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METHODS AVAILABLE FOR CALCULATING CRITICAL SIZES OF SLOW AND RESONANCE ENERGY CHAIN REACTING SYSTEMS

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Methods Available for Calculating Critical Sizes of Slow and Resonance Energy Chain Reacting Systems

The calculation of the critical size of a chain reacting system is one of the central problems in pile technology. At present there are a fairly large number of methods for solving this problem which have been used at different times; however no systematic collection of these has been made. In particular, no attempt has been made to so systematize the calculations that the numerical computations remain, in complicated cases, within reason. The present report is not intended to be such a collection - rather it is intended as an outline, with references, which may be of some use to the mathematics department, whose task it will presumably be to prepare a more comprehensive study.

The methods which have been used can be classified according to the mathematical technique employed, or according to the physical systems to which they apply. Thus, variation methods have been used in many different physical settings; on the other hand, high k piles can be treated from several different mathematical viewpoints. Generally speaking, we shall try to classify the schemes according to the assumptions made regarding the slowing down picture.

A. Mathematical complications arise out of two separate considerations. First, certain geometries are

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naturally harder to deal with than others; and second, even in simple geometries, the spread in energy of the fast neutrons is troublesome. In one group calculations, only the geometric considerations are important. For multi-group calculations even the simplest geometries are difficult.

I. One-Group Model

The one-group model, in which all neutrons are assumed to have the same velocity, reduces to the solution of the wave equation

$$\Delta n + B^2 n = 0 \qquad (1)$$

subject to the boundary condition $n = 0$ on the outer surface of the system. The wave equation is accurate only if the system is large enough for simple diffusion theory to be applicable. This is usually the case in systems of interest to us.

The solutions of the wave equation in many different geometries are well known. We list them under

1. Bare Piles

For simple shapes, such as sphere, slab, cylinder, see CL-574.

For shapes such as elliptic cylinder, cone, etc., which are simply related to

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systems of orthogonal functions, it is usually possible to write the solution as an infinite series of appropriate harmonics. The coefficients are then determined so that the boundary condition, n = 0 on boundary, is satisfied. Since this in general leads to an infinite set of linear equations, the calculation is usually performed by solving successively larger finite sets of linear equations and noting the convergence of the result. By this method the following shapes have been treated:

a. Truncated sphere - F. Murray (CP-1461)

b. Elliptic cylinder - N. Morehouse (unpublished notes which I have)

c. Truncated cone - R. Scalettar, Mon P-33, pg. 16

Solutions for many other shapes must exist in the literature since the critical size problem is identical with the calculation of the fundamental mode of a vibrating cavity whose outer surface is the same as the pile shape. It probably would be worthwhile to resurrect many of these results - in particular the critical size of an ellipsoid.

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The Rayleigh-Ritz variation method is also useful for various odd shaped piles. In this scheme (described in Courant-Hilbert, e.g.) use is made of the fact that

$$B^2 = \frac{\int (\nabla n)^2 \, d\underline{r}}{\int n^2 \, d\underline{r}}$$

is stationary with respect to small variations of the function $n(\underline{r})$. Thus if n is chosen to satisfy the boundary conditions, it is not very important that it also satisfy the wave equation. Applications of this procedure are found, e.g. in Schweinler, Mon P-152, Young and Castle, CP-1456, Scalettar, Mon P-33, p. 16.

If the quantity B^2 is a function of $\underline{r}$, the solution of equation (1) can usually be done only numerically. The critical size can still be calculated by a variation method, however; this has been done by Schweinler, Mon P-152.

If B^2 depends on n, as is the case in a pile operating at high power, the problem becomes non-linear. In this case numerical work must be resorted to. A few special cases have been worked out in which B^2 is a linear function of n: Young and Morehouse, CP-1069. A more extended study of the non-linear problem,

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again with a view to establishing feasible numerical methods would be very worth while.

2. Pile with Reflector

The one group pile with reflector problem is very simple if the geometry is simple. Thus concentric spheres or concentric infinite cylinders are easily solved (CL-574).

On the other hand such a relatively simple looking problem as a cube inside another cube cannot be solved accurately. The reason for this is that the functions appropriate to a cube do not match properly in the corners of the reflector. Thus if $\sin \frac{\pi x}{L_1} \sin \frac{\pi y}{L_2} \cosh \alpha z$ is taken as the solution in the top reflector, and $\sin \frac{\pi x}{L_1} \cosh \alpha y \sin \frac{\pi z}{L_3}$ is taken as the solution in the side reflector, these two functions will overlap along some surface in the corner of the reflector. On this surface the neutron density is continuous but the normal derivative is discontinuous. This corresponds to a solution of the wave equation but with a certain distribution of sources and sinks determined by the nature of the discontinuity in the normal derivative along the surface. Wigner has suggested that this solution, in which there is an extra source, can

be used as a starting point in a method of successive approximations. The next approximations would be to arrange a disposition of sources or sinks which would just balance the original set. These sources will now remove the discontinuity in the derivative, but they will in general spoil the boundary conditions. The details of how one readjusts the boundary conditions have not been worked out.

The problem of concentric ellipsoids can in principle be solved with known functions. It would be a valuable result since any of these "cube in cube" or "cylinder in cylinder" problems can be approximated by the ellipsoid problem.

Another method which has been tried (Mon P-8 - with not too great success) for this problem, is a variant of perturbation theory. In this method, one starts with a uniform pile whose outer surface coincides with the outer surface of the reflector in the actual pile. The perturbed system is obtained from the original one by increasing the buckling of a central piece of the uniform pile until it coincides with the active part of the pile, and at the same time reducing the buckling in the

outer part, corresponding to the reflector. A perturbation calculation is then performed; the result is an approximate characteristic value and function for the system pile + reflector. The success of this method depends on the reflector being rather small; for the perturbation required to convert the uniform pile into reflector is very large, and unless the reflector has a very small statistical weight, the method will not converge. Schweinler has applied this scheme to the concentric sphere problem where the solution is well known- in that case agreement between the approximate and exact theory is good. For the cylinder in cylinder and the sphere in cylinder problem the results, in the particular case tried, diverge. It is not clear why this is so, since the sphere in sphere converges very well. A further investigation of this method would be very worth while.

II. Multi-Group Methods

The schematic handling of the fast neutrons by considering them to diffuse according to a simple diffusion equation without energy loss was suggested by perhaps 6 different people (including a member of the German Uranium group). In the case of a bare pile the use of the multi-group methods

has no advantage over the Fermi-method. However, for a pile with reflector, and particularly if the pile has high multiplication constant, multi-group methods are usually the only feasible way of calculating critical sizes accurately.

The multi-group problem is, mathematically, the following: required to solve the following set of differential equations

$$D_o \Delta n_o - N\sigma_{ao} n_o + k N\sigma_{as} n_s = 0 \qquad (3)$$

$$D_i \Delta n_i - N\sigma_{ai} n_i + N\sigma_{ai-1} n_{i-1} = 0$$

where n_o, n_i represents the neutron density at various energy levels. If the set consists of 2 equations, we speak of a "two-group" theory. The more accurately the slowing down process is described, the larger the number of groups required. For H_2O systems, a two group picture is not too bad; for heavier moderators, at least a three group calculation is needed, although, because the calculation quickly gets very complicated, most calculations have been done with just 2 groups.

The usual problem is to compute the critical radius and the characteristic functions in a system consisting of two regions, pile and reflector. The

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fundamental solutions of equations (3) in e.g., a plane system are a sum of exponentials:

$$n_i = \sum_m A_m g_i e^{-\lambda_m x} \qquad \text{in pile}$$

$$\nu_i = \sum_m B_m h_i e^{-\lambda'_m x} \qquad \text{in reflector}$$

when n_i and ν_i are neutron densities in pile and reflector, gi, hi are known constants and A_m, B_m are arbitrary. At the interface between reflector and pile, density and flow must be continuous. This leads to a set of 2 m equations which are linear and homogeneous. The determinant of these equations will vanish only if the system is just critical, that is, if the pile-reflector interface is at just the right place to make the pile size correct. The problem is therefore, in principle, very simple since it just involves solving a determinantal equation. However, the determinantal equation very rapidly becomes complicated (4-th degree for 2 groups, 6-th degree for 3 groups, etc.) and so one of the most pressing problems is to establish computational schemes which will make the solutions of these linear equations a reasonable task. Various methods for handling these linear equations have been used. These are -

(1) Straightforward solution. This has been used in 2 and 3 group calculations by Wigner, Weinberg,

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Williamson, CP-1461 (2 group, control rods). Friedman and Lloyd, CP-1554 (2 group), CP-1874 (3 group). Volkoff and LeCaine, MT-30 (general treatment.)

(2) Perturbation of Boundary Condition. Wheeler (CP-71 & CP-88) has pointed out that, since the 1 group picture gives good results if the pile is sufficiently large, the effect of the fast group can be treated as a small correction to the boundary conditions. Wigner and Friedman have also indicated how an "equivalent" one group theory can be concoted out of a two group picture (CP-1662, CP-288).

(3) "Back and Forth Methods"- Nordheim (CP-2222, p. 18) has suggested the following computational method for obtaining the characteristic functions in multi-group systems. We illustrate with 2 groups: One starts with the fast group in the reflector, since this group is not coupled to the slow there (assuming there is no multiplication in reflector). One then continues the fast group into the pile by requiring continuity at the boundary. From the fast neutron density in the pile one can compute the density of the slow group inside, and then the density of this group in the reflector. In general the slow group will not vanish, as it should, on the boundary of the reflector; it will vanish, say, inside the

reflector. One then moves the position of the pile-reflector interface in a little and repeats the process. This procedure is repeated again and again, adjusting the position of the interface a little each time, until both the fasts and the slows satisfy all the boundary conditions - in particular, the slows vanish at the outer reflector boundary.

While this seems like a tedious trial and error method, it is actually a very useful scheme, and has been used extensively, especially for 3 group problems. What is needed here is to examine methods for improving the second guess.

(4) Source and Sink Method - A variant of the "Back and Forth" method is to keep the boundary fixed, work in from the reflector fasts, but to observe that, if the pile size is not quite correct, the problem solved is one in which there is a distribution of sources or sinks of a certain strength. From the strength of the source or sink, one should be able to estimate how much the multiplication constant of the whole system needs to be increased or decreased in order to make the system critical without any source or sink. This method has not been tried, (at least by me), but I think it should be

entirely feasible to use the source or sink strength to give a good indication of the required correction.

(5) Perturbation Method - It has been suggested that the perturbation method (Mon P-8, p. 14) can be extended to several groups. Evidently such an extension will be rather complicated - but it is by no means clear that for very many groups this might not provide a relatively feasible computational scheme.

To summarize, the multi-group calculations are, for the most part, in good theoretical shape. What is needed most is a critical study of the mutli-group schemes from a computational standpoint with a view to establishing a very definite procedure which can be used routinely for all critical calculations requiring more than one group.

III. Fermi-Theory

When the number of groups becomes infinite, but the overall mean square distance travelled by a fast neutron remains finite, the multi-group picture is replaced by what is called the Fermi picture. In this case the system of many ordinary differential equations collapses into a pair of equations, one of which is a partial differential equation:

$$\Delta q = \frac{\partial q}{\partial t}$$

$$D \Delta n - \sigma_a n + q(\tau_o) = 0$$

$$q(o) = k \sigma_a n$$

[redacted]

Again the bare pile problem gives no difficulty. However, the pile with reflector problem is very difficult mathematically; it has been solved, in case the pile and reflector have the same moderating properties by Volkoff, MT-21.

IV. General Integral Methods

In its most general from the pile equation for a slow neutron chain reacting system surrounded by a reflector is an integro-differential equation

$$D\Delta n - N\sigma_{a,n} + k\, N\sigma_a \int_c n(\underline{r}')P(\underline{r},\underline{r}')\, d\underline{r}' = 0 \quad (4)$$

where $P(\underline{r},\underline{r}')$ is the probability that a fast neutron produced at $\underline{r}'$ will appear as a slow neutron at $\underline{r}$. The integration is carried out over the active pile since only in this region are fast neutrons produced. Since the Green's function $G(\underline{r},\underline{r}')$ for (4) is known, viz.

$$G(\underline{r},\underline{r}') = \frac{e^{-\left|\frac{r-r'}{L}\right|}}{4\pi L^2 \left|r-r'\right|}, \quad (5)$$

equation (4) can be cast as an integral equation. The most convenient way to do this has been described by Greuling (LA-399); his method is applicable whenever the core and reflector have the same slowing down kernel, $P(\underline{r},\underline{r}')$.

The integral equation for the pile has the form

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$$n(\underline{r}) = \Gamma \int_{\mathcal{E}} \mathcal{F}(\underline{r}-\underline{r}')\, n(\underline{r}')\, dr' \qquad (6)$$

where Γ is essentially the core multiplication constant and $\mathcal{F}(\underline{r}-\underline{r}')$ is, in part, a kernel obtained by taking the convolution of $G(\underline{r}-\underline{r}')$ and $P(\underline{r},\underline{r}')$. The important thing about $\mathcal{F}(\underline{r},\underline{r}')$ is that it can be exhibited as a numerical function provided $P(r,r')$ is known, either from experiment or from theory. Then the integral equation can be solved by successive iteration, or better, by using the fact that

$$\frac{1}{\Gamma} = \frac{\iint n(\underline{r})\mathcal{F}(\underline{r}-\underline{r}')\, n(\underline{r}')\, d\underline{r}'}{\iint n^2(\underline{r})\, d\underline{r}} \qquad (7)$$

is stationary if $n(r)$ satisfies (6). (This may be verified by deriving Euler's equation from the functional $\frac{1}{\Gamma}$. Greuling has used a parabolic approximation to compute $\frac{1}{\Gamma}$, and has tabulated the results for the systems: water core-water tamper.

The advantage of the integral method is very great if the reflector is infinite and has the same moderator as the core. If either of these conditions is not met, I do not know whether the integral method can be made to work. The main difficulty is that the kernel cannot then be written simply as a function of the distance between $\underline{r}$ and $\underline{r}'$. However, by using the group picture one can still express the kernel as the solution of a

coupled set of differential equations. In this case the equation (6) can be replaced by a vector equation

$$\underline{n}(\underline{r}) = \int \underline{\underline{\mathcal{F}}}(\underline{r},\underline{r}', \underline{\Gamma})\, \underline{n}(\underline{r}')\, d\underline{r}' \qquad (8)$$

where $\underline{\underline{\mathcal{F}}}$ is now a Green's matrix. Again a variation problem can be obtained from (8), and, in principle, the eigenvalue vector $\underline{\Gamma}$ can be computed. The problem would then depend on how complicated $\underline{\underline{\mathcal{F}}}$ becomes. I suspect that $\underline{\underline{\mathcal{F}}}$ would be so complicated that there is nothing to be gained by such a mode of attack. However, this is just a conjecture on my part, and I think it might be worth while looking into the method as an alternative to the straightforward group calculation.

V. Passage from Multi-Group Theory to Fermi Theory

The reflector problem with Fermi slowing down has been successfully solved (Volkoff, MT-21) only in case the core and reflector are identical in moderating properties. When the reflector and core are different, no solution has been obtained for the critical problem although Friedman (CP-1073) has obtained it for the distribution from a point source. On the other hand, these problems can be handled by the group method. Furthermore, in the limit of infinitely many groups, the group method and the Fermi method become identical.

It may therefore be conjectured that the following scheme can be used to solve the non-uniform problem with Fermi slowing down. First solve the group problem for n groups, and try to get a general, explicit formula for the characteristic value (i.e., multiplication constant) and the characteristic

functions. Second, try to pass to the limit.

Evidently this is complicated. However, a rather similar limiting process has been carried out (LA-590) in going from the spherical harmonics to the Hopf-Wiener solution of the transport equation, and it may be hoped that in this case too the problem can be solved.

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