(Y F10-66)

AECD-4060

DATE: August 20, 1951
SUBJECT: NUMERICAL TECHNIQUE FOR CRITICALITY CALCULATIONS ON
HYDROGEN MODERATED REACTORS.
TO: Listed Distribution
FROM: J. W. Webster

This report was prepared as a scientific account of Government-sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately-owned rights. The Commission assumes no liability with respect to the use of, or from damages resulting from the use of, any information, apparatus, method, or process disclosed in this report.

Photostat Price \$ 3.30
Microfilm Price \$ 2.40

Available from the
Office of Technical Services
Department of Commerce
Washington 25, D. C.

ANP PHYSICS GROUP
OAK RIDGE NATIONAL LABORATORY
Y-12 Area
Operated by
CARBIDE AND CARBON CHEMICALS COMPANY
A DIVISION OF UNION CARBIDE AND CARBON CORPORATION
Oak Ridge, Tennessee

Contract No. W-7405-eng-26

NUMERICAL TECHNIQUE FOR CRITICALITY CALCULATIONS
ON HYDROGEN MODERATED REACTORS

J. W. Webster

The purpose of this memo is to set down a derivation and numerical technique for a method that can be used for criticality calculations on bare reactors containing hydrogen together with another moderator such as BeO.

The method and notation are that of G. Goertzel (NDA)¹, and D. Selengut (NEPA). In the interest of the computers, the numerical technique², associated notation, and calculation form are modeled after that currently used by the ANP Physics Group for BeO moderated reactors.

¹ G. Goertzel, "CRITICALITY OF HYDROGEN MODERATED REACTORS", TAB-53, 25 July 1950.

² M. J. Nielsen, "BARE PILE ADJOINT SOLUTION", Y-F10-18, pp. 4, 5, 6, 27 October 1950.

The Method

For reactors containing hydrogen and other moderators, a balance equation can be written between the number of neutrons leaving an energy interval E to $E+dE$, above thermal energy, per cubic centimeter, and the number entering as follows:

$$\begin{aligned} & \sigma_{SH}(E) \phi(E) dE + \sigma_a(E) \phi(E) dE + D(E) B^2(E) \phi(E) dE + E \int_0^E \sigma_T(E') \phi(E') dE' \\ & = (E+dE) \int_E^{10^7} \sigma_T(E+dE) \phi(E+dE) + dE \int_E^{10^7} \phi(E') \sigma_{SH}(E') \frac{dE'}{E'} \\ & + \nu_c f(E) dE \left[\int_0^{E_{th}} \sigma_f(E') \phi(E') dE' + \phi_{th} \sigma_{f_{th}} \right] \end{aligned} \quad (1)$$

where the spatial component has been separated out:

For the thermal group the corresponding equation is

$$\sigma_{a_{th}} \phi_{th} + D_{th} B^2 \phi_{th} = E_{th} \int_{E_{th}}^{10^7} \sigma_{T_{th}} \phi(E_{th}) + E_{th} \int_{E_{th}}^{10^7} \phi(E') \sigma_{SH}(E') \frac{dE'}{E'} \quad (2)$$

In equation (1) and (2) the following definitions apply:

- $\sigma_{SH}(E)$ = macroscopic scattering cross-section for hydrogen at energy E .
- $\phi(E)$ = flux per unit energy.
- $\sigma_a(E)$ = macroscopic absorption cross-section for the complete pile mixture including hydrogen.
- $D(E)$ = diffusion constant based on the complete pile mixture including hydrogen.
- $B^2(E)$ = the buckling of the bare reactor, taken to be a function of energy since the extrapolation distance is a function of energy.

- $\sigma_T(E)$ = macroscopic total cross-section of the pile mixture not including hydrogen.
 ν_c = neutrons per fission to make the reactor critical.
 $r(E)$ = distribution function for the normalized fission spectrum.
 $\sigma_f(E)$ = macroscopic fission cross-section.
 ϕ_{th} = the thermal flux.
 $\phi(E_{th})$ = the flux per unit energy at (or just above) thermal energy.

The normalization is used that

$$\nu_c \left[\int_0^{E_{th}} \phi(E') \sigma_f(E') dE' + \phi_{th} \sigma_{f,th} \right] = \nu \quad (3)$$

when ν = actual number of neutrons per fission, i.e. 2.5. This normalization makes $\phi(E)$ the flux per unit energy resulting from 2.5 neutrons being released per second at fission energies in a cubic centimeter. It follows then that the first term on the left side of (1) is the number of neutrons degraded out of the energy interval dE , for one fission per second per cm^3 , by collision with hydrogen. The second term is the number of neutrons absorbed in any pile material including hydrogen having energy in the interval dE , for one fission per sec per cm^3 . Similarly, the third term is the leakage term with same normalization; the fourth gives the neutrons degraded out by collisions with materials other than hydrogen (assumed to take place on a continuous slowing down model). $E \int \sigma_T \phi$ has been found to be more accurate than the usual $E \int \sigma_s \phi$ when appreciable absorption is present. The first term on the right gives the neutrons that entered by continuous slowing down with materials other than hydrogen. As for the second term, since a neutron of energy, E' , which collides with hydrogen has an equal probability of emerging with any energy between 0 and E' , it follows that $\frac{dE}{E'-0}$ is the fraction that emerges with energy in the energy increment of interest, i.e. dE , and hence this probability times $\phi(E') \sigma_{SH} dE'$, the number of collisions with hydrogen

that take place in dE' , integrated over all energies above E gives the number of neutrons that enter dE due to hydrogen collision based as always on one fission per sec. per cm^3 . The last term on the right of (1) becomes the source density for neutrons in the energy range dE , if any, based on a total source of 2.5 neutrons per sec. per cc under the requirement (3).

The thermal equation follows in a similar manner. The neutron entries into the thermal group due to hydrogen collisions are those neutrons that have energy from 0 to E_{th} after collision and hence for neutrons of incident energy E' , the fraction that enter the thermal group is

$$\frac{E_{th}-0}{E'-0}.$$

Now if the change of variable is introduced that

$$u = \ln \frac{10^7}{E},$$

the relations follow that $\phi(E)dE = -\phi(u)du$, $E = 10^7 e^{-u}$, $\frac{du}{dE} = -\frac{1}{E}$ and equation (1) and (2) become

$$\begin{aligned} & -\sigma_{SH}(u) \phi(u) du - \sigma_a(u) \phi(u) du - D(u) B^2(u) \phi(u) du + \int \sigma_T(u) \phi(u) \\ & = + \int \sigma_T(u+du) \phi(u+du) - du e^{-u} \int_0^u \phi(u') \sigma_{SH}(u') e^{u'} du' - \nu f(u) du \end{aligned} \quad (1')$$

and

$$\sigma_{a_{th}} \phi_{th} + \phi_{th} B^2 \phi_{th} = \int \sigma_{T_{th}} \phi(u_{th}) + e^{-u_{th}} \int_0^{u_{th}} \phi(u') \sigma_{SH}(u') e^{u'} du' \quad (2')$$

and expanding $\phi(u+du)$ of the first term on the right side of (1') in two terms of a Taylor's series and subtracting the last term on the left, and dividing out $(-du)$, the result is:

$$\sigma_{SH}(u) \phi(u) + \sigma_a(u) \phi(u) + D(u) B^2(u) \phi(u) = -\frac{\partial [\int_u^\infty \sigma_T \phi(u') du']}{\partial u} + e^{-u} \int_0^u \phi(u') \sigma_{SH}(u') e^{u'} du' + \nu f(u) \quad (1'')$$

and

$$\sigma_{a_{th}} \phi_{th} + D_{th} B^2 \phi_{th} = \int \sigma_{T_{th}} \phi(u_{th}) + e^{-u_{th}} \int_0^{u_{th}} \phi(u') \sigma_{SH}(u') e^{u'} du' \quad (2'')$$

Now the definition is made that

$$\eta(u) = e^{-u} \int_0^u \phi(u') \sigma_{SH}(u') e^{u'} du' .$$

It is to be noted that $\eta(u)$ is the slowing down density at lethargy u due to neutron collisions with hydrogen at all higher energies. Also, the definition is made that

$$q(u) = \int \sigma_T \phi(u)$$

and recalling that σ_T was defined to not include hydrogen it follows that $q(u)$ is the continuous slowing down density at lethargy u due to collisions with materials other than hydrogen.

Upon the substitution of these definitions, equation (1'') and (2'') become

$$\left[\sigma_{SH}(u) + \sigma_a(u) + D(u) B^2(u) \right] \frac{q(u)}{\int \sigma_T \phi(u)} = -\frac{\partial}{\partial u} q(u) + \eta(u) + \nu f(u) \quad (1''')$$

and

$$(\sigma_{a_{th}} + D_{th} B^2) \phi_{th} = q(u_{th}) + \eta(u_{th}) \quad (2''')$$

If $q(u)$ can be determined as a function of lethargy, u , together with $q(u_{th})$ and $\eta(u_{th})$, then the k_{eff} and hence the criticality can be determined from the condition (3), i.e.

$$\int_0^{u_{th}} \frac{\sigma_f(u')}{\int \sigma_T(u')} q(u') du' + \left\{ \frac{\eta(u_{th}) + q(u_{th}) \sigma_{fth}}{\sigma_{ath} + DB_{th}^2} \right\} = \frac{\lambda}{2c} = k_{eff}.$$

When the uranium weight or reactor size (depending upon which one is varied in seeking criticality) has been chosen by trial and error such that $k_{eff} = 1$, then the reactor is critical.

Numerical Technique

To solve for $q(u)$ as a function of u it is noted that $\eta(u)$ satisfies the simple first order differential equation

$$\frac{\partial \eta(u)}{\partial u} + \eta(u) = \phi(u) \sigma_{SH} = \frac{\sigma_{SH} q(u)}{\int \sigma_T} \quad (1''_2)$$

This, coupled with equation (1''') which is now rewritten as (1'''), form two coupled first order differential equations

$$\left[\sigma_{SH}(u) + \sigma_a(u) + D(u) B^2(u) \right] \frac{q(u)}{\int \sigma_T(u)} = - \frac{\partial}{\partial u} q(u) + \eta(u) + \nu f(u). \quad (1''_1)$$

The lethargy scale is divided into intervals, each interval having a particular width U_N with limits U_{n-1} and U_n . Equation (1''') and (1''') are integrated over an interval

$$\begin{aligned} & \int_{U_{n-1}}^{U_n} \left\{ \sigma_{SH}(u) + \sigma_a(u) + D(u) B^2(u) \right\} \frac{q(u)}{\int \sigma_T(u)} du \\ &= \int_{U_{n-1}}^{U_n} - \frac{\partial}{\partial u} q(u) du + \int_{U_{n-1}}^{U_n} \eta(u) du + \int_{U_{n-1}}^{U_n} \nu f(u) du \end{aligned}$$

and

$$\int_{U_{n-1}}^{U_n} \frac{d}{du} \eta(u) du + \int_{U_{n-1}}^{U_n} \eta(u) du = \int_{U_{n-1}}^{U_n} \frac{\sigma_{SH} q(u)}{\sqrt{\sigma_T}} du.$$

Using the approximation:

$$\int_{U_N} A B du = \bar{A} \bar{B} U_N$$

These equations become:

$$\left(\frac{\sigma_{SH} + \sigma_a + DB^2}{\sqrt{\sigma_T}} \right)_N \bar{q}_N U_N = -q_n + q_{n-1} + \bar{\eta}_N U_N + \nu z_N$$

and

$$\eta_n - \eta_{n-1} + \bar{\eta}_N U_N = \left(\frac{\sigma_{SH}}{\sqrt{\sigma_T}} \right)_N \bar{q}_N U_N$$

where

$$z_N = \int_{U_{n-1}}^{U_n} f(u) du.$$

Now the approximations and definitions are made that

$$\frac{q_{n-1} + q_n}{2} = \bar{q}_N \quad (4)$$

$$\frac{\eta_{n-1} + \eta_n}{2} = \bar{\eta}_N$$

$$\left(\frac{\sigma_a + DB^2}{\sqrt{\sigma_T}} \right)_N \frac{U_N}{2} = C_N$$

$$\left(\frac{\overline{\sigma}_{SH}}{\overline{\sigma}_T} \right) \frac{U_N}{2} = H_N.$$

Substituting these expressions, the two equations can be put in the form:

$$\begin{aligned} q_n \left\{ H_N + C_N + 1 \right\} - \frac{U_N}{2} \eta_n &= \nu Z_N - q_{n-1} \left\{ H_N + C_N - 1 \right\} + \frac{U_N}{2} \eta_{n-1}, \\ q_n \left\{ H_N \right\} - \left(1 + \frac{U_N}{2} \right) \eta_n &= -H_N q_{n-1} - \left(1 - \frac{U_N}{2} \right) \eta_{n-1} \dots \end{aligned} \quad (5)$$

Eliminating η_n between these the recursion relation is obtained that

$$q_n = \frac{\nu Z_N \left(1 + \frac{U_N}{2} \right) + q_{n-1} - H_N - C_N \left(1 + \frac{U_N}{2} \right) + \left(1 + \frac{U_N}{2} \right) + U_N \eta_{n-1}}{H_N + \left(1 + \frac{U_N}{2} \right) C_N + \left(\frac{U_N}{2} + 1 \right)}.$$

Knowing q_n from this equation the η_n , needed to obtain q_{n+1} , can be obtained from the equation

$$\eta_n = \frac{2H_N}{1 + \frac{U_N}{2}} q_n + \frac{1 - \frac{U_N}{2}}{1 + \frac{U_N}{2}} \eta_{n-1}$$

which is a rearrangement of equation (5) with the substitution of (4).

To get started on the successive solution the first lethargy interval is taken above the fission spectrum so that

$$\eta_0 = q_0 = 0,$$

and thus

$$q_1 = \frac{\nu Z_1 \left(1 + \frac{U_1}{2} \right)}{H_1 + \left(1 + \frac{U_1}{2} \right) C_1 + \left(\frac{U_1}{2} + 1 \right)},$$

and

$$\eta_1 = \frac{H_1}{1 + \frac{U_1}{2}} q_1 ,$$

from which q_2 and η_2 can be obtained, etc. The test for criticality is then that

$$\sum_N \bar{q}_N \left(\frac{\sigma_f}{\sigma_T} \right)_N + \frac{(q_{th-1} + \eta_{th-1})}{(\sigma_a + \Sigma_{th}^2)} \sigma_{f_{th}} = 1 .$$

The attached sheet shows a sample calculation form that can be used by computers to successively solve the recursion relations, to determine the k_{eff} , and the energy distribution of the flux.

BARE REACTOR CALCULATION (HYDROGEN PRESENT)

CODE _____

GROUP NUMBER	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX	XXI	XXII	XXIII	XXIV	XXV	XXVI	XXVII	VOL FRACTION			
							H_n	$-H_n$ $C_n(1+\frac{U_n}{2})$	H_n $C_n(1+\frac{U_n}{2})$			$(1+\frac{U_n}{2}) \frac{XII}{X}$ $+ C_{n+1} \frac{XII}{X}$	$\frac{XII}{X}$	$\frac{C_{n+1} + C_n}{2}$	$\frac{C_n}{2} \frac{XIII}{X}$ $+ C_{n+1} \frac{XIII}{X}$	$\frac{C_{n+1} + C_n}{2}$	$\frac{C_{n+1} + C_n}{2}$	$2X \frac{XIX}{XII}$	$\frac{C_{n+1} + C_n}{2} \frac{I}{(1+X) \frac{XII}{X}}$	$2X \frac{XIX}{XII}$	$\frac{C_{n+1} + C_n}{2} \frac{II}{(1+X) \frac{XII}{X}}$	$2X \frac{XIX}{XII}$	$\frac{XIII}{XII} + \frac{XIII}{XII}$ $+ \frac{XIII}{XII} + \frac{XIII}{XII}$	$\frac{C_{n+1} + C_n}{2}$ $+ \frac{C_{n+1} + C_n}{2}$	$\frac{XIII}{XII}$	$\frac{XIII}{XII}$	$\frac{XIII}{XII}$				
A	$\frac{H_n}{C_n(1+\frac{U_n}{2})}$	$(\frac{H_n}{C_n(1+\frac{U_n}{2})})^2$	$(\frac{H_n}{C_n(1+\frac{U_n}{2})})^3$	U_{n+2}	$\frac{1-U_n}{1+U_n}$	C_n	$\frac{C_n}{U_{n+1}}$	$\frac{C_n}{1+U_n}$	$(1+\frac{U_n}{2})$	$(1+\frac{U_n}{2})$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$	$\frac{XII}{X}$				
0																															
1				.25							.0525																				
2				.25							.2500																				
3				.25							.5175																				
4				.25							.5775																				
5				.25							.4575																				
6				.25							.2925																				
7				.25							.1675																				
8				.25							.0875																				
9				1.50							.0875																				
10				1.50							0																				
11				.70							0																				
12				.60							0																				
13				.40							0																				
14				.20							0																				
15				.40							0																				
16				.60							0																				
17				.20							0																				
18				.20							0																				
19				.20							0																				
20				.20							0																				
21				.10							0																				
22				.10							0																				
23				.10							0																				
24				.10							0																				
25				.10							0																				
Thermal(18)				1.00							0																				
26				.10							0																				
Thermal(18)				1.00							0																				
27				.10							0																				
28				.10							0																				
29				.10							0																				
30				.10							0																				
31				.10							0																				
Thermal(18)				1.00							0																				
																SUMS (18.4)															
																SUMS (18.5)															
																SUMS (18.6)															
																SUMS (18.7)															
																SUMS (18.8)															
																SUMS (18.9)															
																SUMS (19.0)															
																SUMS (19.1)															
																SUMS (19.2)															
																SUMS (19.3)															
																SUMS (19.4)															
																SUMS (19.5)															
																SUMS (19.6)															
																SUMS (19.7)															
																SUMS (19.8)															
																SUMS (19.9)															
																SUMS (20.0)															
																SUMS (20.1)															
																SUMS (20.2)															
																SUMS (20.3)															
																SUMS (20.4)															
																SUMS (20.5)															
																SUMS (20.6)															
																SUMS (20.7)															
																SUMS (20.8)															
																SUMS (20.9)															
																SUMS (21.0)															
																SUMS (21.1)															
																SUMS (21.2)															
																SUMS (21.3)															
																SUMS (21.4)															
																SUMS (21.5)															
																SUMS (21.6)															
																SUMS (21.7)															
																SUMS (21.8)															
																SUMS (21.9)															
																SUMS (22.0)															
																SUMS (22.1)															
																SUMS (22.2)															
																SUMS (22.3)															
																SUMS (22.4)															
																SUMS (22.5)															
																SUMS (22.6)															
																SUMS (22.7)															
																SUMS (22.8)															
																SUMS (22.9)															
																SUMS (23.0)															
																SUMS (23.1)															
																SUMS (23.2)															
																SUMS (23.3)															
																SUMS (23.4)															
																SUMS (23.5)															
																SUMS (23.6)															
																SUMS (23.7)															
																SUMS (23.8)															
																SUMS (23.9)															
																SUMS (24.0)															
																SUMS (24.1)															
																SUMS (24.2)															
																SUMS (24.3)															
																SUMS (24.4)															
																SUMS (24.5)															
																SUMS (24.6)															
																SUMS (24.7)															
																SUMS (24.8)															
																SUMS (24.9)															
																SUMS (25.0)															
																SUMS (25.1)															
																SUMS (25.2)															
																SUMS (25.3)															
																SUMS (25.4)															
																SUMS (25.5)															
																SUMS (25.6)															
																SUMS (25.7)															
																SUMS (25.8)															
																SUMS (25.9)															
																SUMS (26.0)															
																SUMS (26.1)															
																SUMS (26.2)															
																SUMS (26.3)															
																SUMS (26.4)															

RECEIVED 10 MAR 1963

RECEIVED 10 MAR 1963

934 11