1964

Shim control of heavy-water moderated power reactors by removal of light-water poison

Charles White Sayles
Iowa State University

Recommended Citation

Sayles, Charles White, "Shim control of heavy-water moderated power reactors by removal of light-water poison " (1964). *Retrospective Theses and Dissertations*. 3007.
https://lib.dr.iastate.edu/rtd/3007

SAYLES, Charles White, 1937–
SHIM CONTROL OF HEAVY-WATER MODERATED
POWER REACTORS BY REMOVAL OF LIGHT-
WATER POISON.

Iowa State University of Science and Technology
Ph.D., 1964
Engineering, chemical

University Microfilms, Inc., Ann Arbor, Michigan

SHIM CONTROL OF HEAVY-WATER MODERATED POWER REACTORS BY REMOVAL OF LIGHT-WATER POISON

by

Charles White Sayles

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:

In Charge of Major Work

Head of Major Department

Dean of Graduate College

Iowa State University
Of Science and Technology
Ames, Iowa

1964

TABLE OF CONTENTS

I. INTRODUCTION

The progress of heavy-water reactor development can be traced along two lines, the development of heavy water and then the development of nuclear reactors.

A knowledge of the existence of heavy water dates back to 1932, when Urey and his co-workers (27) discovered deuterium by fractional distillation of liquid hydrogen. At first deuterium (heavy hydrogen) and D_2O (heavy water) were scientific curiosities and were used by researchers as tracers in biochemistry and in the study of the properties of the isotopes. This interest created a demand for small quantities of this material, which was then produced commercially as a by-product in the electrolytic production of hydrogen and oxygen.

In 1940, interest in heavy water for nuclear reactors caused research and development work to be started on the large scale production of heavy water. As a result of this work, several plants for the production of heavy water by distillation were built. Because these plants were expensive to operate and because the main emphasis in reactor development then was with graphite reactors, these distillation plants were shut down at the end of the war.

In 1949, renewed interest in heavy water caused the Atomic Energy Commission to start research on alternate methods of heavy-water production. This work led to a gas-liquid exchange process for the separation of deuterium from ordinary hydrogen.

The basic element of the gas-liquid exchange process is a pair of contacting towers (4). One tower operates at a temperature of 30° to 40°C.

Water passes downward through first the cold tower and then downward through the hot tower and is contacted with H_2S (hydrogen sulfide) gas. This gas-liquid exchange process gives a better separation than does distillation, and for low concentrations of deuterium it is more economical.

In 1950, the AEC ordered the construction of new facilities for the production of heavy water. These new facilities used gas-liquid exchange process for enriching the D_2O content from 0.015 mol per cent in natural water to 10 to 15 mol per cent. This water was further enriched in a distillation system until the D_2O concentration was 93 to 96 mol per cent. Final enrichment was obtained by electrolysis. Two of these new facilities were built primarily to provide heavy water for the plutonium production reactors built and operated for the AEC by the duPont Company at Savannah River, South Carolina. One was at Savannah River and the other at Dana, Indiana. The Savannah River Plant is still in operation. The Dana Plant, which was built by remodeling one of the World War II plants, was shut down because it was less efficient.

From the earliest days of nuclear reactor development it was realized that there were advantages in the use of heavy water as a neutron moderator (38). The deuterium of heavy water is second only to hydrogen in its ability to moderate neutrons, and its capture cross section is considerably less. Although it was the superior moderator it was available in only limited amounts and for this reason the main emphasis of early reactor development was placed on graphite reactors.

A few experimental reactors were built using heavy water as a moderator. The first of these, CP-3, was built at the Argonne Laboratory and went critical on May 15, 1944 (36). Other experimental reactors built were the Norwegian-Dutch (JEEP), the Canadian NRX and ZEEP reactors, and the French ZOE (19). All of these reactors used natural uranium fuel and further demonstrated the use of heavy water as a moderator.

When the additional plutonium production reactors were built in the early 1950's, they were reactors which used heavy water as a moderator.

The use of heavy-water reactors for the production of electrical power has received considerable attention. The advantage of heavy-water moderated power reactors is the fact that they can be used with natural or slightly enriched uranium fuel. In the United States several companies are working on the development of heavy-water moderated power reactors. The only heavy-water moderated power reactor in the United States is the Carolina Virginia Tube Reactor (7) located at Parr Shoals, South Carolina. This reactor, designed by Westinghouse's Atomic Power Division for the Carolina Virginia Nuclear Power Associates, uses fuel enriched in uranium-235 to 1.5% and 2.0% and produces 17 electrical megawatts (8).

An extensive study of heavy water moderated and cooled power reactors has been conducted by duPont (2). This work has been directed toward finding the optimized concept from a wide range of heavy-water moderated natural uranium fueled reactor designs. Others doing work in the United States on heavy-water power reactors are Atomics International and Nuclear Development Corporation.

In Canada there are two heavy-water reactors for power production. These are the NPD-2 and the CANDU (2).

Although heavy water reactors do offer the advantage of the use of natural uranium fuel, their development in the United States has lagged that of light-water reactors which must use enriched fuel. The reason for this lag of heavy-water moderated power reactors has been the availability of the enriched uranium fuels and the expense of the heavy-water. From the start of the power reactor development, enriched uranium has been available, and the first power reactors built used this enriched fuel. Because of the experience with these early light-water moderated power reactors, improvements have resulted, and today these reactors can be built in the United States more economically than any other reactors. Thus for any other reactor system to become competitive within this country, the costs associated with that reactor type must be reduced.

Outside the United States where enriched uranium fuels are not readily available there is a greater incentive for the use of natural uranium. In these countries, heavy-water moderated power reactors are becoming competitive.

It is the purpose of this thesis to investigate the possibilities of shim control of heavy-water moderated power reactors by removal of a light-water poison and to ascertain whether or not this method of shim control can result in a decrease in net power costs.

II. REVIEW OF LITERATURE

There are three kinds of control needed for thermal nuclear reactors. These are shut-down control, regulating control, and shim control.

Shut-down control is the method that is used only to stop the nuclear chain reaction within the reactor. For most nuclear power reactors shut-down control is achieved by safety rods. These are rods containing a material with a very high neutron capture cross section. Upon insertion of these rods within the reactor, the effective multiplication factor, k_{eff}, is reduced to a value below 1.0000 and the neutron level decreases. Frequently nuclear reactors have a back up emergency shut-down control for scramming the reactor in the event of some malfunction. This could be the dumping of the reactor moderator or the insertion of additional poison.

Regulating control of a nuclear reactor is the control that is used to change the power level of a reactor and keep it operating at some power level. The amount of excess reactivity contained within the regulating control is very small. This prevents sudden changes in reactivity that would cause the reactor to become prompt critical. Regulating control is achieved by means of a regulating rod.

Shim control of a nuclear reactor is that control used to adjust the effects of long term reactivity changes within the reactor. These reactivity changes come from the gradual increase of fission products and changes in the isotopic concentration of fissionable materials. These changes in reactivity are more than can be controlled by the regulating rods, and shim control is provided. In most reactors shim control is provided by means of shim rods which contain a neutron poison material. As fission products build up within the reactor and the number of fissionable isotopes decreases the shim rods are slowly withdrawn so the reactor remains just critical.

In power reactors shim rods must be replaced at regular intervals, frequently at the end of each fuel cycle. The reason for this is that the poison isotope within the shim rod has been depleted, and the shim rod can not provide the amount of control that is necessary.

Because of the frequency that a large number of expensive shim rods must be replaced, an alternate method of shim control could prove advantageous.

For some heavy-water reactors that have been proposed (33) twenty-five shim rods are specified. The cost of these shim rods in 1959 was $24,100 per rod (34). Thus any method which can be used for shim control that does not require shim rods is worthy of investigation.

This thesis proposes that the shim control be attained by poisoning the heavy-water moderator and coolant with a variable amount of light-water. The control would be obtained by removing the light-water from the heavy water with a distillation system. This system would be similar to the one used to maintain the required heavy-water concentration in a heavy-water moderated power reactor.

The advantages of this system are several. First, the expensive shim rods would not have to be replaced at the end of each fuel cycle. Secondly, the presence of shim control rods cause the flux distribution to be disturbed throughout the reactor resulting in a higher maximum to average flux ratio. The lower maximum-to-average flux ratio obtained by removal of light-water poison allows a higher burnup of the fuel. This means a longer fuel cycle and a better utilization of the fuel.

The disadvantages of this system are a larger distillation unit, a larger heavy water inventory, and a lower conversion ratio. A larger distillation unit is needed because more light water must be removed. Normally the only light water that is to be removed is the light water that has leaked into the heavy water system. But with this system of control much more light water is needed for control than would leak into the heavy water. The removal of the greater amount of light water requires a larger distillation system.

Since the distillation does not completely separate the light water, but only gives a mixture with a higher light water concentration than is in the reactor system, a large amount of heavy water is removed with the light water.

The lower conversion ratio of fertile atoms to fissionable atoms comes from a higher resonance escape probability. This conversion ratio is a measure of the amount of plutonium formed, and since fewer neutrons are captured in the U-238 resonances, fewer atoms of the plutonium isotopes are formed. The effect of this is a slight reduction in the long term reactivity, and a smaller amount of plutonium produced.

Other methods of shim control that do not use control rods have been proposed. The most notable are the spectral shift, a burnable poison, a soluble poison, and the control by variation of the moderator level.

The spectral shift concept has been developed by Babcock and Wilcox Company (39). With this method of shim control, reactivity is gained by the addition of light water to the moderator that has an initial D_2O concentration of approximately 80 per cent. The lattice of a spectral shift reactor is under moderated. Therefore the addition of light water, which has a greater slowing down poer, causes an increase in reactivity. This comes from a downward shift of the neutron energy spectrum. The current spectral shift reactors are designed for an enrighment of 4% U235. At this enrichment of U235, there is no initial increase in reactivity due to the increase of plutonium so that the shim control is obtained by only the addition of light water. At the end of the fuel cycle enough light water has been added to reduce the heavy water concentration to approximately 20 per cent. (Actually the spectral shift reactor core is more nearly that of a light-water reactor than it is to a heavy-water reactor.) There is no on-site distillation unit associated with a spectral shift reactor. The heavy water that is removed is sent off-site for upgrading to the initial D_2O concentration. The light water that leaks into the reactor is not a problem since light water is being added at all times.

The advantage of shim control by the removal of a light-water poison is that natural uranium fuel can be used.

When a burnable poison is used for shim control a material of high neutron cross section is placed within the reactor fuel. The reactivity is gained for shim control by the gradual depletion of this neutron poison. The main disadvantage of this method is its inflexibility. This method can control only a decreasing reactivity. As with the spectral shift concept, this method can only be used with reactor that are least least slightly enriched with U-235. Because of the initial increase in reactivity with natural uranium this method can not be used. Also there is no outside control of the reactivity added by removal of the poison. Frequently when this method is used, it serves to decrease the initial reactivity to a value that can be controlled by shim rods.

When a soluble poison is used for shim control it is added to the liquid coolant or moderator. It has the advantage over a burnable poison, in that it can be added at any time during the fuel cycle. And by some means, such as ion exchange or other chemical techniques, can be removed from the reactor system. The disadvantages of this method are the changes it makes in the nature of the coolant or moderator. The addition of a soluble neutron poison to the coolant or moderator may make it more corrosive, and it is more difficult to maintain the purity of the liquid. Corrosion is frequently controlled by adjusting the liquid to a proper pH value. The pH value that is optimum for corrosion control may not be the one that is optimum for maintaining the solubility of the neutron poison. The soluble neutron poison may make it difficult to maintain the purity of the coolant or moderator more difficult, because methods used to remove the undesired impurities may also remove the soluble poison.

The advantage of light water as a neutron poison over some soluble poison is that light water is completely compatible with heavy water.

The Canadians are using moderator level control for two of their heavy-water reactors, the NPD and the CANDU. By adjusting the level of the moderator the leakage of neutron from the reactor is changed. An increase in moderator level decreases the leakage and causes the reactivity to increase. Although this method does not require the control rods of the normal heavy-water reactor, it does not produce a uniform vertical flux distribution and the optimum maximum-to-average flux for the long term reactivity considerations.

When the methods of burnable poison, soluble poison, and moderator level adjustment are used, the problem of leakage of light water into the reactor still exists and a method must be provided to maintain the D_2O concentration.

Klug and Zwiefel (28) have made a study of H_2O-D_2O reactors in hope of finding a reactor that could be controlled by adjusting the H_2O-D_2O mixture. They determined the infinite multiplication factor, k_∞, as a function of H_2O concentration for various metal-to-water ratios and for various fuel element diameters. It is their contention that if k reached a maximum value greater than 1.000 at some intermediate H_2O concentration, this could be used for reactor control. For natural uranium fuel they did not find such a k_∞ peak, but they did find one for a low enriched fuel.

When shim control is attained by light water removal it is not necessary to operate in a region where k_∞ has a peak value. It is only necessary that k_∞ vary as a function of light water concentration.

The work of the author has been to take a model of a heavy-water nuclear reactor and show that it can be shim controlled by light water removal. This is done by calculating the excess reactivity and its time variation with standard techniques. This time variation of the excess reactivity is related to a time dependent H_2O concentration and the reactor size and the distillation system and requirements and size are determined. A comparison is then made between shim control by removal of a light-water poison and shim control by control rods or some other means.

III. THE NUCLEAR REACTOR MODEL

To study this problem a reactor model was chosen to demonstrate the feasibility of shim control by removal of a light-water poison. It was desired to choose a model that would be representative of proposed heavy-water moderated power reactor and at the same time be simple enough to be described simply by analytical methods.

In keeping with the current trends in the size of proposed heavy-water moderated power reactors, the thermal output of the reactor was chosen as 1000 megawatts, and a 25% thermal efficiency gave an electrical output of 250 megawatts. These values are in agreement with those of heavy-water moderated power reactors studied by Sargent and Lundy Engineers (33) and duPont (2).

Although there are several heavy-water reactor types (2, 3) those that were studied by Sargent and Lundy and duPont were chosen because they are more nearly the size that would be used to produce economical power and also more information is available on them.

The team of Sargent and Lundy and duPont investigated four types of heavy-water moderated and cooled power reactors; a boiling D_2O reactor a direct cycle pressure tube reactor, a pressurized D_2O indirect cycle pressure vessel reactor, and a pressurized D_2O indirect cycle pressure tube reactor. Of these four types, the latter is chosen. This choice is arbitrary, but any result from this type of reactor could be considered as applicable for the others.

The fuel selected is natural uranium dioxide. The oxide is chosen over the metal because of the higher temperature that can be obtained with the oxide fuel. Based on values of fuel element pitch and number (2, 33) the size of this reactor could be determined. Thus the fuel elements are considered to be on an 11 inch triangular pitch, and the total number of fuel elements is 330. In the proposed reactors of Sargent and Lundy and duPont, the pitch is 11.1 inches and the number of fuel elements for their 200 electrical megawatt plant is 284 and for their 300 electrical megawatt plant it is 356.

A layout of an one-sixth segment of the reactor core is shown in Figure 1. The middle seven fuel elements have been removed. This removal reduces the number of fuel elements required and also reduces the maximum-to-average flux within the reactor.

This model of the reactor has a one foot radial and vertical reflector, which is the same as the reactors proposed by both Sargent and Lundy and duPont. The active core height for this reactor is 19.00 feet, the active diameter is 18.7 feet, and the total fuel loading is 76 metric tons of uranium.

The element is similar to the type of element in the proposed reactors of Sargent and Lundy and duPont. The fuel element is housed in a Zircalloy-2 pressure tube housing that has an inside diameter of 4.650 inches and a wall thickness of 0.162 inch. The fuel is in the form of 0.500 inch diameter fuel rods clad with 0.025 inch Zircalloy-2. There are 37 rods to a fuel element. These rods are spaced 0.652 inch center to center in a hexagonal array. A cross section of a fuel element is shown in Figure 2.

The coolant for this reactor is a mixture of D_2O and H_2O with the same composition as the moderator. The average operating temperature of

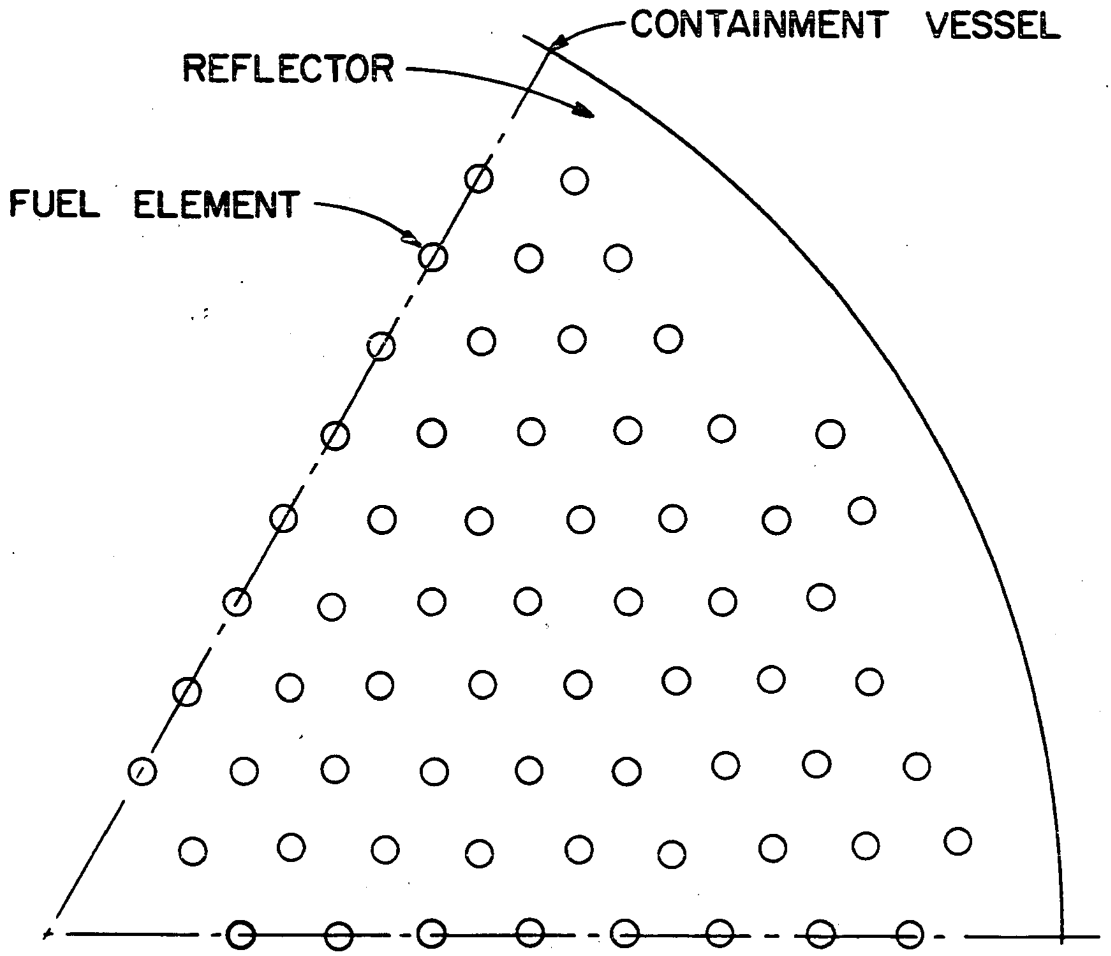

FIGURE 1. ONE-SIXTH SEGMENT OF REACTOR CORE.

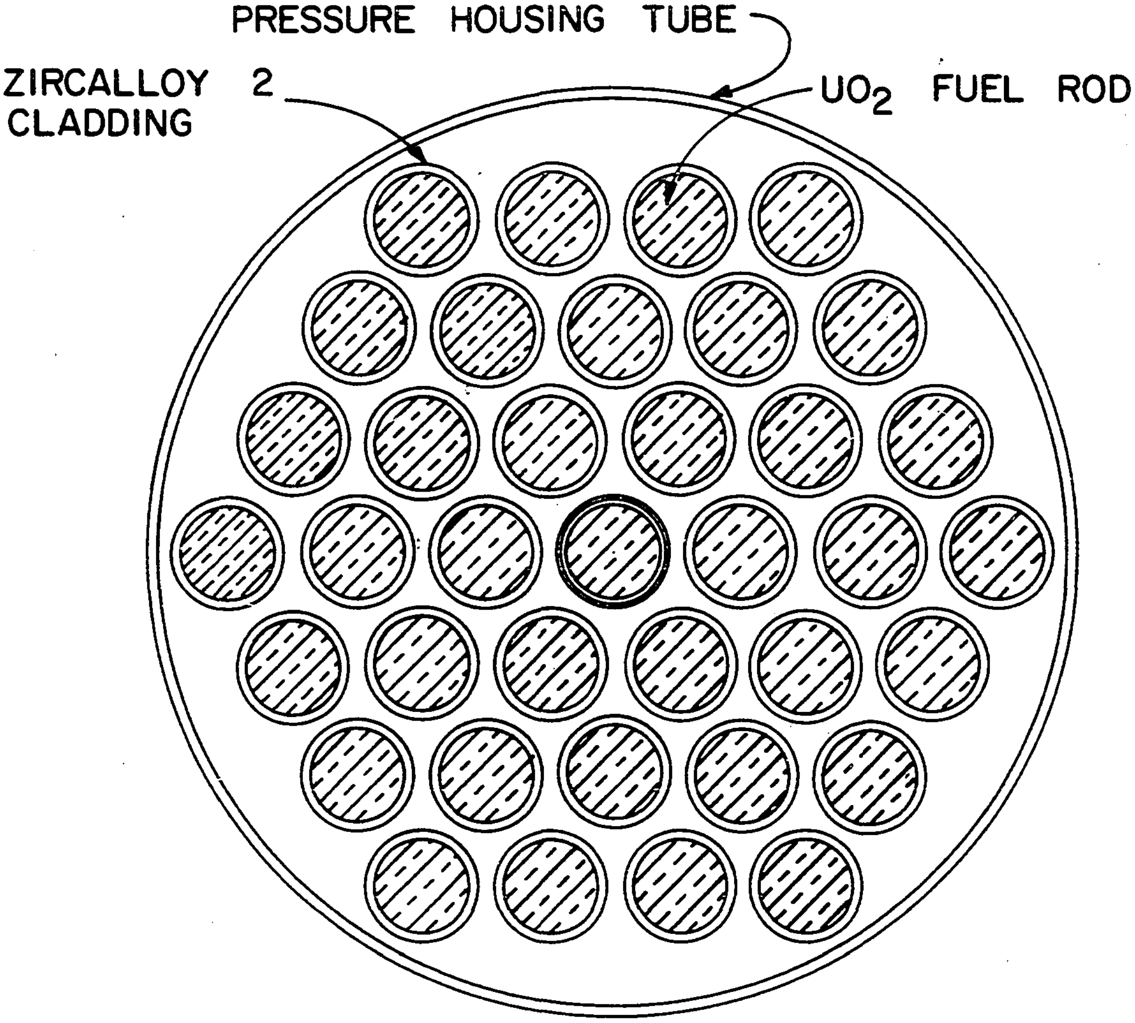

FIGURE 2. CROSS SECTION OF FUEL ELEMENT.

the coolant is 240°C (464°F). The average temperature of the moderator is 68°C (155°F), and the average temperature of the fuel is 927°C (1701°F).

The amount of moderator required for this reactor system is determined from an average of the values for the Sargent and Lundy reactor (33) plus the amount needed for the distillation. The average of 200 electrical megawatt and the 300 electrical megawatt reactors of Sargent and Lundy is 368.5 metric tons of moderator. The value is considered a minimum amount for the reactor and the steam generating facilities. An additional 412 metric tons of heavy water are required for the distillation scheme to be described later.

A summary of the characteristics of this reactor along with those of the reactor proposed by Sargent and Lundy are given in Table I.

Table 1. Summary of design data for various reactor power plants

Reactor	Reactor Model	200 Mw_e(33)	300 Mw_e(33)
Total thermal power, megawatts	1000	835	1145
Net plant power, Mw_e	250	217	300
Net plant efficiency	25.0	26.0	26.0
Reactor core			
Active diameter, feet	18.7	16.8	18.7
Active height, feet	19.0	17.5	20.5
Lattice pitch, inches	11.0	11.1	11.1
Number of fuel elements	330	284	356
Reflector thickness, feet	1.0	1.0	1.0

Table 1. (Continued)

Reactor	Reactor Model	200 Mw_e(33)	300 Mw_e(33)
Pressure tube material	Zr-2	Zr-2	Zr-2
I.D. of pressure tube, inches	4.650	4.650	4.650
Wall thickness, inches	.162	.162	.162
Primary coolant temperature °F	464	483	483
Core loading metric tons U	76	62.2	91.2
D_2O inventory, metric tons	780	326.5	410

IV. CALCULATION OF REACTIVITY

Of basic importance in the study of the feasibility of shim control of heavy-water moderated power reactors is a knowledge of the excess reactivity of the reactor. For it is from such knowledge that the amount of control needed can be determined. The criticality of a reactor is defined by the Fermi critical equation (20, 40), Equation 1.

$$k_{eff} = \frac{k_{\infty}\ e^{-B^2\tau}}{1 + L^2B^2} \qquad (1)$$

where

k_{∞} is the infinite multiplication factor

B^2 is the buckling and B is the lowest eigenvalue of the critical equation

τ is the average age of thermal neutrons

L is the diffusion length

and k_{eff} is the effective multiplication factor.

The reactivity is defined by Equation 2.

$$\rho = \frac{k_{ex}}{k_{eff}} = \frac{k_{eff} - 1}{k_{eff}} \qquad (2)$$

where

ρ is the reactivity

and k_{ex} is the excess multiplication factor.

The factors that make up k_{eff} are the lattice parameters and are dependent upon the materials and geometry of the reactor. Various methods and recipes are used to calculate the lattice parameters needed in this study.

The infinite multiplication factor is defined by Equation 3 (31).

$$k = \eta\varepsilon pf \tag{3}$$

where

η is the thermal reproduction factor

ε is the fast fission factor

p is the resonance escape probability

and f is the thermal utilization.

This relationship is known as the four factor formula. The four factors; η, ε, p, and f must be defined so that they are dimensionally consistent and the infinite multiplication factor, k_∞ is defined as the ratio of thermal neutrons absorbed in one generation to the number of thermal neutrons absorbed in the next generation. In this study, η, the thermal reproduction factor is defined as the number of fast neutrons produced per absorption of a neutron in any part of the fuel element. The fast fission factor, ε, is defined as the total number of fast neutrons produced by fission due to neutrons of all energies divided by the number of fast neutrons produced by fission due to thermal neutrons. The resonance escape probability, p, is defined as the fraction of fast neutrons that are slowed to thermal energies without being captured. The thermal utilization is defined as the ratio of the number of neutrons absorbed within the fuel element to the number of neutrons absorbed within the reactor.

In Equation 1, the term $e^{-B^2\tau}$ is the fast leakage and this is the fraction of neutrons that leak from the reactor while they are being thermalized. In the same equation the factor $(1 + L^2B^2)^{-1}$ is the fraction of thermal neutrons that leak from the reactor. The total leakage is the product of the fast leakage factor and the thermal leakage factor and is given by Equation 4.

$$\text{Total leakage} = \frac{e^{-B^2\tau}}{1 + L^2B^2} \quad . \tag{4}$$

The methods used to calculate each of the lattice parameters are discussed below.

A. Infinite Multiplication Factor

The infinite multiplication factor is calculated using the four factor formula relationship in Equation 3.

B. Thermal Reproduction Factor

The thermal reproduction factor is the ratio of fast neutrons produced to the number of neutrons absorbed within the fuel element and is expressed in Equation 5.

$$\eta = \frac{\nu\Sigma f}{\Sigma_a} \tag{5}$$

where

η is the number of neutrons produced per fission

Σ_f is the homogenized macroscopic fission cross section

and Σa is the homogenized macroscopic absorption cross section.

The values of ν used for the various fissionable isotopes are given below in Table 2.

Table 2. ν values for certain fissionable isotopes

Isotope	ν (23)
Uranium-235	2.47
Plutonium-239	2.88
Plutonium-241	2.91

The macroscopic cross sections for the fuel element are given by Equation 6.

$$\Sigma_i = f_{fuel}(N_{25}\,\sigma_{25i} + N_{28}\,\sigma_{28i} + N_O\,\sigma_{Oi} + \ldots \qquad (6)$$

$$+ f_{coolant}(N_H\,\sigma_{Hi} + N_D\,\sigma_{Di} + N_O\,\sigma_{Oi})$$

$$+ f_{clad}\,N_{zr}\,\sigma_{Zr}$$

where

f_{fuel} is the volume fraction of fuel, .396

$f_{coolant}$ is the volume fraction of coolant, .546

f_{clad} is the volume fraction of cladding, .148

N is the atomic number density of the isotopes

σ is the microscopic cross section for reaction i with the isotope.

The subscripts are as follows:

25 is the uranium 235 isotope

28 is the uranium 238 isotope

O is oxygen

H is hydrogen

D is deuterium

and Zr is zirconium.

(For a discussion of microscopic cross sections see Appendix A.) Elements included in the fuel fraction of the fuel element are uranium (isotopes 235 and 238), oxygen, xenon 135, samarium 149, plutonium (isotopes 239, 240, and 241), and the fission products of Uranium-235, Plutonium-239, and Plutonium-241.

C. Fast Fission Factor

The fast fission factor is determined using a method developed by Fleishman and Soodak (16). This method is based on the original work of Spinrad (38). Spinrad defines the fast effect as the number of fast neutrons escaping into the moderator from the fuel to the number of fast neutrons produced from thermal neutron induced fission. This method divides the fast neutrons remaining in the reactor into three groups:

Group 1 Neutrons with energies above 1.4 Mev (the fission threshold for Uranium-238.)

Group 2 Fission neutrons with energies less than 1.4 Mev

Group 3 Neutrons that have scattered from group 1 to energies below 1.4 Mev.

Equation 7 is the equation for the fast effect.

$$1 - \varepsilon = C_1G_1 - C_2L_2 - C_3L_3 \qquad (7)$$

where

C_1 is the number of collisions in Group 1 per original fission

G_1 is the gain in number of neutrons per collision in Group 1

and L_1 is the loss in neutron number per collision of a Group 1 neutron.

The relationship for the collision numbers are given by Equations 8, 9, and 10.

$$C_1 = \frac{f_1 P_1}{1 - P_1 \left(\frac{\nu_1 \, f_1 \, \Sigma_{1f} + \Sigma_{11}}{\Sigma_{1t}} \right)} \tag{8}$$

$$C_2 = \frac{f_2 P_2}{1 - P_2 \, \frac{\Sigma_{22}}{\Sigma_{2t}}} \left(1 + \frac{\nu_1 \, \Sigma_{1f}}{\Sigma_{1t}} \, C_1 \right) \tag{9}$$

$$C_3 = \frac{P_3}{1 - P_3 \, \frac{\Sigma_{33}}{\Sigma_{3t}}} \; \frac{\Sigma_{13}}{\Sigma_{1t}} \; C_1 \tag{10}$$

The equations for the gain and losses are given by Equations 11, 12, and 13.

$$G_1 = \frac{(\nu_1 - 1) \, \Sigma_{1f} \; - \Sigma_{1c}}{\Sigma_{1t}} \tag{11}$$

$$L_2 = \frac{\Sigma_{2c}}{\Sigma_{2t}} \tag{12}$$

$$L_3 = \frac{\Sigma_{3c}}{\Sigma_{3t}} \tag{13}$$

In the above equations f_i is the fraction of fission neutrons in group i, (f_1 = .561) and f_2 = .439 for Uranium-235), the P's are collision probabilities obtained from the work of Case (8). The Σ's are macroscopic cross sections, identified by the subscripts f, c, or t for fission, capture, or transport within the respective energy groups. ν is the number of neutrons per fission.

In calculation the fast effect the cross sections used for UO_2, Zr, and D_2O are those given by Soodak and Sullivan (37). The values of the cross sections for H_2O used in this investigation are obtained by examining the fast group cross sections for hydrogen and oxygen given in the

Reactor Physics Constants (1).

In applying the method of Fleishman and Soodak (16) to complex fuel elements moderated with D_2O, Crandall (12) suggests that the fuel elements can be homogenized. When this is done the same volume fractions that are used in the determination of the homogenic macroscopic fuel element cross sections (see page 20) are used.

D. Resonance Escape Probability

The resonance escape probability for a heterogenous reactor is defined (20) by Equation 14.

$$p = \exp\left(- \frac{N_o V_o \phi_o}{V_1 \ \xi_1 \ \Sigma_{s1} \ \phi_1} \int (\sigma_{ao})_{eff} \frac{dE'}{E'} \right) \qquad (14)$$

where

N_o is the number density of the resonance absorber (U-238)

V_o is the volume of the resonance absorber

V_1 is the volume of the moderator

$\xi_1 \Sigma_{s1}$ is the slowing down power of the moderator

ϕ_o is the average flux in the absorber

ϕ_1 is the average flux in the moderator

$\int (\sigma_{ao})_{eff} \frac{dE'}{E'}$ is known as the resonance integral.

The main problem in calculating the resonance escape probability is that of determining the effective resonance integral. The resonance integral is given (32) by Equation 15.

$$R.I._o = A + B \left(\frac{S_{eff}}{M} \right)^{1/2} \qquad (15)$$

where

A is a term representing the volume absorption in the fuel

B is a term related to the surface absorption

S_{eff} is the effective surface of the fuel, given by Equations 16 and 17

and M is the mass of the fuel element.

The following equations give the effective surface for a cluster of fuel rods.

$$S_{eff} = S_{cl} + \gamma(S_o - S_{cl}) \tag{16}$$

$$\gamma = 2\, \Sigma_s\, \rho\, P_o(\Sigma_s\, \rho) \tag{17}$$

In these equations S_{cl} is the surface of the smallest hexagon inclosing the fuel cluster. (This surface in the past was frequently called the rubber band surface.) S_o is surface area of all fuel rods of radius within the fuel element. Σ_s is the macroscopic scattering cross section of neutrons at the resonance energy within the rod. P_o is the non-collision probability with the rod, and is defined by Equation 18.

$$P_o = 1 - P_c \tag{18}$$

where P_c is the collision probability discussed in connection with fast effect.

The neutron energy range of the resonance integrals is from 4 to 100 ev. Crandall (12) states that experiments at Savannah River indicate that the resonance absorption energy can be assumed to be 30 ev. Using this energy of 30 ev, the microscopic scattering cross sections are obtained from Reactor Physics Constants (1).

The values of A and B for UO_2 moderated by D_2O have been determined by Hellstrand (21). The resonance integral in barns is given by Equation 19.

$$R.I._o = \left[4.15 + 26.6 \left(\frac{S}{M}\right)^{1/2}\right] b \qquad (19)$$

The effective resonance integral is for fuel at room temperature. In power reactors the effect of Doppler broadening of the absorption integrals must be taken into account. Hellstrand (22) gives the following expression in Equation 20 for the effect of the Doppler coefficient.

$$R.I. = R.I._o \left[1 + \beta(\sqrt{T} - \sqrt{T_o})\right] \qquad (20)$$

where for UO_2

$$\beta = (0.58 + 0.5\, S/M) \times 10^{-2}.$$

This effective resonance integral Equation 14 becomes Equation 21.

$$p \approx \exp\left(- \frac{N_o V_o}{\xi \Sigma_1 V_1} R.I.\right) \qquad (21)$$

With Equation 21 in complex fuel element geometries the moderator is assumed to be not only the moderator, but also the cladding and the coolant.

E. Thermal Utilization Factor

The thermal utilization factor, f, in this investigation is calculated by the use of Equation 22. This equation is an approximation derived from the use of integral transport theory (1).

$$\frac{1}{f} - 1 = \frac{b^2 - a^2}{a^2} \frac{\Sigma_{mc}}{\Sigma_{fc}} G + \kappa_m^2 b^2 C + \frac{b^2 - a^2}{a} \Sigma_{mc} \left(\frac{3}{2}\lambda + 1\right) \qquad (22)$$

where

Σ_{mt} is the total cross section of the moderator

Σ_{mc} is the capture cross section of the moderator

Σ_{fc} is the capture cross section within the fuel element

Σ_{ft} is the total cross section with the fuel element

$\kappa_m^2 = 3\ \Sigma_{mt} \cdot \Sigma_{mc}$

$$C = \frac{1}{2}\left(\frac{b^2/a^2}{\frac{b^2}{a^2} - 1}\ \ln\frac{b}{a} - \frac{3}{4} + \frac{1}{4a^2/b^2}\right)$$

and $G = \frac{\phi(a)}{\phi f}$, where ϕ_f is the average flux in the fuel element. The approximation used for G is given in Equation 23.

$$G = 1 + \frac{\Sigma_{fc}}{\Sigma_{ft}}\ B(a\Sigma_{ft}) \tag{23}$$

where

$$B(x) = \frac{1}{1-P_c}\left(x^2\left[I_o(x)K_o(x) + I_1(x)K_1(x)\right] + xI_o(x)K_1(x) - x\right)-1$$

I_o, K_o, I_1, K_1 are Bessel functions and P is the collision probability.

In Equations 22 and 23 a is the radius of a fuel element, and b is the radius of a unit cell. The values of λ and B are tabulated as a function of $a\Sigma_{ft}$ in Reactor Physics Constants (1).

In these calculations the fuel element has been homogenized to include everything within the fuel element housing tube. For a discussion of cross sections and number densities used in this set of calculations see Appendix A.

F. Fast Leakage Factor

The fast leakage factor e^{-B^2} is determined from the geometric buckling B_g^2 and the age to thermal of the neutrons. The buckling is related to the size of the reactor through Equation 24.

$$B_g^2 = B_r^2 + B_H^2 = \left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2 \qquad (24)$$

where

B_r is the radial geometric buckling

B_H is the axial geometric buckling

R is the radius of core + reflector savings

H is the height of the core + 2 times reflector savings.

The reflector savings, δ, is given (40) by Equation 25.

$$\delta = \frac{D_I}{D_{II}\,\kappa_{II}} \tanh \kappa_{II} T \qquad (25)$$

where

D_I is the diffusion coefficient of the homogenized core $(3\ \Sigma_{tr})^{-1}$

D_{II} is the diffusion coefficient of the reflector

$\kappa_{II}^2 = 3\ \Sigma_a \Sigma_{tr}$

Σ_{tr} is the macroscopic transport cross section

Σ_a is the macroscopic absorption cross section

and T is the thickness of the reflector.

According to the definition of Fermi (31), the age is defined in Equation 26.

$$\tau = \int_{u_0}^{u} \frac{D\,du}{\xi\Sigma} \qquad (26)$$

In calculation of the age in D_2O reactors Soodak and Sullivan divide the age into two parts (37) as in Equation 27.

$$\tau = \tau_1 + \tau_2 \tag{27}$$

where

τ_1 is the age in D_2O down to .1 Mev, 38 cm^2

τ_2 is the remaining age to thermal

τ_2 can be expressed by Equation 28.

$$\frac{D}{\xi\ \Sigma_s}\ \Delta u = \frac{\Delta u}{3\Sigma_{tr}\xi\Sigma_s} \tag{28}$$

where

Δu is the lethargy between .1 Mev and thermal

Σ_{tr} and Σ_s are macroscopic transport and scattering cross sections

and ξ is the logarithmic energy decrement.

Soodak and Sullivan (37) determine Δu by assuming the age to thermal for D_2O to be 120 cm^2. The values of macroscopic cross section are obtained by homogenizing the entire reactor core. This is possible since the fast flux is assumed to be flat across the unit cell (12). The microscopic cross sections of Soodak and Sullivan (37) are used in these age calculations.

G. Thermal Leakage Factor

To calculate the thermal leakage factor, $(1 + L^2B^2)^{-1}$ once the buckling is known, it is necessary only to determine the thermal diffusion length. The diffusion length, L, is defined by Equation 29 (20).

$$L = \sqrt{\frac{D}{\Sigma a}}$$

where

D is the diffusion coefficient for neutrons

and Σ_a is the macroscopic cross section for absorption. Weinberg and Wigner (40) show that the diffusion coefficient can be approximated as in Equation 30.

$$D = \frac{\Sigma s}{3\Sigma\Sigma_{tr}} \approx \frac{1}{3\ \Sigma_{tr}} \tag{30}$$

where

Σ_s is the macroscopic scattering cross section

Σ_{tr} is the macroscopic transport cross section

Σ is the total macroscopic cross section

Therefore from Equations 29 and 30, L^2 can be expressed as in Equation 31.

$$L^2 \approx \frac{1}{3\ \Sigma_{tr}\ \Sigma_a} \tag{31}$$

In calculating the thermal leakage using this relationship for thermal diffusion length the macroscopic cross section was based on the entire reactor core being homogenized. When this technique is used the values obtained are in agreement with those of Soodak and Sullivan (37).

By the use of the factors described above the effective multiplication can be calculated using Equation 1.

V. PREDICTION OF LONG TERM REACTIVITY CHANGES

In the study of nuclear reactor shim control over the entire fuel cycle it is necessary to know the time variation of the amount of excess reactivity. In high power nuclear reactors the reactivity changes because of the change in concentrations of fissionable isotopes and the build up of fission products.

In low enriched or natural uranium fuel reactors the build of plutonium isotopes initially causes the amount of excess reactivity to increase. The first plutonium isotope, Pu-239, is formed from the following nuclear reaction.

$$U^{238} + {}_0n^1 \longrightarrow U^{239} \xrightarrow{\beta} Np^{239} \xrightarrow{\beta} Pu^{239}$$

The next isotope of plutonium, Pu^{240}, is formed by the subsequent non-fission capture of a neutron in Pu^{239}. Pu^{241} is formed by the capture of a neutron in Pu^{240}.

The initial increase in reactivity is due to the Pu^{239} and Pu^{241} isotopes. These isotopes are fissionable, and the more of these isotopes are formed, the more the excess reactivity will increase. For natural uranium fuel reactors these plutonium isotopes initially build up faster than the U-235 atoms are depleted.

The conversion ratio is defined as the number of fissionable atoms produced per fissionable atom destroyed. Equation 32 (5) defines the conversion ratio.

$$C = \frac{N_g\sigma_g}{N_f\sigma_f} + \eta\varepsilon P_1(1-p) \qquad (32)$$

where

N_g is the number of furtile atoms per cubic centimeter

N_f is the number of fissionable atoms per cubic centimeter

σ_g is the microscopic cross section of the furtile isotope

σ_f is the cross section of the fissionable isotope

η is the thermal reproduction factor

ε is the fast fission factor

P_1 is the non-leakage probability of neutrons slowing down to the energy of the fertile isotope resonances

and (1-p) is the resonance capture probability.

For the reactor described in Chapter III with a D_2O concentration of 0.96 the conversion ratio is 0.7565. For the same reactor with a D_2O concentration of 0.9975, the conversion ratio is 0.7823. The later case would be the normally shim controlled nuclear reactor.

The amount of excess reactivity eventually begins to decrease as the plutonium atoms reach their equilibrium concentrations and the number of fission products increases.

To determine the time dependency of the excess reactivity it is necessary to know the time variation of the important isotopes with the fuel. Benedict and Pigford (5) derive the relationships given in Equation 34 through 44 for these isotopes, as a function of integrated flux, θ, where θ is defined by Equation 33.

$$\theta = \int_0^t \phi(t)\, dt. \tag{33}$$

For Uranium 235

$$N_{25} = N_{25}^{\circ} \exp(-\sigma_{25}\theta) \tag{34}$$

For Plutonium 239

$$N_{49} = C_1 + C_2\exp(-\sigma_{25}\theta) - (C_1 + C_2)\exp(-\gamma\sigma_{49}\theta) \qquad (35)$$

where C_1, C_2, and γ are defined by Equations 36, 37, and 38.

$$C_1 = N^\circ_{28}\ \sigma_{28}/\gamma\sigma_{49}. \qquad (36)$$

$$C_1 = N^\circ_{25}\ \sigma_{25}\ \eta_{25}\ P_1(1-p)/(\gamma\sigma_{49} - {}_{25}). \qquad (37)$$

$$\gamma = 1 - \eta_{49}\varepsilon\ P_1(1-p)\ . \qquad (38)$$

For Plutonium 240.

$$N_{40} - C_3 + C_4\exp(-\sigma_{25}\theta) + C_5\exp(-\gamma\sigma_{49}\theta) - (C_3 + C_4 + C_5)\exp(-\sigma_{40}\theta). \qquad (39)$$

where C_3, C_4, and C_5 are defined by Equations 40, 41, and 42.

$$C_3 = N_{28}\sigma_{28}\alpha_{49}/\sigma_{40}\gamma(1 + \alpha_{49})\ . \qquad (40)$$

$$C_4 = \frac{N^\circ_{25}\eta_{25}\ \varepsilon P_1(1-p)\ \sigma_{25}\ \sigma_{49}\ \alpha_{49}}{(1 + \alpha_{49})(\sigma_{25} - \gamma\sigma_{49})(\sigma_{25} - \sigma_{40})}\ . \qquad (41)$$

$$C_5 = \frac{C_3\ \sigma_{40}}{\gamma\sigma_{49} - \sigma_{40}} - \frac{C_4(\sigma_{25} - \sigma_{40})}{\gamma\sigma_{49} - \sigma_{40}}\ . \qquad (42)$$

For the fission products of U-235 and Pu-239, the concentrations are given by Equations 43 and 44.

$$N_F(25) = \frac{N^\circ 25}{1 + \alpha_{25}}\left(1 - \exp(-\sigma_{25}\theta)\right). \qquad (43)$$

$$N_F(49) = \frac{\sigma_{49}}{1 + \sigma_{49}} C_1 + \frac{C_2 \; 1 - \exp(-\sigma 25\theta)}{\sigma_{25}} \qquad (44)$$

$$- (C_1 + C_2) \frac{1 - \exp(-\lambda\sigma_{49}\theta)}{\sigma_{49}} \; .$$

Two other important isotopes are those of Xenon 135 and Samarium 149. The concentrations of these two isotopes are given by Equations 45 and 46.

$$N_{Xe} = \frac{N_f \; \sigma_f \; \phi \; (yXe \; + y_I)}{\lambda_{Xe} \; + \; \sigma_{Xe}\phi} \qquad (45)$$

$$N_{Sm} = \frac{N_f \; \sigma_f \; \phi y_{Sm}}{\phi\sigma_{Sm}} = \frac{N_f \; \sigma \; f y_{Sm}}{\sigma_{Sm}} \qquad (46)$$

where y is the fission yield.

In the above equations the subscripts have the following meaning:

25 is U-235

28 is Pu-239

49 is Pu-239

40 is Pu-240

41 is Pu 241

Xe is Xenon 135

Sm is Samarium 149

and f is fissionable atoms.

Benedict and Pigford (5) also give equations for the number densities of U 236, Pu 241, and the fission products of Pu 241, but these equations were not used for these reactivity studies. The effect of U 236 is considered in the fission product cross section of the U 235 fission products (24). In natural uranium fueled reactors very little Pu-241 is formed. A simpler approximation for the amount of Pu-241 and its fission products is used based on the concentration of Pu-240.

The values of microscopic cross section and U-235 and U-238 number densities that are used in this investigation are given in Appendix A.

The calculation of the long term reactivity of a heavy water reactor system where the light concentration varies is complicated by the fact that the fast fission factor, resonance escape probability and the non-leakage of epi-resonance neutrons are all functions of light water concentration. For this reason number densities of the plutonium isotopes could not be determined directly, but had to be based on some averaged values of ε, p, and P_1.

The primary purpose of predicting the time dependency of reactivity is to determine the amount of shim control required. When the shim is controlled by light water, the purpose is to then determine the time dependency of the light water concentration. The required concentration of light water can be found by making a series of reactivity calculations at various times after the start of the fuel cycle. Then the correct concentration is the one where the reactor will be just critical. These criticality calculations are made using techniques described in Section IV. The reactor is just critical when k_{eff} is equal to 1.0000.

The following technique is used to adjust the values of ε, p, and P_1 for making plutonium isotope concentration calculations. The fuel cycle is divided into a number of time increments. For the first time increment the values of ε, p, and P_1 used are those for the initial critical reactor. These values are associated with an H_2O concentration of 3.69 mol per cent. The values of the fast effect is 1.02302, resonance escape probability is 0.9092, and the fast neutron non-leakage is 0.9925. With these values plutonium concentrations at the end of the first time increment are calculated, the criticality is determined by the techniques of Chapter IV, and from these numbers is determined the just critical H_2O concentration. For this case the concentration is 4.28 mol per cent. The values of ε, p, and P_1 for the second time increment are the time weighted averages of the values for the previous time increments and the values associated with the present H_2O concentration. Again using the averaged values of ε, p, and P_1, new concentrations of the plutonium isotopes are determined, the criticalities calculated, and the just critical H_2O concentration found for the end of the second time increment. The procedure is repeated to the end of the fuel cycle.

The time increments used are taken in terms of integrated flux times, θ, as given by Equation 33. θ has the dimensions of cm^{-2}, and the increments used are 10^{20} cm^{-2}, 2×10^{20} cm^{-2}, and 2.5×10^{20} cm^{-2}. The final value of θ was 30.0×10^{20} cm^{-2}.

The actual time of an increment can be found from the intermediate flux time by knowing the average flux over a time interval. The average flux can be determined from Equation 47.

$$\Phi_{fuel} = \frac{\text{fission rate}}{V_{fuel}\,\Sigma_f} \qquad (47)$$

where

Φ_{fuel} is the average flux with the fuel

V_{fuel} is the volume of the fuel

Σ_f is the macroscopic fission cross section.

The fission rate is dependent upon the reactor power. The fission rate per watt is 3.1×10^{10} (19). Thus for a total reactor power of 1000 megawatts the fission rate is 3.1×10^{19} sec^{-1}. For 330 fuel elements with a volume of 26,800 cm^3 each, the average initial flux is $8.68 \times 10^{13}/cm^2$ sec.

The concentrations of the various isotopes within the fuel element are given in Table 3 and Figure 3. The concentration of H_2O necessary to make the reactor just critical are given in Figure 4. It is from this information in Figure 4 that the requirements for the distillation system for shim control are determined.

In order that shim control by the removal of a light-water poison be compared with other methods of shim control, the amount of excess reactivity as a function of time is determined for a heavy water reactor. This reactor is assumed to be similar to the reactor model discussed in Chapter III, except that it operates with a constant D_2O concentration of 99.75 mol per cent. The techniques of calculating the amount of excess reactivity is similar to the technique discussed in this chapter. The main differences are that the values of ε, p, and P_1 are assumed constant and it is not necessary to find the just critical concentration of H_2O. The excess reactivity as a function of integrated flux time is shown in Figure 5.

Table 3. Averaged isotope concentration in fuel

Integrated flux 10^{20}cm^{-2}	U 235 10^{20}cm^{-3}	Pu 239 10^{20}cm^{-3}	Pu 240 10^{20}cm^{-3}	Pu 241 10^{20}cm^{-3}	F.P. U 235 10^{20}cm^{-3}
0.0	1.595	0.0000	0.00000	0.00000	0.00000
1.0	1.549	0.0338	0.00063	0.00001	0.03920
2.0	1.509	0.0637	0.00241	0.00009	0.07726
4.0	1.412	0.1122	0.00857	0.00051	0.15006
6.0	1.336	0.1506	0.01722	0.00148	0.2187
8.0	1.259	0.1797	0.02746	0.00311	0.2835
10.0	1.187	0.2022	0.03872	0.00503	0.3444
12.0	1.119	0.2196	0.05046	0.00741	0.4019
14.0	1.055	0.2332	0.06234	0.01020	0.4561
16.0	0.9945	0.2456	0.07407	0.01331	0.5072
18.0	0.9373	0.2513	0.08544	0.01662	0.5553
20.0	0.8837	0.2570	0.09621	0.02009	0.6007
22.5	0.8205	0.2620	0.1093	0.02454	0.6672
25.0	0.7625	0.2653	0.1210	0.02838	0.7032
27.5	0.7085	0.2657	0.1327	0.03839	0.7637
30.0	0.6578	0.2673	0.1433	0.04144	0.8074

Table 3. (Continued)

Integrated flux 10^{20}cm^{-2}	FP Pu239 10^{20}cm^{-3}	FP Pu241 10^{20}cm^{-3}	Xe135 10^{16}cm^{-3}	Sm149 10^{20}cm^{-3}	Actual time days
0.0	0.00000	0.00000	0.01787[a]	0.000222[a]	0.0
1.0	0.00174	0.00000	0.1787	0.000222	13.3
2.0	0.00537	0.00000	0.1823	0.000231	27.1
4.0	0.02500	0.00005	0.1913	0.000242	56.0
6.0	0.05122	0.00021	0.1982	0.000252	86.2
8.0	0.08443	0.00035	0.2042	0.000262	117.4
10.0	0.1230	0.00064	0.2058	0.000262	149.0
12.0	0.1657	0.00097	0.2058	0.000262	180.8
14.0	0.2098	0.00344	0.2058	0.000267	212.7
16.0	0.2623	0.00528	0.2063	0.000265	244.4
18.0	0.3107	0.00761	0.2063	0.000264	275.9
20.0	0.3626	0.01048	0.2034	0.000260	307.1
22.5	0.4288	0.01436	0.2018	0.000258	345.7
25.0	0.4966	0.01896	0.1971	0.000254	383.1
27.5	0.5654	0.02477	0.1946	0.000248	420.1
30.0	0.6346	0.03170	0.1940	0.000246	457.0

[a] These values are equilibrium values and are reached a few hours after reactor starts up.

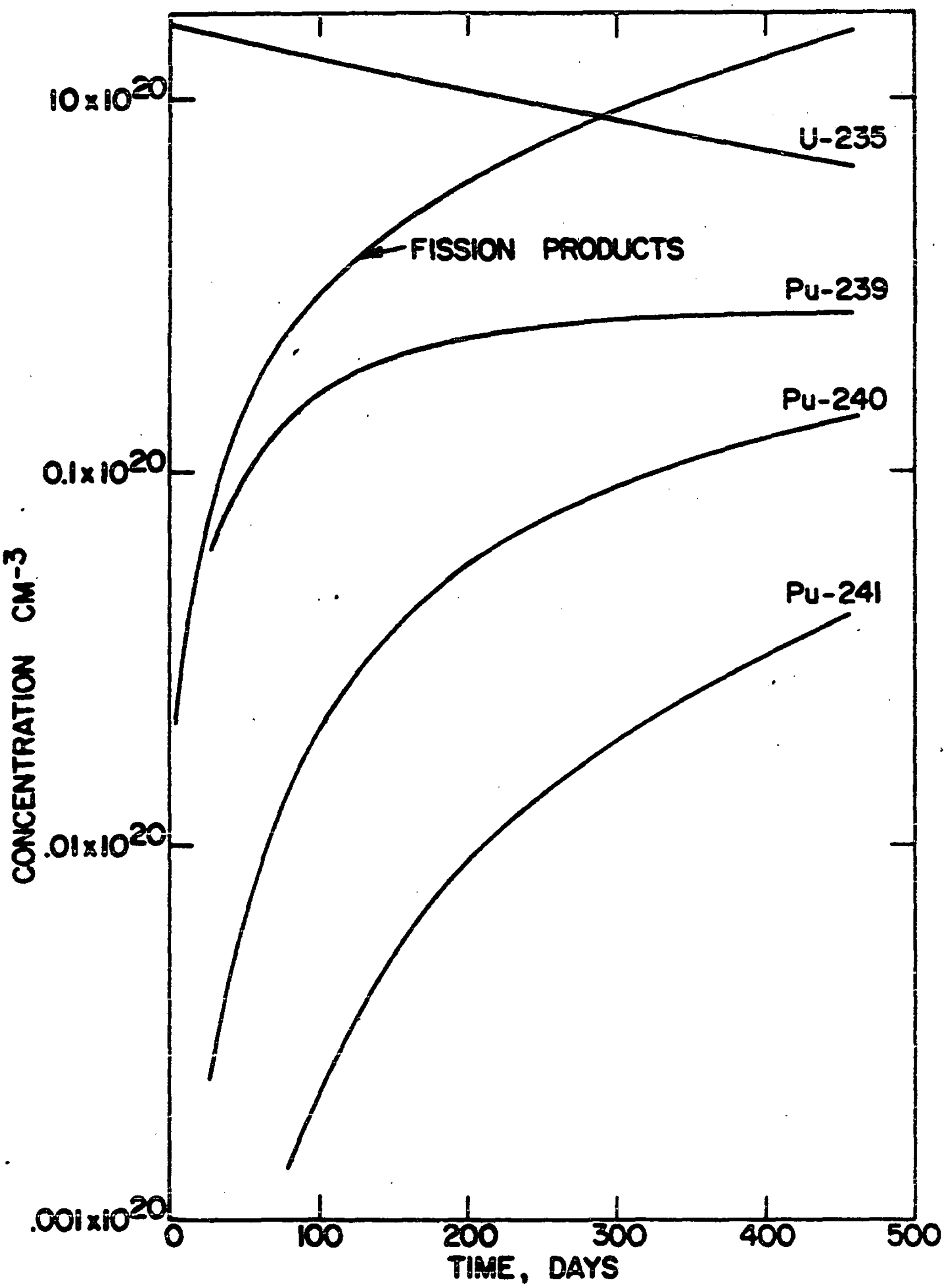

FIGURE 3. ISOTOPE CONCENTRATION VS. TIME.

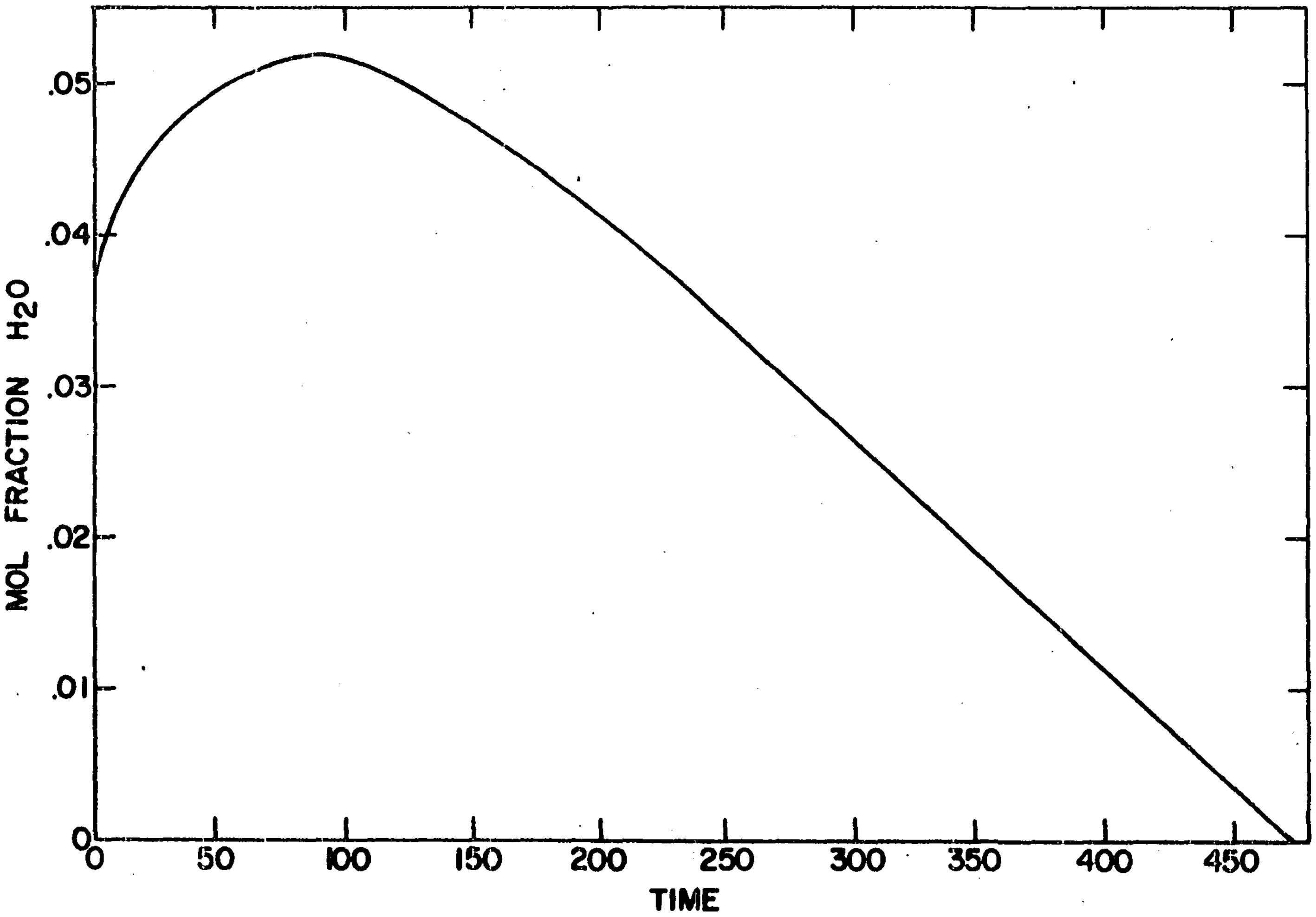

FIGURE 4. CONCENTRATION H_2O WITH TIME.

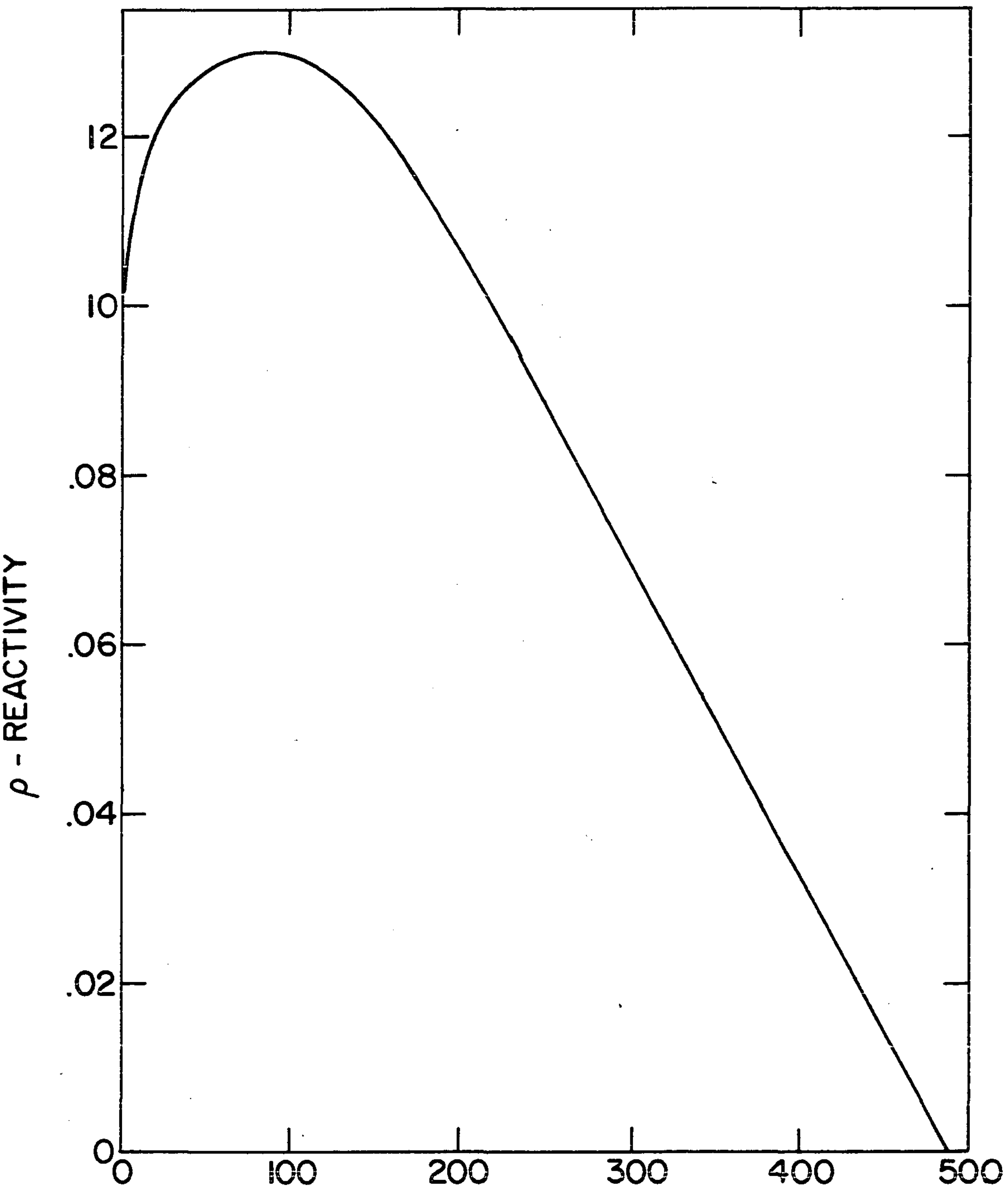

FIGURE 5. REACTIVITY VS. TIME FOR REACTOR WITH 99.75 MOL % D_2O.

VI. THE DISTILLATION UNIT

Within the larger heavy-water moderated nuclear power plants, such as the production reactors at Savannah River (6), the CANDU reactor (29), and power plants proposed by Sargent and Lundy (33), a distillation unit is integrated with the heavy-water system of the reactor to reconstitute the heavy water. A thorough description of the system used at Savannah River is given by Bertsche (6). With these reactors, the purpose of the distillation system is to remove light water that has leaked into the heavy-water system. The light water is eliminated by fractional distillation of the heavy-light water mixture.

At the Savannah River plant (6, 35) this distillation is done by removing a side stream of 7 gallons per minute from the reactor to the distillation system. The distillation system consists of two columns connected in series. Each column is operated under a vacuum and has 90 sieve plates. The system has a rectifying section, in which the light water is increased from a feed concentration of approximately 0.25 mol per cent H_2O to 12 mol per cent H_2O, and a stripping section in which the light-water concentration is decreased to 0.23 mol per cent H_2O. These systems were designed for a product rate of 1150 to 1250 pounds per year of H_2O at a feed concentration of 99.75 per cent D_2O to the bottom plate, an overhead draw off rate of 1.5 pounds per hour, a vacuum of 100 mm hg at the condensers, and a boil-up rate between 3000 and 4000 pounds per hour.

The distillation system for the heavy-water power reactors proposed by Sargent and Lundy are designed to remove one pound of water per day from the reactor. This system consists of two 90 foot columns packed with 1 inch berl saddles. The rectifying section produces a mixture of 25 per cent light water and 75 per cent heavy water.

A distillation system that is used for shim control differs in three ways from the distillation systems mentioned above. First the shim control distillation systems are larger than the usual distillation system associated with a reactor. This larger distillation system is necessary since more light water must be removed. Secondly, where the usual distillation system operates at nearly constant feed composition and rate, the shim controlling distillation system must handle a range of feed compositions and rates. And thirdly, shim control distillation must supply the reactor with heavy water than can have a concentration that is either greater than that of the reactor or less than that of the reactor. The last condition comes from the fact that in low enriched power reactors, there is an initial increase in reactivity due to the build up of the plutonium isotopes. During this part of the fuel cycle light water is effectively added to the system to compensate build up. Later in the fuel cycle as fission products build up the reactivity decreases and the light water must be removed. The light water can be added to the system by returning to the reactor only the overheads products of the rectifying section which has a lower D_2O concentration and a higher H_2O The light water is removed by returning to the reactor the bottoms product of the stripping section, which has a lower H_2O concentration. A flow sheet of the scheme that has been devised to do this is shown in Figure 6. This distillation system has three series connected, 83 bubble-cap plates. The feed from the reactor enters between the first and second columns. The first column is the stripping section and the

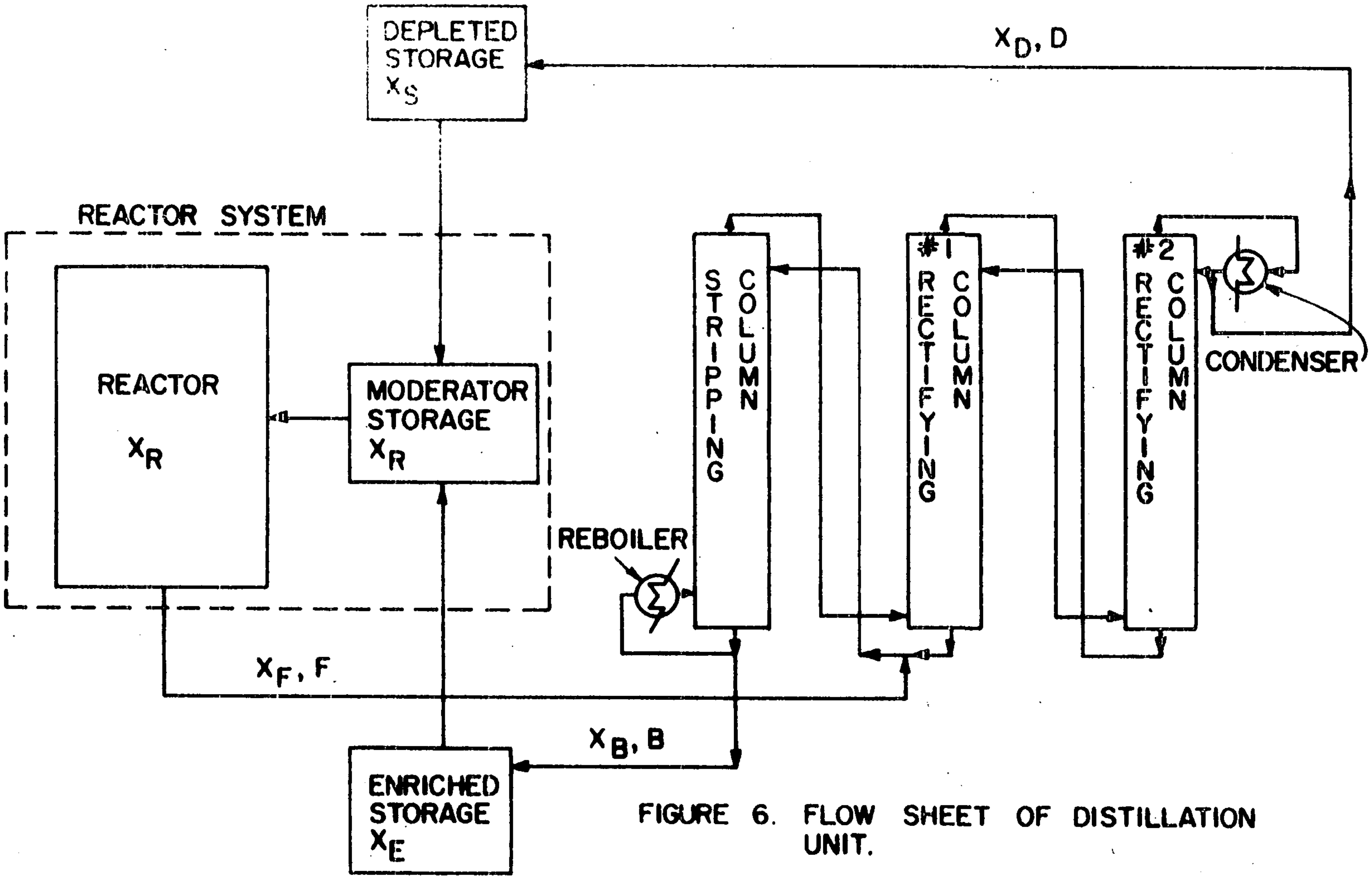

FIGURE 6. FLOW SHEET OF DISTILLATION UNIT.

second and third columns are the rectifying section. The bottoms product from the stripping section is piped to an enriched storage tank. The enriched storage will hold a light-heavy water mixture that has a higher D_2O concentration than does the reactor. The overheads product from the rectifying section is piped to the depleted storage which contains a light-heavy water mixture with a concentration of heavy water less than that of the reactor.

The moderator storage contains a light-heavy water mixture that has the same heavy water concentration as the reactor. This storage contains the amount of moderator that is in excess of the amount needed in the reactor core itself. The amount in the excess moderator storage varies during the fuel cycle and at one time its contents approach empty.

To shim control the reactor the distillation system is operated in the following manner. At the start of the fuel cycle most of the water will be in the reactor and the excess moderator storage. The enriched storage will be empty and within the depleted storage will be a 56 mol per cent H_2O light-heavy water mixture. The amount contained initially in the depleted storage will be the amount of light water needed to counter the initial build up of reactivity.

As the fuel cycle starts, a side stream is drawn from the reactor system and is sent to the distillation system. The fraction enriched in D_2O is sent to the enriched storage for use later in the fuel cycle, and the fraction depleted in D_2O is sent to the deplete storage for use in shim control during the period of reactivity increase within the reactor. The shim control is obtained by controlling the flow rate from the depleted storage to the reactor. If the initial amount contained within the depleted storage is correctly chosen, the volume of the depleted storage will approach empty at some time during the period of reactivity increase. After approaching empty the volume contained in the depleted storage will again increase. The reason for this is that at the time the rate of reactivity build-up has decreased to a point where the amount of additional light water needed to shim control is less than is being supplied by the distillation system.

When the reactivity within the reactor ceases to increase and reaches its peak, the flow from the depleted storage to the reactor is stopped and the flow from the enriched storage is started. From this time to the end of the fuel cycle shim control is obtained by controlling the flow from the enriched storage to the reactor.

As the excess reactivity within the reactor begins to decrease the amount of flow from the enriched storage to the reactor is less than the flow from the distillation system to the enriched storage. During this time the amount within the excess moderator storage decreases while the amount within the enriched storage increases. Later during the cycle the rate of change of reactivity increases and the flow from the enriched storage to the reactor is greater than the flow from the distillation system to the enriched storage. During this part of the cycle the amount in the excess moderator storage increase while the amount in the enriched storage decreases. Finally at the end of the fuel cycle the enriched storage is empty.

During the part of the fuel cycle in which the excess reactivity is decreasing, the amount of liquid in the depleted storage has been increasing. As the spent uranium fuel is removed from the reactor and fresh fuel loaded into the core, some of the water from the depleted storage is drained into the moderator system of the reactor until the enrichment of H_2O is enough for the initial shim control. When this is done the amount remaining in the depleted storage will be equal to the amount initially within this storage and is ready to be used for shim control of the initial increase of excess reactivity.

This completes the fuel cycle and the distillation required to accomplish the shim control. The only heavy-water that needs to be added to the system is that to replace leakage. Furthermore none of the depleted D_2O has to be sent to an off-site installation for upgrading to a higher D_2O enrichment. A discussion of the distillation system calculations and flow rates is given in the next section.

VII. DISTILLATION CALCULATIONS

In designing distillation columns for the separation of light and heavy water certain physical properties of the system must be known. One of the most important of these properties is that of relative volatility.

The relative volatility, α, is defined (17) in Equation 48.

$$\alpha_{ab} = \left(\frac{y_a}{x_a}\right)\left(\frac{1 - x_a}{1 - y_a}\right) = \frac{P_a}{P_b} \tag{48}$$

where

α is the relative volatility of componet a relative to component b

x_a is the mol fraction of a in the liquid

y_a is the mol fraction of a in the vapor

P_a is the vapor pressure of a

and P_b is the vapor pressure of b.

The relative volatility is independent of concentration for ideal solutions that obey Raoult's law. Raoult's law is given by Equation 49.

$$p_a = x_a P_a \tag{49}$$

where

p_a is the partial pressure of component a in the vapor.

Thus the relative volatility is a measure of separation that would be obtained in the single partial evaporation of a liquid and the condensation of its vapors. A second separation can be obtained by reevaporating the condensate and condensing the vapor. A distillation column is a series of condensations and re-evaporations to obtain the separation of two or more components.

Whenever water contains both hydrogen and deuterium three compounds exist in equilibrium with each other. These three compounds are H_2O, HDO, and D_2O. Their nature is such that their equilibrium is quickly formed through the reaction below.

$$H_2O + D_2O = 2\ HDO$$

Figure 7 shows the concentration of H_2O, HDO, and D_2O as a function of D_2O concentration. In this figure it is seen that at low concentrations of D_2O the main components are H_2O and HDO. At high concentration of D_2O the main components are HDO and D_2O. It is only in the middle concentrations of D_2O that all three compounds exist to an appreciable extent. Thus in the low concentrations of D_2O the relative volatility is the relative volatility of H_2O and HDO, and in the high range of D_2O concentration it is the relative volatility of HDO and D_2O.

Benedict and Pigford (5) state that the relationship of the vapor pressures of H_2O, HDO, and D_2O is that of Equation 50.

$$\frac{P_{H_2O}}{P_{HDO}} = \frac{P_{HDO}}{P_{D_2O}} \qquad (50)$$

Equation 50 means that the relative volatilities of the two are equal, and then the separation factors at the high and low D_2O enrichments are the same. Bebbington and Thayer (4) suggest that this relative volatility can be used over the entire range of D_2O concentrations. For although the actual relative volatility deviates from this near the middle concentration ranges and this makes for a slight over design, the difference is not of practical importance.

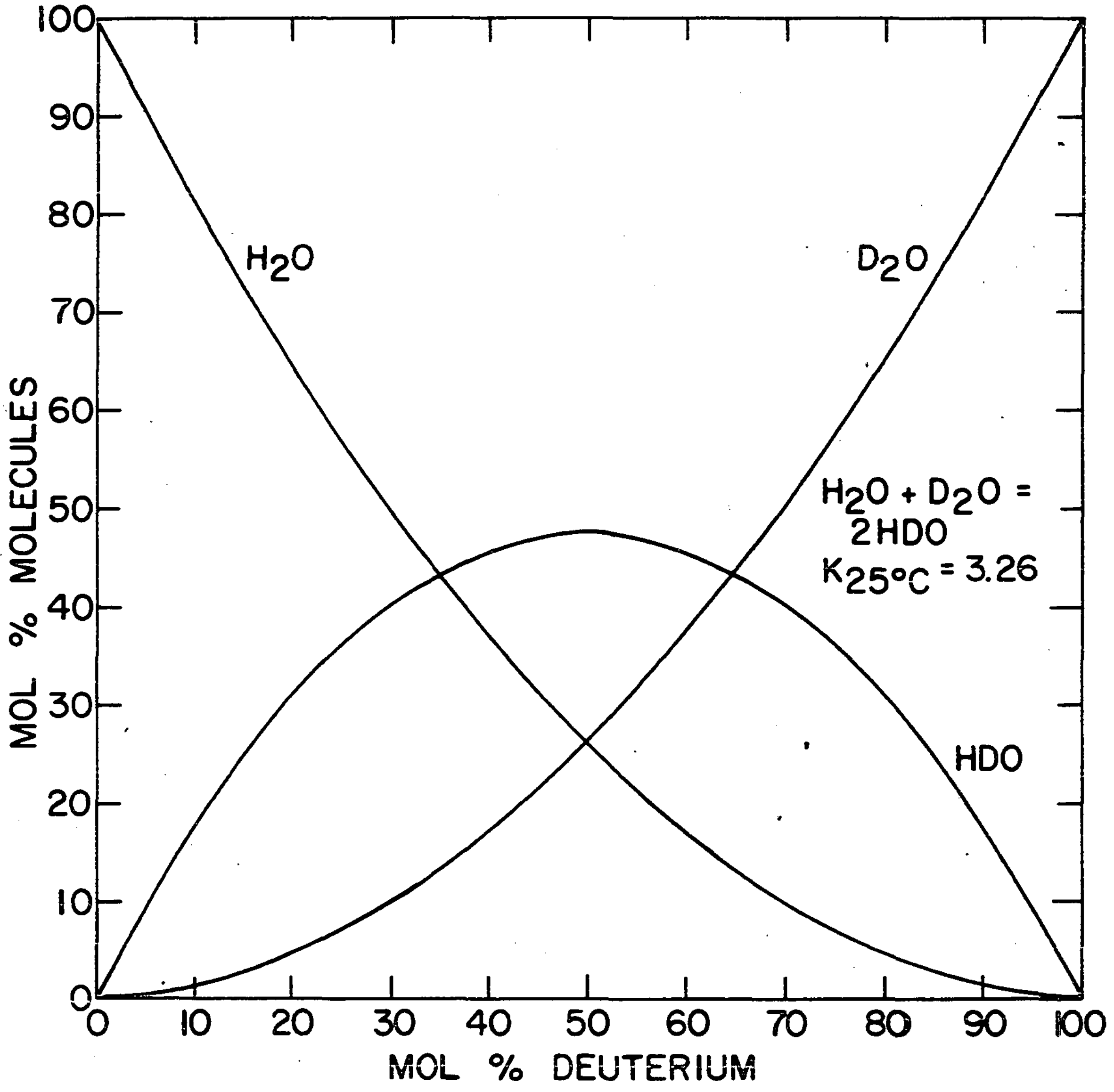

FIGURE 7. EQUILIBRIUM CONCENTRATIONS OF H_2O, D_2O, AND HDO VS. OVER-ALL CONCENTRATION OF D_2O IN WATER.

For the purposes of the discussion and notation the hydrogen concentration of water will be expressed in mol per cent H_2O and the deuterium concentration in mol per cent D_2O.

In determining a value for α, it is assumed that the average operating pressure with each distillation column is 100 mm Hg. Bertsche (6) suggests that this is about the optimum operating condition for this kind of distillation. From the data given by Kirshenbaum (27) a pressure of 100 mm Hg for D_2O corresponds to a temperature of approximately 52°C. At this temperature the relative volatility is 1.051.

Because this value of relative volatility is close to one, significant separation can only be obtained at high reflux ratios. The reflux ratio, R is defined by Equation 51.

$$R = \frac{L_0}{D} \qquad (51)$$

where

L_0 is amount of liquid returned from the condenser to the top of the distillation column

and D is the amount of overheads product withdrawn from the condenser.

A value of 1600 was chosen for the reflux ratio for these calculations in this investigation. The comparable value of reflux ratios in the reactor integrated distillation systems at the Savannah River Plant is 1999.0.

The number of theoretical states required is determined by using the McCabe-Thiele technique (30). For purposes of illustration a McCabe-Thiele diagram is shown in Figure 8. (In general use the McCabe-Thiele method lends itself readily to solution by graphical techniques. But

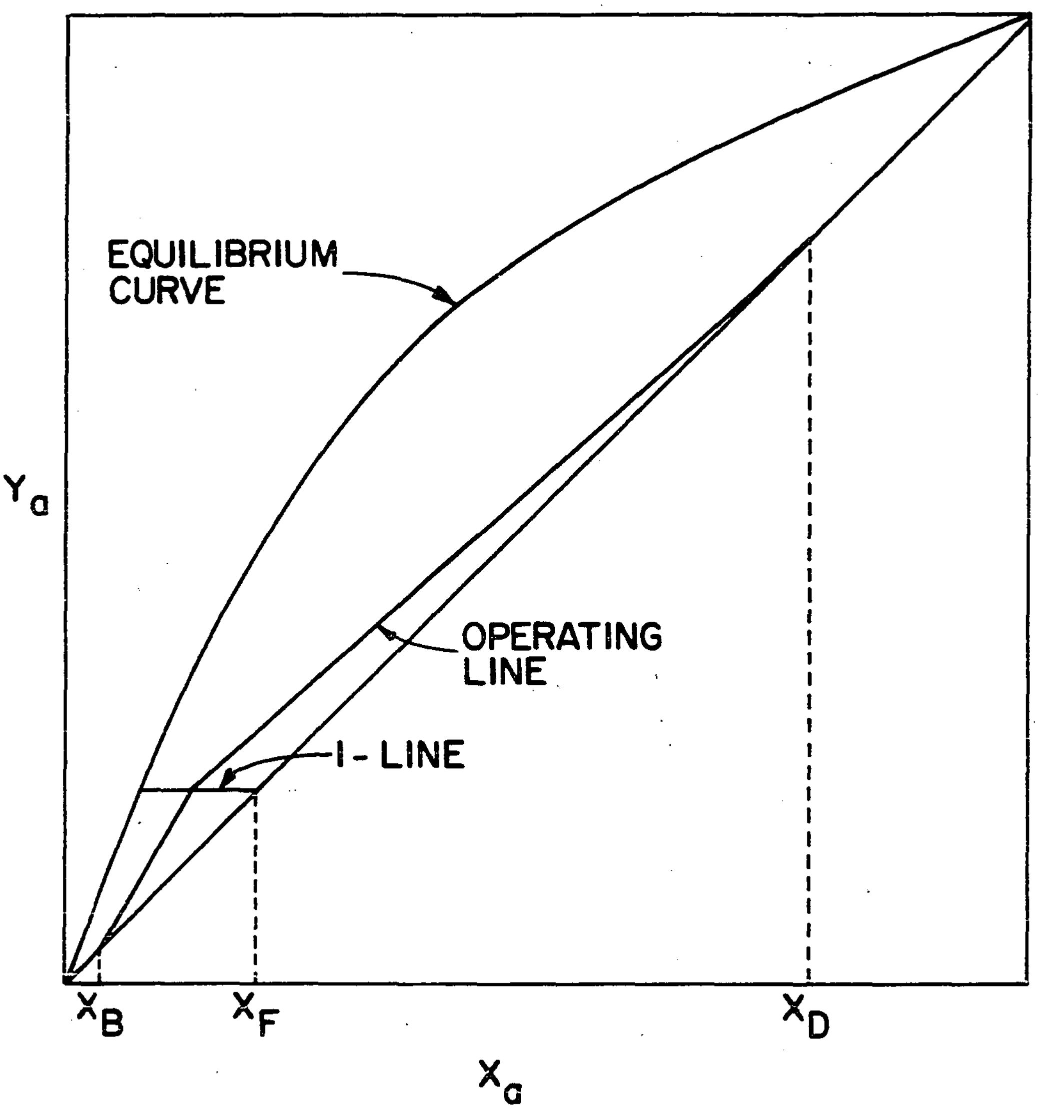

FIGURE 8. AN ILLUSTRATIVE McCABE THIELE DIAGRAM.

because of the low value of $\alpha - 1$, the number of stages is determined by an analytical McCabe-Thiele technique. In Figure 8, the value of α is not the one used in this investigation.)

The number of plates is determined by considering a vapor feed composition of 1 mol per cent H_2O. The i-line, which represents the feed composition is from the x = y line to the equilibrium curve. The equation for the equilibrium curve is given in Equation 52, which is derived from Equation 48.

$$y_{eq} = \frac{\dfrac{\alpha x}{1 - x}}{1 + \dfrac{\alpha x}{1 - x}} = \frac{\alpha x}{1 + (\alpha - 1)x} \qquad (52)$$

where

y_{eq} is the equilibrium mol fraction of H_2O in the vapor

x is the mol fraction of H_2O in the liquid.

The i-line intersects the equilibrium curve at a liquid concentration of 0.96 mol per cent H_2O. An operating line for the stipping section is chosen so as to bisect the i-line between 0.96 and 1.00 mol per cent, or at a concentration of 0.98 mol per cent H_2O. The slope, m, of an operating line in the stipping section is given by Equation 53.

$$m = \frac{R}{R + 1} \qquad (53)$$

This operating line intersects the x = y line at a concentration of 32.96 mol per cent H_2O. This is the value at x_D in Figure 8. The equation for this operating line is given in Equation 54.

$$y_{op} = x_D - m(x_D - x) = .000206 + .999375\ x_{op} \qquad (54)$$

where

y_{op} is the mol fraction of H_2O in the vapor at operating conditions

x_{op} is the mol fraction of H_2O in the liquid at operating conditions.

For this case the calculation of the number of stages is done by starting on the operating line at x_{op} equal to 0.0098. With this value of x, a value of y on the equilibrium curve is obtained by Equation 52. The equilibrium value y is 0.010207 and is equal to operating line value of y. This equality represents the condensing of the vapors rising from the first stage. From this value of y_{op} a value of x_{op} from Equation 54 is determined to be 0.010007. This completes the calculation of the first stage. For the second stage and subsequent stages this procedure is repeated until the concentration of H_2O becomes 0.3296 mol fraction. Table 4 shows the steps involved in this calculation. From Table 4 the total number of theoretical stages is seen to be 117.

The number of stages in the rectifying section is one-half the number in the stripping section or 58. The separation obtained in this section is determined in a way similar to that used to determine the number of stages in the stripping section. In the analysis of this section, the operating line is arbitrarily constructed between x = 0.98 mol per cent H_2O on the i-line and the point x = 0.2 mol per cent H_2O on the x = y line. The relationship for this operating line is given by Equation 55.

$$y_{op} = 1.02974x - .00005454 \ . \qquad (55)$$

Starting with a y value of 1 mol per cent H_2O (this corresponds to an x value of 0.98 mol per cent H_2O in the previous discussion) similar

Table 4. McCabe-Thiele calculation in stripping section

Stage	x	$y_{eq} = y_{op}$	Stage	x	$y_{eq} = y_{op}$	Stage	x	$y_{eq} = y_{op}$
1	.0098	.01021	40	.0250	.02603	79	.0950	.09860
2	.0100	.01050	41	.0258	.02685	80	.0984	.10211
3	.0103	.01084	42	.0266	.02769	81	.1019	.10573
4	.0105	.01093	43	.0274	.02852	82	.1055	.10945
5	.0107	.01114	44	.0283	.02945	83	.1093	.11337
6	.0109	.01135	45	.0292	.03039	84	.1132	.11740
7	.0111	.01156	46	.0302	.03143	85	.1172	.12152
8	.0113	.01177	47	.0312	.03247	86	.1213	.12574
9	.0115	.01198	48	.0322	.03351	87	.1256	.13018
10	.0117	.01219	49	.0333	.03465	88	.1300	.13472
11	.0119	.01239	50	.0344	.03579	89	.1327	.13751
12	.0121	.01260	51	.0356	.03704	90	.1373	.14225
13	.0124	.01291	52	.0368	.03829	91	.1421	.14704
14	.0127	.01323	53	.0381	.03964	92	.1469	.15213
15	.0130	.01353	54	.0394	.04099	93	.1520	.15738
16	.0133	.01385	55	.0408	.04244	94	.1572	.16273
17	.0136	.01416	56	.0422	.04389	95	.1626	.16828
18	.0139	.01448	57	.0437	.04545	96	.1681	.17393
19	.0142	.01479	58	.0452	.04699	97	.1738	.17979
20	.0145	.01510	59	.0468	.04867	98	.1796	.18563
21	.0149	.01552	60	.0484	.05033	99	.1856	.19190
22	.0153	.01593	61	.0501	.05209	100	.1918	.19826
23	.0157	.01635	62	.0519	.05396	101	.1981	.20464
24	.0160	.01666	63	.0537	.05583	102	.2046	.21138
25	.0164	.01708	64	.0558	.05801	103	.2113	.21924
26	.0168	.01749	65	.0578	.06008	104	.2181	.22520
27	.0172	.01791	66	.0599	.06226	105	.2251	.23235
28	.0177	.01843	67	.0620	.06445	106	.2322	.23962
29	.0182	.01895	68	.0642	.06672	107	.2395	.24707
30	.0187	.01947	69	.0665	.06910	108	.2470	.25664
31	.0192	.01999	70	.0689	.07159	109	.2565	.26442
32	.0197	.02051	71	.0714	.07418	110	.2643	.27238
33	.0203	.02113	72	.0740	.07687	111	.2723	.28053
34	.0209	.02176	73	.0767	.07966	112	.2804	.28878
35	.0215	.02238	74	.0795	.08256	113	.2887	.29722
36	.0221	.02307	75	.0824	.08556	114	.2972	.30586
37	.0228	.02373	76	.0854	.08867	115	.3058	.31460
38	.0235	.02446	77	.0885	.09188	116	.3145	.32344
39	.0242	.02519	78	.0917	.09518	117	.3234	.33247
						118	.3325	

steps are taken. From Equation 52 an equilibrium x value of 0.009601 is obtained. This is equated to an operating x. The operating x is used in Equation 55 to obtain a value of y which becomes the initial value. This process is continued until 58 are stepped off. (The 58 stages correspond to the one tower in the rectifying section while in the stripping section there are two towers.) The results of this procedure are given in Table 5. In this table it is seen that the final concentration of the bottoms product is 0.1996 mol per cent H_2O.

Bertsche (6) defines an enrichment factor, E, by Equation 56.

$$E = \frac{\frac{y_T}{1-y_T}}{\frac{y_B}{1-y_B}} \qquad (56)$$

where

y_T is the concentration of the more volatile component in the overheads

and y_B is the concentration of the more volatile component in the bottoms product.

For the stripping section of this distillation system the value of y_T can be considered the overheads product concentration, 32.96 mol per cent H_2O and y_B is the feed concentration, 1.0 mol per cent H_2O. Likewise for the rectifying section y_T is the feed concentration, 1 mol per cent H_2O and y_B is the bottoms concentration 0.2 mol per cent. Using these values in Equation 56, the enrichment factor in the stripping section is 48.5 and in the rectifying section it is 5.02. Bertsche further states (6) that enrichment factor does not change if all other operating properties of the column remain the same. Thus through the use of the enrichment factor, it is possible to quickly calculate by means of Equation 56 the overheads and bottoms product concentrations for

Table 5. McCabe-Thiele calculation in the rectifying

Stage	y	$x_{eq} = x_{op}$	Stage	y	$x_{eq} = x_{op}$
1	0.01000	0.00960	30	0.00517	0.00496
2	0.00989	0.00950	31	0.00504	0.00484
3	0.00969	0.00930	32	0.00491	0.00471
4	0.00949	0.00911	33	0.00478	0.00459
5	0.00929	0.00892	34	0.00465	0.00446
6	0.00910	0.00874	35	0.00452	0.00434
7	0.00891	0.00855	36	0.00439	0.00421
8	0.00872	0.00837	37	0.00426	0.00409
9	0.00853	0.00819	38	0.00414	0.00397
10	0.00834	0.00801	39	0.00402	0.00386
11	0.00816	0.00783	40	0.00390	0.00374
12	0.00798	0.00766	41	0.00378	0.00363
13	0.00781	0.00750	42	0.00367	0.00352
14	0.00763	0.00732	43	0.00356	0.00342
15	0.00746	0.00716	44	0.00345	0.00331
16	0.00729	0.00700	45	0.00334	0.00321
17	0.00712	0.00684	46	0.00323	0.00310
18	0.00696	0.00668	47	0.00313	0.00300
19	0.00680	0.00653	48	0.00303	0.00291
20	0.00664	0.00637	49	0.00293	0.00281
21	0.00648	0.00622	50	0.00283	0.00272
22	0.00632	0.00607	51	0.00273	0.00262
23	0.00617	0.00592	52	0.00263	0.00252
24	0.00602	0.00578	53	0.00253	0.00243
25	0.00587	0.00564	54	0.00244	0.00234
26	0.00573	0.00550	55	0.00235	0.00226
27	0.00559	0.00537	56	0.00226	0.00217
28	0.00545	0.00523	57	0.00217	0.00208
29	0.00531	0.00510	58	0.00208	0.001996
			59	0.001993	

various feed compositions without having to go through lengthy McCabe-Thiele calculations. Using the two aforementioned enrichment factors the overheads product concentration, y_D and the bottoms product concentration y_B are determined for various feed concentrations. Table 6 gives values of these concentrations that are used for this distillation system.

Table 6 also gives the ratio of the feed rate to overheads products rate and the bottoms product rate to the overheads feed rate. These rates are determined from material balances in Equations 57 and 58.

Overall balance around distillation unit.

$$F = B + D \tag{57}$$

where

F is the feed rate

B is the bottoms product rate

D is the overheads product rate.

H_2O balance around distillation unit.

$$x_F F = x_B B + x_D D \tag{58}$$

where

x_F is the mol fraction of H_2O in the feed

x_B is the mol fraction of H_2O in the bottoms product

x_D is the mol fraction of H_2O in the overheads product.

Combining Equations 57 and 58 the ratios of B/D and F/D are given by Equations 59 and 60.

$$\frac{B}{D} = \frac{x_D - x_F}{x_F - x_B} \tag{59}$$

Table 6. Distillation unit stream compositions and rates

x_F	x_B	x_D	B/D	F/D
0.03985	0.00820	0.6681	19.858	20.858
0.04465	0.00922	0.6939	18.324	19.324
0.04830	0.01001	0.7111	17.309	18.309
0.05105	0.01006	0.7229	16.612	17.612
0.05090	0.01057	0.7223	16.648	17.648
0.04855	0.01006	0.7122	17.242	18.242
0.04565	0.00944	0.6988	18.037	19.037
0.04195	0.00885	0.6799	19.274	20.274
0.03750	0.00770	0.6539	20.686	21.686
0.03265	0.00668	0.6208	22.645	23.646
0.02780	0.00566	0.5810	24.993	25.993
0.02340	0.00475	0.5375	27.565	28.565
0.01655	0.00334	0.4494	32.768	33.768
0.01085	0.00218	0.3473	38.802	39.802
0.00600	0.00120	0.2264	45.941	46.941

$$\frac{F}{D} = \frac{x_D - x_B}{x_F - x_B} \qquad (60)$$

The rates required for this distillation system can now be determined from the data in Table 6 and a knowledge of the concentration of light water within the reactor system as a function of time. The variation of light water concentration as a function of time is given in

Figure 4.

The rate equations can be obtained by a material balance between the reactor system and the distillation system. Figure 6 shows a simplified flow sheet of a distillation system for shim control of a nuclear reactor. The material balances are made on this system. The excess moderator or storage and the contents of the moderator and coolant with reactor will be considered as the reactor inventory. At any time, t, after the start of a fuel cycle the amounts of liquid in the reactor, the enriched storage, and the depleted storage are given by Equations 61, 62, and 63.

$$R(t) = R(o) - \int_o^t F(t)dt + \int_o^t H(t)dt + \int_o^t T(t)dt \qquad (61)$$

$$E(t) = E(o) + \int_o^t B(t)dt - \int_o^t H(t)dt \qquad (62)$$

$$S(t) = S(o) + \int_o^t D(t)dt - \int_o^t T(t)dt \qquad (63)$$

where

$R(t)$ is the reactory inventory at time t

$E(t)$ is the enriched storage inventory at time t

$S(t)$ is the depleted storage inventory at time t

$F(t)$ is the feed rate to the distillation system at time t

$D(t)$ is the overhead products rate at time t

$B(t)$ is the bottoms product rate at time t

$H(t)$ is the flow from enriched storage to the reactor

$T(t)$ is the flow from depleted storage to the reactor.

The mol fraction concentration of H_2O at any time t in the reactor, the enriched storage, and the depleted storage are given by Equations 64, 65, and 66.

$$x_E(t) = \frac{R(o)x_R(o) - \int x_R(t)F(t)dt + \int x_S(t)T(t)dt + \int x_E(t)H(t)dt}{R(t)} \qquad (64)$$

$$x_E(t) = \frac{x_E(o)S(o) + \int x_B D(t)dt - \int x_E(t)T(t)dt}{E(t)} \qquad (65)$$

$$x_s(t) = \frac{x_S(o)S(o) + \int x_D D(t)dt - \int x_S(t)T(t)dt}{S(t)} \qquad (66)$$

where x(t) is the mol fraction concentration of H_2O.

In the above equations the subscripts R, S, E, B, D, and F indicate reactor system, depleted storage, enriched storage, distillation bottoms product, distillation overheads product, and feed. The feed concentration, x_F, is the same as the concentration within the reactor, x_R.

The relationships for the flow rates from the enriched storage to the reactor, H(t), and the flow rate from the depleted storage to the reactor, T(t), can be obtained by combining Equations 61 and 64.

$$\int R(o) \left[x_R(t) - x_R(o)\right] dt - \int F(t)\left[x\,(t) - x_R(t)\right] dt + \int H(t) \left[x_R(t) - x_E(t)\right] dt + \int T(t) \left[x_R(t) - x_s(t)\right] dt = o \qquad (67)$$

Upon differentiating Equation 67, Equation 68 is obtained.

$$R(o) \left[x_R(t) - x_R(o)\right] + H(t) \left[x_R(t) - x_E(t)\right]$$
$$+ T(t) \left[x_R(t) - x_S(t)\right] = 0 . \qquad (68)$$

In the operation of this system for shim control, flow to the reactor system at any time will be either from the enriched storage or the depleted storage, but not from both. Therefore when H(t) has a non-zero value T(t) is zero, and when T(t) has a non-zero value H(t) is zero. Thus, H(t) and T(t) can be expressed by Equations 69 and 70.

$$H(t) = R_o \frac{x_F(t) - x_F(o)}{x_E(t) - x_F(t)} \qquad (69)$$

$$T(t) = R_o \frac{x_F(t) - x_F(o)}{x_S(t) - x_F(t)} \qquad (70)$$

To keep the reflux patio of the system constant the overheads product must be removed at a constant rate, i.e., D is constant. If this rate is too low enough light water will not be removed and the fuel cycle will end too quickly. If the rate is too high all of the moderator will be removed from the reactor and again the fuel cycle will be ended early.

To illustrate the above effect in shim control by distillation, three ratios of yearly overhead product removal to initial reactor system inventory are studied. These three ratios were 0.065, 0.060, and 0.056. These studies are made in the manner described below.

The first step in these studies is to divide the fuel cycle into a series of time intervals. The length of these time intervals varied from 13 to 39 days depending on the rate of chance of the H_2O concentration with time. During these time intervals the concentration of H_2O is assumed to vary linearly, so that a numerical average can be taken as the average H_2O concentration in the feed. Using the average H_2O concentration in the feed, x_F, average values of H_2O concentration in the overheads product, x_D, the bottoms product, x_B, and the feed rates and bottoms product as a function of initial reactor inventory can be determined from Table 6. (Actually the values of x_F listed in Table 6 are the average values of H_2O concentration used.) Using the values from Table 6, the values of reactor system inventory, depleted storage and enriched storage can be determined. (The depleted storage and enriched storage and their part in shim control is discussed in Chapter VI.)

Over each of the time intervals the various rates and concentrations are assumed to be independent of time, so that Equations 61, 62, 63, 65, 66, 69 and 70 can be modified to become Equations 71 through 77.

$$R(t_2) = R(t_1) - F\Delta t + H\Delta t + T\Delta t \tag{71}$$

$$E(t_2) = E(t_1) + B\Delta t - H\Delta t \tag{72}$$

$$S(t_2) = S(t_1) + D\Delta t - T\Delta t \tag{73}$$

$$x_E(t_2) = \frac{x_E(t_1)E(t_1) + x_B B\Delta t - x_E(t_1)H\Delta t}{E(t_2)} \tag{74}$$

$$x_S(t_2) = \frac{x_S(t_1)S(t_1) + x_D D\Delta t - x_S(t_1)T\Delta t}{S(t_2)} \tag{75}$$

$$H = R(t_1)\,\frac{x_F(t_2) - x_F(t_1)}{x_E(t_2) - x_F(t_2)} \tag{76}$$

$$T = R(t_1)\frac{x_F(t_2) - x_F(t_1)}{x_S(t_2) - x_F(t_2)} . \qquad (77)$$

In these equations Δt is $\overset{t}{\underset{o}{}}$ dt.

It can be shown that for values of HΔt less than $E(t_1)$ + BΔt or TΔt less than $S(t_1)$ + DΔt, Equations 74 and 75 can be written as Equation 78 and 79.

$$x_E(t_2) = \frac{x_E(t_1)E(t_1) + x_B B\Delta t}{E(t_1) + B\Delta t} \qquad (78)$$

$$x_S(t_2) = \frac{x_E(t_1)S(t_1) + x_D D\Delta t}{S(t_1) + D\Delta t} \qquad (79)$$

The fraction of liquid in reactor system, the enriched storage and the depleted storage for each to the three ratios of yearly overheads product to reactor inventory are given in Table 7. Figure 9 shows the fraction of the heavy water in the reactor system for each of the three ratios.

The ratio 0.065 is too high and after 376 days all of the moderator is removed from the reactor. The ratio 0.056 is too low and after 398 days all of the moderator is removed from the enriched storage so that shim control is no longer possible. With a 0.060 ratio of yearly overheads product to reactor inventory it is possible to obtain a fuel cycle length of 433 days. It is this ratio that is used in this demonstration.

The amount of water in the initial reactor inventory now can be determined. The reactor must always contain at least 368.5 metric tons of a light-heavy water mixture. This amount is needed to assure enough moderator and coolant for the operating reactor. According to Figure 9

Table 7. Fractions of heavy water in reactor system, enriched storage, and depleted storage

Time days	Ratio 0.056			Ratio 0.060			Ratio 0.065		
	R	S	E	R	S	E	R	S	E
0	0.9868	0.0132	0.0000	0.9878	0.0122	0.0000	0.9875	0.0124	0.0000
13	0.9482	0.0058	0.0452	0.9540	0.0042	0.0418	0.9570	0.0042	0.0388
27	0.9067	0.0023	0.0902	0.9161	0.0005	0.0832	0.9222	0.0004	0.0773
56	0.8183	0.0027	0.1782	0.8347	0.0006	0.1647	0.8470	0.0001	0.1529
86	0.7280	0.0056	0.2656	0.7512	0.0034	0.2454	0.7698	0.0024	0.2278
117	0.6670	0.111	0.3211	0.6992	0.0084	0.2923	0.7255	0.0071	0.2674
149	0.6084	0.0167	0.3796	0.6452	0.0136	0.3412	0.6804	0.0119	0.3077
181	0.5498	0.0223	0.4322	0.5994	0.0188	0.3819	0.6458	0.0167	0.3375
213	0.4951	0.0279	0.4813	0.5613	0.0239	0.4148	0.6225	0.0215	0.3559
244	0.4475	0.0333	0.5234	0.5365	0.0290	0.4346	0.6182	0.0262	0.3556
276	0.3868	0.0389	0.5785	0.5082	0.0341	0.4576	0.6190	0.0310	0.3500
307	0.3142	0.0444	0.6457	0.4824	0.0391	0.4784	0.6344	0.0356	0.3300
346	0.1784	0.0512	0.7746	0.4502	0.0454	0.5043	0.6902	0.0415	0.2683
383	0.0000[a]	0.0565	0.9435	0.4450	0.0515	0.5098	0.8503	0.0471	0.1024
420				0.5832	0.0575	0.3648	0.9492	0.0508	0.0000[b]
433				0.9404	0.0596	0.0000			

[a] The reactor inventory is depleted in 376 days.

[b] The enriched storage is emptied in 398 days.

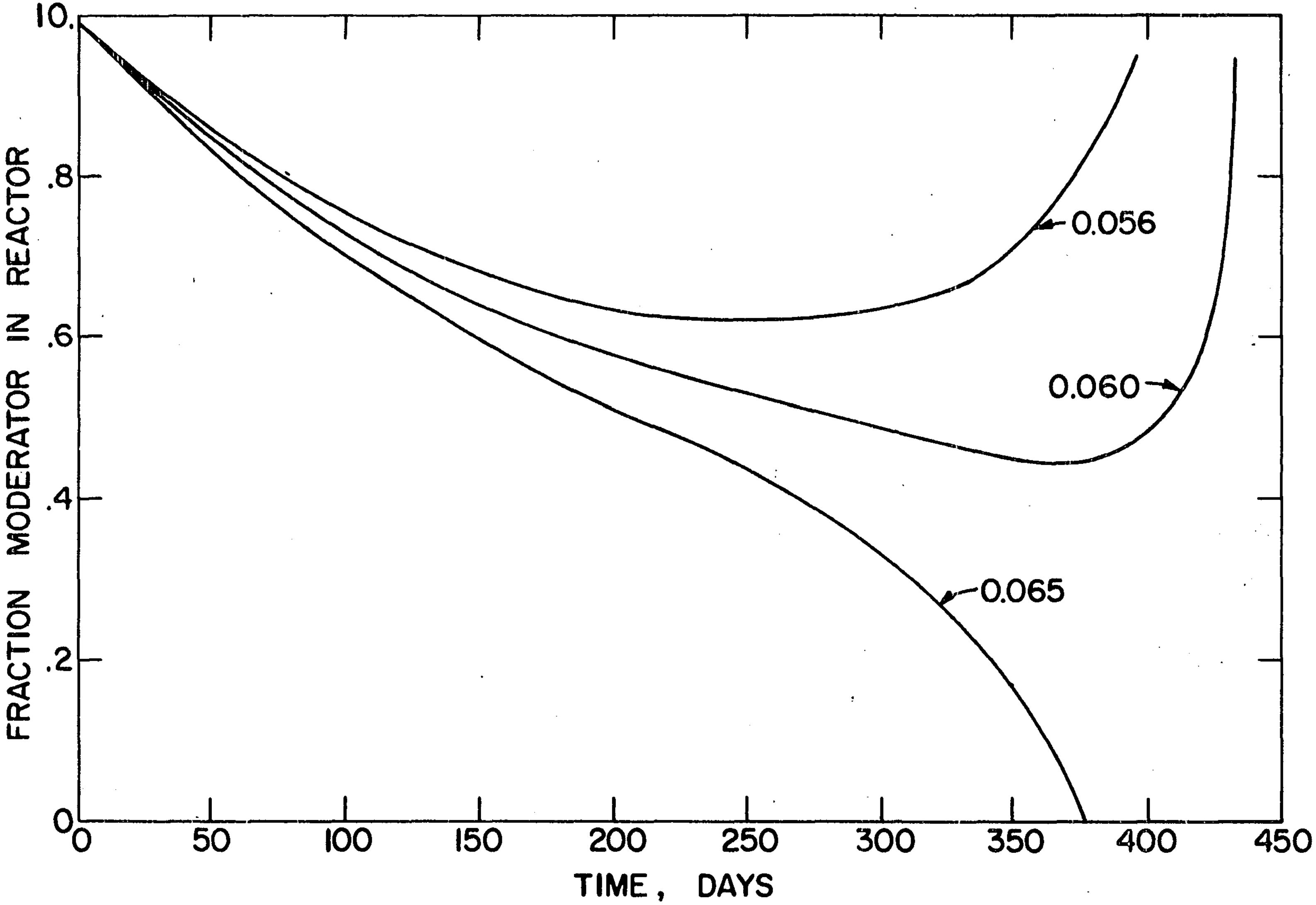

FIGURE 9. FRACTION OF MODERATOR IN REACTOR FOR VARIOUS RATIOS OF OVERHEAD TO INVENTORY.

for the ratio of 0.060, the minimum fraction in the reactor system is 0.44 and this occurs at 366 days after the start of the fuel cycle. Thus to maintain the minimum of 368.5 metric tons with the reactor system, the initial reactor inventory must be 780 metric tons of heavy water.

The overheads product rate is determined from the 0.060 ratios and the initial reactor inventory. This rate is 11.72 pounds per hour. For a reflux ratio of 1600, the reboilers must vaporize 18,750 pounds per hour. The flow rates of B, F, H, and T are given in Table 8.

Table 8. Distillation unit flow rates

Time (days)	B (lbs/hr)	F (lbs/hr)	H (lbs/hr)	T (lbs/hr)
0-13	262	274	0	58.5
13-27	224	236	0	31.8
27-56	211	223	0	11.9
56-86	203	215	0	5.4
86-117	203	215	89	0
117-149	211	223	96	0
149-181	220	232	124	0
181-213	236	248	159	0
213-244	232	264	206	0
244-276	290	302	222	0
276-307	305	317	254	0
307-346	336	348	289	0
346-383	400	412	392	0
383-420	479	491	725	0
420-434	540	552	2720	0

Bebbington and Thayer (4) indicate that for this type of column the optimum vapor velocity is 13.3 ft/sec or at these pressures 270 $\frac{\text{lbs}}{\text{hr.sq.ft.}}$. For a total vapor flow of 18,750 pounds per hour the cross section of the tower is 69.6 sq.ft. This corresponds to tower diameter of 9.42 feet.

For bubble cap towers used in D_2O distillation the overall plate efficiency is 70% (4). Thus for the three towers of 58 theoretical plates each, each tower will have 83 actual plates. As a comparison, the production of heavy water at the Dana Plant in Dana, Indiana, towers are used that are 10.5 feet in diameter with 72 plates, and also towers 8.0 feet in diameter with 83 plates.

VIII. CHARACTERISTICS OF SHIM CONTROL BY LIGHT WATER REMOVAL

From the results of the preceding chapters it is seen that shim control of heavy-water moderated power reactors by removal of a light-water poison is possible. The distillation system required for a 250 electrical megawatt nuclear power plant is described in Chapters VI and VII.

For this particular system criticality can be maintained for 433 days. This is based on the reactor operating at a thermal power of 1000 megawatts. For a fuel loading of 76 metric tons of uranium, a burn up of 5,700 megawatt days per ton of uranium is obtained. Based on the plutonium concentration at the end of the fuel cycle, 159 kilograms of plutonium are produced and are available for use as plutonium credit.

The radial flux distribution is given in Figure 10. From this figure the maximum-to-average flux is determined to be 1.63505. The flux distribution was determined by a computer code AIM-6 (15) which is described in Appendix B.

Part of the study of the feasibility of shim control by light water removal will be a comparison with other methods of shim control. For heavy-water reactors of this type, estimates of burn up have been obtained (2). For a 200 megawatt electric nuclear power plant a burn up of 6800 megawatts a day per metric ton of uranium was obtained. And for a 300 megawatt electric nuclear power plant the burn up is estimated to be 7800 megawatt days per ton. These two estimates are for a four zone refueling scheme. This means that one-fourth of the fuel is replaced at a time. This zone refueling increases the attainable burn up. In studies

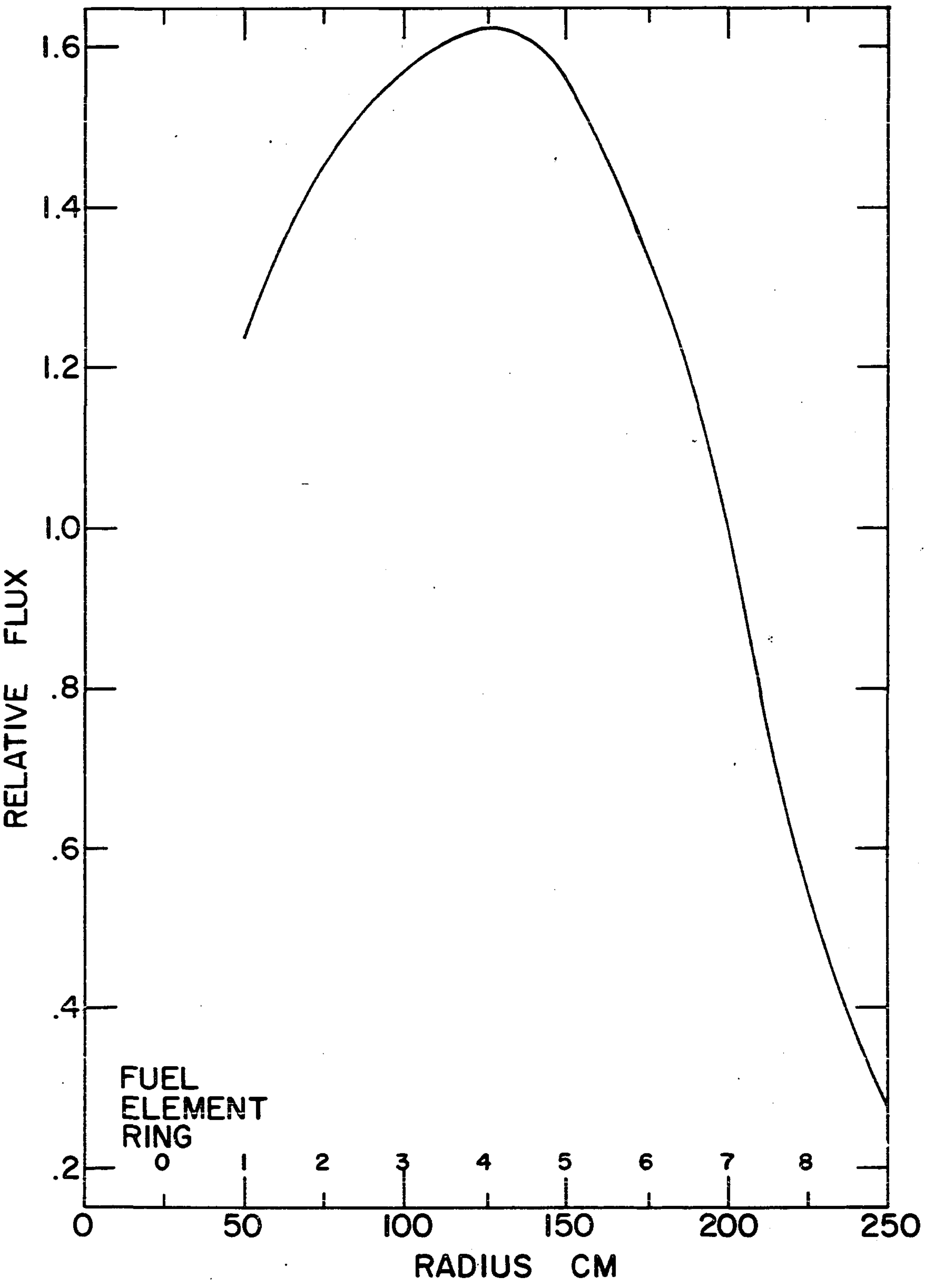

FIGURE 10. RELATIVE FLUX IN FUEL ELEMENTS.

by Sargent and Lundy (33). the burn up in this type of reactor is increased approximately 45% by changing from batch refueling to a three zone refueling technique. The reactor model chosen for this study is assumed to be batch refueled. Such an assumption simplifies the criticality calculations. If the refueling were to be changed to a three zone refueling scheme and the burn up was assumed to be increased by 45%, then the attainable burn up would be 8,250 megawatt days per ton of uranium.

Because the estimated burn up is a function of the technique used in its calculation, another comparison of burn up can be made using the same techniques of calculation as are used in this demonstration. In this comparison a reactor model similar to that described in Section III is chosen except that the D_2O concentration is maintained at a constant 99.75 mol per cent. These calculations are described on page 35 and the results presented in Figure 5. The length of time that criticality can be maintained with such a reactor is 466 days. For fuel loading of 76 metric tons of uranium and a thermal power level of 1000 megawatts the burn up attainable is 6,150 megawatt days per metric ton of uranium. This reactor produces 164 kilograms of plutonium. This value of burn up and plutonium production are probably high since in their calculation no account is made of the disturbance of the neutron fluxes caused by the shim control rods.

The economic feasibility of shim control by light water removal is dependent on five main factors. These are

1) Control rod cost

2) Distillation equipment cost

3) D_2O inventory cost

4) Attainable burn up

5) Plutonium credit.

Of these only the first three will be considered here. The last two, burn up and plutonium credit will be assumed the same until further information is available. There are also some lesser costs that will be neglected. Among these lesser items are operating cost for the distillation system and in-leakage of light water to the system. The distillation operating cost work in favor of shim control by rods. The smaller distillation unit would result in less operating expense. On the other hand, in-leakage of water works in favor of shim control by light water removal. Because a greater amount of light water can leak into this system certain tolerances can be lessened. (Sargent and Lundy (34) have determined that a savings of .06 mil/kwhr could be realized from a 95% D_2O concentration compared to a 99.75 per cent D_2O concentration. The main savings is in the fact that more light water could leak into the reactor.)

The cost comparisons of the two methods of shim control is based on the costs prevailing in 1959, the date of the cost of the shim rod controlled reactor.

The cost of a bubble cap distillation tower 9 feet 6 inches in diameter, made of ordinary steel is $1200 per plate based on an Engineering News Record Index(ENR) of 400 (9). The ENR Index in July 1959, was 804.61 (10). Thus for an 83 plate distillation tower the installed cost in 1959 was $200,000. (The October, 1963, ENR Index was 914.88 (11), so the 1963 cost is $228,000.) The total cost of three such towers and the associated condensers, tanks, and instrumentation is \$840,000. The depreciation rate on nuclear plants is 14% per year, therefore the yearly cost is \$117,500.

The comparable cost associated with the rod controlled reactor must include not only the distillation cost but also the costs of the rods. The 1959 cost of the distillation unit is \$164,700 (33), or \$23,000 annually. The costs of the rods is \$24,100 a piece (34). A 1000 thermal megawatt reactor of this type will require 23 shim rods (33). The control rod cost is \$555,000 per set. If the control rods last for one fuel cycle, then for a 433 day fuel cycle, and a load factor of .8, the lifetime is 1.48 years. The annual cost is \$375,000. (Sargent and Lundy (34) give the life of control rods as approximately one year.) Based on the depreciation of equipment cost and the cost of control rods, the annual cost of shim control by shim rods is \$398,000. This compares with shim control by light water removal cost of \$117,500.

However, the value of the 368.5 metric tons of heavy water required in the shim rod controlled reactor is \$22,700,000 based on a D_2O price of \$28 per pound (34). The value of 780 metric tons of 97.31 mol per cent D_2O is \$45,000,000 based on a price of \$26.60 per pound. In cost estimation, the AEC requires the D_2O be depreciated at a rate of 12.5 per cent per year. Then the inventory charges for the rod controlled reactor are only \$2,840,000 per year compared with \$5,640,000 per year for a reactor shim controlled by light water removal. This is a net disadvantage for the light water removal technique of \$2,519,500 per year or 1.42 mil per kilowatt hour.

Another consideration of interest is the temperature and void coefficients of reactivity. For this reactor system two temperature coefficients of reactivity were examined. Temperature coefficients of reactivity are determined by making two reactivity calculations. One is made at a reference temperature and the second at a temperature 100°C higher.

The number densities of the liquids are changed properly and the microscopic cross sections are recalculated by the methods of Appendix A. The first temperature coefficient considered only an increase in the temperature of the fuel elements and the associated coolant. This temperature coefficient as a function of light water enrichment is given in Figure 11. This temperature coefficient is always negative.

The second coefficients considered a temperature rise that is assumed to be the same for both moderator and fuel-coolant. These coefficients are presented in Figure 12. Part of these coefficients are positive and this is because of contribution of the moderator. The assumption that the temperature rise in the moderator is equal to the temperature rise of the fuel and coolant is overly conservative. The large heat capacity of the moderator as compared with fuel and coolant where the heat is being generated would make the temperature rise within the moderator only a small fraction of the temperature rise within the fuel and coolant. If this fact had been taken into consideration the overall temperature coefficients would have been negative.

The void coefficient of the coolant is determined by reducing the number density of the coolant by a given percentage, and then based on this reduced coolant number density the reactivity of the system is recalculated. The void coefficient of the coolant is shown in Figure 13.

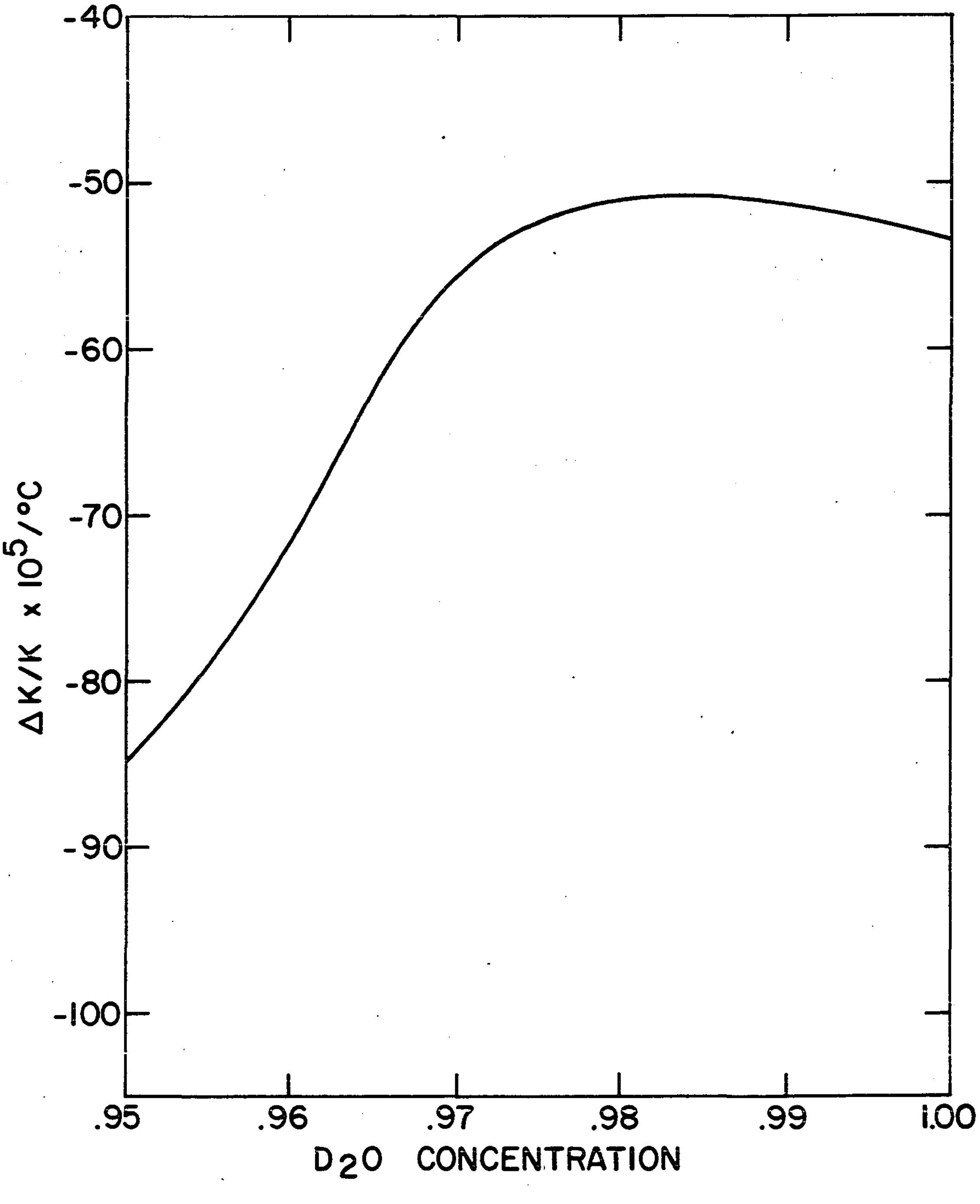

FIGURE 11. TEMPERATURE COEFFICIENT OF REACTIVITY FOR TEMPERATURE RISE IN FUEL AND COOLANT.

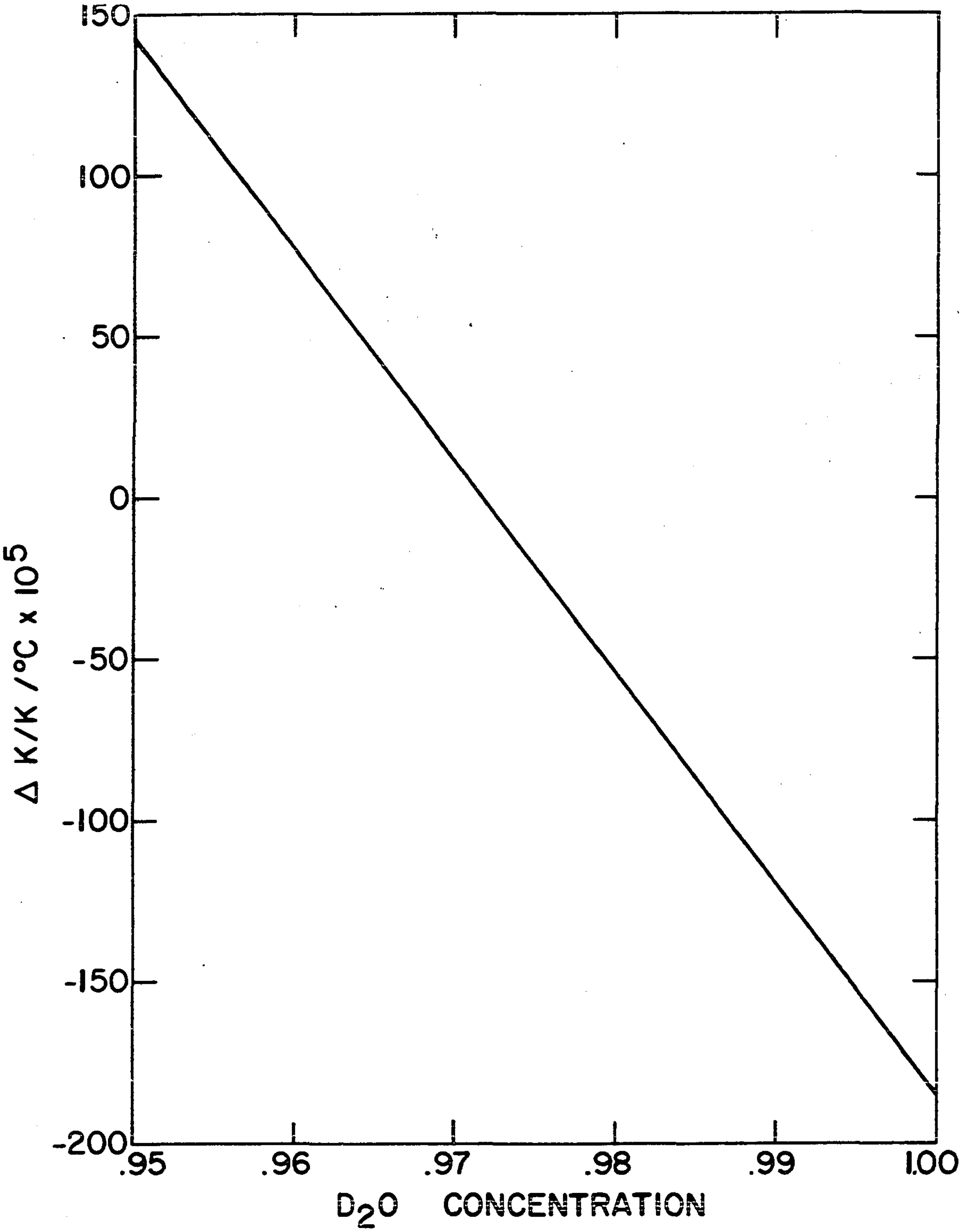

FIGURE 12. TEMPERATURE COEFFICIENT OF REACTIVITY UNIFORM TEMPERATURE RISE.

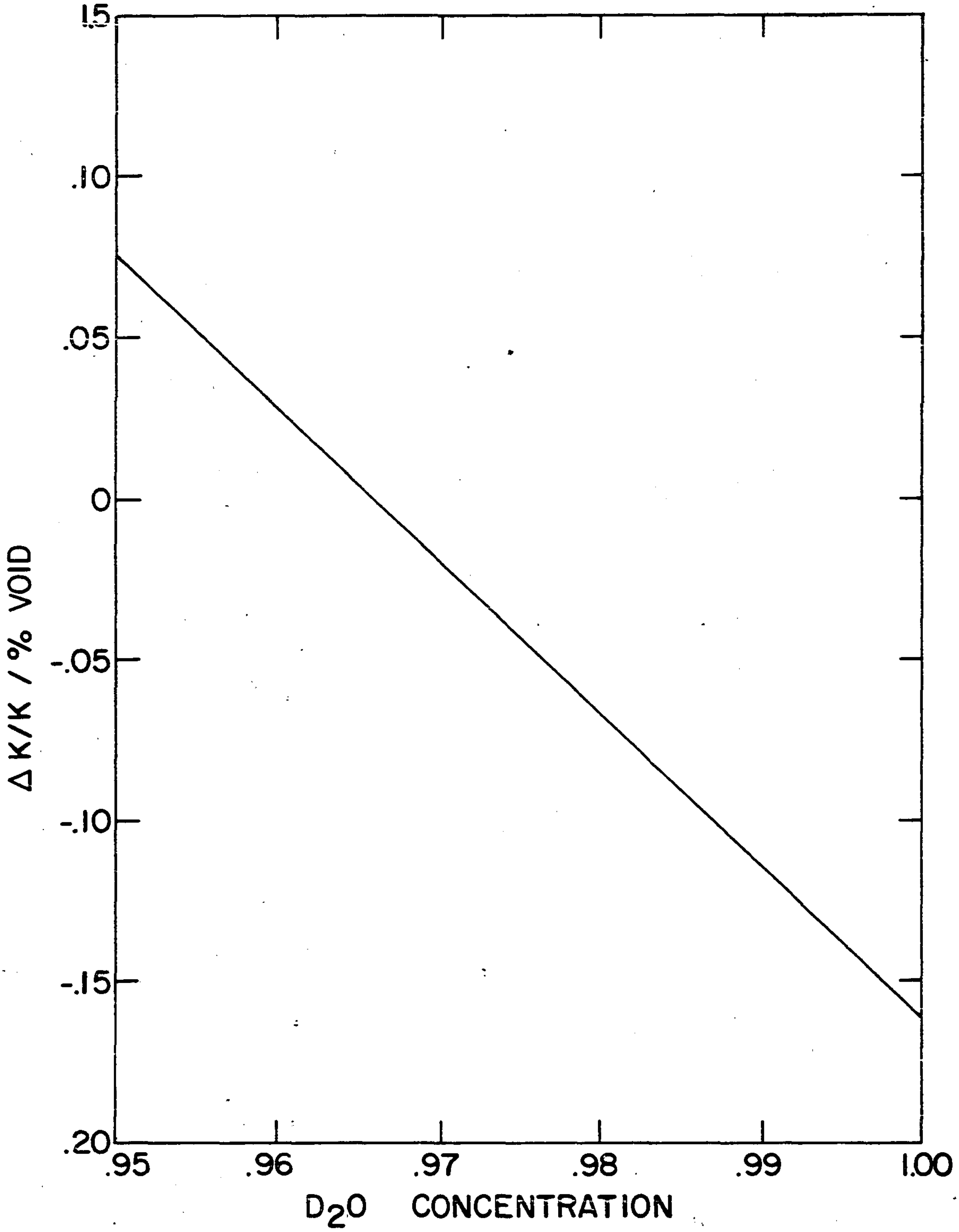

FIGURE 13. COOLENT VOID COEFFICIENT OF REACTIVITY.

Although it is positive it is small (31) and when coupled to the negative temperature coefficient should present no difficult control problems.

IX. CONCLUSIONS AND RECOMMENDATIONS

In the previous section it was shown that although shim control of heavy-water reactors is possible by removing a light-water poison, it is not economically advantageous with the distillation technique proposed here. The main disadvantage is the greater amount of D_2O inventory required, and if some way can be found to reduce the inventory, this method of shim control may have an economic advantage.

It is recommended that in any future study of this problem a multizone refueling scheme be considered. This would have two promising effects. First, it would increase the attainable burn up. Second, the use of multizone refueling would reduce the amount of excess reactivity that must be controlled. This would reduce the distillation requirements and hence the D_2O inventory requirements.

Another method to reduce the heavy water inventory would be to use the same distillation system for shim controlling several reactors in a power complex. These reactors would have their refueling cycles out of phase with each other. In this way the enriched D_2O storage of one reactor would be used as the moderator for another reactor. This would spread the extra inventory cost over several reactors and increase the economic feasibility.

Before this system of shim control could be used in a power reactor further study should be made into the reactor kinetics. The main purpose of this study would be to make sure that moderator temperature coefficients and coolant void coefficients have no adverse effect on reactor stability.

X. REFERENCES

1. Argonne National Laboratory. Reactor physics constants. U. S. Atomic Energy Commission Report ANL-5800. [Argonne National Laboratory, Lamont, Illinois] 1958.

2. Babcock, D. F. Heavy water moderated power reactors. U. S. Atomic Energy Commission Report DP-480. (E. I. duPont deNemours and Co., Wilmington, Delaware) 1960.

3. ________, R. R. Hood, L. Isakoff, J. C. Jensen, D. S. St. John, and J. W. Wade. An evaluation of heavy-water-moderated power reactors. U. S. Atomic Energy Commission Report DP-830. (E. I. duPont deNemours and Co., Wilmington, Delaware) 1963.

4. Bebbington, W. P. and V. R. Thayer, ed. Production of heavy water Savannah River and Dana Plants. U. S. Atomic Energy Commission Report DP-400. (E. I. duPont deNemours and Co., Wilmington, Delaware) 1959.

5. Benedict, M. and T. H. Pigford. Nuclear chemical engineering. New York, N. Y., McGraw Hill Book Company, Inc. 1957.

6. Bertsche, E. C. Distillation of light water from heavy water moderator. U. S. Atomic Energy Commission Report DP-325. (E. I. du Pont deNemours and Co., Wilmington, Delaware) 1958.

7. Carolinas Virginia Nuclear Power Associates. Final hazards summary report, Carolina Virginia Tube Reactor. 4 vols. U. S. Atomic Energy Commission Report CVNA-90. (Carolinas Virginia Nuclear Power Associates, Columbia, South Carolina) 1961.

8. Case, K. M., F. deHoffman, and G. Placzek. Introduction to the theory of neutron diffusion. Washington, D. C., Government Printing Office. 1953.

9. Chilton, C. H. Cost data correlated. Chemical Engineering 56, No. 6: 97-106. June 1949.

10. Construction scoreboard. Engineering News Record 163, No. 1: 73. July 2, 1959.

11. Construction scoreboard. Engineering News Record 171, No. 17: 61. October 24, 1963.

12. Crandall, J. L. Status of the United States effort in D_2O reactor physics. U. S. Atomic Energy Commission Report DP-787. (E. I. duPont deNemours and Co., Wilmington, Delaware) 1962.

13. Daniels, F. and R. A. Alberty. Physical chemistry. New York, N. Y., John Wiley and Sons, Inc. 1955.

14. Davis, M. V. and D. T. Hauser. Thermal-neutron data for the elements. Nucleonics 16, No. 3: 87-89. March 1958.

15. Flass, H. P. and D. C. Baller. The AIM-6 code. Canoga Park, California., Atomics International. 1961.

16. Fleishman, M. R. and H. Soodak. Methods and cross sections for calculating the fast effect. Nuclear Science and Engineering. 7: 217-227. 1960.

17. Foust, A. S., L. A. Wenzel, C. W. Clump, L. Maus and L. B. Anderson. Principles of unit operations. New York, N. Y., John Wiley and Sons, Inc. 1960.

18. Friedlander, G. and J. W. Kennedy. Nuclear and radio-chemistry. New York, N. Y., John Wiley and Sons, Inc. 1955.

19. Glasstone, S. Principles of nuclear reactor engineering. Princeton, N. J., D. Van Nostrand Company, Inc. 1955.

20. ________ and M. C. Edlund. The elements of nuclear reactor theory. Princeton, N. J., D. Van Nostrand Company, Inc. 1952.

21. Hellstrand, E. Measurements of the effective resonance integral in uranium metal and oxide in different geometries. Journal of Applied Physics 28: 1493-1502. 1957.

22. ________, P. Blomberg, and S. Horner. The temperature coefficient of the resonance integral for uranium metal and oxide. Nuclear Science and Engineering 8: 497-506. 1960.

23. Hughes, D. J. and R. B. Schwartz. Neutron cross sections. 2nd ed. U. S. Atomic Energy Commission Report BNL-325. [Brookhaven National Laboratory, Upton, N. Y.] 1958.

24. Hurst, D. G., J. M. Kennedy, and W. H. Walker. Cross sections and yields of pseudo-fission products. U. S. Atomic Energy Commission Report CRRP-760. (Chalk River Project, Chalk River, Ontario, Canada) 1958.

25. International Business Machines Corporation. General information manual Fortran. New York, N. Y., International Business Machines Corporation. 1961.

26. Keenan, J. H. and F. G. Keyes. Thermodynamic properties of steam. 1st ed. New York, N. Y., John Wiley and Sons, Inc. 1936.

27. Kirshenbaum, I. Physical properties and analysis of heavy water. New York, N. Y., McGraw Hill Book Company, Inc. 1951.

28. Klug, N. P. and P. F. Zwiefel. An H_2O-D_2O moderated reactor. Nuclear Science and Engineering 7: 541-544. 1960.

29. Lewis, W.B. Basic considerations of the full scale heavy water and natural uranium power plant (Atomic Energy of Canada Limited, Chalk River Project, Chalk River, Ontario, Canada) U. S. Atomic Energy Commission Report DM-57. 1959.

30. McCabe, W. L. and J. C. Smith. Unit operations of chemical engineering. New York, N. Y., McGraw Hill Book Company, Inc. 1956.

31. Murray, R. L. Nuclear reactor physics. Englewood Cliffs, N. J., Prentice-Hall, Inc. 1957.

32. Pershagen, B., G. Andersson and I. Carlvik. Calculation of lattice parameters for uranium rod clusters in heavy water and correlation with experiments. International Conference on the Peaceful Uses of Atomic Energy, 2nd, Geneva, 1958, Proceedings 12: 341-350. 1958.

33. Sargent and Lundy Engineers. Evaluation and design of heavy water moderated power reactor plants. U. S. Atomic Energy Commission Report TID-8530. [Technical Information Service, AEC]. 1960.

34. Sargent and Lundy Engineers and Nuclear Development Corporation of America. Heavy water moderated power reactor plant design study. Parts 1 and 2. U. S. Atomic Energy Commission Report TID8503. [Technical Information Service, AEC]. 1959.

35. Scotten, W. C., ed. Recovery of degraded heavy water at the Savannah River Plant. U. S. Atomic Energy Commission Report DP-470. (E. I. duPont deNemours and Company, Aiken, South Carolina). 1960.

36. Smyth, H. D. Atomic energy for military purposes. Princeton, N. J., Princeton University Press. 1946.

37. Soodak, H. and R. Sullivan. A method for calculating the reactivity of D_2O moderated natural uranium lattices with clustered rod fuel elements. U. S. Atomic Energy Report NDA-2131-38. [Nuclear Development Associates, Inc., White Plains, N. J.] 1961.

38. Spinrad, B. I. Fast effect in lattices reactors. Nuclear Science and Engineering 1: 455-460. 1956.

39. Wehmeyer, D. B., J. M. Doederlein, K. E. Roach, and W. A. Wittkopf. Spectral shift control reactor basic physics program. 2 parts. U. S. Atomic Energy Commission Report BAW-1230. [Babcock and Wilcox, New York]. 1962.

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

XI. ACKNOWLEDGEMENTS

The author would like to express his gratitude to Dr. Glenn Murphy, Anston Marston Distinguished Professor and Head of the Nuclear Engineering Department of Iowa State University of Science and Technology for his advice and guidance given during this investigation.

The author would also like to thank Mr. Ben C. Rusche of the E. I. duPont deNemours Company's Savannah River Laboratory who first suggested this topic and who provided information on some of the properties of heavy water.

Also the author would like to thank Mr. Howard Jesperson of the Iowa State University Computation Center for the guidance he gave in the converting the AIM-6 code to use with the IBM-7074.

XII. APPENDIX A

A. Number Densities

The number density of an element is the number of nucleii of that element per unit of volume. The number density is given by Equation 80.

$$N_i = \frac{\rho\, x_i}{N_{Av}\, A_i} \tag{80}$$

where

N_i is the number density of the element, number/cm^3

ρ is the physical density of the material, gm/cm^3

x_i is the atomic fraction of i

A_i is the atomic number of i

N_{Av} is Avargadro's number 6.02 x 10^{23} atoms/mol (13).

In determining the number densities of mixtures of light and heavy water one finds that only a limited amount of data is available on the density of pure D_2O. Kirshenbaum (27) gives the density of pure D_2O at 25°C as 1.10775 ± .00016. The variation of density with temperature is given only for temperatures up to about 40°C. A ratio of D_2O density at 240°C to its density at 20°C of 0.8118 is used by Savannah River Laboratory, according to B. C. Rusche, Savannah River Laboratory, Aiken, South Carolina. (Private communication, letter concerning properties of heavy water. May 14, 1963) To find densities at other temperatures interpolation or extrapolation is used.

The density of light-heavy water mixtures is obtained by interpolation. The densities of light water are taken from Keenan and Keyes (26).

In obtaining the actual number density of the water mixtures, the first step is to obtain the overall molecular density of oxygen number density. Not only are both atom densities of hydrogen and deuterium obtained from this number, but also number densities of H_2O and D_2O. These number densities are determined for temperatures of 68°C, 168°C, and 340°C. As an example the number densities at 68°C are presented in Table 9.

Table 9. Number densities of light-heavy water mixture[a] at 68°C

X_{D_2O}	N_D	N_H	N_O	N_{D_2O}	N_{H_2O}
0.94	0.06036	0.003853	0.03211	0.03018	0.001927
0.95	0.06099	0.003210	0.03210	0.03050	0.001605
0.96	0.06120	0.002568	0.03209	0.03060	0.001289
0.97	0.06225	0.001925	0.03209	0.03112	0.000967
0.98	0.06288	0.001283	0.03208	0.03144	0.000641
0.99	0.06350	0.000641	0.03207	0.03175	0.000321
1.00	0.06413	0.000000	0.03207	0.03207	0.000000

The number densities with the fuel elements are taken at room temperature. For although the density changes, so does the dimensions, and the number of atoms remains the same. Within the fuel itself, only the number densities of the two uranium isotopes and oxygen need be determined. The number densities of plutonium and fission products are determined from the techniques in Chapter V. The initial number densities of non-water elements are based on the values of Davis and Hauser

(14) and are given in Table 10.

Table 10. Initial number densities of non-water elements at 28°C

Element	Number density
Zirconium	$0.0423 \times 10^{24}/cm^3$
Oxygen	$0.0444 \times 10^{24}/cm^3$
Uranium-238	$0.0221 \times 10^{24}/cm^3$
Uranium-235	$1.595 \times 10^{20}/cm^3$

B. Cross Sections

The thermal neutron flux is assumed to have a Maxwellian distribution of energies. For a Maxwellian energy distribution the average microscopic absorption cross section for those elements that follow the "1/v" law is given in Equation 81 (20).

$$\sigma_a (T_2) = \frac{\sqrt{\pi}}{2} \quad \sigma_a(T_1) \sqrt{\frac{T_1}{T_2}} \qquad (81)$$

where

$\sigma_a (T_2)$ is the average cross section at temperature T_2

$\sigma_a (T_1)$ is the cross section of neutrons with energy kT_1.

The 2200 m/sec cross section are used as the reference cross sections. These cross sections come from either Davis and Hauser (14), Friedlander and Kennedy (18), or Benedict and Pigford (5), or Hughes and Schwartz (23).

For those elements that do not follow the "1/v" law, a non-"1/v" correction must be applied. For Uranium 235 Benedict and Pigford (5) give a value of 0.981. This factor is applied to both absorption and fission cross sections.

For the plutonium isotopes Pu-239, Pu-240, and Pu-241 which do not follow the "1/v" law, the absorption and fission cross section are determined by averaging the Maxwellian energy distribution for temperature of 1200°K and 1300°K over the values of cross section obtained from Hughes (23).

The absorption cross sections for fission products are a function of flux time and the fissionable isotope from which the fission products come. These cross sections as a function have been experimentally determined by Hurst, Kennedy, and Walker (24). The cross section for fission products of U-235 and Pu-241 contain within them the contributions of isotopes U-236 and Pu-242 respectively.

At thermal energies the scattering cross section is assumed to be independent of energy. The transport cross section is the sum of the absorption and scattering cross sections.

The microscopic cross sections that are calculated are presented in Table 11.

Table 11. Microscopic cross sections in barns

Element	Temperature	σ_a	σ_s	σ_t	σ_f
H_2O	68°C	0.528	103	103.5	
	168°C	0.48	103	103.5	
	240°C	0.448	103	103.4	
	340°C	0.408	103	103.4	
D_2O	68°C	0.0008	13.6	13.6	
	168°C	0.0007	13.6	13.6	
	240°C	0.0007	13.6	13.6	
	340°C	0.0006	13.6	13.6	
Zr	240°C	0.12	8	8.12	
	340°C	0.11	8	8.11	
Xe 135	1200°K	1.2×10^6		1.2×10^6	
	1300°K	1.1×10^6		1.1×10^6	
Sm 149	1200°K	2.36×10^4		2.36×10^4	
	1300°K	2.28×10^4		2.28×10^4	
O	1200°K	0.00001	4.2	4.2	
	1300°K	0.00001	4.2	4.2	
U-238	1200°K	1.205	8.3	9.5	
	1300°K	1.157	8.3	9.4	
U-235	1200°K	295	8.3	303	252
	1300°K	276	8.3	283	238
Pu-239	1200°K	1371	10	1381	879
Pu-240	1200°K	445	10	455	
Pu-241	1200°K	1170	10	1180	849

XIII. APPENDIX B

The AIM-6 code (15) is a multigroup, one dimensional diffusion code written by Atomics International in FORTRAN for an IBM 704 or 709 type machine with a core memory of 32,000. The Atomics International version of this program can handle problems with 101 space points, 18 neutron energy groups, downscattering to lower groups from 17 groups, 20 regions of different materials with up to 10 elements or isotopes per region.

Since this program is written in FORTRAN (25) it can be easily adapted to other machines using the FORTRAN programing system. At Iowa State University there is an IBM-7074 computing machine and it was decided to convert the AIM-6 code to use on this machine. The IBM-7074 differs from the IBM-704 or 709 in several ways. When using the AIM-6 code there are two main differences. First the IBM-7074 has only 20,000 storage locations within its memory. Second the IBM-7074 is not capable of performing an operation called "chain". These two differences make the AIM-6 code not so easily converted to use on the IBM-7074.

The first difference caused the most changes to be made in the AIM-6 code. The most significant change made in the AIM-6 was reducing the number of energy groups from 18 to six. Then to get all the program into the 20,000 memory locations of the IBM-7074, all of the variables had to be re-assigned to new locations.

The "chain" operation is used for large programs. The program is written in a number of smaller sections. Each section is called a chain. When the program is run it is placed on tape. The chains are read from the tape into memory one at a time and that part of the program is operated. When the part is finished the next chain is called from tape into memory replacing the previous section. This procedure is repeated until the end of the last chain. When the last chain is completed, the tape is rewound, and the first chain is read from the tape into memory to start the second problem.

The Atomic International version of AIM-6 is divided into a two section chain. To adapt AIM-6 for the IBM-7074, the AI version was divided into two separate programs. The first one and its data are read into memory. When the operations of this program are completed, the variables that have been calculated are read from the memory to an auxiliary tape. The second program is read into the memory. The first operation of the second program is to read the variables from the auxiliary tape back into memory.

Although this procedure does allow the AIM-6 to be used on the ISU computer, only one problem at a time can be run. Both programs must be reloaded for each problem.

The input data for this code is described in the AIM-6 program description (15). Because of the modifications made on this code, there are four changes in the required input data.

First, the six group microscopic cross sections for 19 different elements must be included. This data is prepared as a package which is loaded immediately after the program and just before the data described in the program description (15). In the cross section library there is one card for each energy group of each element. Each card contains eight cross sections. They are the absorption cross section, the fission cross section times "ν", the scattering cross section, and then five cross sections for scattering from a higher energy group.

Although all elements or groups may not be used; nevertheless, 114 cards must be included in the library.

The second change required in the input data is the atomic weights of the elements in the cross section library. The atomic weights are listed with the "floating point data." These weights are placed in locations 1997 through 2015 of the "floating point data." (See the program description (15) for details of "floating point data").

The third change required in the input data is the fission spectrum. This spectrum is provided by the fraction of neutrons born in each energy group. These fractions must be included with the "floating point data," and are placed in locations 7124 through 7129 of the "floating point data."

The fourth change in the input data is the lethargy of each energy group. The lethargies are included in the "floating point data," and are placed in locations 1216 through 1221.

This modified version of the AIM-6 code is used for the determination of the flux distribution with the reactor model. The reactor is considered to be a cylinder. The fuel elements are homogenized into rings, which include uranium, oxygen, zirconium, xenon, and samarium. The moderator and coolant are also homogenized into rings, and consist of hydrogen, deuterium, and oxygen. Thus the model has 9 fuel rings and 10 moderator rings.

Four neutron energy groups are used. (The cross sections of groups 5 and 6 are made zero in the library.) The cross sections used are listed in Table 12. The input data used in these calculations is listed in Table 13.

(The microscopic cross sections and number densities of xenon and samarium are adjusted so that the correct macroscopic cross section is obtained. This is necessary due to the limit of significant figures in the number densities. The number densities are used as data in terms of numbers times 10^{24}. Only 6 figures are carried, so the minimum number density is 10^{18}. Although xenon and samarium concentrations are less than 10^{18}, they have very large cross sections. Therefore the real number densities of these isotopes are increased by some factor and the cross sections decreased by the same factor. In this way the correct macroscopic cross sections are obtained.)

Table 12. Cross section library for AIM-6 code

Element	Group	σ_a	$\nu\sigma_f$	σ_t	σ_{tr1}	σ_{tr2}	σ_{tr3}
U-235	1	1.44	3.5238	6.539			
	2	2.90	5.4923	9.5244	1.92		
	3	47.1	74.78	24.0			
	4	295.2	623.7	303.5			
	5						
	6						
U-238	1	0.43565	0.987392	5.68233			
	2	0.403300	0.000331	1.92			
	3	0.328		8.53			
	4	1.205		9.5			
	5						
	6						
H	1	0.00040		1.54			
	2	0.00040		2.6575	1.475		
	3	0.01236		6.348		2.085	
	4	0.264		49.65			2.13103
	5						
	6						
D	1			1.305			

Table 12. (Continued)

Element	Group	σ_a	$\nu\sigma_f$	σ_t	σ_{tr1}	σ_{tr2}	σ_{tr3}
	2			2.3204	0.3679		
	3			2.27606		0.46562	
	4	0.0004		4.7			0.59465
	5						
	6						
Pu-239	1-6	This element not used, place 6 blank cards					
Pu-240	1-6	This element not used, place 6 blank cards					
Xe-135	1-3						
	4	1.2		1.2			
	5						
	6						
Sm-149	1-3						
	4	1.0		1.0			
	5						
	6						
F.P. 25	1-6	This element not used, place 6 blank cards					
F.P. 49	1-6	This element not used, place 6 blank cards					
Pu-241	1-6	This element not used, place 6 blank cards					
0	1	0.0247		2.5386			
	2			3.618	0.2085		
	3			3.798		0.0955	
	4	0.00001		4.2			0.049
	5						
	6						
	1-6	13th element not specified, place 6 blank cards					
	1-6	14th element not specified, place 6 blank cards					
	1-6	15th element not specified, place 6 blank cards					
Zr	1			3.841			
	2			7.8391	0.583		
	3	0.0077		6.384		0.05	
	4	0.12		8.12			0.02
	5						
	6						
	1-6	17th element not specified, place 6 blank cards					
	1-6	18th element not specified, place 6 blank cards					
	1-6	19th element not specified, place 6 blank cards					

Table 13. Input data for AIM-6 code

Number	Description	Remarks
+ 1	MTEST	No changes to library
0	DTEST	Simple diffusion coefficient
19 4 3 2	M,NOG,NDS,MA	Regions, groups, downscattering, materials
1 2 1 2 1 2	R1,R2,R3,...	The material in each region
1 2 1 2 1 2	....	
1 2 1 2 1 2	....	
1 2 1 2 1	..... R19	
3 1	Load Instr.	Number densities of material 1
3.0025678		Number density of element 3,H
4.061205		Number density of element 4,D
12.032094		Number density of element 12,0
5 11	Load Instr.	Number densities of material 2
2.016113		No. density of element 2, U-238
1.00011629		No. density of element 1, U-235
7.0017029		No. density of element 7, Xe
8.000523		No. density of element 8, Sm
12.032517		No. density of element 12, 0
11 16	Load Instr.	Material 2 No. densities con't.
16.011460		No. density of element 16, Zr
1 CONC. SEARCH ZERO BURNUP UNIFORM XE-SM		Alphanumeric card
5 1	Load Instr.	
2	Geometry	Cylinder
1	Origin	d /dr = 0
1	Edge	= 0
1	Convergence	Eigenvalue convergence
1		Simple extrapolation
5 6	Load Instr.	
2		Print eigenvalue and fluxes
1		Print every point
1		Source specified by region
1		Constant buckling all regions
1		Buckling group independent

Table 13. (Continued)

Number		Description	Remarks
5	11	Load Instr.	
	2		Print input and cross sections
	2		Print date
	19		Number of regions
	89		Number of points
	4		Number of groups
5	16	Load Instr.	
	3		Number of downscatterings
	11		Interface region 1
	15		Interface region 2
	19		Interface region 3
	23		Interface region 4
5	21	Load Instr.	
	27		Interface region 5
	31		Interface region 6
	35		Interface region 7
	39		Interface region 8
	43		Interface region 9
5	26	Load Instr.	
	47		Interface region 10
	51		Interface region 11
	55		Interface region 12
	59		Interface region 13
	63		Interface region 14
5	31	Load Instr.	
	67		Interface region 15
	71		Interface region 16
	75		Interface region 17
	79		Interface region 18
	89		Interface region 19
3	37	Load Instr.	
	1		Flux normalized by point
	4		Normalized on group 4
	1		Normalized on point 1
5	41	Load Instr.	
	4		Print 4 groups

Table 13. (Continued)

Number		Description	Remarks
	1		Print group 1
	2		Print group 2
	3		Print group 3
	4		Print group 4
3	61	Load Instr.	
	1		Element number of fissile element
	0		Median energy option not used
	2		Element No. of fertile element
2	70	Load Instr.	
	2		Conc. Search on 2 elements
	0		Direction of Conc. change
11	76	Load Instr.	
	1		Concentration Search
2	1	Load Instr.	
.0001			Convergence for flux
.001			Convergence for criticality
1	24	Load Instr.	
.000101106			Buckling
5	44	Load Instr.	
.0			Initial source guess region 1
.117			Initial source guess region 2
.0			Initial source guess region 3
.139			Initial source guess region 4
.0			Initial source guess region 5
5	49	Load Instr.	
.156			Initial source guess region 6
.0			Initial source guess region 7
.154			Initial source guess region 8
.0			Initial source guess region 9
.148			Initial source guess region 10
5	54	Load Instr.	Initial source guess region 11
.0			Initial source guess region 11
.117			Initial source guess region 12
.0			Initial source guess region 13
.095			Initial source guess region 14
.0			Initial source guess region 15

Table 13. (Continued)

Number	Description	Remarks
4 49	Load Instr.	
.05		Initial source guess region 16
.0		Initial source guess region 17
.026		Initial source guess region 18
.0		Initial source guess region 19
5 164	Load Instr.	
5.0		Increment width region 1
.675		Increment width region 2
5.65		Increment width region 3
.682		Increment width region 4
5.65		Increment width region 5
5 169	Load Instr.	
.690		Increment width region 6
5.65		Increment width region 7
.689		Increment width region 8
5.65		Increment width region 9
.694		Increment width region 10
5 174	Load Instr.	
5.65		Increment width region 11
.691		Increment width region 12
5.65		Increment width region 13
.692		Increment width region 14
5.65		Increment width region 15
4 179	Load Instr.	
.692		Increment width region 16
5.65		Increment width region 17
.761		Increment width region 18
3.048		Increment width region 19
4 1216	Load Instr.	
2.50		Group 1 lethargy
7.50		Group 2 lethargy
16.6		Group 3 lethargy
20.0		Group 4 lethargy
4 1997	Load Instr.	
235.1175		Atomic weight element No. 1
238.12522		Atomic weight element No. 2
1.008145		Atomic weight element No. 3
2.01474		Atomic weight element No. 4

Table 13. (Continued)

Number	Description	Remarks
4 2001	Load Instr.	
239.0		Atomic weight element No. 5
240.0		Atomic weight element No. 6
135.0		Atomic weight element No. 7
149.00		Atomic weight element No. 8
4 2005	Load Instr.	
116.5		Atomic weight element No. 9
118.0		Atomic weight element No. 10
241.0		Atomic weight element No. 11
16.0		Atomic weight element No. 12
4 2009	Load Instr.	
26.99021		Atomic weight element No. 13
55.85		Atomic weight element No. 14
39.1		Atomic weight element No. 15
91.22		Atomic weight element No. 16
3 2013	Load Instr.	
92.9353		Atomic weight element No. 17
88.92		Atomic weight element No. 18
52.01		Atomic weight element No. 19
4 7124	Load Instr.	
.7524		Fission neutron fraction group 1
.2454		Fission neutron fraction group 2
.000		Fission neutron fraction group 3
.000		Fission neutron fraction group 4
11 8197	Load Instr.	
.990		Conc. adjustment factor
1 JULY 1963 S AMPLE PROBLEM FOR AIM-6 CO NCENTRATION S ARCH	Alphanumeric Card	This card is for the second program. This is the only data card for the second program.