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REACTOR CELL PARAMETERS IN MULTIGROUP COLLISION PROBABILITY THEORY

by

L. AMYOT

1966

Joint Nuclear Research Center
Ispra Establishment - Italy

Reactor Physics Department
Reactor Theory and Analysis

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SUMMARY

A consistent set of definitions of the reactor cell parameters is presented and discussed in the framework of the multigroup, multi-region collision probability technique. The assumptions implied in the fundamental neutron balance and, in particular, the link with more general integral transport theory, are examined in the light of the recent literature on the subject.

Introduction

There exists at the present time no privileged set of lattice parameters capable of describing adequately every type of systems encountered in practice, nor perhaps can there be in view of the wide variety of designs, fuel compositions, reactor sizes suggesting an equally vast diversity of convenient, simplified models. A deeper explanation of this situation may be found in the fact that a complete representation in terms of observable events is impossible or at least unpractical. Ideally, however, a theoretical model should be able to predict all measurable quantities, not only the bulk reactor parameters but also the detailed reaction rates, in terms of which the multiplying properties of a lattice may be gauged. Within the limits of economic considerations, it is therefore desirable that a calculation method be built as close as possible around a system of neutron balance equations through which the competition between the several phenomena determining the fate of a typical neutron may be studied.

It is an essential merit of multigroup, multiregion techniques that they allow just this sort of detailed accounting. In principle, once the balance equations have been solved, all parameters defined in terms of collision rates are immediately expressible. The main drawback, of course, is that this happy situation is not achieved without much expenditure in machine-time, be it with Monte-Carlo or most deterministic methods, especially if the system to be analyzed is very heterogeneous. The vigorous growth and multifarious applications of collision probability techniques during the last decade are mainly due to their ability to reproduce with astonishing accuracy and at a far lower cost many dearly bought results of the classical methods. Their domain of validity is strictly limited and they will be of no advantage if a very refined picture is desired, since they can only yield integral values. However, not many differential parameters are of direct interest in practical reactor design.

In the present report, a consistent set of definitions of the reactor cell parameters is presented in the framework of the multigroup, multiregion collision probability technique.

Manuscript received on July 6, 1966

1. The Neutron Balance Equation

The integral form of the Boltzmann equation, as applied to a neutron gas was first established by Peierls [1] as long ago as 1939. In spite of this early start and chiefly because of the mathematical difficulties involved in the treatment of practical geometries, the Peierls equation, as it is often called, has not been so widely used, except in special cases, as the familiar integro-differential form [2]. However, the last few years have shown a renewal of interest, prompted mainly by the rapid development of collision probability techniques [3], [4], which combine the advantages of simplicity and surprising accuracy. This new usefulness could only be gained at the price of a few assumptions which limit the range of application but, at the same time, point the way to eventual improvements. In the following paragraphs, the neutron balance equation which serves as a basis for lattice calculations using the concept of first collision probability is derived step by step from the general integral transport equation and the hypotheses introduced in the process are pointed out.

The neutron flux in an arbitrary system is a solution of the equation [5]

$$\phi(\vec{x},E,\vec{\Omega},t) = \int_0^\infty ds\, H(\vec{x}-s\vec{\Omega},E,\vec{\Omega},t-\tfrac{s}{v}) \exp\left[-\int_0^s ds'\, \Sigma(\vec{x}-s'\vec{\Omega},E)\right] \qquad (1)$$

where

$\phi(\vec{x},E,\vec{\Omega},t)$ = number of neutrons in the unit volume around $\vec{x}$, the unit solid angle about $\vec{\Omega}$ and the unit energy range about E which, in unit time around time t, will cross a unit surface area, normal to the direction $\vec{\Omega}$, on the unit sphere surrounding $\vec{x}$;

$H(\vec{x},E,\vec{\Omega},t)$ = number of neutron of energy E emitted at time t, per unit volume, angle and energy at the point $\vec{x}$ and along direction $\vec{\Omega}$;

$\Sigma(\vec{x},E)$ = total neutron cross section of the medium at point $\vec{x}$ and energy E.

Equation (1) states that the flux is obtained by looking backward from point $\vec{x}$ at time t, along direction $\vec{\Omega}$ and summing the product of the sources along $\vec{\Omega}$ and the probability of surviving the flight to point $\vec{x}$. The source neutrons represented by the function H may be

supplied by some external means independent of the system (such as a Ra - Be source) or as a result of fission and scattering events involving neutrons of the population considered. If, for the sake of convenience, the delayed neutron emitters are considered as external sources, and attention is focused on the virgin prompt and scattered components of the neutron distribution, we may write [6]

$$H(\vec{x},E,\vec{\Omega},t) = S(\vec{x},E,\vec{\Omega},t) + \int_0^\infty dE' \int_{(4\pi)} d\vec{\Omega}' \, \nu(\vec{x},E'\to E,\vec{\Omega}) \, \Sigma_f(\vec{x},E') \, \phi(\vec{x},E',\vec{\Omega}',t) \qquad (2)$$

$$+ \int_0^\infty dE' \int_{(4\pi)} d\vec{\Omega}' \, \Sigma_s(\vec{x},E'\to E,\vec{\Omega}'\to\vec{\Omega}) \, \phi(\vec{x},E',\vec{\Omega}',t)$$

where

$S(\vec{x},E,\vec{\Omega},t)$ = number of neutrons of energy E generated by external sources (including delayed neutron emitters) at time t, per unit volume, angle and energy at the point $\vec{x}$ and along direction $\vec{\Omega}$;

$\nu(\vec{x},E'\to E,\vec{\Omega})$ = number of prompt neutrons of energy E produced at point and along direction $\vec{\Omega}$ per fission taking place at energy E' ;

$\Sigma_s(\vec{x},E'\to E,\vec{\Omega}'\to\vec{\Omega})$ = cross section at point $\vec{x}$ for changing the neutron energy and direction E' , $\vec{\Omega}'$, into an energy and direction E, $\vec{\Omega}$;

$\Sigma_f(\vec{x},E')$ = fission cross section at point $\vec{x}$ and energy E' .

Time dependent problems can always be at least formally reduced to stationary ones provided, as is implicitly assumed in equs.(1), (2), that the properties of the medium do not change with time [7], [8]. The steady state Peierls equation is therefore of very general interest and, in view of the applications envisaged in the present paper, the time variable will be dropped in the following development. In practice, a stationary distribution of the neutron flux may be obtained either in a subcritical assembly fed by a permanent external source or in a critical reactor, where the chain reaction is self-sustaining without any contribution from external sources. Only the second case will be considered here. We have then

$$\phi(\vec{x},E,\vec{\Omega}) = \int_0^\infty d\rho \int_0^\infty dE' \int_{(4\pi)} d\vec{\Omega}' \left[\nu(\vec{x}-\rho\vec{\Omega},E'\to E,\vec{\Omega}) \, \Sigma_f(\vec{x}-\rho\vec{\Omega},E') + \Sigma_s(\vec{x}-\rho\vec{\Omega},E'\to E,\vec{\Omega}'\to\vec{\Omega}) \right] \qquad (3)$$

$$\cdot \, \phi(\vec{x}-\rho\vec{\Omega},E',\vec{\Omega}') \, \exp\left[-\int_0^\rho d\rho' \, \Sigma(\vec{x}-\rho'\vec{\Omega},E) \right]$$

From the mathematical point of view, the new equation offers the advantage of being homogeneous and thus more easily tractable. Another consequence of eliminating the external source terms is that the absolute value of the flux may no longer be determined from the transport equation alone.

Most frequently, the integral equation (3) is approximated for solution by introducing a multigroup energy structure. Because of the interdependence of the energy loss and the angular deviation and, more importantly, due to the space-energy correlation this procedure is not rigorously justified. It creates the problem of defining suitable averages for the nuclear properties of the medium. The choice of the approximate technique will be greatly influenced by the nature of the system under study and the position of a given group on the scale of energy. The actual width of the groups will of course be a major limiting factor for the range of validity of any set of group constants. This is especially true in the resonance region where the energy variation may be very large and abrupt. The problem will be considered in more detail in latter sections.

While a degree of separability between spectral and spatial effects must be assumed in the calculation of every group parameter, the problem of the transfer cross section is essentially more complex because of its directional aspect. A device commonly used to meet this difficulty is to expand both the flux and the transfer cross section in spherical harmonics. Although it has been shown [9] that, for a given order of expansion in spherical harmonics, the integral transport group equation is inherently more accurate than the corresponding and better known integro-differential form, the machine-time required with even a moderately high order of expansion would be prohibitively long for routine calculations. Fortunately, the general treatment is seldom warranted.

Anisotropic scattering assumes increasing importance at higher energies where the presence of a forward bias may affect neutron diffusion and leakage to a significant extent. The effect on reactivity will then be particularly large in fast and intermediate reactors. It turns out, however, that a suitable transport approximation, leading to an isotropic type solution, generally will yield acceptable results even in such systems [10] , [11] . With

very light moderating nuclides, v.g. hydrogen or deuterium, some attention must be paid to scattering anisotropy in the thermal range. Up to a point, the effect is mitigated by the randomness of thermal motion and the effective increase in mass of the target nuclides due to molecular binding . At most, linear anisotropy may have to be considered [12], [13], but, here again, a diagonal transport correction is ordinarily sufficient [14].

The great advantage of the integral formulation is that for isotropic scattering the angular flux need not be computed. Thus, in energy group n, the transport scalar flux at point $\vec{x}$ is given by

$$\phi_m(\vec{x}) = \int_{(4\pi)} d\vec{\Omega} \int_0^\infty d\rho \cdot \sum_m \left[\nu_{m\to m}(\vec{x}-\rho\vec{\Omega}) \Sigma_{f,m}(\vec{x}-\rho\vec{\Omega}) + \Sigma_{s,m\to m}(\vec{x}-\rho\vec{\Omega}) \right] \cdot \frac{\phi_m(\vec{x}-\rho\vec{\Omega})}{4\pi} \cdot \exp\left[-\int_0^\rho d\rho' \Sigma_m(\vec{x}-\rho'\vec{\Omega}) \right] \qquad (4)$$

where the group transfer cross section $\Sigma_{s,m\to m}$ may be assumed to be transport corrected and all nuclear parameters are supposed to be properly averaged over energy. This is actually the type of equation that is solved in the THERMOS code [14]. The expression on the right-hand side may be simplified by transforming the line integrals to a volume integral through the substitution

$$\vec{x}' = \vec{x} - \rho\vec{\Omega}$$

$$d\vec{x}' = |\vec{x}-\vec{x}'|^2 \, d\rho \, d\vec{\Omega}$$

the result being

$$\phi_m(\vec{x}) = \int_{(V)} d\vec{x}' \sum_m \left[\nu_{m\to m}(\vec{x}') \Sigma_{f,m}(\vec{x}') + \Sigma_{s,m\to m}(\vec{x}') \right] \phi_m(\vec{x}') \cdot \frac{e^{-\tau_m(\vec{x}',\vec{x})}}{4\pi |\vec{x}-\vec{x}'|^2} \qquad (5)$$

where $\tau_m(\vec{x}',\vec{x})$ is the "optical distance" between the two points $\vec{x}'$ and $\vec{x}$ for group m neutrons.

In real situations, the medium of propagation is always made up of a number of homogeneous regions of finite extension, in each of which the nuclear cross sections may be taken as constant. The integration over the variable $\vec{x}'$ in equation (5) may thus be decomposed into a sum of integrals extended over the κ partial volumes V_j constituting the physical system. Defining the average group n flux in region j as

$$\phi_{j,m} = \frac{1}{V_j} \int_{(V_j)} d\vec{x} \cdot \phi_m(\vec{x}) \tag{6}$$

and the average emission density of group n neutrons in region j as

$$H_{j,m} = \frac{1}{V_j} \int_{(V_j)} d\vec{x}' \sum_m \left[\nu_{m\to m}(\vec{x}') \Sigma_{f,m}(\vec{x}') + \Sigma_{s,m\to m}(\vec{x}') \right] \phi_m(\vec{x}') \tag{7}$$

the total collision rate in region j for group n neutrons is obtained from the following balance equation

$$V_j \Sigma_{j,m} \phi_{j,m} = \sum_{i=1}^{K} V_i P_{i\to j,m} H_{i,m} \tag{8}$$

with the abbreviation

$$P_{i\to j,m} = \frac{\Sigma_{j,m} \int_{(V_j)} d\vec{x} \int_{(V_i)} d\vec{x}' \cdot \frac{e^{-\tau_m(\vec{x}',\vec{x})}}{4\pi |\vec{x}-\vec{x}'|^2} \cdot \sum_m \left[\nu_{m\to m}(\vec{x}') \Sigma_{f,m}(\vec{x}') + \Sigma_{s,m\to m}(\vec{x}') \right] \phi_{i,m}(\vec{x}')}{\int_{(V_i)} d\vec{x}' \cdot \sum_m \left[\nu_{m\to m}(\vec{x}') \Sigma_{f,m}(\vec{x}') + \Sigma_{s,m\to m}(\vec{x}') \right] \phi_m(\vec{x}')} \tag{9}$$

The symbol $P_{i\to j,m}$ denotes the probability for a group n neutron emitted in region i to suffer its first collision in region j .

It may be appropriate to add that there now are in existence various generalized definitions of the first collision probability which will take direct account of scattering anisotropy [23], [24]. However, it will be assumed here that an equivalent transport corrected scheme has been established.

Except perhaps as a convenient shorthand notation, the concept of collision probability would be of far less practical advantage were it not for the fact that the interactions $P_{i\to j,m}$ are rather insensitive to the spatial distribution of the source neutrons. Although parabolic and more complex distributions have been considered in particular cases [15], the most widely used approximation is to assume that the emission density is uniformly distributed in region i. This condition holds the better, the smaller the dimensions of the partial volumes and the nuclear cross sections of the materials they contain. There results

$$P_{i \to j,m} = \frac{\Sigma_{j,m}}{V_i} \int_{(V_j)} d\vec{x} \int_{(V_i)} d\vec{x}' \cdot \frac{e^{-\tau_m(\vec{x}',\vec{x})}}{4\pi |\vec{x}-\vec{x}'|^2} \qquad (10)$$

The neutron behaviour in a critical system, may therefore be described by a matrix of linear algebraic equations of type (8) which are easily solved for group fluxes in every region, once the group constants have been determined from a preliminary spectrum calculation and the collision probabilities have been evaluated by performing the integrations over space indicated in equ. (10).

2. The Wigner-Seitz Model

2.1 The Unit Cell

The criticality equation for a finite system gives the relation between the nuclear properties of an assembly and the size and shape of the reactor which must hold if the chain-reaction within the system is to be self-perpetuating at a constant intensity. Nearly always, the overall physical dimension of the assembly are such that a direct solution of the problem,using a system of collision balance equations of the type just described, is a practical impossibility. It is also unnecessary, since the detailed flux distribution may usually be separated into the product of a macroscopic function, subject to a simpler representation, and a microscopic function, which alone must be studied with great detail and accuracy as to its variation with space and energy. A more refined picture [16] would show that, in addition to this product, the general expression of the flux at any point inside a reactor, contains a perturbation term proportional to the gradient of the macroscopic flux; however this is a small correction which may safely be neglected in most approximations.

There logically follows a two-step procedure. Few-group parameters are first evaluated for a limited number of homogenized regions through preliminary multigroup-multiregion calculations which take into account the detailed neutron distribution in space and energy in restricted portions of the system. These nuclear parameters are then supplied as input to a second (quite commonly, diffusion theory) calculation applied to the whole system, but this time

with a much coarser space-energy point network.

For homogeneous reactors,the problem is, of course, considerably simplified by the absence of a fine structure of the flux. To some extent, this is also true of fast reactors, where the core dimensions often are of the same order of magnitude as the average neutron mean free path. Intermediate and thermal cores, on the other hand, appear, from the neutronic point of view, as uniform masses of moderating materials in which control or/and fuel elements are dispersed in discrete lumps of absorbing and fissile matter. Far from the heterogeneities, the flux in the moderator varies smoothly with position and energy, but strong local distortions are created by the sources and sinks. The so-called "heterogeneous" method will allow, it is true, a direct calculation of the point fluxes anywhere in the moderator but only after the nuclear parameters attached to the various singularities and the moderator have been obtained through a suitable space-energy averaging over the fine group fluxes [17]. Full advantage of the decomposition into microscopic and macroscopic fluxes is taken in the competing and long since classical Wigner-Seitz cell method.

Originally developed for the theory of crystals, the Wigner-Seitz method assumes that the reactor core may be divided into a number of cells centered around the lumped sources and sinks. Usually, the interaction between control and fuel elements is not considered directly, but the core is viewed as two superimposed arrays of fuel cells and control supercells. The reactivity of the lattice is first evaluated and homogenized few-group core parameters are derived with the control elements supposed to be completely withdrawn. The reactivity worth of the control elements is then estimated by considering each control element as associated with a given volume of homogenized core material. This technique has been shown to handle adequately the cases involving relatively large numbers of evenly distributed control elements [18]. Although the uncontrolled reactor core model is somewhat idealized, it permits such a simplification of the theory that it is almost universally used for not too heterogeneous assemblies.

In practice, the fuel elements are distributed in a fairly regular lattice made up of a small number of different types of cells.

Generally, there may be a juxtaposition of several zones with different compositions or a superposition of two or more networks, each one being made up of identical cells. Finally, the geometrical configuration of the lattice may be one-, two- or three-dimensional according to the shape of the fuel elements (v.g. plates, rods or spheres).

In agreement with the postulated separability of the microscopic and macroscopic fluxes, the Wigner-Seitz Theory assumes that the lattice pattern is repeated to infinity. Thus small reactors, where a relatively large number of fuel elements lie in the vicinity of the boundaries and, in particular, the influence of the reflector is felt deep in the core, are not treated adequately by the cell method: they rightly belong to the realm of the heterogeneous method. The same reasoning applies to multi-zoned configurations if the unit cell compositions vary markedly and the dimensions of the zones are such that too many elements are close to surfaces of discontinuity. The difficulty of defining suitable boundary conditions between neighbouring cells of different composition will also exclude mixed lattices if the unit cells are not closely similar. The Wigner-Seitz theory finds, therefore, its ideal field of application in the analysis of large reactors made up of identical cells.

Three-dimensional periodic structures present the drawback that in such assemblies, fuel loading and discharging operations are necessarily awkward. For this reason, except in the very early experimental piles contructed during the war, reactor designers have elected to build one- or two-dimensional periodic lattices, using either plates or variants of cylindrical shapes for the fuel elements. Plane lattices are normally associated with small reactors with highly enriched fuel. Thus, lattices with two-dimensional periodicity constitute by far the largest class of practical systems and all further discussion will be concerned with these configurations even though Wigner-Seitz theory covers one- and three-dimensional arrays just as well.

The very nature of the cell geometry entails an essential distinction between the lattice plane and the direction normal to it which may be of importance in studying neutron migration: this effect of anisotropy will be considered later. In Wigner-Seitz theory the unit cell is assumed to extend indefinitely along the third dimension. It may be

noted that the resulting replacement of the finite reactor problem by an infinite medium problem in which the flux and source distributions inside the reactor are analytically extended throughout space is justified by the so-called second fundamental theorem of reactor physics [5], the validity of which has been demonstrated for any reactor made up of a large number of identical cells [19]. A last remark concerning the longitudinal dimension of the unit cell in Wigner-Seitz theory: the composition of the lattice is supposed to remain perfectly uniform along this direction. While this allows a considerable simplification in the theory, since the flux may now be taken as constant along any normal to the lattice plane, it also introduces the problem of the end effects. For ease of manipulation and to facilitate mechanical support, the fuel channels, especially in power reactors, are usually filled with a string of rods, each one of which is terminated by joints. There results a fine structure of the axial flux which is not directly taken into account in the Wigner-Seitz method.

Only three types of geometrically regular figures will completely fill a plane: the triangle, the square and the hexagon. All three boundary shapes are used in practical lattice design. Provided suitable conditions are imposed on the neutron flux and current at the boundaries of a unit cell, it is possible, in principle, to represent the periodicity of the lattice and, therefore, to evaluate the reactivity of a lattice by considering the neutron balance in a single cell. Unfortunately, for cells with circular fuel channels but rectilinear outer boundaries, the disparity in the geometries poses a serious problem, and it is only quite recently [12] that rigorous expressions have been established for collision and escape probabilities in realistic cell configurations. To obviate this difficulty, it is usual for routine calculation purposes, to replace the actual lattice cell by an equivalent cylindrical cell with the same volume ratio of moderator to fuel. In addition, the cylindrical boundary is often assumed to be perfectly reflecting. For close-packed lattices, this idealization of the real situation may lead to serious errors [20]. By making use of exact expressions for the interaction probabilities in regular lattices, the effect of the transformation to cylindrical geometry has recently been studied by several authors [21], [22]. It has been found that a much improved representation of the true flux distribu-

tion is obtained with the equivalent cylindrical cell model if the neutrons are supposed to be reflected isotropically at the external boundary.

If cell-to-cell interaction may not always be neglected, because of its effect on the moderator-to-fuel flux ratio, it is unlikely, in most cases, to perturb significantly the flux distribution inside the fuel channel. This is fortunate, in view of the wealth of exotic as well as more conventional shapes produced by the engineer's imagination. In practice, two types of situations may be encountered. Quite frequently, the components are so finely and uniformly distributed that, at least in some energy range, the fuel assembly may be considered as homogeneous. It can then be represented in an equivalent array of concentric cylindrical annuli where lattice periodicity is taken into account without difficulty [25]. When, on the other hand, the heterogeneous distribution of the fuel plays a significant part, it is often permissible to treat the fuel channel in isolation by imposing a suitable boundary condition at the moderator interface, without introducing lattice periodicity in the analysis of the hyperfine structure. This assumption underlies many of the techniques devised for the calculation of collision probabilities in pin clusters and other complex-shaped fuel elements [26], [27]. As a matter of fact, even circular or tubular fuel geometries are sometimes handled in this way when, in the thermal range, diffusion theory is used in the moderator [28]. However, if such a simplified treatment is not allowable, the possibility still exists of using a more general numerical technique developed for the study of arbitrary geometries, where suitable cell boundary conditions may be applied without difficulty [29].

2.2. Definition of Criticality

The solution of the system of neutron balance equations for the equivalent unit cell, with appropriate collision probabilities, will yield the average flux in every group and every region of the corresponding infinite lattice. The multiplying properties of the lattice can then be characterized by the intensive quantity k-inf, the infinite

medium multiplication factor, which is simply expressed as the ratio of the average production rate to the average absorption rate in the equivalent unit cell [5]:

$$k_\infty = \frac{\sum_j \sum_m (\nu\Sigma_f)_{j,m} \phi_{j,m} V_j}{\sum_j \sum_m (\Sigma_a)_{j,m} \phi_{j,m} V_j} \tag{11}$$

where the summations extend over all groups n and regions j of the equivalent unit cell.

In a homogeneous bare reactor, the first fundamental theorem of reactor physics states that the spatial distribution $\psi(x)$ is the principal solution of the wave equation

$$\nabla^2 \psi(x) + B^2 \psi(x) = 0 \tag{12}$$

Since the neutron distribution is supposed to be separable in space and energy, the geometrical buckling B^2 will be the same in every group. It is generally assumed that the large-scale flux behaviour in a heterogeneous reactor obeys the same laws.

Just as the mean absorption and fission characteristics, it is possible, by using the concept of geometrical buckling, to define the average diffusion properties of a unit cell and, from this knowledge, to derive the net leakage $\mathcal{L}_n$ of group n neutrons from the cell [30]. Thus, we have

$$\mathcal{L}_n = D_n B^2 \phi_n V \tag{13}$$

where D_n is the diffusion coefficient for group n neutrons in the unit cell; ϕ_n is the average group n neutron flux in the cell:

$$\phi_n = \frac{\sum_j \phi_{j,n} V_j}{\sum_j V_j} \tag{14}$$

and

$$V = \sum_j V_j$$

This suggests that the criticality equation for the equivalent bare reactor be written as

$$1 = \frac{\sum_j \sum_m (\nu\Sigma_f)_{j,m} \phi_{j,m} V_j}{\sum_j \sum_m (\Sigma_a)_{j,m} \phi_{j,m} V_j + \sum_m D_m B^2 \phi_m V} \tag{15}$$

which just states that, in a critical assembly, the total neutron production rate is exactly equal to the neutron loss rate due to absorption and leakage. To be fully consistent and to correct, in some measure, for the competition between neutron leakage and absorption events, the neutron balance equations (8) should now read

$$\sum_{j=1}^{K} V_j \Sigma_{j,m} \phi_{j,m} + D_m B^2 \phi_m V = \sum_{j=1}^{K} \sum_{i=1}^{K} V_i P_{i-j,m} H_{i,m} \qquad (16)$$

The value of the buckling which will make an assembly of given composition and lattice design just critical can be found by an iterative solution of the system (15), (16).

While the definition of the multiplication factor based on the detailed neutron balance combines the advantages of conceptual simplicity and generality, an alternate formulation grounded on the idea of neutron life-cycle is usually adopted in the literature. According to the second point of view, the multiplication factor in a given system is given by the ratio of the number of neutrons of one generation to the number of the preceding generation. It has been shown that the life-cycle and the neutron balance multiplication factors are rigorously equivalent [5] .

Through a somewhat artificial and not always unambiguous decomposition, the life-cycle of an average neutron in an infinite lattice may be divided into several phases each of which is adequately treated by a system of simplified balance equations. There results a set of detailed parameters providing an easily visualized picture of the overall neutron behaviour and, which is more important, more or less directly accessible to measurements. Thus, the four-factor formula has enjoyed a highly successful career in the field of heavy water and graphite reactor lattices using natural or slightly enriched uranium. In such systems, there exists a rather well defined separation of neutron events into three energy regions, the thermal range being dominated by U-235 fission, the fast range by U-238 fission and the epithermal range by slowing down in the moderator and resonance capture in U-238. Furthermore, the relatively large pitches reduce the possibility of interaction between fuel rods for non-thermal neutrons, which leads to considerable simplifications in the expressions for the individual parameters.

The domain of validity of the four-factor formula is of course, limited by the ideal nature of a model where the side processes of the neutron life cycle are often left out or, at best, receive a rather crude treatment. In particular, it will not take epithermal fission into account. To solve this problem, which may have some importance at smaller pitches especially with enriched fuel, a common device has been the introduction of additional parameters [31], [32]. The necessary modifications to the definitions of the original four factors are thus kept at a minimum. However, if the detailed neutron balance is to be faithfully reproduced in these condensed expressions and if the interactions between the many competing events are to be included, the classical definitions must yet be recast.

A possible formulation of the infinite medium multiplication factor, from the neutron life-cycle viewpoint, is [33]

$$k_\infty = \varepsilon \left[p (\eta f)_{th} + (1-p) (\eta f)_{epi} \right] \tag{17}$$

For a large, predominantly thermal reactor, the criticality equation is traditionally defined in an equivalent two-group formalism as

$$1 = \frac{k_\infty}{(1+L^2B^2)(1+\tau B^2)} \tag{18}$$

It has been shown that, with the exception of the one-group model, the various characteristic equations in current use are practically equivalent [34].

The signification of the various symbols in the equations (17), (18) is given in the following sections.

3. The Intensive Parameters

The quantities entering the definition of the multiplication factor in an infinite medium having the same small-scale composition as that of the reactor under consideration are often called intensive or intra-cell parameters. In the present section, a consistent set of definitions will be given for these parameters in the framework of collision probability theory, using the neutron balance equations (8). Unless otherwise stated, the unit cell will be assumed throughout to be divided into the same geometrical regions.

3.1. High Energy Range

The flux normalization for the whole energy spectrum is obtained by arbitrarily stating that the total number of neutrons produced per unit time in the reactor by thermal and epithermal fissions is equal to unity. Let us suppose that we have p fast groups, q epithermal groups and r thermal groups, the highest energy group being group 1. We may then write

$$\sum_{m=p+q}^{p+q+r} \sum_{m=1}^{p+q} \sum_{j} (\nu\Sigma_f)_{j,m+m} \phi_{j,m} V_j = 1 \qquad (19)$$

where, as before, the index j refers to a cell region.

In reality, the virgin fission neutron spectrum vanishes to insignificance outside a not very wide band of energy, roughly co-extensive with what is normally thought of as the high energy range. The lower boundary of this energy region has fluctuated in the literature all the way from the fast fission threshold to the top of the U-238 resonance region. It may not be desirable to extend the fast neutron range too far down. While the scattered neutron flux tends, after a few collisions, to assume a uniform distributions, the virgin neutron flux is strongly localized in the fuel regions. Thus, at lower energies, even complex-shaped fuel elements may reasonably be presented in a simpler geometry of concentric cylindrical annuli but, in the vicinity of the Mev-range, the rod geometry must be more closely approximated especially with air-cooled elements. For the sake of simplicity and because the structure of the neutron balance equations in the high energy range is not altered essentially by this choice, it will be supposed here that the fast neutron region is exactly co-extensive with the energy range in which the U-235 fission spectrum normalized to unity stays above a prescribed level of significance.

Since scattering-up from the epithermal and thermal range is of no practical importance, the "external" source $q_{j,m}$ in each fast group may be obtained from

$$\sum_{m=1}^{p} \sum_{j} q_{j,m} V_j = \sum_{m=p+1}^{p+q+r} \sum_{m=1}^{p} \sum_{j} (\nu\Sigma_f)_{j,m+m} \phi_{j,m} V_j = 1 \qquad (20)$$

Of course, at the start of the calculations, the flux distribution in the epithermal and thermal ranges is completely unknown. However, a reasonable initial assumption is to take the source desnity as constant in every fuel region and zero everywhere else, so that

$$\sum_{m=1}^{p} \sum_{j} q_{j,m}^{(1)} V_j = 1 \qquad (21)$$

The fission neutron spectrum is implicitly supposed to be known. Once a complete neutron cycle has been investigated, a new estimate may be found for the fast source distribution by using equation (20) and a second iteration performed. The effect of the fast source non-uniformity is relatively small, so that a third iteration is not expected to be necessary. In what follows, it will be supposed that convergence has already been attained.

The neutron balance equations in the high energy region may be written as

$$\Sigma_{j,m} \phi_{j,m} V_j = \sum_{m=1}^{p} \sum_{i} \left[\Sigma_{i,m} \cdot q_{i,m \to m} \phi_{i,m} + q_{i,m} \right] V_i \cdot P_{i \to j,m} \quad (1 \leq m \leq p) \qquad (22)$$

where the transfer coefficient $q_{i,m \to m}$ is given by

$$q_{i,m \to m} = \frac{\Sigma_{el,i,m \to m} + \Sigma_{inel,i,m \to m} + 2\Sigma_{(n,2n),i,m \to m} + (\nu\Sigma_f)_{i,m \to m}}{\Sigma_{i,m}} \qquad (23)$$

and the source density $q_{i,m}$ by equation (20).

The input cross sections for the fast and epithermal broad groups are easily obtained through a preliminary calculation with one of the many computer codes solving, in a rather large number of ine groups, the neutron balance equations for a homogeneous medium [35] - [37] . Depending on the reactor type under study, and the desired accuracy, various procedures may be adopted.

If the population of non-thermal neutrons is relatively large, as in intermediate reactors, it is often worth-while to perform a homogeneous calculation before each fine structure analysis. Furthermore, the cell problem will then be attacked with a sizable number of broad groups. On the contrary, for a natural uranium thermal reactor, it could very well be sufficient to compute once and for all a set of broad group cross sections in a typical lattice and to examine the microscopic flux in a very coarse energy structure.

At any rate, it is usually found that, in the high energy region, the calculated absorption and fission rates are not very sensitive to the detailed spectrum shape, so that a small number of broad groups will generally be enough. One [38] and two-group [39] - [41] structures are quite common.

Following Carlvik and Pershagen [42], [43], the fast multiplication factor, ε, is here defined as the number of neutron slowing down past the lower limit of the high energy region per neutron produced in thermal and epithermal fission:

$$\varepsilon = \sum_{m=1}^{p} \sum_{m=p+1}^{p+q+r} \sum_{i} q_{i,m\to m} \Sigma_{i,m} \phi_{i,m} V_i \qquad (24)$$

This definition will automatically include the effects of back-scattering from the moderator and cell-to-cell interaction. It will also take into account the heterogeneous distribution of the fuel and the non-uniformity in the fast flux distribution. The only conditions are the use of a sufficiently fine spatial grid and the availability of simple calculation methods for the collision probabilities. In particular, in the analysis of cluster-fueled cells, there arises the problem, already discussed above, of combining a formalism adapted to the description of pin-to-pin interactions in the fuel element with a second series of expressions developed for the treatment of annular systems such as the idealized moderator in the equivalent unit cell.

Another quantity of major interest in the high energy region is the ratio of fast fissions in U-238 to fission in U-235, denoted by δ_{28}. We have

$$\delta_{28} = \frac{\sum_{m=1}^{p} \sum_{i} \Sigma_{f,i,m}^{28} \phi_{i,m} V_i}{\sum_{m=1}^{p+q+r} \sum_{i} \Sigma_{f,i,m}^{25} \phi_{i,m} V_i} \qquad (25)$$

which, for natural uranium fueled reactors, is closely approximated by

$$\delta_{28} \simeq \nu_{th}^{25} \sum_{m=1}^{p} \sum_{i} \Sigma_{f,i,m}^{28} \phi_{i,m} V_i \qquad (26)$$

where ν_{U}^{25} is the average number of neutrons produced in thermal U-235 fissions.

It should be noted that, since the present definition of the fast effect, ε, depends on the overall neutron balance in the lattice, there can be no simple relationship between ε and δ_{28} as in the cases where the fast fission factor is calculated for a fuel element considered in isolation as a bare reactor [5].

3.2. Intermediate Energy Range

As the term implies, the intermediate energy range extends from the lower energy limit of the fast neutron region down to the upper limit of the thermal range, which is loosely defined as a point above which up-scattering events and the effects of chemical binding of the moderator atoms lose all significence.

Formally, the neutron balance equations for the intermediate range are very similar to the relations pertaining to the high energy region. However the transfer coefficients $q_{i,m\to m}$ no longer include (n, 2n) nor virgin fission neutron contributions, and the source densities are now given by

$$q_{j,m} = \sum_{m=1}^{\phi} \Sigma_{j,m} \cdot g_{j,m\to m}\, \phi_{j,m} \qquad (27)$$

Thus, we have

$$\Sigma_{j,m}\phi_{j,m}V_j = \sum_{m=\phi+1}^{\tilde{m}} \sum_i \left[\Sigma_{i,m} \cdot g_{i,m\to m}\, \phi_{i,m} + q_{i,m} \right] V_i P_{i\to j,m} \quad (\phi < m \leq \phi+\eta) \qquad (28)$$

All cross sections are obtained in the same way as in the high energy reginn, except those of the resonance nuclides. Indeed, the calculation of the broad group cross sections for the resonance nuclides constitutes the main stumbling-block for the multigroup collision probability technique. For special studies, when one can afford to use a very large number of groups and regions, the problem is amenable to a classical treatment [44]. Since, in this case, the local variations in space and energy of the cross sections and fluxes are not too large, one may average the basic cross sections over a simple and approximate flux spectrum. However, the transition from these very fine group cross sections to relatively broad group constants is not ob-

vious. Certainly, the effects of fuel lumping are far too important to allow a simple weighting over a homogenized core spectrum such as is used for smoother cross sections.

Most calculation methods presently in use for the determination of the broad epithermal group constants of resonance nuclides are based on the concept of the effective resonance integral [45]-[49], i.e. an effective absorption cross section such that, multiplied by the unperturbed $1/E$ flux and the atomic density of the resonance nuclide, it will yield the correct number of neutrons captured in a given resonance per unit volume and unit time. Though never wholly exact, a number of correspondence relations of varying complexity have been developed in an attempt to equate the resonance integral pertaining to a heterogeneous fuel configuration to the resonance integral in an equivalent homogenous system [50]. It has thus been shown [51] that the detailed geometrical shape of the fuel assembly will enter the expression of the resonance integral mainly in the condensed form of an effective fuel surface area S_{eff}, so that a representation of the f form

$$I_{n,m} = A_n + B_n \sqrt{\frac{S_{eff}}{M}} \qquad (29)$$

where A_n and B_n are group constants depending only on the nature of the resonance nuclide, is often justifiable.

While for an isolated fuel rod, the effective surface area is exactly equal to the geometrical surface area, the mutual shadowing between the separate parts of a complex-shaped fuel element will result in a depletion of the incident current which is conveniently treated as an effective reduction of the surface-area. The correction factor is often called the internal Dancoff coefficient and has been explicitely formulated for a large number of geometries [54] - [56]. As for the mutual shielding of neighbouring fuel elements in a close-packed lattice, in collision probability theory based on the Wigner-Seitz model it is most naturally introduced through an appropriate cell boundary condition.

The effective resonance integral may alternately be evaluated by direct numerical integration of the slowing down equation in a more or less approximate representation of the real geometry [52], [53] . However, at the present time, even this sophisticated approach commonly retains two assumptions which may be of some importance. A single collision with a moderator atom is supposed to remove a neutron from the resonance being considered: this is the narrow resonance approximation for the moderator. Furthermore, the flux is taken as uniformly distributed both in the fuel and the moderator. Now, it has, in fact, been found possible [51], [59] to correlate the results obtained from the Zut-Tuz code which incorporates Nordheim's numerical technique with a simple analytical formula of type (29). Whether an equally simple representation will still apply when the restrictions just mentioned are removed from the more exact theoretical model remains to be seen. Recent comparisons with Monte Carlo results suggest, indeed, rather strongly the need for an improved treatment of the neutron slowing down in the moderator and spatial distribution across the cell, especially at small lattice pitches and for large fuel elements [60]., [61] .

It is customary to study separately the effect of each individual resonance, the flux being assumed to recover its asymptotic behaviour in the intervening energy intervals. While this procedure is justified for heavy absorbers such as U-238 where, in the resolved range, the resonances are relatively far apart, its validity is more doubtful in the case of fissionable nuclides in which the level spacings are much smaller [57], [58] . In addition to this effect, interference between U-235 and U-278 resonances may play a significant part in lattices using enriched fuel. In natural uranium reactors, since the resonance peaks of U-235 are roughly ten times lower than those of U-238 and the concentration is over a hundred times smaller, only the U-238 resonance absorption need be considered in great detail.

Once the resonance integral for every energy group has been obtained, the corresponding resonance cross sections are derived, ideally, by applying a correction factor which takes into account the divergence of the real flux from the asymptotic 1/E law. Typically, the flux depression factor reduces the effective U-238 cross sections by about 10 %. While an effect of this magnitude is not negligible, it is still

small enough to admit an approximate treatment. A reasonable procedure would be to evaluate first the flux distribution is the epithermal range in the absence of absorption. A second calculation might then be performed with absorption, the U-238 resonance cross section being defined as equal to

$$\sigma_{res,j,m}^{28\,(0)} = \frac{\tilde{I}_{nj,m}}{\Delta u_m} \tag{30}$$

An initial guess of the flux depression factor in region j and group n is given by $\frac{\phi_{j,m}^{(1)}}{\phi_{j,m}^{\infty}}$, where $\phi_{j,m}^{\infty}$ is the group n neutron flux in region j in the absence of absorption and $\phi_{j,m}^{(1)}$ is the value of the same quantity obtained with absorption present. The new value

$$\sigma_{res,j,m}^{28\,(1)} = \sigma_{res,j,m}^{28\,(0)} \cdot \frac{\phi_{j,m}^{\infty}}{\phi_{j,m}^{(1)}} \tag{31}$$

may now be fed into a third flux calculation and the iterations continued until

$$\frac{\sigma_{res,j,m}^{28\,(N)}}{\sigma_{res,j,m}^{28\,(N-1)}} \simeq 1 \tag{32}$$

The cross section library being completed and the detailed neutron balance established, the epithermal parameters are now readily evaluated. The probability p that a neutron will escape absorption while slowing down through the intermediate energy region is simply expressed as

$$p = \frac{\sum_{m=1}^{p} \sum_{m=p+1}^{p+q} \sum_{i} q_{i,m\to m} \cdot \Sigma_{i,m} \phi_{i,m} V_i}{\sum_{m=1}^{p} \sum_{m=p+1}^{p+q+r} \sum_{i} q_{i,m\to m} \cdot \Sigma_{i,m} \phi_{i,m} V_i} \tag{32}$$

The denominator is seen to be exactly equal to ϵ as defined through equation (24); the numerator, completely analogous in form, represents the total number of neutron slowing down into the thermal range.

Next, the epithermal multiplication factor $(\eta f)_{epi}$ may be defined as the number of neutrons produced in epithermal fission per neutron absorbed in the intermediate energy range:

$$(\eta\mathfrak{f})_{p+1} = \frac{\sum_{m=p+1}^{p+q} \sum_{i} (\nu\Sigma_f)_{i,m} \phi_{i,m} V_i}{\sum_{m=1}^{p} \sum_{m=p+1}^{p+q+r} \sum_{i} g_{i,m\to m} \Sigma_{i,m} \phi_{i,m} V_i - \sum_{m=1}^{p+1} \sum_{m=p+q+1}^{p+q+r} \sum_{i} g_{i,m\to m} \Sigma_{i,m} \phi_{i,m} V_i} \qquad (33)$$

As mentioned above, it is a distinct advantage of a consistent multi-group scheme such as the one presented here that, provided the energy structure is fine enough, all cell parameters expressible in terms of reaction rates are immediately given once the neutron balance equations have been solved. At least in principle, this is true even of quantities like the cadmium and relative conversion ratios which involve fluxes pertaining to different energy regions.

3.3 Thermal Energy Range

The only formal distinction between the neutron balance equations for the thermal energy region and the corresponding relationship for the epithermal range is due to the presence of up-scattering terms. Quite generally, we may write

$$\Sigma_{j,m} \phi_{j,m} V_j = \sum_{m=p+q+1}^{p+q+r} \sum_{i} \left[\Sigma_{i,m} g_{i,m\to m} \phi_{i,m} + q_{i,m} \right] V_i P_{i\to j,m} \qquad (p+q < m \leq p+q+r) \qquad (34)$$

where

$$q_{j,m} = \sum_{m=1}^{p+q} \Sigma_{j,m} \cdot g_{j,m\to m} \phi_{j,m} V_j \qquad (35)$$

The calculation of thermal spectra is, at present, a very active field of research [62] - [64]. In addition to the fundamental work directed towards the formulation of accurate scattering laws for the various moderating materials, much effort is being devoted to an improved understanding of the neutron distribution in heterogeneous lattices. Selective absorption in the fuel and rethermalization in the coolant entail the need for a careful treatment of the space-energy correlation. Thus, just as in the resonance range, it is often necessary that the basic cross sections be weighted over a spatially dependent spectrum in a more or less approximate representation of the cell geometry.

In the light of these considerations, a three-step procedure might be adopted for routine calculation. Basic cross sections could

first be averaged over an homogenized core spectrum [66] in a very fine group structure. A many-broad-group but few-region problem might then be performed using equations of type (34) or (4). Finally, a one-group, many-region calculation would yield a detailed picture of the spatial behaviour. In general, the first step need only be executed once for a given type of lattice. As for the second step, it should be remembered that the collision probability technique goes over to the integral transport solution as the number of spatial zones increases. Besides, recent progress sustains the hope that a phenomenomenological model may soon provide a simple and reliable description of spatially dependent spectra even in irradiated lattices with complex-shaped fuel elements, thus, in effect, short-circuiting this part of the problem with a considerable saving in machine-time [67].

The validity of the single-group representation for the detailed spatial distribution is fairly well established [14], [66]. Comparisons with Monte-Carlo results and experimental values have shown that it will yield reasonably accurate values for the disadvantage factor and the various thermal parameters. However, in very weakly absorbing regions, the mean flux is extremely sensitive to any change in the self-collision probability, since, in the one-group model, the flux in region j reduces to

$$\phi_j = \frac{\sum_{i \neq j} \left[\Sigma_{a,i} \phi_i + q_i\right] V_i P_{i \to j}}{\Sigma_j V_j \left(1 - \frac{\Sigma_{a,j}}{\Sigma_j} P_{j \to j}\right)} \qquad (36)$$

Thus, a large number of regions must always be used in the moderator, if it is to be treated with collision probability theory. For this reason, in the thermal range, one will often prefer to use diffusion theory away from the fuel moderator boundary, since, fortunately, this simpler technique then becomes asymptoticaly valid [3].

From a knowledge of the microscopic flux distribution, the value of the thermal multiplication factor $(\eta f)_{th}$ is immediately deduced, the factor $(\eta f)_{th}$ being classically defined as the number of neutrons produced in thermal fission per neutron absorbed in the

thermal range. In general, with r thermal groups, we have

$$(\eta f)_m = \frac{\sum_{m=p+q+r} \sum_i (\nu\Sigma_f)_{i,m} \phi_{i,m} V_i}{\sum_{m=p+q+r} \sum_i (\Sigma_a)_{i,m} \phi_{i,m} V_i} \qquad (37)$$

4. The Extensive Parameters

Although they are only used in connection with the macroscopic flux distribution, the so-called extensive parameters are entirely determined by the properties of the unit lattice cell.

The migration area, which represents the average distance traveled by a neutron between birth and capture and thus determines the total quantity of leakage from the critical reactor, is conveniently divided into two parts. The first phase of a neutron lifetime being typically spent in the slowing down process from fission to thermal energy, the mean neutron displacement through the high and intermediate energy ranges is a strong function of the moderating properties of the medium and appropriately defined in terms of the slowing down area τ . Once the average neutron has become thermalized, it will migrate through the lattice until absorbed: this last stage of its existence is summarily described in the definition of the thermal diffusion area, L^2 .

4.1. The Slowing Down Area

The slowing down area in a homogeneous medium is readily evaluated as the second moment of the slowing down kernel [5] . Since most of the neutrons are slowed down in the moderator, this suggests that the neutron age in a lattice could be reasonably well approximated by multiplying the slowing down area in the infinite moderator, obtained through a preliminary spectrum calculation [37] , by a correcting factor taking into account the heterogeneous distributions of the various cell materials. Thus, for every fast and intermediate group, we have

$$\tau_m = \tau^m_m \cdot g_m \qquad (38)$$

As, in most practical cases, the heterogeneity factor q_m is not very far from unity, no large error will be incurred by using in its derivation the approximate Fermi age theory. In such a case, the slowing down area in a narrow-energy range may be expressed as the ratio of the average diffusion coefficient to the average"slowing-down" cross section, and we may write

$$q_m = \frac{D_m^{m'}}{D_m} \cdot \frac{\Sigma_{sD,m}}{\Sigma_{sD,m}^{m}} \tag{39}$$

where D_m^m, $\Sigma_{sD,m}^m$ are moderator properties and $D_m, \Sigma_{sD,m}$ are averaged over the unit cell.

In the definition of the slowing down cross section, allowance must be made for inelastic scattering, for instance, by writing

$$\Sigma_{sD,l,m} = N_l \left[\xi_l \sigma_{el,l,n} + \sigma_{inl,l,m} \overline{\Delta u}_{l,m} \right] \tag{40}$$

where $\overline{\Delta u}_{l,m}$ is the average lethargy increment per inelastic scattering event for nuclide l in neutron group n. As for the diffusion coefficient D_m it has been shown 30 that a proper space-**averaging** procedure is given by

$$D_m = \frac{1}{3} \cdot \frac{\sum_i \sum_j V_i \phi_{i,n} \lambda_{j,m} P_{i \to j,m}}{\sum_i \sum_j V_i \phi_{i,m}} \tag{41}$$

λ_j being the transport cross section in region j.

Lattice anisotropy is taken into account by defining radial and axial diffusion coefficients, through the introduction of directional probabilities. Thus, the diffusion coefficient along direction k is obtained by substituting $P_{i,j,k}$ to P_{ij} in equation (41). If Ω_k is the directional coefficient which identifies the component in the k-direction of the average first-collision probability P_{ij} we have

$$P_{i,j,k} = \frac{3}{\lambda_j V_i} \int_{(V_j)} d\vec{x} \int_{(V_i)} d\vec{x}' \cdot \frac{e^{-\tau(\vec{x}', \vec{x})}}{4\pi |\vec{x} - \vec{x}'|^2} \cdot \Omega_k^2 \tag{42}$$

$$P_{ij} = \frac{1}{3} \sum_k P_{i,j,k} \tag{43}$$

Explicit expressions are available in the literature for these directional quantities in a geometry of concentric cylindrical annuli [68] , or in a pin cluster geometry [30], [27].

4.2. The Thermal Diffusion Area

The programme of evaluation of the thermal diffusion area L^2 is essentially the same as for the slowing down area. If, for the sake of simplicity, the thermal range is assumed to be described as a single energy group, we may write

$$L^2 = \frac{D_a}{\Sigma_{a,a}} \tag{44}$$

where the average thermal absorption cross section is given by

$$\Sigma_{a,a} = \frac{\sum_i \Sigma_{a,i,a}\, \phi_{i,a}\, V_i}{\sum_i \phi_{i,a}\, V_i} \tag{45}$$

and the cell-averaged diffusion coefficient is obtained through an equation of the form (41). If so desired lattice anisotropy may be introduced in just the same way as in the fast and epithermal energy regions.

Here, as in the evaluation of τ , the separability of leakage and absorption (or slowing down) effects is taken for granted, although this assumption is not necessary.

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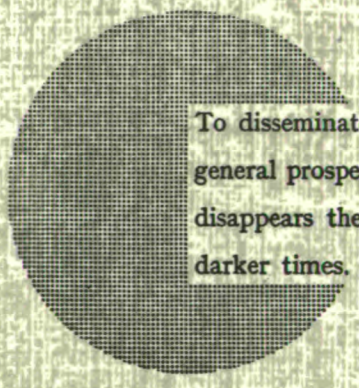

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Alfred Nobel

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