1969

Coupling effects in fast reactors using the Monte Carlo technique

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FLANAGAN, George Fergus, 1944-
COUPLING EFFECTS IN FAST REACTORS
USING THE MONTE CARLO TECHNIQUE.

Iowa State University, Ph.D., 1969
Engineering, nuclear

COUPLING EFFECTS IN FAST REACTORS
USING THE MONTE CARLO TECHNIQUE

by

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A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

Major Subject: Nuclear Engineering

Approved:

Signature was redacted for privacy.

In Charge of Major Work

Signature was redacted for privacy.

Head of Major Department

Signature was redacted for privacy.

Dean of Graduate College

Iowa State University
Ames, Iowa

1969

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I. INTRODUCTION

Considerable interest has recently been shown in coupled reactors. The term "coupled" is generally taken to mean that in each of the reactors which are "coupled", neutrons are emitted by fissions induced by neutrons produced in other reactors. In 1967, a conference was held at Texas A&M University which dealt entirely with coupled reactor kinetics.

Application to the areas of coupled fast-thermal assemblies, Argonaut type reactors, coupled nuclear rocket engines, and modular cores for large power reactors is discussed in several papers (12, 13, 18, 25).

In his paper on coupled fast reactors, W. H. Hannum (12) discusses the various aspects, both pro and con, for use of a fast coupled reactor. These aspects can be divided into six general areas. The six areas are neutron tailoring in space and energy including high blanket power tailoring, improved reactivity coefficients, neutron lifetime increase, higher loading, powerpeaking, and control and instrumentation. Mr. Hannum (12) concludes that only the first and last can be considered as advantageous. The latter is of special interest to those concerned with system safety, since large coupled fast reactors generally have negative temperature coefficients. However, in the last year this advantage has been weighed against the problems involved in design and building of large coupled systems. These included economic as well as technical problems. This was one of the considerations involved in the switch by Westinghouse[1] and Atomics International[2] from a modular system to a single core design.

Even though the coupling may not be of as much importance to the commercial field as first thought, it is still important in research and in the space field.

In the research area nearly all zero power reactors and other critical facilities are of a modular core design thus making coupling important.

In the space area the current thought is to couple the present nuclear rockets in order to obtain larger thrusts instead of constructing a larger engine. As an example, at the present time 250,000-750,000 pounds of thrust are required to attain earth orbit departure with a reasonable payload. The NERVA engine has a thrust of 200,000-500,000 pounds, so in order to attain earth orbit departure, 1-3 engines would be required. Although coupling in rocket engines is loose, i.e. 0.25¢ or less, it must be

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[1]Dyos, M. Walte Mill Site, Westinghouse Electric Corp., Pittsburth, Penn. Fast demonstration plant description. Private communication. 1969.

[2]Lancet, R. Atomics International, Canoga Park, California. Fast reactor safety. Private communication. 1969.

taken into account for control and safety design (18).

Several analytical models have been proposed for the coupled system. The most familiar of these was proposed by R. Avery (2). In this approach which will be more thoroughly discussed in the next section, the coupling is treated using the formalism of constucting ratios of integral parameters in order to define such quantities as lifetime, reactivity etc. Further refinements to Avery's model have been introduced by Cockrell and Perez (6). In addition to the spatial coupling included in Avery's model, the Cockrell-Perez model introduces spectral coupling. Again the specific parameters involved are defined by ratios of integrals. Both the Avery and the Cockrell-Perez models involve solutions of the integro-differential form of the Boltzmann neutron transport equations from which the point kinetics equations for the coupled system are derived.

In both formulations an effective multiplication constant for coupling between cores is defined as the expectation value that a neutron in reactor j gives rise to a next generation fission neutron in reactor i. This term, usually written as k_{ij}, appears as a coefficient in the point kinetics equations in coupled form. It is the calculation of these coupling coefficients and the variation of such with the criticality of the reactor which is the prime consideration of this work.

These coefficients are generally calculated by a ratio of importance weighted fluxes. However, it is proposed to calculate the coupling parameters using a Monte Carlo technique and their basic definitions.

The Monte Carlo technique, as employed here, follows a neutron through the assembly from its release until it is absorbed or escapes. The neutron's path length between interactions, and the types of interactions (fission, capture, and scattering) which it undergoes are determined by the materials, neutron cross sections, and angular distributions for various reactions. Since the origin and the destination of each neutron is known using Monte Carlo, this technique resolves itself nicely to the statistical prediction of coupling coefficients.

Detailed descriptions of the Avery model and of the particular Monte Carlo program used in this work follow in the next two sections.

An overall description and comparison of the Avery, Cockrell-Perez, and several other major coupling models are given by F. T. Adler, S. J. Gage, and G. C. Hopkins (1) in the appendix of the Proceedings of the Symposium on Coupled Reactor Kinetics which was held at Texas A&M in 1967.

II. MODELS OF COUPLED REACTORS

A. Basic Definitions and Theory of the Avery Model

The general formulation of the reactor equations as given by the time, space, and energy dependent Boltzmann equation may be applied to the coupled system.

The system is characterized in terms of explicit integral parameters defined below (2).

K'_{ij}	the expectation value that a fission neutron in reactor j gives rise to a next generation fission neutron in reactor i
L_{ij}	the average prompt neutron lifetime for the above process
$1-K'_{ii}=\Delta_i$	a measure of the subcriticality of reactor i without the contribution of the other reactors
S_i	the total fission neutron source in reactor i
S_{ij}	the total fission neutron source in reactor i which results from fissions caused by neutrons which originate in reactor j.
N_{jk}	the number of neutrons, properly weighted, in the system which originated in reactor k and are destined to produce next generation neutrons in reactor j
C_{ki}	the properly weighted measure of the number of delayed neutron emitters of the ith group

in reactor k

β, β_i, and λ_i have the usual kinetic definitions.

An asterisk superscript on any of the above quantities indicates the adjoint formulation.

If there are N reactors in the entire system then,

$$S_i = \sum_{j=1}^{N} S_{ij} \tag{1}$$

and the expectation values for a critical system can be defined by the following ratios

$$\frac{S_{ii}}{S_i} = K'_{ii} \tag{2a}$$

$$\frac{S_{ij}}{S_j} = K'_{ij} \tag{2b}$$

For simplicity consider a two reactor system in which it follows from Equation 1.

$$S_{11} + S_{12} = S_1 \tag{3a}$$

$$S_{21} + S_{22} = S_2 \tag{3b}$$

and upon substitution of Equations 2a and 2b, 3a and 3b become

$$K'_{11}S_1 + K'_{12}S_2 = S_1 \tag{4a}$$

$$K'_{21}S_1 + K'_{22}S_2 = S_2 \tag{4b}$$

For a critical system a solution for Equations 4a and 4b must exist for non negative values of S_i. The criticality condition can be expressed in matrix notation as

$$\begin{vmatrix} (K'_{11}-1) & K'_{12} \\ K'_{21} & (K'_{22}-1) \end{vmatrix} = 0 \tag{5}$$

or

$$K'_{12}K'_{21} = \Delta_1\Delta_2 \tag{6a}$$

Also, if criticality holds, a ratio of sources S_1 and S_2 can be expressed as

$$\frac{S_1}{S_2} = \frac{K'_{12}}{\Delta_1} = \frac{\Delta_2}{K'_{21}} \tag{6 b}$$

For a non-critical system one introduces the fictitious value of the number of neutrons per fission ν_c needed to maintain criticality. Therefore for a non-critical system $\nu \neq \nu_c$ and the neutron source in one generation will result in the next generation with a magnitude which differs by a factor K where $K = \frac{\nu}{\nu_c}$

A quantity ρ is also introduced where

$$\rho = K-1 = K_{ex} = \frac{\delta\nu}{\nu} = \frac{\nu-\nu_c}{\nu} \tag{7}$$

The coupling coefficients are used in the coupled point reactor kinetics equations. In the equations below, D is the number of delayed neutron groups.

In terms of the defined quantities the point reactor equations become

$$L_{jk} \frac{dS_{jk}}{dt} = K'_{jk}(1-\beta) \sum_{m=1}^{N} S_{km} - S_{jk} + K'_{jk} \sum_{i=1}^{D} \lambda_i C_{ki} \qquad (8)$$

$$\frac{dC_{ki}}{dt} = \beta_i \sum_{m=1}^{N} S_{km} - \lambda_i C_{ki} \qquad (9\text{-}21)$$

If one defines the following quantities a correlation to a general formulation of the reactor equations can be developed. Exact definitions of the various coupling parameters mentioned earlier can be obtained and these can then be explicitly evaluated. The parameters defined will be the steady state values (2).

$\phi(r,v)$ — the neutron flux as a function of position and velocity

$\phi^*(r,v)$ — the adjoint flux as a function of position and velocity

$\nu\Sigma_f(r,v)$ — the product of the average number of neutrons emitted per fission and the macroscopic fission cross section (the product may be a function of position and of incoming neutron velocity)

$[\nu\Sigma_f(r,v)]_j$ — the part of $\nu\Sigma_f(r,v)$ which prescribes the reactor j; where

$$\sum_j [\nu\Sigma_f(r,v)]_j = \nu\Sigma_f(r,v)$$

$x(v)$ — the normalized fission spectrum where

$$\int x(v)dv = 1$$

$\phi_j(r,v)$ — the part of the steady state flux that results from neutrons from the reactor j where

$$\sum_j \phi_j(r,v) = \phi(r,v)$$

$\phi_j^*(r,v)$ — the part of the importance function which is contributed by neutrons which will cause their next fission in reactor j.

Correlating the coupling parameters with the general quantities just defined S_j and C_{jk} become

$$S_j = \int\int[\nu\Sigma_f(r,v)]_j\ \phi(r,v)\,dr\,dv \tag{22}$$

$$C_{ji} = \frac{\beta_i}{\lambda_i}\int\int[\nu\Sigma_f(r,v)]_j\ \phi(r,v)\,dr\,dv \tag{23}$$

In order to divide the total source in reactor j into partial sources, one takes the fraction of the total importance arising from fission neutrons in reactor j which results from neutrons from the various other reactors.

$$S_{jk} = \frac{\int\int[\nu\Sigma_f(r,v)]_j\phi(r,v)\,dr\,dv \times \int\int\int x(v)\phi^*(r,\acute{v})[\nu\Sigma_f(r,v)]_j\phi_k(r,v)\,dr\,d\acute{v}\,dv}{\int\int\int x(\acute{v})\phi^*(r,\acute{v})[\nu\Sigma_f(r,v)]_j\phi(r,v)\,dr\,d\acute{v}\,dv} \tag{24}$$

This definition allows one to assign the same average importance to all the partial sources as was done previously i.e.,

$$N_{jk}^* = N_{jL}^* = N_j^* \tag{25}$$

The coupling coefficient was defined as

$$K_{jk} = \frac{S_{jk}}{S_k} \tag{26}$$

Therefore, using Equations 22, 24, and 26 one obtains an expression for K_{jk}

$$K_{jk} = \frac{\iint [\nu\Sigma_f(r,v)]_j \phi(r,v)\,dr\,dv}{\iint [\nu\Sigma_f(r,v)]_k \phi(r,v)\,dr\,dv}$$

$$\times \frac{\iiint \chi(\acute{v})\phi^*(r,\acute{v})[\nu\Sigma_f(r,v)]_j \phi_k(r,v)\,dr\,d\acute{v}\,dv}{\iiint \chi(\acute{v})\phi^*(r,\acute{v})[\nu\Sigma_f(r,v)]_j \phi(r,v)\,dr\,d\acute{v}\,dv} \qquad (27)$$

$N_j{}^*S_{jk}$ can be interpreted as the total importance of the fission neutrons in reactor j which result from neutrons born in reactor k. Therefore

$$N_j{}^*S_{jk} = \iiint \chi(\acute{v})\phi^*(r,\acute{v})[\nu\Sigma_f(r,v)]_j \phi_k(r,v)\,dr\,d\acute{v}\,dv \qquad (28)$$

and solving for $N_j{}^*$ using Equation 23 for S_{jk}

$$N_j{}^* = \frac{\iiint \chi(\acute{v})\phi^*(r,\acute{v})[\nu\Sigma_f(r,v)]_j \phi(r,v)\,dr\,d\acute{v}\,dv}{\iint [\nu\Sigma_f(r,v)]_j \phi(r,v)\,dr\,dv} \qquad (29)$$

The overall neutron lifetime L is given by the usual definition of the total importance divided by the rate of production of importance.

$$L = \frac{\iint \frac{\phi^*(r,v)\phi(r,v)}{v}\,dr\,dv}{\iiint \chi(\acute{v})\phi^*(r,\acute{v})\,\nu\Sigma_f(r,v)\phi(r,v)\,dr\,d\acute{v}\,dv} \qquad (30)$$

realizing

$$\sum_j \phi_j^* = \phi^*$$

and

$$\sum_k \phi'_k = \phi$$

one can express Equation 30 as

$$L = \frac{\sum_{jk} \iint \frac{\phi_j^*(r,v)\phi_k(r,v)}{v} drdv}{\iiint x(\acute{v})\phi^*(r,\acute{v})\nu\Sigma_f\phi(r,v)drd\acute{v}dv} \tag{31}$$

In order to obtain the partial lifetimes one simply drops the double summation sign in Equation 31.

$$L_{jk} = \frac{\iint \frac{\phi_j^*(r,v)\phi_k(r,v)}{v} drdv}{\iiint x(\acute{v})\phi^*(r,\acute{v})[\nu\Sigma_f(r,v)]\phi_k(r,v)dr,d\acute{v}dv} \tag{32}$$

This definition of L_{jk} is in keeping with the definition of N_{jk} i.e., $N_{jk} = S_{jk}L_{jk}$.

The fluxes are obtained in the usual manner using various numerical techniques for solution of the Boltzmann transport equation. However, in small fast systems where the leakage terms (and therefore the coupling) are important, the boundary conditions can easily be defined only in a simple one dimensional problem.

B. Coupling Model Used with the Monte Carlo Technique

The coupling coefficients as used in this work are defined as follows:

K_{ij} the normalized expectation value that a fission neutron in reactor j gives rise to a next-generation fission neutron in reactor i

S_i the total fission neutron source in reactor i

S_{ij} the fission neutron source in reactor i which results from fissions caused by neutrons which originate in reactor j

If there are N reactors in the system then

$$S_i = \sum_{j=1}^{N} S_{ij}$$

and the normalized coupling coefficients are calculated using the following ratios.

$$K_{ii} = \frac{S_{ii}}{S_i}$$

$$K_{ij} = S_{ij}/S_j$$

For a critical reactor this definition agrees with that used in the Avery model. However, for the non-critical reactor, the coupling coefficients calculated in this work are the Avery coefficients divided by the criticality factor i.e. $K_{ij} = K'_{ij}/K$.

A logical method of obtaining these coupling coefficients is by use of a Monte Carlo technique, where the neutrons are followed from their production to their removal from the assembly. The coupling coefficient, K_{ij}, can be obtained by taking the ratio of all the fission neutrons produced in reactor i which originated in reactor j to the total number of neutrons originating in reactor j.

The coupling coefficients used in this work should not vary with changes in criticality due to cross section or density changes since they are normalized by dividing by the criticality factor. If the geometry is changed one could expect a variation in the coupling coefficients due to changes in leakage.

III. THE MONTE CARLO METHOD AND ITS APPLICATION IN THE "O5R" CODE

A. Historical Background

The Monte Carlo method originated during the 1940's as a result of work done by J. von Neumann and S. Ulam at Los Alamos. However, virtually nothing appeared in print until 1949. In that year, a symposium was held on Monte Carlo methods at Los Angeles under the sponsorship of the Rand Corporation and the National Bureau of Standards in cooperation with Oak Ridge National Laboratory. The proceedings of this symposium were published by the National Bureau of Standards (24) in 1951.

A second symposium was held at the University of Florida in 1954. It was sponsored by Wright Air Development Center of the Air Research and Development Command (21).

Since the first publication the interest in the field has grown. With the advent of bigger and faster computing machines in recent years, the full capabilities of the method are now being more nearly realized. As an example, in a recent article in Nuclear Applications, the O5R Monte Carlo code at Oak Ridge was used to calculate the flux distribution in a SNAP reactor and the results were in excellent agreement with experimentally measured values (32). There have been several articles which describe both theoretical and applied work using Monte Carlo (4, 5, 10, 16, 19, 20, 21, 24) and no further background will be given here.

B. General Description

The code used in this work was the O5R Monte Carlo Code. It was developed by R. R. Coveyou, J. G. Sullivan and H. P. Carter at Oak Ridge National Laboratory in Oak Ridge, Tennessee (8).

The O5R code system was designed to calculate any quantity related to neutron transport in a reactor or shielding problem.

Sources may have arbitrary spatial, energy, and angular distributions via a subroutine written by the user. Arbitrary three dimensional geometries bounded by quadric surfaces and a maximum of sixteen media may be included in the problem. Anisotropic scattering can be included for both elastic and inelastic processes. The code is applicable to fissionable as well as non fissionable media. Also included are several variance reduction techniques such as Russian roulette and splitting.

A calculation generally consists of two main operations. First, the O5R-generator is used to generate histories and produce "collision tapes" on which are written any or all of 34 distinct parameters which describe the collision.

Secondly, these tapes are processed separately by an "analysis" routine written by the user.

A batch system of processing is employed to obtain a detailed table of cross sections in fast memory. The cross sections in memory at one time encompass only a small energy range. All collisions of a batch for which these cross sections are needed are generated before reading another group of cross sections from a tape. O5R can handle an energy range extending from 77.13 MeV to 0.07×10^{-3}eV.

The cross sections are prepared for use in O5R by a special routine XSECT. This code performs a variety of manipulations such as preparing, updating, and editing a master cross section tape; in addition it performs cross section arithmetic.

C. Generation of Histories

The source data are generated by a routine SOURCE written by the user. The assembly used in this work consists of two coupled bare slabs of uranium. In order to speed convergence a cosine distribution in the X and Y direction and a uniform distribution in the Z direction were used with a fission spectrum distribution of energies. The angular distribution was chosen to be isotropic for the source neutrons.

Inelastic collisions are treated using an evaporation model (11, 33). The temperature of the compound nucleus is a constant times the square root of the incident neutron energy. This temperature is used as the most probable temperature of a modified Maxwell Boltzmann distribution (27) from which an energy for the scattered neutron is chosen using random numbers.

The neutron histories are generated in the following manner (Appendix B).

First, the neutron is assigned a NAME, which is an integer which distinguishes it from every other neutron in the batch. An initial speed and direction are also assigned, as are the spatial coordinates X, Y, and Z of its birth and an initial weight (usually equal to 1.0). The quantities may be arbitrarily assigned by the user using the SOURCE subroutine or may result from the distributions of fissions from the previous batch in fissioning systems. Finally, the geometry routine, GEOM, determines in which medium the neutron lies.

During the slowing down process, the number of mean free flight times (path length divided by velocity) that the neutron is to travel is chosen from an exponential distribution. From a consideration of the cross sections and the geometry, a tentative position for the next collision is chosen. If the flight path lies entirely within the medium of origin, the tentative position is adopted as the site of the next collision. If, however, the flight path crosses a medium boundary the position of the boundary crossing is found, and the distance to this crossing point is subtracted from the original path length. The boundary crossing point then becomes the starting point for the continuation of the flight. The flight distance within the new medium is the original distance less the distance traveled to the medium crossing. This process continues until a flight path lying entirely within a single medium is found or until the neutron escapes.

At the collision point a new weight is computed by multiplying the old weight by the survival probability i.e., the non-absorption probability. For this case fissions are considered as scattering events, therefore fission is involved in the calculation of the non-absorption probability.

The nuclide from which the neutron is to scatter is chosen by considering the scattering cross sections of all nuclides of the medium of the collision point. As noted previously all collisions are scattering events.

From the mass of the scatterer, the neutron velocity in the laboratory system before the collision, the type (elastic or inelastic) of scattering, and a selection from an angular distribution associated with the scatterer; a new velocity is found.

The energy corresponding to the new velocity of the neutron is compared to an arbitrary cut-off energy. If the energy is greater than the cut-off energy the slowing down process continues, if it is less than the cut-off value the slowing down is concluded and the neutron enters the thermal group. Several treatments of the thermal case can be optionally handled by O5R i.e., the one velocity model, the independent gas model, or a model created by the user. Since the system being investigated in this work is a fast system no thermal treatment is specified. The few neutrons reaching the cut-off energy are lost.

A random number generator is included in the O5R code which supplies various distributions and pseudorandom numbers. The following distributions are available for use in all subprograms including those programs written by the user.

R=FLTRNF(DUM)	Uniformly distributed on the interval (0,1)
R=SFLRAF(DUM)	Uniformly distributed on the interval (-1,1)
R=EXPRNF(DUM)	Expontentially distributed : $P(R)\ dR = e^{-R} dR$
CALL AZIRN(Sin,Cos)	A random azimuthal angle. The sine and cosine of ϕ, where ϕ is uniformly distributed on the interval $(0,2\pi)$.

CALL POLRN(Sin,Cos)	The sine and cosine of Θ where $\cos\Theta$ is uniformly distributed on the interval (-1,1). A random polar angle.
CALL GTISO(X,Y,X)	An isotropic unit vector $X=\cos\Theta$, $Y=\cos\phi\sin\Theta$, $Z=\sin\phi\sin\Theta$ where Θ is a random polar angle and ϕ is a random azimuthal angle.
R=RNMAXF(T)	Maxwellian energy distribution : $P(R)dR=(4/T^3\pi)^{1/2}R^{1/2}e^{-R/T}dR$
R=FISRNF(DUM)	A neutron speed squared from the Watt fission spectrum : $P(R)dR=C\ e^{-R/T}$ $\sinh(2/EE_f/T)$, where T=0.965 X 1.913220092 X 10^{18} and E=0.523 X 1.913220092 X 10^{18}. Where the constant 1.913220092 X 10^{18} is the conversion factor from MeV to cm^2/sec^2.

Since absorption is not allowed in O5R, the fissions which eventually produce the source neutrons for the second and successive batches are treated as follows.

At each collision point a fission weight WATEF is calculated. This is the probability of a fission neutron being produced i.e., $\nu\Sigma_f(E)/\Sigma_{tot}(E)$. Where Σ_{tot} is the total cross section including absorption. The fission weight is compared to the product of a floating point random number between 0 and 1.0 and an arbitrarily chosen weight assigned to neutrons created by fissions (usually 1.0). If the fission weight is less than the product, no fissions are assumed to occur and control is returned to the main program. If, however, the fission weight is greater than the product of the random number and the assigned weight, a fission is said to occur and a neutron having the preassigned weight and the coordinates of the collision point is stored on the fission tape.

At the end of each batch the neutrons on the fission tape are retrieved. The weights are normalized so that the total weight of the neutrons is equal to the total weight of the neutrons in the initial batch. The energy of these neutrons is that of the Watt spectrum and this energy is assigned by the previously described random number routine.

In addition to the method of assigning fission neutrons for each batch, the O5R code also accumulates the sum of the product ($\nu\Sigma_f/\Sigma_{tot}$ * WATE) over all collisions where WATE is the non-absorption probability mentioned above. This accumulated weight FTOTAL is used in the calculation of the multiplication constant.

One of the most distinctive features of O5R is its highly detailed representation of neutron cross section data. The entire energy range, from 77.13 MeV to 0.08 X 10^{-3} eV, is first divided into forty supergroups by energy boundaries a factor of two apart. Each supergroup is then subdivided into n subgroups of equal energy width, where n is any number between 1 and 512.

Cross sections are assumed constant across each subgroup. This choice of representation reproduces fairly well the general tendency of cross sections to vary somewhat more regularly with lethargy than with energy, yet it takes into account the ease of working with equal energy spacings within a supergroup. The memory address of the particular cross section needed is obtained by a linear energy transformation.

The O5R internally uses the speed squared instead of the energy, thus the unusual limits of energy. The value 77.13 MeV is 2^{67} cm^2/sec^2 where 0.07×10^{-3} eV is equal to 2^{27} cm^2/sec^2 (28).

The neutrons are processed in parallel through each supergroup with only the cross sections for the supergroup being processed held in memory at any one time in order to conserve memory space. The parallel processing involves following each neutron as far as possible with the data in the memory. The neutron is then laid aside until all others are processed similarly. When all are processed the data for the next lower energy group are brought into memory and the above processing continues.

The second unique feature of the O5R is the geometry routine. This is especially important in the general coupling problem due to the unwieldy geometry of large coupled assemblies. The O5R can handle calculations involving sixteen media with permissible boundaries being any shape which can be described by quadric surfaces either singly or combined. The routine which handles the tracing and tallying of neutron paths through the system is GEOM.

The first step in the description of a system for the GEOM routine is to enclose the entire system in a rectangular parallelepiped with faces parallel to the coordinate planes.

This parallelepiped is divided into smaller parallelepipeds called zones whose faces are again parallel to the coordinate planes.

The zones are once again divided into smaller parallelepipeds called blocks, with boundaries parallel to the coordinate axes but extending only across individual zones. The planes used as boundaries for zones or blocks need not be boundaries between media, however, it is advantageous to make any boundaries separating media which are parallel to the coordinate axes boundaries of blocks or zones as well.

Boundaries between media which are not block or zone boundaries may be any quadric surfaces. The quadric surface is defined by the zeros of a quadratic function. This surface divides all space into two sectors. In one sector the function will be positive, and in the other it will be negative.

Each block can contain up to eighteen surfaces as medium boundaries. The positive and negative portions of the block are called sectors, however, each sector must contain only one medium. Two sectors containing the same medium are allowed to join.

O5R includes two voids. The first, the external void (assigned the medium number 0), represents all space outside the enclosing parallelepiped. If a neutron enters the external void it escapes from the system.

The second, the internal void (represented by the medium number 1000), is treated as a medium where the mean free path of the neutron is infinite. A neutron entering the internal void traverses it entirely and the path length in the void is considered to be zero.

O5R also provides for a system of regions for the application of weight standards. The regions exhibit the same divisions into blocks and zones as for the media geometry, but division of a block is independent of the media divisions.

In this work no region geometry was considered since weight standards were not applied, and all areas of the assembly possess equal weights.

The geometry data are read into the GEOM routine in the following manner (7):

List of boundaries of zones in increasing order along
the X axis
List of boundaries of zones in increasing order along
the Y axis
List of boundaries of zones in increasing order along
the Z axis

For each zone (l,m,n)

List of block boundaries in increasing order in X
List of block boundaries in increasing order in Y
List of block boundaries in increasing order in Z

For each block of the zone

List of media numbers in the block, sector by
sector
List of surface numbers appearing in the block

For each sector

List of indices marking the position of the sector
with respect to the surfaces of the block
(+1,-1,0)

*Possible data of statistical regions

List of regions
List of boundary surfaces numbers in the block

For each region

List of incides marking the position of the region
with respect to the boundary surfaces of regions
of the block

List of quadratic functions describing the surfaces in
the order of surface number in the blocks above

*Not used if region geometry is not included in the
problem.

A detailed description of the operation of the geometry subroutine GEOM is given in the operating manual for the O5R code (28).

D. Input Parameters for O5R

The following variables must be supplied to O5R in card form. In addition to these variables listed below, two tapes written by the routine XSECT are required. The first is the system data tape which contains (a) the mean-free-flight times for each energy subgroup interval, (b) the non-absorption probability for each subgroup interval, and (c) the cumulative scattering probabilities. The second tape is the PHI tape containing data used in the anisotropic scattering routine of O5R. The values on this tape are calculated using a technique developed by R. R. Coveyou (8), a summary of the technique is discussed in Appendix A.

The card input data variables are as follows:

NSTRT	The number of neutrons initially in each batch
NMOST	The maximum number of neutrons permitted to appear during the run of one batch
NITS	The number of batches in the run
NQUIT	The number of runs
EBOT	The energy, in eV, below which neutrons are considered to be in the thermal group
NTHRML	The option for treatment of thermal neutrons as mentioned in part B of this section
MEDIA	The total number (less than sixteen) of media exclusive of voids in the system

NCONT1 The logical number of the system data tape

NCONT2 The logical number of a copy of the system data tape. This is used to avoid wasting machine time in rewinding NCONT1

NSTAPE The logical number of the data tape used in one of the thermal neutron options, ignored in the case of no thermal neutrons

A set of the following five variables is required for each medium in the system.

LF1 The type of scattering used for each scatterer in the medium

ASSES The atomic mass, in amu, of each scatterer in the medium. The mass of an inelastic scatterer is represented by zero mass

SLOTH, SLOPS, SLOFS Data used in the one velocity thermal neutron option

The following ten variables are for source neutrons, the values assigned are overridden by data generated by SOURCE.

ESOUR The source energy in eV

UINP, VINP, WINP The direction cosines of the source neutrons, a value of zero for each will denote an isotropic distribution of source neutrons

WTSTRT The statistical weight assigned to each neutron

XSTRT, YSTRT, ZSTRT The coordinates of the initial position of all neutrons in units of centimeters

NMED — The medium number within which the above coordinates lie

NREG — The region number within which the starting coordinates lie

The following parameters specify output parameters.

NHISTR — The logical number assigned to the first collision tape may be assigned. When the first tape is filled the logical number NHISTR is advanced by 1 and the recording of collisions continues until NHISMX is reached or the problem is terminated

NBIND — An index indicating which of the 36 output parameters are to be recorded. This list will be given in part E of this section

RANDM — The octal representation of the initial parameter in the random number generation routine. The starting random number should end in 1 or 5 in order for the period of the random number sequence to be maximum

Finally the following five parameters are needed to complete the input data.

NSOUR — An index which in fissionable media offers an option with respect to the source for batches after the initial batch. If NSOUR ≤ 0, the original source will be used for all batch. If NSOUR ≥ 1, the source for these second and succeeding batches will be the neutrons resulting from fissions taking place during the transport of the preceding batch

MFISTP The logical number of the tape for storing fission neutron parameters during a batch

FWLOW The arbitrary weight to be assigned to neutrons produced by fissions (usually equal to 1.0)

NPTAPE The logical number of the PHI tape mentioned earlier

NTYPE An index which indicates whether biasing of angular scattering is to be considered

Further variables are required if variance reduction techniques are to be used. However, for the problem under consideration in this paper, no further input data are needed.

E. Output Parameters

The following parameters may be obtained for each collision.

NCOLL An integer identifying the type of "collision" to which the parameters apply

NCOLL=1 source neutron data

NCOLL=2 real collision of a neutron with a nuclide

NCOLL=3 neutron killed by Russian roulette

NCOLL=4 neutron escapes from the system

NCOLL=5 application of weight standards has caused the neutron to split. The data for the original neutron is given

NCOLL=6 the data for the new neutron due to splitting is given

NCOLL=7 neutron crosses a medium boundary

NCOLL=8 neutron survives Russian roulette and its weight increases accordingly

NCOLL=9 optional, for use by the user

NAME An integer which identifies the neutron having the collision

SPDSQ The speed squared of the neutron after a collision

U The neutron velocity in the X direction, after the collision

V The neutron velocity in the Y direction, after the collision

W The neutron velocity in the Z direction, after the collision

WATE The neutron weight after the collision

SPOLD The speed squared before the collision

UOLD The neutron velocity in the X direction, before the collision

VOLD The neutron velocity in the Y direction, before the collision

WOLD The neutron velocity in the Z direction, before the collision

XOLD The X coordinate of the previously recorded event

YOLD The Y coordinate of the previously recorded event

ZOLD The Z coordinate of the previously recorded event

OLDWT The neutron weight before the collision

THETM The mean free flight time to the collision

PSIE The non-absorption probability at the site of the collision

ETAUSD The number of mean free paths used to arrive at the collision point from the last collision point

NGROUP An integer specifying the energy supergroup within which SPOLD lies

LELEM An integer identifying the nuclide collided with

NREG The region in which the collision took place

NMED An integer identifying the medium in which the collision occurred

NAMEX An integer identifying the neutron from which the current neutron was produced if it was produced by splitting

WATEF The fission weight produced at the collision point (WATEF=OLDWT*$\nu\Sigma_v/\Sigma_{tot}$)

BLZNT	A packed word giving the block and zone of X, Y, and Z
BLZON	A packed word giving the block and zone location of XOLD, YOLD, and ZOLD
LAMBDA	The mean free path in the medium before the collision
SO	The speed of the neutron before the collision
S1	The speed of the neutron after the collision
ETHATH	The time taken to arrive at the collision point from the previous collision point
FONE	The average value of the cosine of the scattering angle in the center-of-mass system
EXTRA1	Not used at the present, for user option
EXTRA2	Not used at the present, for user option

IV. PROBLEM DESCRIPTION

A. The Assembly

The assembly used in this work consisted of two 27.94 cm diameter cylinders each 6.676 cm thick. The two cylinders were spaced 36.94 cm apart along the Z axis as shown in Figure 1.

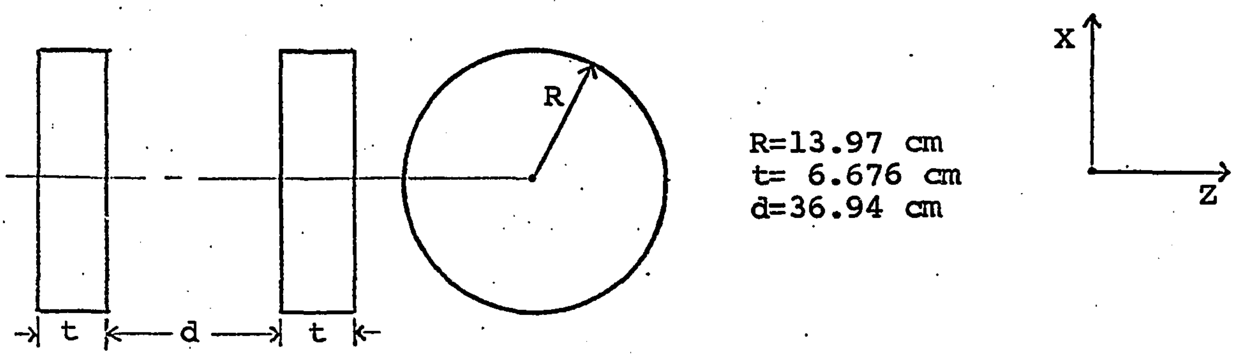

Figure 1. Configuration and orientation of the assembly

As can be seen from Figure 1, the rectangular coordinate system was chosen with the Y axis outwardly perpendicular to the page. This corresponds to a simple fast critical facility in three dimensions.

The reason for the selection of the above configuration is two fold.

First, an assembly such as the above was used by John Mihalczo (22) at Oak Ridge as an experimental assembly to measure the kinetic effects of coupled reactors. Mr. Mihalczo used the O5R Monte Carlo code to calculate coupling coefficients in the assembly. These were then used in solving the coupled point reactor kinetics equations to obtain theoretical results which were compared to experimental data. Thus, for one set of data a comparison of results can be made. However, neither the technique involved in the calculation of the coefficients, the parameters used, nor the variation of the coefficients with criticality were given in detail in the above paper. The experimental determination of the coupling coefficients appears to be difficult and no experimental results are available for comparison at this time. This paper, therefore, will emphasize the technique used for calculation of the coupling coefficients and their dependence on the criticality of the system.

The second reason for applying the code to a simple system was to conserve computer fast memory space and therefore computer expense. The more complicated the geometry the greater the amount of memory space needed for storage of boundary data and medium cross sections, also the greater the time required to trace the neutron paths. The expansion to a more complicated system simply involves changing the geometry input cards described in section C of Part III.

In the first run, each of the uranium slabs was enriched to 93.15% in U-235. This run corresponds to the O5R calculation made by J. Mihalczo at Oak Ridge. A comparison of results follows in Part VI.

The upper energy limit chosen for the problem was the same as the upper limit of the Watt fission spectrum i.e. 10 MeV. The lower end of fast reactor spectra, 500 eV, was chosen as the lower limit or cut-off energy in this problem. This energy encompasses 17 supergroups. After checking BNL-325 (15, 31) for the variation of cross sections with energy in the energy range of 10 MeV - 500 eV, 128 subgroups per supergroup were used. This corresponds to 2,176 energy groups in a usual multigroup calculation.

As was mentioned earlier, the initial spatial distribution of source neutrons was that of a cosine in the X and Y directions, and a uniform distribution in the Z direction. The energy distribution was taken from the Watt spectrum.

After the first run the spatial distribution for each batch was taken from the fissions produced by the preceding batch. For new runs, the fissions from the last batch in the preceding run were used as a source of neutrons. This speeds convergence and improves running times. Convergence as used here means that the neutrons in each successive batch approach a particular spatial distribution in the assembly. The more closely the first batch approximates the distribution the faster the convergence and the shorter the running times.

B. Input and Output Data

Each run requires five tapes; two are input tapes, the system data tape and the PHI tape, which were described previously. A third tape is used to store information from neutrons resulting from fissions. The last two tapes contain the output of the O5R.

For this problem, fourteen of the possible thirty-six output parameters available for each collision were chosen. These include the type of collision, the name of the neutron, the speed squared, the X, Y, and Z coordinates, the weight, the old X, Y, and Z coordinates, the mean-free flight time, the medium in which the collision occurred, the fission weight, and the time taken to arrive at the collision point from the previous collision point.

The above are recorded for four types of events, an escape, the source data, a real collision, and a boundary crossing.

Not all of the parameters are needed for calculation of the coupling coefficients. However, if one wishes to calculate other collision parameters, the O5R will not need to be run again, but only the collision tape and an analysis routine will be necessary.

The cross section data used in the computation were taken from the Oak Ridge National Laborabory cross section library (9). These data include a value for the total, the elastic, and the inelastic cross sections as well as the product of the average number of neutrons emitted per fission, ν, and the fission cross section, σ_f.

Also, included in the set of cross sections for U-235 and U-238 were fourteen terms in a Legendre expansion of the anisotropic elastic scattering cross section.

All of the data are available in an energy range of 15 MeV down to 0.017 eV.

The cross sections in the Oak Ridge library are comparable to the approved set available in the ENDF/B library (34), however, the Oak Ridge set have been adjusted in order to correlate experimental and theoretical predictions. It was the feeling of the author that the Oak Ridge library represented a more reliable set of data than the ENDF/B file.

The normalized and slightly modified Maxwell-Boltzmann velocity distribution used for the evaporation model for inelastic scattering was taken from A. E. Profio's "PULSE" Monte Carlo code (27). The integral (cumulative) distribution and the density function are shown in Figures 2 and 3.

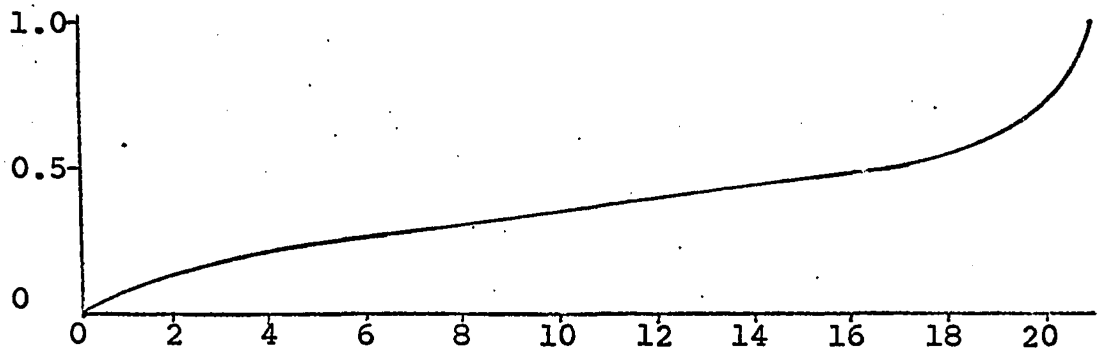

Figure 2. Cumulative probability function for inelastic scattering evaporation model

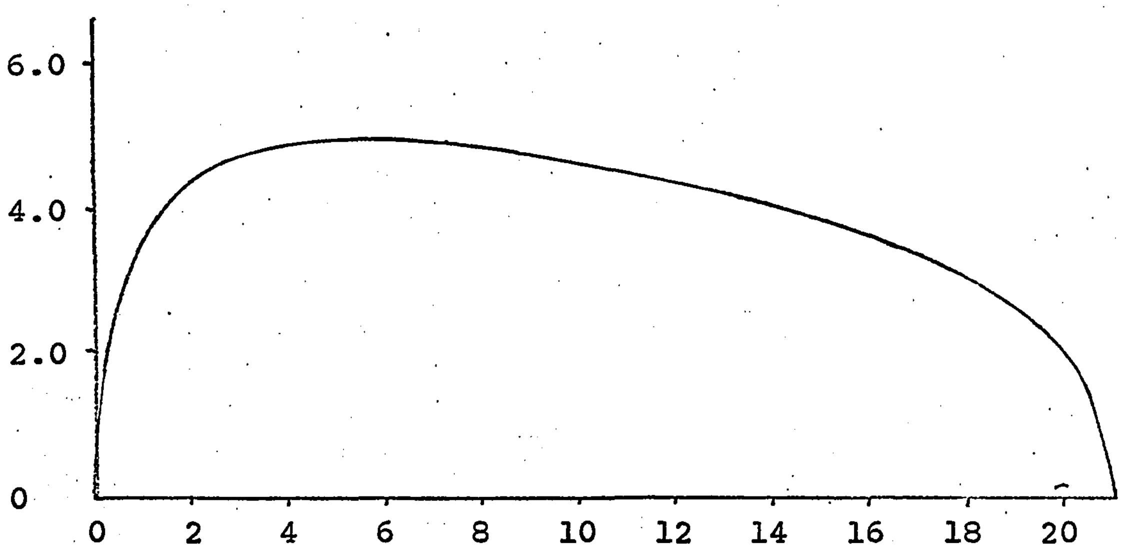

Figure 3. Density function for inelastic scattering evaporation model

V. ANALYSIS OF DATA

The analysis of data consists of two parts. First, the expectation value $\overline{K}$ defining the criticality of the entire system is calculated along with a variance. Secondly, the individual coupling coefficients, K_{11}, K_{22}, K_{12}, and K_{21}, are calculated.

In the analysis of data for the calculation, the following quantities are used.

FWATE the fission probability of each neutron at the end of the batch

WATE the non-absorption probability of each neutron at the end of the batch

N the number of neutrons in a batch

M the number of batches in a run

$\overline{K}$ the expectation value for the entire system (the criticality factor)

σ the standard deviation of $\overline{K}$

Using these quantities, the calculation of $\overline{K}$ is carried out as follows.

First, the non-absorption probability and fission weights are summed over all neutrons in a batch.

$$\text{SWATE} = \sum_{1}^{N} \text{WATE}$$

$$SFWATE = \sum_{1}^{N} FWATE$$

For each batch a partial expectation value is calculated.

$$K = SFWATE/SWATE$$

as is the square of the expectation value

$$K^2 = (SFWATE/SWATE)^2$$

The expectation value is calculated by summing the value of K over all batches and dividing by the total number of batches.

$$\overline{K} = \frac{\sum_{1}^{M} K}{M} = \frac{\sum_{1}^{M} \frac{SFWATE}{SWATE}}{M}$$

The variance of $\overline{K}$, σ^2, is calculated in the usual manner.

$$\sigma^2 = \frac{[(\sum_{1}^{M} K^2)/M - \overline{K}^2]}{M - 1} = \frac{[\overline{K^2} - \overline{K}^2]}{M - 1}$$

The standard deviation is the square root of the variance.

$$\sigma = (\sigma^2)^{1/2} = \left\{\frac{[(\sum_{1}^{M} K^2)/M - \overline{K}^2]}{M - 1}\right\}$$

$$= \frac{[\overline{K^2} - \overline{K}^2]^{1/2}}{\sqrt{M - 1}}$$

The calculation of the coupling coefficients is based on the definitions in Section B of Chapter II. That is, the coupling coefficients are a ratio of source neutrons in one reactor originating in another reactor to the total source of neutrons in the original reactor.

When a neutron from one assembly crosses the internal void to the other assembly it contributes to the fission probability and also to the non-absorption probability in the second assembly during the time it remains in the second assembly.

If the same neutron again crosses the internal void back to the assembly from which it came, it again contributes to the fissioning probability in the original assembly and also to the non-absorption probability in the original assembly.

Therefore, if one defines the following variables, as expectation value for the coupling coefficient can be calculated.

FKij The fission weight of neutrons in reactor i which originated in reactor j. For $i \neq j$, this includes the fission weight of neutrons which have crossed the boundary between regions i and j an odd number of times. For $i=j$, the neutrons have either not crossed the boundary between i and j or have crossed an even number of times.

Nij The number of collisions in a batch of neutrons in reactor i which originated in reactor j. Again for $i \neq j$ Nij includes the sum of the number of collisions of neutrons which crosses the boundary between i and j an odd number of times. For $i=j$ Nij includes the sum of the number of collisions of neutrons which either have not crossed the boundary or have crossed an even number of times.

For the two reactor case, the partial source terms of Avery's model can be defined for each batch.

$$S11 = \sum_{1}^{N11} FK11$$

$$S12 = \sum_{1}^{N12} FK12$$

$$S21 = \sum_{1}^{N21} FK21$$

$$S22 = \sum_{1}^{N22} FK22$$

The total source for each batch is calculated by summing the appropriate partial sources.

$$S1 = S11 + S12$$

$$S2 = S21 + S22$$

The partial coupling coefficients are defined as the ratio of the partial sources to the total source in each assembly.

$$K11 = S11/S1$$

$$K12 = S12/S2$$

$$K21 = S21/S1$$

$$K22 = S22/S2$$

For a run containing M batches, the expectation values which are the coupling coefficients can be expressed as the following.

$$\overline{K11} = \frac{(\sum_{1}^{M} K11)}{M}$$

$$\overline{K12} = \frac{(\sum_{1}^{M} K12)}{M}$$

$$\overline{K21} = \frac{(\sum_{1}^{M} K21)}{M}$$

$$\overline{K22} = \frac{(\sum_{1}^{M} K22)}{M}$$

VI. RESULTS AND DISCUSSION

The primary purpose of this work as stated earlier was two fold. First, to make the O5R package and its associated routines operational on the Iowa State University IBM 360/65 computer. Secondly, to develop a method of computing coupling coefficients patterned after the definitions of Avery (Equations 2a and 2b). Avery's definitions are for a critical reactor, however, the definitions were extended to include non-critical systems in this work and the variation of these newly defined coefficients with criticality were investigated.

The majority of the time was spent in attaining the first goal. This included changing many of the routines, writing new ones, preparing input-output tapes, and tying together the entire O5R package consisting of 68 subroutines, 9 assembler language routines, and 6 object routines. Also, the cross section routine, XSECT, was modified to be compatible with the O5R package.

Once this goal was accomplished, several runs were made using the geometrical arrangement described in section A of chapter IV. The criticality was changed in each run by changing the enrichment ratio in each slab. The first run used a cosine distribution in the X and Y directions and a uniform distribution in the Z direction for each slab. All the runs after the first used the fission neutrons from the previous run as a source.

A summary of results appears in Table 1. The only data

Table 1. O5R results

	Run #1	Run #2
Thickness of each slab in cm	6.676	6.676
Separation distance in cm	36.94	36.94
Enrichment in atomic percent	93.15	95.5
Number of batches/run	13	20
Number of histories/batch	200	200
Criticality factor $\overline{K}$	0.9933	1.138
K11 coupling coefficient in $	141.0	142.5
K22 coupling coefficient in $	145.1	142.9
K12 coupling coefficient in $	5.801	4.123
K21 coupling coefficient in $	4.452	4.068
Standard deviation in %	2.9	1.83
Time/run (min:sec)	1:15	3:25

[a]Calculated by J. Mihalczo (22).

Run #3	Run #4	Run #5	Run #6	Oak Ridge Results[a]
6.676	8.6	6.676	6.676	6.676
36.94	36.94	50.0	50.0	--
90.0	90.0	95.5	93.15	93.15
20	20	20	20	--
200	200	200	200	--
0.875	0.941	1.097	0.9901	.901
141.8	142.1	147.5	145.7	--
143.0	142.4	147.2	147.1	--
4.124	4.123	2.133	2.134	--
4.072	4.081	2.150	2.148	3.5
1.81	1.85	1.88	1.81	5
2:01	2:35	3:31	2:39	--

available for comparison are listed in the last column. The calculation was made by J. Mihalczo (22) at Oak Ridge using the O5R code. The enrichment and slab thickness is the same as that used in Run #1; however, as can be easily seen the results do not compare favorably. This may be due to two reasons. First, no information as to the type of analysis, number of runs, number of histories, source of cross sections, nor number of energy groups used by Mihalczo were available. These of course are essential for duplication of results. Secondly, there is a distinct possibility that the values calculated at Oak Ridge may have been for an assembly with the two slabs spaced at a distance larger than the 36.94 cm used here, thus the lower value of criticality and coupling. The coupling coefficients calculated here are of the correct magnitude for such an assembly even though exact agreement with other calculations is not found.

The criticality ranges from far subcritical through critical to super critical. In this wide range the coupling coefficients remain constant well within statistical accuracy as can be seen by reading horizontally across the table for any coupling coefficient in Runs #1 through #3.

In all cases except Run #1, the coupling is symetrical i.e., $K_{11} = K_{22}$, and $K_{12} = K_{21}$. This can be expected since the assembly used was symetrical in geometry and enrichment. This is another check as to the reliability of the results.

Runs #5 and #6 were made with a separation of 50 cm to check the variation of the coupling coefficient in an assembly using a different geometrical arrangement. Again, the coupling coefficients appear constant for variations in criticality due to density changes. This lack of variation in the coupling coefficients does not appear to be unique to a particular geometrical arrangement over the ranges of criticality used in this work.

Run #4 was made to check an assumption made by Mihalczo (22). In his experiments with Rossi-α, Mr. Mihalczo assumes the coupling coefficients remain constant with a change in the slab thickness (and therefore a change in criticality) as long as the separation distance remains constant. Run #4 appears to confirm this assumption although further runs are necessary for a complete verification.

Mihalczo's assumption appears to have a valid basis if one considers the physical problem. The fuel slabs used in this work are 6.676 cm in thickness, or two to three mean free paths where a mean free path for this assembly is about 2.5 cm. On the average a neutron which has entered the interior void has suffered a collision in the fuel region within two or three cm of the interior interface. It is the combination of the angle at which these neutrons left the scattering reaction and the distance between slabs which determines which neutrons reach the other slab and thus determines the coupling coefficient. If material is added to the outside of the slab leaving the interior separation distance the same, no change in coupling should occur. Those neutrons arising in this added material or the average suffer at least two collisions before reaching the area within one mean free path of interior interface. The collisions are independent and if the neutrons do arrive in the area within one mean free path of the interior interface their origin is lost thus the effect of the addition of the material is not felt. Of course some neutrons will penetrate the interior interface and cross the void without having suffered any collisions. The number involved in this type of phenomenon issmall since the probability of traveling such a distance without any collision is small. Any gain in coupling due to neutrons in the added material which crossed to the other slab without a collision is offset by the increase in the number leaking out due to the same phenomena.

The run times listed include only the actual CPU (Central Processing Unit) times, they do not include the time for analysis of data nor time used for preparing the cross section input tapes. These are in the order of 1 and 3 minutes respectively.

The short run time can be expected in a fast assembly such as the one used here since there is considerable leakage and neutrons are generally not followed for more than 10-20 collisions before leaking out of the system since, as mentioned earlier, the approximate mean free path for the material and enrichments used in the assembly is 2.5 cm.

The deviation of Run #1 from Runs #2 and #3 can be explained as follows. First, not as many histories were used since this was the first time the code was run, and a conservative number of histories was chosen to avoid using excessive computer time. Secondly, and more important, the source was that supplied by the user and many histories were run before convergence. Thus the unsymmetrical coefficients and large standard deviation.

The sum of the coupling coefficients, K_{11} and K_{12}, is approximately $1.0/\beta$ for any run. This is also true for the sum of K_{21} and K_{22} for any run. Thus the values as calculated are normalized and are independent of the criticality of the system. The values compare to the Avery coupling coefficients only if the reactor is exactly critical. The Avery coefficients can be obtained by multiplying the coefficients of this work by the criticality factor of the noncritical system.

In the physical situation one would not expect the Avery self-coupling term, K_{ii}, to change with increased separation distance. Runs #5 and #2 differ only in their separation distance. If the values of K_{11} and K_{22} for these runs are multiplied by the appropriate criticality factor to obtain the Avery coefficients, the K'_{ii}'s obtained are found to be essentially constant. The cross-coupling coefficients however show a marked sensitivity to separation distance.

The β used in the calculations in Table 1 was 0.00672, the same as used in the Oak Ridge calculation (22).

VII. CONCLUSIONS AND RECOMMENDATIONS

A. Conclusions

Several conclusions can be drawn from the data expressed in Table 1.

First, it is feasible, both economically and mathematically, to calculate the coupling coefficients by the Monte Carlo technique using the basic definitions of a coupling model. Using the O5R code, reasonable results with an error of no more than 3% can be obtained in running times of 3 minutes or less.

These coefficients remain invariant with variations of the criticality factor ranging from 0.87-1.138, and this invariance does not appear to be unique to a particular geometrical arrangement. This conclusion is especially important in reactor design. It implies that the coupling coefficients which appear in the point reactor kinetics equations are not a function of the criticality of the system. Therefore, once the design of the reactor is decided, the coupling coefficients need only be calculated once, say for the "critical" condition. These "critical" values can then be used in other calculations involving a change in criticality without recalculation.

It should be noted the coefficients which appear here were calculated using the new definitions similar to those presented in the Avery model for a critical system. For both critical and non-critical systems, the definitions used in this work give a normalized coefficient which is independent of criticality.

This model gives a very simple representation of spatial coupling. The values listed in Table 1 should not be used for calculations involving other coupling models. An analysis of the same O5R output can be made using another model as a basis and these new values for coupling coefficients used in any calculation based on that particular model.

The values obtained from calculations based on any other model should not be expected to correlate with these calculated in this paper.

B. Recommendations for Future Work

There are numerous problems and topics for future work associated with the O5R now that it has been made operational at Iowa State. Some of these will be mentioned below.

First, several other quantities associated with coupled reactors can be calculated and comparison made to published experimental results. These include a coupling lifetime calculation, neutron flux determination in coupled reactors, calculation of spectral-spatial coupling coefficients such as suggested in the Cockrell-Perez coupling model (6), perturbation studies in coupled reactors, and application of coupling calculations to a specific reactor or critical assembly. This later suggestion may prove important in design of fast reactors. Monte Carlo and especially the O5R can give detailed values for design parameters due to the detailed cross section handling capabilities.

Second, O5R can be used to obtain comparative checks on experiments performed using the Iowa State University neutron generator.

Third, the static features of O5R can be combined with the time dependent features of the PULSE code which was also made operational at Iowa State by the author. Together a general time dependent code could be developed which could handle pulsed neutron problems.

This latter suggestion is of special importance since the Iowa State Nuclear Engineering Department has recently purchased a neutron generator for pulsing the UTR-10 reactor. A modified time dependent O5R code offers an excellent method to check experimental results. The source can be approximated by writing a new source generation routine which generates a delta function corresponding to that generated by the neutron generator. The detector response can also be taken into account by introducing a medium containing the detector material at the appropriate location in the UTR-10. The number of neutrons entering this detector medium can be statistically found and compared to the actual experimental measurements. This model more nearly approximates the physical situation than the usual modal models, which require a sinusoidal source and which cannot model detector response. Also, a three dimensional study can be made which is not possible except with very elaborate modal technique.

It should be noted that the O5R code can be used to model the latter problem without modification if proper use is made of the output data concerning neutron flight times. However, a time modified code would allow more versatility.

It is also possible to make further use of the output tapes resulting from the five O5R runs made in this work. These tapes contain fourteen parameters for each collision. The parameters can be used for calculation of coupling lifetimes, spectral-spatial coupling coefficients, and flux distributions for the geometrical configuration used here. These calculations can be done by an analysis routine without running the O5R.

The Avery coefficients, although not explicitly defined except for a critical system, can be calculated directly using Monte Carlo by taking the ratio of S_{ij} of batch k to the total source S_j of the previous batch (k-1). With this method of calculating the coefficients, they would add up to the criticality factor as is required in the Avery formulation, and are thus dependent on the criticality.

If one is interested in the Monte Carlo technique itself, the O5R can be used as a model for developing a new code which would calculated adjoint or importance fluxes. These could then be used along with the actual fluxes obtained by O5R for evaluation of importance weighted quantities.

Also, investigation of various inelastic and source routines for use in O5R would be of great value to future users.

Finally, the cross section code and cross section library can be used as a source of detailed cross sections for various materials in a variety of problems.

It is the feeling of the author that as computers become larger and faster, Monte Carlo methods will replace some of the more conventional analysis methods presently in use. This reason being Monte Carlo more nearly approximates the actual physical problem including three dimensional geometry and detector response which is of special importance when correlating theoretical and experimental results.

VIII. BIBLIOGRAPHY

1. Adler, F. T., Gage, S. J., and Hopkins, G. C. Spatial and spectral coupling effects in multicore reactor systems. The National Topical Meeting on Coupled Reactor Kinetics Proc. 1967: 521-556. 1967.

2. Avery, R. Theory of coupled reactors. In U.N. (2nd Geneva) Conference on Peaceful Uses of Atomic Energy. Vol. 12. Pp. 182-191. New York, New York, United Nations. 1958.

3. Baldwin, G. C. Kinetics of a reactor composed of two loosely coupled cores. Nuclear Science and Engineering 6: 320-327. 1957.

4. Cashwell, E. D., Everet, C. J., and Rechard, O. W. Practical manual on the Monte Carlo method of random walk problems. U.S. Atomic Energy Commission Report LA-2120 (Los Alamos Scientific Lab., Los Alamos, New Mexico). 1957.

5. Clark, M., Jr. and Hansen, K. E. Methods of numerical analysis. New York, New York, Academic Press. 1964.

6. Cockrell, R. G. and Perez, R. B. On the kinetic theory of spatial and spectral coupling of the reactor neutron field. Symposium on Neutron Dynamics and Control Proc. 1966: 323-341. 1966.

7. Coseau, Y. Geometric treatment of trajectories in the O5R program. Fantenay-aux-Roses, France, CEN/FAR Electronic Computer Division Report No. 17. 1966.

8. Coveyou, R. R., Sullivan, J. G., and Carter, H. P. O5R, a general purpose Monte Carlo neutron transport code. Oak Ridge, Tennessee, Oak Ridge National Lab. Radiation Shielding Information Center. 1968.

9. Cross Section Library (BCD). Oak Ridge, Tennessee, Oak Ridge National Lab. Radiation Shielding Information Center. 1968.

10. Cupini, E., Molinari, V. G., and Solinias, G. Time-dependent neutron thermalization by the Monte Carlo method. Nukleonik 9: 295-300. 1967.

11. Hanna, G. C. and Clark, R. C. Neutron evaporation in the 14 MeV neutron fission of uranium. Canadian Journal of Physics 39: 967-973. 1961.

12. Hannum, W. H. and Probulos, J. J., Jr. Why coupled fast breeder reactors? National Topical Meeting on Coupled Reactor Kinetics Proc. 1967: 118-125. 1967.

13. Hendrickson, R. A. and Danofsky, R. A. Measurement of the reactivity coefficient in the Iowa State UTR-10. National Topical Meeting on Coupled Reactor Kinetics Proc. 1967: 506-515. 1967.

14. Henkel, R. L. Fission by fast neutrons. In Marian, J. B. and Fowler, J. L., eds. Fast neutron physics. Vol. 2. Pp. 2001-2050. New York, New York, Interscience Publishers. 1963.

15. Hughes, D. J. and Schwartz, R. B. Neutron cross sections. U.S. Atomic Energy Commission Report BNL-325 (Brookhaven National Lab., Upton, New York) Supplement Number 2. 1958.

16. Irving, D. C., Freestone, R. M., Jr., and Kam, F. B. K. O5R: a general Monte Carlo neutron transport code. U.S. Atomic Energy Commission Report ORNL-3622 (Oak Ridge National Lab., Oak Ridge, Tennessee). 1965.

17. Irving, D. C., Kinney, W. E., and Rea, P. LEGENDRE, a program to calculate Lengendre coefficients from angular distributions. U.S. Atomic Energy Commission Report ORNL-1241 (Oak Ridge National Lab., Oak Ridge, Tennessee). 1965.

18. Johnson, P. G. Coupled reactors in nuclear rocket application. National Topical Meeting on Coupled Reactor Kinetics Proc. 1967: 11-19. 1967.

19. Kahn, H. Applications of Monte Carlo. U.S. Atomic Energy Commission Report AECU-3259 (Division of Technical Information Extension, AEC). 1956.

20. Mayne, A. J. Monte Carlo methods for solving neutron problems. U.S. Atomic Energy Commission Report AWRE-18155 (Great Britian Atomic Weapons Research Establishment, Aldermaston, Berks, England). 1955.

21. Meyer, H. A., ed. Symposium on Monte Carlo methods: held at the University of Florida, conducted by Wright Air Development Command, 1954. New York, New York, John Wiley and Sons, Inc. c1956.

22. Mihalczo, J. T. Rossi-α and pulsed neutron measurements in subcritical coupled uranium-metal cylinders. National Topical Meeting on Coupled Reactors Proc. 1967: 484-499. 1967.

23. Miller, L. B. Monte Carlo analysis of reactivity coefficients in fast reactors; general theory and applications. U.S. Atomic Energy Commission Report ANL-7307 (Argonne National Lab., Argonne, Illinois). 1967.

24. Monte Carlo method: Proceedings of a symposium held at Los Angeles, conducted by RAND Corp. and the National Bureau of Standards, with the cooperation of the Oak Ridge National Lab. U.S. Department of Commerce National Bureau of Standards Applied Mathematics Series No. 12. 1951.

25. Pluta, P. R., Hubschmann, W. G., and Lill, G. W. Kinetics of coupled thermal-fast spectrum power reactors. National Topical Meeting on Coupled Reactors Proc. 1967: 360-372. 1967.

26. Proceedings of the conference on the application of computing methods to reactor problems. U.S. Atomic Energy Commission Report ANL-7050 (Argonne National Lab., Argonne, Illinois). 1965.

27. Profio, A. E. PULSE, an IBM 7094 program for calculation of fast neutron kinetics by Monte Carlo: progress report Oct. 1963. Cambridge, Massachusetts, Department of Nuclear Engineering, Massachusetts Institute of Technology. 1963.

28. RSIC computer code collection O5R general purpose Monte Carlo neutron transport code. Oak Ridge, Tennessee, Oak Ridge National Lab., Neutron Physics Division. 1968.

29. Smith, A. B. Inelastic neutron scattering: a compendium. Conference on Neutron Cross Section Technology, 1966. U.S. Atomic Energy Commission Report CONF-660303 (Division of Technical Information Extension, AEC): 577-598. 1966.

30. Smith, A. B. Scattering of fast neutrons from natural uranium. Nuclear Physics 47: 633-651. 1963.

31. Stehn, J. R., Goldberg, M. D., Weiner-Chasman, R., Mughabghab, S. F., Magurno, B. A., and May, V. M. Neutron cross sections. U.S. Atomic Energy Commission Report BNL-325 (Brookhaven National Lab., Upton, New York) Supplement Number 2, Vol. 3. 1955.

32. Straker, E. A. and Mackeuthaler, T. J. Measured and calculated absolute power and fission distribution in the TSF-SNAP reactor. Nuclear Applications 6: 274-278. 1969.

33. Weinberg, A. M. and Wigner, E. P. The physical theory of neutron chain reactors. Chicago, Illinois, The University of Chicago Press. 1958.

34. Wittkopf, W. A., Roy, D. H., and Livolsi, A. Z. U-238 neutron cross section data for the ENDF/B. Lynchburg, Virginia, Babcock and Wilcox Co. 1967.

IX. ACKNOWLEDGMENTS

The author wishes to thank the following for their assistance toward the completion of this dissertation. Dr. R. A. Danofsky of the Iowa State Nuclear Engineering Department for his advice, direction, and consultation; Dr. Glenn Murphy head of the Iowa State University Nuclear Engineering Department for his assistance and advice in this work; and Mrs. Gaile Nazemi of the Iowa State University Computation Center for her programming assistance. The author also wishes to thank the National Aeronautics and Space Administration for the fellowship which provided funds for his graduate education.

In addition to the above mentioned people, the author wishes to give special acknowledgment to his parents, Mr. and Mrs. Fergus Flanagan, for their encouragement, support, and assistance throughout his entire college career.

X. APPENDIX A

The Coveyou Technique for Treatment of Anisotropic Scattering

In most heavy materials, the elastic scattering of neutrons becomes anisotropic at energies above 100 keV. The degree of anisotropy increases with increasing energy.

For some problems the anisotropic scattering can be approximated with very simple techniques, such as the use of a transport cross section in the diffusion approximation. However, a more accurate calculation is sometimes necessary especially in problems involving distributions deep within thick shields, or at the other extreme, in very small critical assemblies.

With Monte Carlo, angular distributions can be included to as high a degree of accuracy as desired, however, the higher the degree of accuracy, the more costly the solution since the selection of a scattering angle becomes an elaborate procedure requiring large amounts of computer time.

The Coveyou technique presented in this Appendix gives the same accuracy as that obtained by a selection from a Legendre expansion but requires considerably less computer time.

The derivation of the technique (8) follows.

First, one expresses the distribution function $F(\mu)$, of the cosine of the scattering angle μ, as a Legendre series

$$F(\mu) = \sum_{L=0}^{n} \frac{2L+1}{2} f_L P_L(\mu) + \sum_{L=n+1}^{\infty} \frac{2L+1}{2} f_L P_L(\mu) \tag{1}$$

where

$$f_L = \int_{-1}^{1} F(\mu)\ P_L(\mu)\ d\mu \tag{2}$$

In Equation 1 only the finite sum is known, while the sum from n+1 to infinity is unknown.

Now, consider a second distribution $G(\mu)$.

$$G(\mu) = \sum_{K=0}^{n} \phi_k\ \delta(\mu - \theta_k) \tag{3}$$

Expanding the δ function gives

$$G(\mu) = \sum_{K=0}^{n} \phi_k \left\{ \sum_{L=0}^{\infty} \frac{2L+1}{2} P_L(\theta_k)\ P_L(\mu) \right\} \tag{4}$$

$$= \sum_{L=0}^{n} \frac{2L+1}{2} \left\{ \sum_{K=0}^{n} \phi_k\ P_L(\theta)_k) \right\} P_L(\mu)$$

$$+ \sum_{L=n+1}^{\infty} \frac{2L+1}{2} \left\{ \sum_{K=0}^{n} \phi_k\ P_L(\theta_k) \right\} P_L(\mu) \tag{5}$$

Define f_L as a function of θ_k

$$f_L = \sum_{K=0}^{n} \phi_k\ P_L(\theta_k) \tag{6}$$

With the definition of f_L, Equations 1 and 5 are accurate to the same order of approximation when both are truncated at n.

Now, in order to obtain θ_k, multiply Equation 6 by $(2L+1)/2P_L(\theta_k)$ and sum over L from 0 to n:

$$\sum_{K=0}^{n} \phi_k \sum_{L=0}^{n} \frac{2L+1}{2} P_L(\theta_k) P_L(\phi_j) = \sum_{L=0}^{n} \frac{2L+1}{2} f_L P_L(\theta_j) \tag{7}$$

where the right hand side is obtained by interchanging summation signs and using Equation 6.

From the orthogonality relation which will be derived later, one obtains the following equation.

$$\sum_{L=0}^{n} \frac{2L+1}{2} P_L(\mu') P_L(\mu)$$

$$= \frac{n+1}{2}\left[\frac{P_{n+1}(\mu')P_n(\mu) - P_n(\mu')P_{n+1}(\mu)}{\mu' - \mu}\right] \tag{8}$$

Now if the n+1 values of θ_k are the roots of $P_{n+1}(\mu)$; i.e.,

$$P_{n+1}(\theta_k) = 0 \tag{9}$$

and this value is used in the right hand side of Equation 8 it then becomes

$$\sum_{L=0}^{n} \frac{2L+1}{2} P_L(\Theta_k) P_L(\Theta_j) = 0 \qquad K \neq j \tag{10}$$

This condition enables one to solve Equation 7 for $\emptyset_j$.

$$\emptyset_j = \frac{\sum_{L=0}^{n} \frac{2L+1}{2} f_L P_L(\Theta_j)}{\sum_{L=0}^{n} \frac{2L+1}{2} [P_L(\Theta_j)]^2} \tag{11}$$

If $F(\mu)$ is a normalized distribution,

$$\int_{-1}^{1} F(\mu)d\mu = 1 = \sum_{K=0}^{n} \emptyset_k$$

If all the $\emptyset_k$'s are positive as in the problem in this thesis, then a value of μ is chosen from one of the Θ_k's by choosing a random number, R, and letting $\mu = \Theta_j$ if

$$\sum_{K=0}^{j-1} \emptyset_k < R \leq \sum_{K=0}^{j} \emptyset_k \tag{12}$$

If any of the $\emptyset_k$'s are negative, the selection technique must be modified.

The orthogonality relation is derived by first considering the equation

$$I = (2L+1) P_L(\mu') P_L(\mu) (\mu' - \mu) \tag{13a}$$

$$= (2L+1) [P_L(\mu) \mu' P_L(\mu') - P_L(\mu') \mu P_L(\mu)] \tag{13b}$$

Use is now made of the recursion relation

$$\mu' P_L(\mu') = \frac{1}{2L+1}\{(L-1)P_{L+1}(\mu') + L\,P_{L-1}(\mu')\} \qquad (14)$$

The expression in Equation 13b can be rewritten using Equation 14 for $\mu'\,P(\mu')$ and $\mu\,P(\mu')$.

$$I = P_L(\mu)[(L+1)P_{L+1}(\mu') + L\,P_{L-1}(\mu')]$$

$$+ P_L(\mu)[(L+1)P_{L+1}(\mu) + L\,P_{L-1}(\mu)] \qquad (15)$$

Factor and rearrange the terms having coefficients $(L+1)$ and L.

$$I = (L+1)[P_{L+1}(\mu')P_L(\mu) - P_L(\mu')P_{L+1}(\mu)]$$

$$- L[P_L(\mu')P_{L-1}(\mu) - P_{L-1}(\mu')P_L(\mu)] \qquad (16)$$

$$= j_L(\mu',\mu) - j_{L-1}(\mu',\mu) \qquad (17)$$

where

$$j_L(\mu'-\mu) = L+1[P_{L+1}(\mu')P_L(\mu) - P_L(\mu')P_{L+1}(\mu)] \qquad (18)$$

using Equation 13a and 17, one obtains

$$(\mu'-\mu)(2L+1)P_L(\mu')P_L(\mu) = j_L(\mu',\mu) - j_{L-1}(\mu',\mu) \qquad (19)$$

Sum over all L from 1 to n.

$$(\mu'-\mu)\sum_{n=1}^{n}(2L+1)P_L(\mu')P_L(\mu) = \sum_{L=1}^{n} j_L(\mu'-\mu) - j_{L-1}(\mu',\mu)$$

$$(20)$$

$$= \sum_{L=1}^{n} j_L(\mu', \mu) - \sum_{L=0}^{n-1} j_L(\mu', \mu) \qquad (21)$$

$$= j_n(\mu', \mu) - (\mu' - \mu) \qquad (22)$$

Hence, taking $(\mu'-\mu)$ to the left side and summing from L=0 to n one gets

$$(\mu' - \mu) = \sum_{L=0}^{n} (2L+1) P_L(\mu') P_L(\mu) = j_n(\mu', \mu) \qquad (23)$$

or using the definition of $j_n(\mu', \mu)$

$$\sum_{L=0}^{n} (2L+1) P_L(\mu') P_L(\mu) = n+1\left[\frac{P_{n+1}(\mu')P_n(\mu) - P_n(\mu')P_{n+1}(\mu)}{\mu' - \mu}\right] \qquad (24)$$

which is the orthogonality relationship in Equation 9.

The Coveyou technique requires that the Legendre coefficients, f_L, be carried on the master cross section tape.

These coefficients are calculated by the program LEGENDRE which was written by D. C. Irving, W. E. Kinney, and P. Rea (17) of Oak Ridge. This program is not included in the O5R package, however, the cross section library used in the solution of O5R contained the values of f_L calculated by LEGENDRE for a fourteen term expansion. The program LEGENDRE uses an angular distribution at equally spaced values, from -1 to +1, of the cosine of scattering for the calculation of the f_L's.

XI. APPENDIX B

A Simplified Flow Chart of the Monte Carlo Operation

Figure 3 contains a simplified flow chart showing the major operations and decisions involved in the operation of the O5R code. A more detailed flow diagram is contained in the operation manual for the O5R (28).

Some of the abbreviations used in the chart are listed below:

STRT	Start of the run
N	Integer identifying the neutron
BNDRY	Medium boundary
WT	The weight of the neutron N
VEL	The velocity of neutron N
EGRP	The energy group being processed
NMAX	The maximum number of neutrons in a batch
Dist.	Distance in cm
FWATE	Fission weight of neutron N after a collision
FTOTAL	Accumulated fission weight of neutron N
ECUT	Lowest energy in the slowing down process
STORE	Instruction meaning to store neutron data in computer memory or on tape
BANK	Instruction meaning to store neutron data on tape for input in the next batch

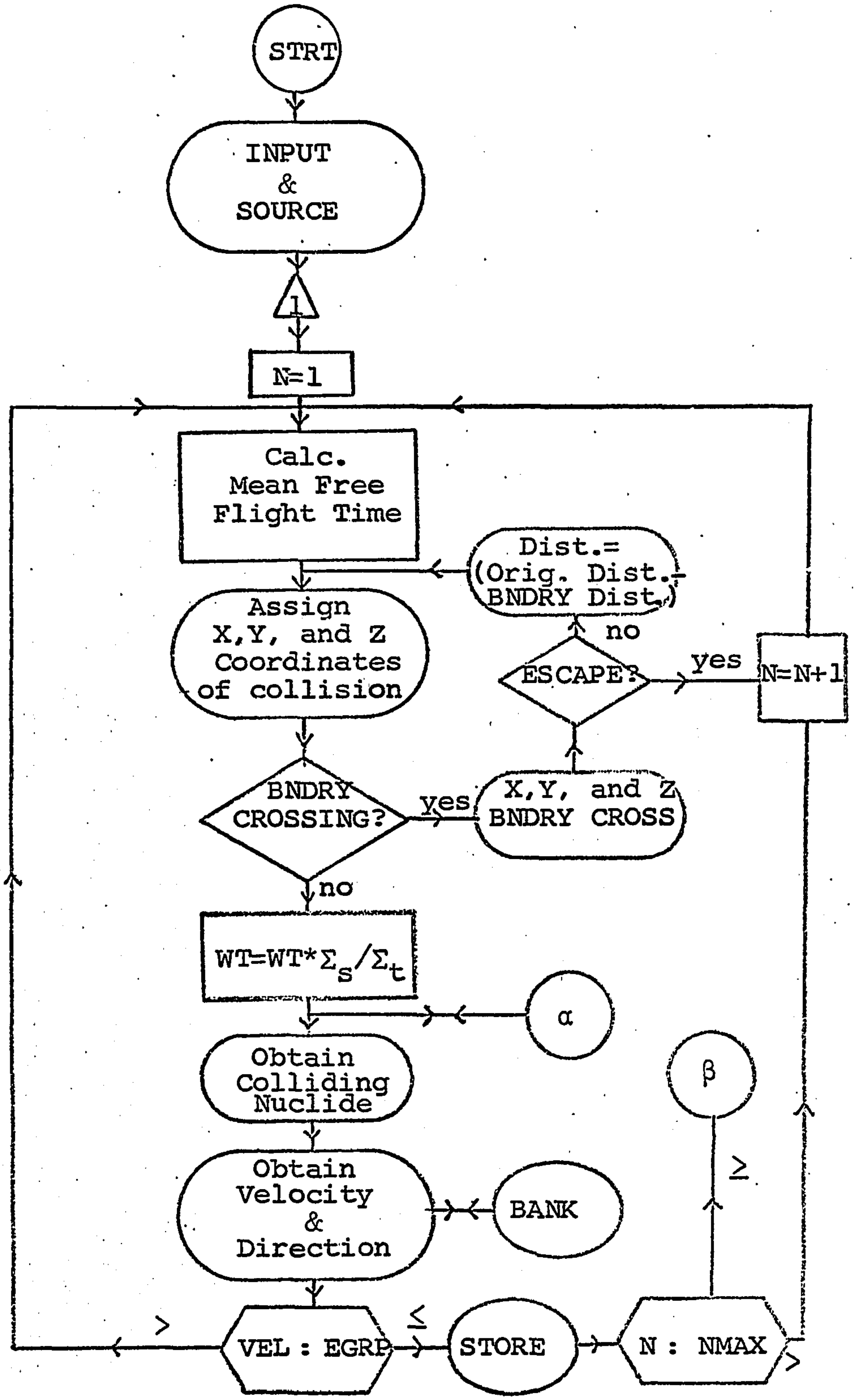

Figure 4. O5R flow chart

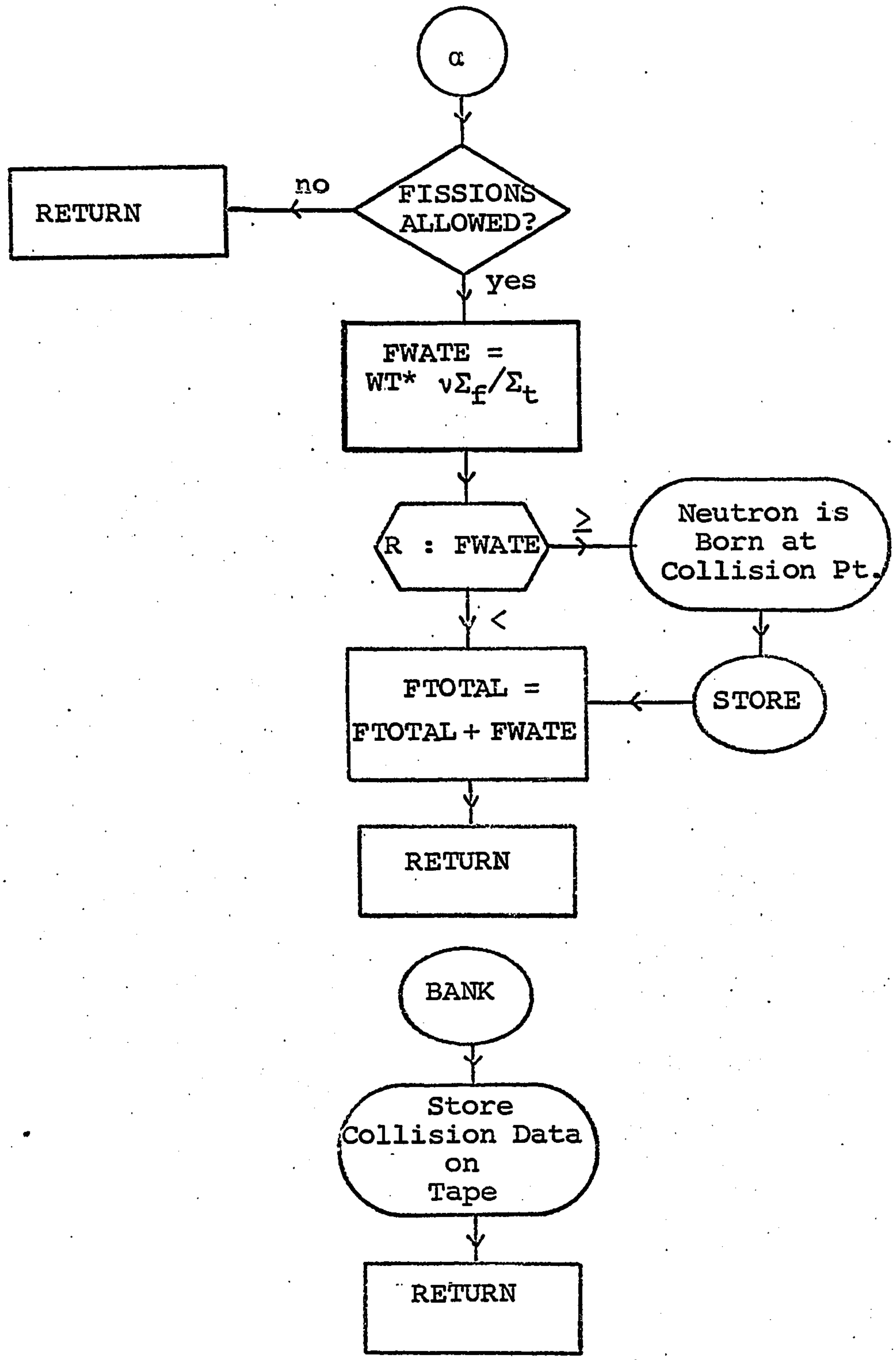

Figure 4 (Continued)

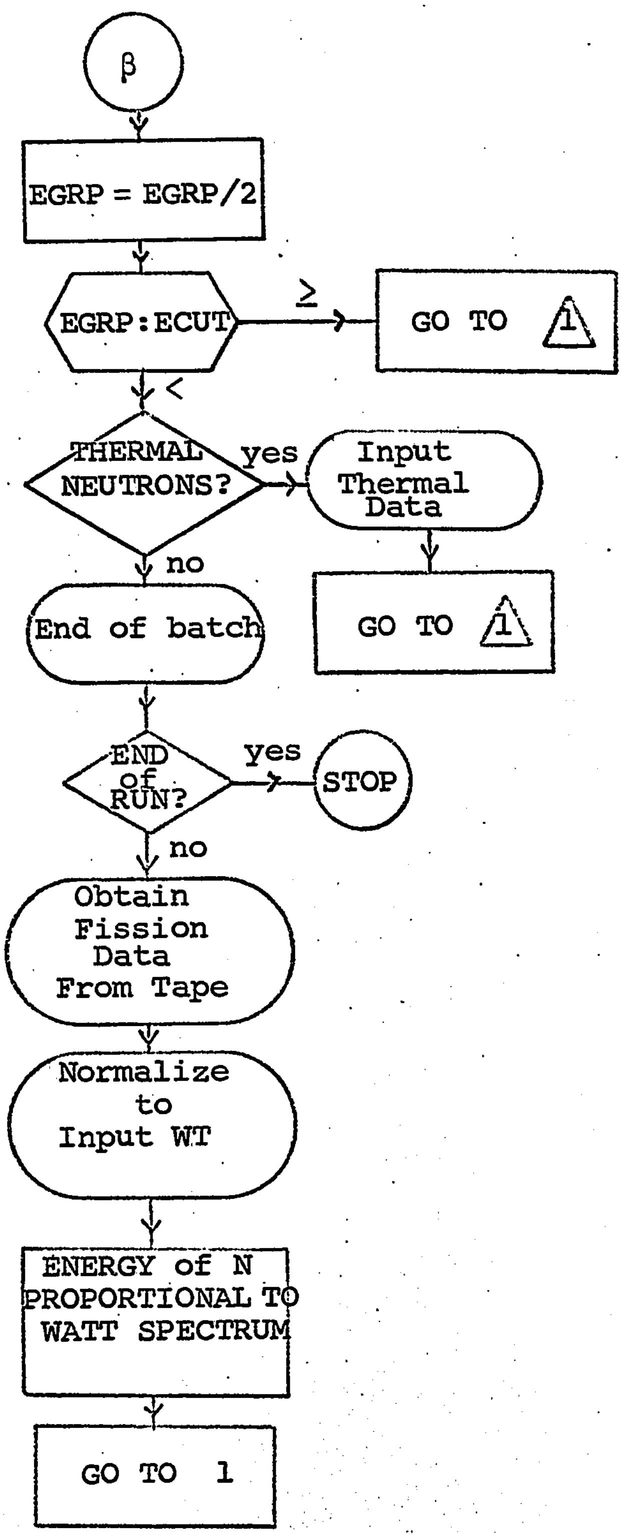

Figure 4 (Continued)