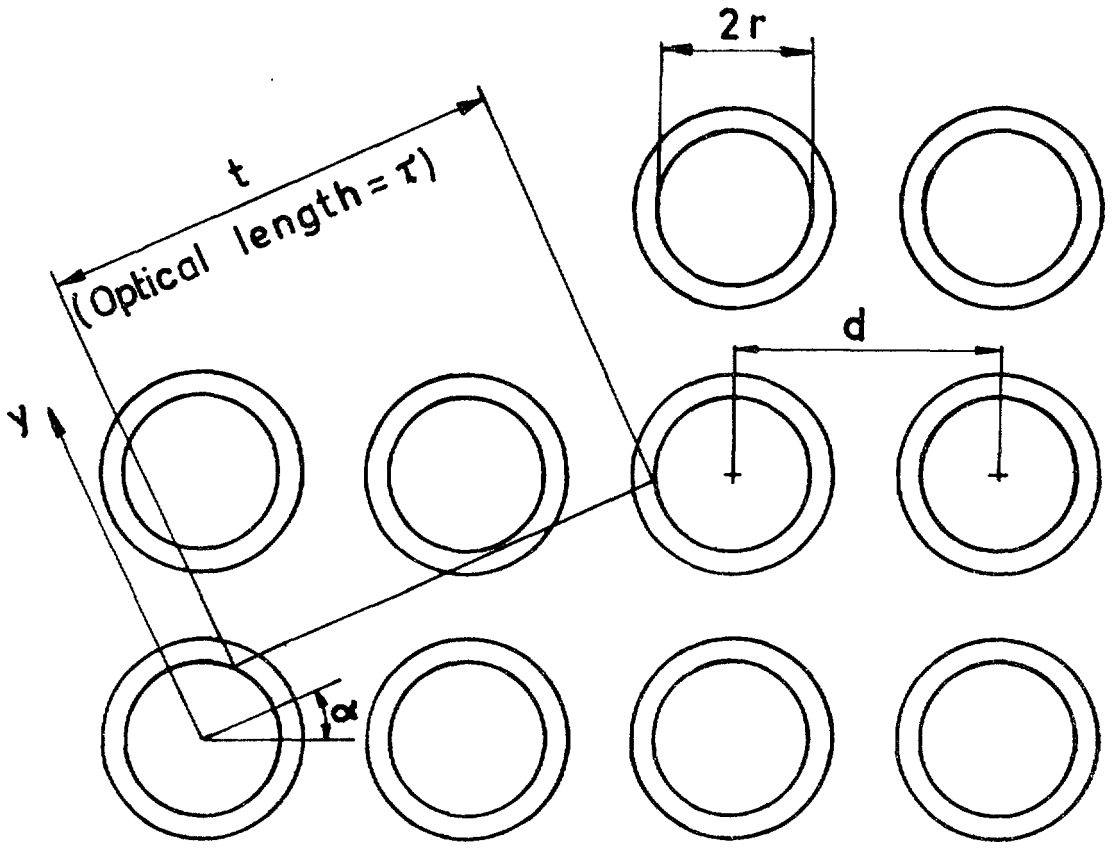

Figure 1

Notations used for the calculation of the Dancoff correction in a lattice

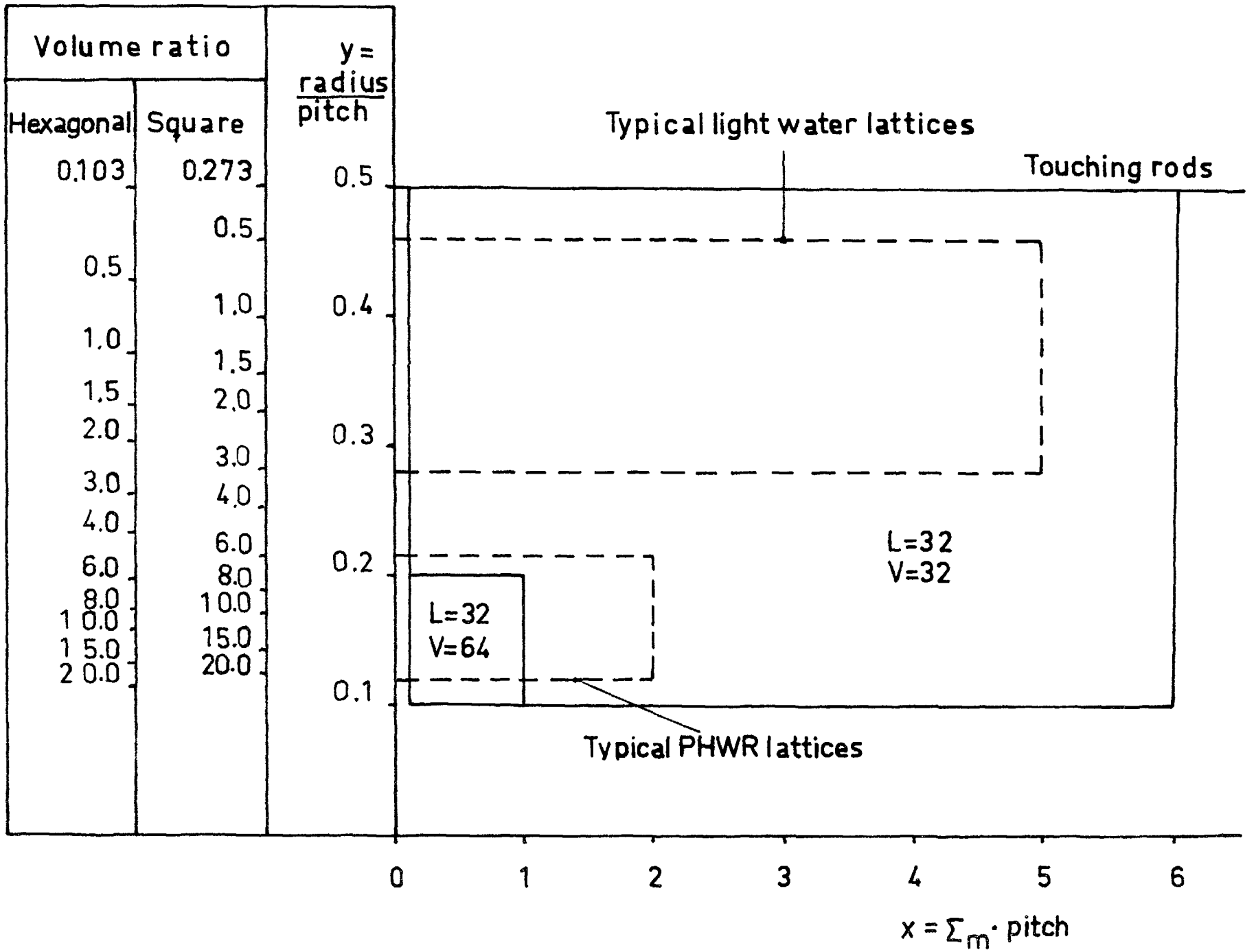

Figure 2

Parameter variation

The present calculations cover the regions inside the large rectangle

Figure 3. C as a function of $\Sigma\bar{\ell}$ for small volume ratios and small $\Sigma\bar{\ell}$. Square lattice

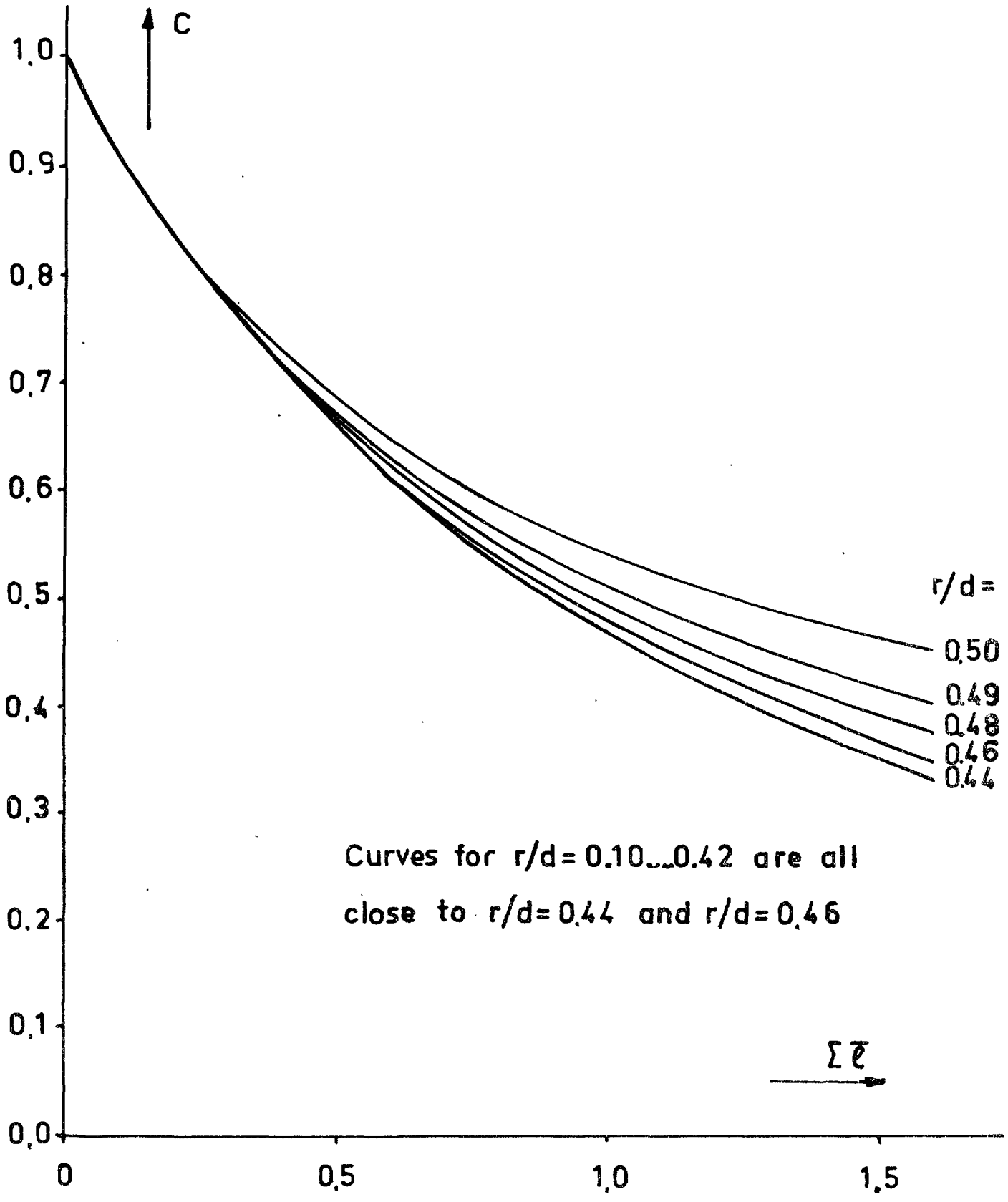

Figure 4. Investigation of Bonalumi's formula