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HTGR SAFETY RESEARCH PROGRAM
QUARTERLY PROGRESS REPORT

for

APRIL - JUNE 1975

I. INTRODUCTION

The Los Alamos Scientific Laboratory (LASL) is carrying out a broad program of research in High-Temperature Gas-Cooled Reactor (HTGR) safety technology under the direction of the Reactor Safety Research Division of the United States Nuclear Regulatory Commission. The present LASL program includes the following task areas:

- Fission Product Technology
- Primary Coolant Impurities
- Structural Evaluation
- Safety Instrumentation and Control Systems
- Accident Delineation
- Phenomena Modeling and Systems Analysis

This program was started in March 1974 and is a continuing effort. Previously, progress has been reported in a series of informal monthly progress reports. This present report is the third in a series of formal quarterly progress reports.

II. SUMMARY

Calculations of core temperatures and consequent fractional ^{131}I releases during the loss of forced cooling (LOFC) accident have been examined for sensitivity to the size of element used in the AYER heat conduction code. Three cases were compared: 1) the basic element size used in earlier calculations, 2) an element size a factor of four smaller, 3) an element size a factor of four larger. The results of the

comparison show that the sensitivity to element size is not great and that the basic element size provides a good balance between computing accuracy and time.

A simple gas transport model has been developed to partially account for the hold up of fission products within the PCRV during the Maximum Hypothetical Fission Product Release (MHFPR) accident. Using this model to replace the usual assumption that fission products released from the core are completely and instantly transported into the containment building results in a significant decrease in the rate at which an isotope is released from the containment building into the atmosphere and a significant decrease in the total release of short-lived fission products.

The complex transport behavior of cesium in graphite is being studied. One portion of the problem, fast surface diffusion, can be examined by means of computer dynamic simulation of the transport of one cesium atom across a graphite surface. The derivation of a potential energy function for this motion is described in subsequent sections, together with calculational results which show possibly fortuitous agreement with experiment.

The OXIDE-3 code has been rewritten in a different style which reduces code length and running time. The new version, tentatively labeled OXIDE-3A is now operational,

but requires some further work. LASL review of OXIDE-3 has been discussed with General Atomic Company (GAC) personnel. We believe that the conversion effort has shown that there are no significant programming errors in OXIDE-3.

Work has continued on complex equilibrium calculations including development of the computer code QUIL. Calculations of the equilibria to be expected in the presence of cesium have just begun. A number of calculational results are reported and analyzed. These efforts indicate that, as a first approximation, equilibria of the carbon-steam system can be treated by consideration of the major species (H_2 , H_2O , CO , CO_2 , CH_4) only.

The experimental set up for using electrical resistance measurements to follow the kinetics of gas-metal reactions has been improved to increase the sensitivity of the measurements. An experiment to determine the oxidation of pure Ni in air was repeated with excellent results; however, two subsequent experiments involving more complex reactions met with limited success. It appears that the use of electrical resistance measurements without supplementary data to determine the kinetics of gas-metal reactions is limited to cases where only surface oxidation occurs or to cases where surface oxidation plus internal changes occur simultaneously.

A computer code which computes constitutive relationships for plain and reinforced concrete from basic materials data has been obtained, made operational on LASL computers, and incorporated into NONSAP. This code appears to be the most advanced one available for representing the complex behavior of reinforced concrete.

Application of NONSAP is currently restricted by the lack of several features in the code. Work is underway to provide a number of needed features and others will soon be attacked.

Dowel pins and slots have been added to the two-dimensional core seismic analytical model. A movie illustrating the affects of the pins under single-frequency horizontal excitation has been prepared.

Studies have been undertaken to estimate stiffness of the core block, locating pin, and locating pin slot. Results are reported for the first two in subsequent sections.

The use of the computer program SIMEAR for providing earthquake excitation to the core block model has been attempted during this quarter. It was found that acceleration, velocity, and displacement time histories furnished by SIMEAR were independent and consequently produced incredible results. Current application of SIMEAR input uses only the acceleration time history.

Scaling law studies for physical models of core seismic response have been extended. The results of studies of four systems are reported.

The improved version of the LASL Afterglow Impurities Monitor was completed and operated at Fort St. Vrain on May 28 and 29, 1975. On May 28th, the monitor indicated 504 ppmV water in the primary coolant. A level of 25 ppmV was measured on May 29th.

The reactivity worths of several HTGR control rod configurations were calculated with a two-dimensional model cross section provided by GAC. Where comparison data are available, there is good agreement between these calculations and previous GAC and one-dimensional LASL calculations.

The reactivity change resulting from the failure of the three graphite posts supporting the central refueling region and a consequent 2-m drop of the refueling region has been calculated to be small and negative regardless of the position of the central control-rod pair.

Neutronic kinetics parameters calculated for the Fulton Generating Station are in good agreement with those reported in the PSAR.

Independent LASL cross-section preparation for homogeneous HTGR media has progressed to the point that neutronic calculations using these cross sections are in reasonable agreement with calculations based on GAC cross sections, taking into account the expected effect of core heterogeneity. The source of error for earlier attempts to generate HTGR cross sections at LASL has been identified and eliminated.

CHAP code development is continuing.

III. TASK 1, FISSION PRODUCT TECHNOLOGY

A. Parameter Study on Temperatures and Iodine Release (J. H. Fu and G. E. Cort)

1. Objectives of the Study

One problem of concern in the HTGR safety study is the time-dependent temperature of the reactor core, resulting in release of fission products from fuel particles, during the loss of forced circulation (LOFC) accident. Previously, the iodine release problem was analyzed using a simplified uniform core temperature model.¹ This simplified model revealed the essential concepts about the fission product release calculation techniques. In addition, the problem was analyzed in detail using an AYER heat conduction model.² The AYER heat conduction model is a modified version of the LASL AYER heat conduction computer code³ which uses the finite element method⁴ (FEM) as the computation scheme. The present calculations are based on this heat conduction model.

The purposes of this study are to examine the variations in computed results, such as the temperature of the reactor core and fractional ¹³¹I release, as a function of the variation of the size of the element used in the finite element method, and to search for a set of optimal

size parameters which will furnish both computational efficiency and relatively accurate results.

2. Size Parameter Ranges

In previous AYER heat conduction model studies, the selected input size parameter led to the use of 361 annulus-ring elements in total, of which 112 elements were in the reactor core. In the present study, three different size parameters have been investigated:

- Case A - The size of an element in the active core is four times larger than that used in the previous study. The total number of elements in the reactor core is 28, and the total number of elements used in the finite element method calculation is 180.
- Case B - The size parameter of the previous study is used.
- Case C - The size of an element in the active core is equal to one-fourth that of previous study. There are 448 elements in the reactor core, and a total of 918 annulus-ring elements are used in the finite element method calculation.

The size parameters used in the finite element method calculations for these three cases are summarized in Table I.

3. Calculations

The time-dependent core temperatures and the fractional ¹³¹I releases were calculated for the three cases described. In each case, the calculations covered a period of 12 h after the onset of the LOFC accident. The time increments used in the calculations were: 1) every 300 s up to 900 s, 2) every 900 s up to 2 h, and 3) every hour up to 12 h. Assumptions, physical parameters, and initial

TABLE I

SIZE PARAMETERS USED
IN THE FINITE ELEMENT METHOD CALCULATIONS

Case	Number of Elements in the Active Core	Total Number of Elements Used in FEM	Total Number of Nodes Used in the FEM
A	28	180	208
B	112	361	400
C	448	918	980

and boundary conditions used in the present study are similar to those used in previous studies. Some of the important ones are:

- The HTGR has been operating at a constant power of 3000 MW_t prior to the LOFC accident.
- The irradiation history of fuel particles in the reactor core is four years.
- The temperature range for fuel particles to fail is from 1303 to 1673 K, and the fraction of fuel particles is a linear function of the local temperature of the reactor core within this range.⁵
- It is assumed that 10% of the fuel particles have failed prior to the LOFC accident.
- The fission product iodine is released only from failed fuel particles with the release rate given by the usual Arrhenius relation (Ref. 5, Fig. 5-3) i.e.

$$\text{Rate of Release for } ^{131}\text{I} = 6796.7 \exp(-22075.5/T).$$

- The initial temperature of the reactor core is 1100 K.
- The afterheat generation rate in each finite element in the reactor core is proportional to the decay power. For convenience of comparison the proportionality constant has been assigned a

value of unity in the present study.

The calculated temperatures for the three cases are given in Table II, and the average temperatures are plotted versus time in Fig. 1. Only a single curve has been plotted for the maximum temperature of the reactor core because the differences in the maximum temperatures for these cases are too small to be separated on the plot. A comparison of the extremes (Case A and Case C) shows that the maximum difference in the average temperature is only 2%. This difference occurs at the end of the time period of the calculations; i.e., at 12 h.

Table III is a comparison of the fractional ¹³¹I release for the three cases during the first 12 h after the onset of the accident. In Fig. 2, the ¹³¹I release data are plotted against time after the onset of the LOFC accident. The results of the earlier simplified uniform core temperature model¹ are plotted as Case D for comparison.

Finally, a comparison of computation times on the CDC 7600 required in these three cases is given in Table IV; the computation time for Case C is longer than that for Case A by more than sixfold.

TABLE II

MAXIMUM AND AVERAGE TEMPERATURES OF THE REACTOR CORE
FOR THE THREE CASES LISTED IN TABLE I
VERSUS TIME AFTER ONSET OF THE LOFC ACCIDENT

Time (hour)	Average Temperature (K)			Maximum Temperature (K)		
	Case A	Case B	Case C	Case A	Case B	Case C
0.083	1137.1	1139.8	1141.6	1146.1	1146.0	1146.0
0.167	1164.2	1168.0	1170.4	1178.7	1178.6	1178.6
0.250	1188.0	1192.7	1195.7	1207.8	1207.6	1207.5
0.500	1245.4	1252.0	1256.0	1279.0	1278.4	1278.4
0.750	1295.6	1303.6	1308.3	1342.0	1340.9	1340.9
1.000	1341.1	1350.4	1355.8	1399.5	1398.4	1398.4
1.250	1383.4	1393.9	1399.9	1453.4	1452.6	1452.6
1.500	1423.3	1434.8	1441.4	1504.5	1504.1	1504.1
1.750	1461.0	1473.6	1480.7	1553.5	1553.5	1553.5
2.000	1497.0	1510.6	1518.2	1601.1	1601.1	1601.1
3.000	1620.6	1637.6	1646.4	1770.5	1770.6	1770.6
4.000	1730.2	1750.4	1760.1	1926.0	1926.3	1926.3
5.000	1829.7	1852.8	1863.0	2072.1	2072.6	2072.7
6.000	1921.2	1946.7	1957.4	2210.5	2211.4	2211.6
7.000	2006.0	2033.8	2044.8	2342.6	2344.0	2344.3
8.000	2085.3	2115.0	2126.2	2469.3	2471.2	2471.7
9.000	2159.8	2191.2	2202.7	2591.4	2594.2	2594.9
10.000	2230.3	2263.3	2274.9	2709.5	2713.3	2714.2
11.000	2297.2	2331.7	2343.5	2824.1	2828.8	2830.0
12.000	2361.0	2396.8	2408.7	2935.3	2941.1	2942.6

TABLE III

FRACTIONAL IODINE RELEASED FROM THE FAILED FUEL PARTICLES
IN THE REACTOR CORE DURING THE LOFC ACCIDENT
FOR THOSE THREE CASES LISTED IN TABLE I

Time After Onset of the Accident (hour)	Fractional $^{131}_{53}\text{I}$ Released		
	Case A	Case B	Case C
0.083	2.124×10^{-7}	2.227×10^{-7}	2.290×10^{-7}
0.167	5.519×10^{-7}	5.844×10^{-7}	6.047×10^{-7}
0.250	1.059×10^{-6}	1.131×10^{-6}	1.177×10^{-6}
0.500	4.860×10^{-6}	5.319×10^{-6}	5.599×10^{-6}
0.750	1.705×10^{-5}	2.062×10^{-5}	2.233×10^{-5}
1.000	5.744×10^{-5}	6.998×10^{-5}	7.682×10^{-5}
1.250	1.575×10^{-4}	1.915×10^{-4}	2.098×10^{-4}
1.500	3.660×10^{-4}	4.449×10^{-4}	4.861×10^{-4}
1.750	7.553×10^{-4}	9.189×10^{-4}	1.001×10^{-3}
2.000	1.427×10^{-3}	1.738×10^{-3}	1.890×10^{-3}
3.000	1.311×10^{-2}	1.566×10^{-2}	1.686×10^{-2}
4.000	4.235×10^{-2}	4.995×10^{-2}	5.329×10^{-2}
5.000	9.844×10^{-2}	1.154×10^{-1}	1.224×10^{-1}
6.000	1.859×10^{-1}	2.157×10^{-1}	2.276×10^{-1}
7.000	2.973×10^{-1}	3.388×10^{-1}	3.554×10^{-1}
8.000	4.136×10^{-1}	4.594×10^{-1}	4.786×10^{-1}
9.000	5.167×10^{-1}	5.562×10^{-1}	5.749×10^{-1}
10.000	5.999×10^{-1}	6.236×10^{-1}	6.421×10^{-1}
11.000	6.651×10^{-1}	6.785×10^{-1}	6.898×10^{-1}
12.000	7.154×10^{-1}	7.205×10^{-1}	7.269×10^{-1}

Fig. 1. The maximum and average temperatures of the reactor core versus time after onset of the LOFC accident.

Fig. 2. Fractional ^{131}I release versus time after onset of the LOFC accident

TABLE IV

COMPUTATION TIME FOR THE
THREE CASES LISTED IN TABLE I

Size Parameter	Computation Time (s)
Case A	19.31
Case B	36.07
Case C	130.58

4. Summary

The purpose of this study was to examine the variations in calculated reactor core temperature and fractional iodine release caused by varying the size of parameters used in the AYER heat conduction model calculations. During the time period covered by the present

calculations, the maximum variation in the temperature of the reactor core (between the extreme cases A and C) is only 2%; however, the computation times for the extremes differ by more than sixfold. Based on these comparisons, the element size used in the previous studies² (Case B) appears to be an adequate compromise between competing goals of computational accuracy and efficient computer usage.

B. Fission Product Transport from the PCRVR (J. E. Foley)

1. Introduction

A simple gas transport model was developed so that the time-dependent release of fission products from the PCRVR during the MHFPR accident could be calculated. In the fission product release computer programs currently being used for

release calculation (e.g. AYER² and SORS⁵), it is assumed that fission products which are volatilized from the core are transported instantaneously into the containment building through the penetration failure which caused the accident. The gas transport model was developed so that the time-dependent transport of fission products from the PCRV could be included in the release calculations. The model is applicable only to single PCRV penetration failures; it does not apply to failures that establish a natural circulation flow between the PCRV and the containment building.

The gas inside the PCRV depressurizes at the onset of the MHFPR accident and an equilibrium pressure is established between the residual gas inside the PCRV and the gas inside the containment building. In the gas transport model described here, it is assumed that the subsequent flow of gas into the containment building is produced by an expansion of the residual gas inside the PCRV as the gas temperature (T) rises due to core decay heat.

2. Identification of PCRV Leak Rate

It will be assumed that the gas inside the PCRV obeys the ideal gas law. It will be assumed further that, after the initial depressurization of the PCRV, the pressures inside and outside the PCRV are the same and that they remain constant during the time period of interest. This assumption is justified because the pressure inside the containment building for the Summit Plant, for example, is calculated to decrease only ~ 1 psi from ~ 25 psia at 2 h to ~ 24 psia at 18 h following the onset of the MHFPR accident;⁶ i.e., the containment building pressure remains nearly constant with time. This assumption allows us to decouple the PCRV from the containment building and to analyze the PCRV flow independently.

The time-dependent change in the amount of gas inside the PCRV is given by

$$\frac{dN}{dt} = \left(\frac{\partial N}{\partial T} \right) \left(\frac{dT}{dt} \right), \quad (1)$$

$$= - \left(\frac{PV}{RT^2} \right) \left(\frac{dT}{dt} \right). \quad (2)$$

This equation can be rewritten in a more convenient form:

$$\frac{dN}{dt} = - \left(\frac{1}{T} \right) \left(\frac{dT}{dt} \right) N. \quad (3)$$

The leak rate (fractional release rate) of the PCRV is thus identified in Eq. (3) as

$$L(t) = \frac{1}{T} \frac{dT}{dt}. \quad (4)$$

3. Fission Product Leakage from the PCRV

The fission products which are volatilized from the core and become gasborne are assumed to be well mixed with the coolant gas inside the PCRV. The rate of change in the amount (n) of the gasborne isotope is given by

$$\frac{dn(t)}{dt} = S(t) - [\lambda + L(t)] n(t) \quad (5)$$

where

- S is the source term of the isotope in the coolant gas (equal to the rate at which the isotope is volatilized from the core),
- λ is the radioactive decay constant of the isotope,
- L is the leak rate of the PCRV defined by Eq. (4).

Plateout of the isotope on surfaces interior to the PCRV has been ignored, but it could be included by setting $\lambda = \lambda + P$ where P is a fractional rate for plateout.

Equation 5 is of the same form as that used in Ref. 1, Eq. (13) to describe fission product release from a containment building. Thus, the same formulation that is used to calculate the time-dependent leakage from the containment building can be used for this problem.

If the source term $S(t)$ and the leak rate $L(T)$ are considered to be constants during short time intervals of length Δt , then the amount of the gasborne isotope released (R_i) into the containment building from the PCRV during the i^{th} time interval is given by Eq. (16) of Ref. 1, i.e.,

$$R_i = \frac{L_i}{\lambda_i^*} (n_{i-1} - \frac{S_i}{\lambda_i^*}) (1 - e^{-\lambda_i^* \Delta t}) + L_i \frac{S_i}{\lambda_i^*} \Delta t \quad (6)$$

where

- n_{i-1} is the amount (C_i , moles, atoms, etc) of the isotope gasborne inside the PCRV at the end of the $(i-1)^{\text{st}}$ time interval (at time t_{i-1}),
- L_i is the leak rate of the PCRV during the time interval,
- λ_i^* equals $\lambda + L_i$.

The source term S_i is the average rate of release of the isotope from the core during the time interval; it can be identified as the release rate from the core obtained using either the LASL AYER or the GAC SORS computer programs.

4. Calculations

^{131}I is used as the example for these calculations, but the analysis could be applied equally well to any other isotope. The assumptions used for the AYER calculations are similar to, but not exactly the same as, those used for the parametric study discussed earlier. Because of slight differences in the assumptions, the temperatures and release rates presented in this section are slightly different from those presented earlier. These slight differences are not important for this discussion.

It will be assumed that the coolant gas temperature is equal to the average core temperature; this assumption results in gas temperatures that are too

high, but these temperatures are sufficiently accurate for this analysis.

The time-dependent leak rate, defined by Eq. (4), is calculated using the temperature data from the AYER calculations. It is assumed that the average core temperature increases linearly over 1-h time intervals. During the 4- to 5-h time interval ($i=5$), for example, the average gas temperature is 1804.8 K and the temperature rise is 106.7 K (from 1751.5 K to 1858.2 K); therefore, the leak rate of the PCRV during the time interval is

$$L_5 = \frac{106.7 \text{ K/h}}{1804.8 \text{ K}} = 0.0591 \text{ h}^{-1}.$$

Thus, 5.91% of the gasborne fission products inside the PCRV leak into the containment building during the time interval 4- to 5-h after the onset of the MHFPR accident. The PCRV leak rates for the other time intervals are calculated in the same way; they are given in Table V.

The source terms S_i for ^{131}I for each time interval are given in Table VI; these values are based on a total core inventory of ^{131}I of 7.78×10^7 Ci for a 3000 MW_t reactor (Ref. 1, Appendix A).

5. Results of the Calculations

The calculated time-dependent release curves of ^{131}I from the PCRV are shown in Fig. 3 for: 1) the release of the fission products directly from the core to the containment building, and 2) the release using the PCRV leak rate of $\frac{1}{T} \frac{dT}{dt}$ given in Table V. It is seen that the rate of release of the isotope from the PCRV is significantly slower using the $\frac{1}{T} \frac{dT}{dt}$ leak rate than it is using the direct release model.

The analysis was extended to include calculations of the time-dependent release of the isotope into the environment from the containment building. The time-dependent release rates into the containment building from the PCRV were used for

TABLE V
LEAK RATE OF PCRV

Time Interval (h)	Avg. Temp. (K)	dT (K)	Leak Rate (h ⁻¹)
0-1	1220.3	240.6	0.197
1-2	1419.8	158.5	0.112
2-3	1566.2	134.2	0.0857
3-4	1692.4	118.2	0.0698
4-5	1804.8	106.7	0.0591
5-6	1907.0	97.6	0.0512
6-7	2000.8	90.1	0.0450
7-8	2087.2	82.6	0.0396
8-9	2167.3	77.6	0.0358
9-10	2242.8	73.4	0.0327
10-11	2314.3	69.6	0.0301
11-12	2382.3	66.4	0.0279
12-13	2447.2	63.4	0.0259
13-14	2509.2	60.7	0.0242
14-15	2568.8	58.4	0.0227
15-16	2626.2	56.3	0.0214
16-17	2681.4	54.3	0.0203
17-18	2733.1	49.0	0.0179

TABLE VI
¹³¹I RELEASE FROM CORE

Time Interval (h)	Fractional Release Rate (h ⁻¹)	Release Rate (Ci/h)
0-1	2.570×10^{-5}	1.999×10^3
1-2	2.034×10^{-3}	1.582×10^5
2-3	1.344×10^{-2}	1.046×10^6
3-4	3.720×10^{-2}	2.894×10^6
4-5	7.330×10^{-2}	5.703×10^6
5-6	1.110×10^{-1}	8.636×10^6
6-7	1.270×10^{-1}	9.881×10^6
7-8	1.230×10^{-1}	9.569×10^6
8-9	8.900×10^{-2}	6.924×10^6
9-10	6.400×10^{-2}	4.979×10^6
10-11	4.900×10^{-2}	3.812×10^6
11-12	4.000×10^{-2}	3.112×10^6
12-13	3.300×10^{-2}	2.567×10^6
13-14	2.700×10^{-2}	2.101×10^6
14-15	2.400×10^{-2}	1.867×10^6
15-16	1.900×10^{-2}	1.478×10^6
16-17	1.700×10^{-2}	1.323×10^6
17-18	1.500×10^{-2}	1.167×10^6

Fig. 3. Time-dependent release of ¹³¹I from the PCRV during the MHFPR accident.

the source terms of the isotope inside the containment building. The leakage from the containment building was then determined using Eq. (6),* as described in Ref. 1, p. 6-8. It was assumed that all of the iodine released from the core (except for that which undergoes radioactive decay) is available for release from the containment building, i.e., the arbitrary 25% factor for availability (Ref. 1, p. 6) was not used (this factor can be included by multiplying the release values by 0.25). The time-dependent release curves for ¹³¹I from the containment building were calculated for the two cases given in Fig. 3; they are shown in Fig. 4. It is seen that the use of the $\frac{1}{T} \frac{dT}{dt}$ PCRV leak rate results

* The leak rate of the containment building was assumed to be 0.1%/day and the clean-up rate for the containment cleanup system was assumed to be 0.9 h⁻¹.

Fig. 4. Time-dependent release of ^{131}I from the containment building during the MHFPR accident.

in a significant decrease in the rate at which ^{131}I is released to the atmosphere. The total amount of ^{131}I released to the atmosphere decreases if the $\frac{1}{T} \frac{dT}{dt}$ PCRVR leak rate is used because of the additional time for radioactive decay resulting from the holdup time of the isotope inside the PCRVR. For short-lived isotopes the additional holdup results in a significant decrease in the amount of the isotope released; for long-lived isotopes, the additional holdup results in little decrease in the total amount released to the atmosphere, although the time required for the release is spread out over a longer period of time.

6. Summary

Including the gas transport model for the PCRVR in the fission product release calculations results in a significant decrease in the rate at which an isotope is released from the PCRVR during

the MHFPR accident. The additional hold up time of the isotope inside the PCRVR results in a significant decrease in the total amount of the short-lived isotopes released to the atmosphere. The total amount of the long-lived isotopes released does not decrease significantly.

The slower release rate offers some advantage in satisfying the CFR Title 10, Part 100 criteria⁷ for both the 2-h Exclusion Area Boundary (EAB) dose and the Low Population Zone (LPZ) dose. If the gas transport model is ignored (direct release from the core to the containment), then most of the ^{131}I release occurs during the time period 4h - 12h following the onset of the MHFPR accident (see Fig. 4) and, because this is the time period for the worst atmospheric transport conditions^{8,9} [the time period for largest atmospheric diffusion factors ($\frac{\lambda}{Q}$)], the calculated thyroid dose will be its maximum value. On the other hand, if the gas transport model is used, most of the release of the long-lived isotopes occurs at times > 12 h when better atmospheric conditions prevail, and thus the calculated population dose is lower. A long, slow release of an isotope results in a lower overall calculated dose than does a short, fast release of the same total amount.

C. The Interaction Between Cesium and Graphite for Use in the Study of Surface Phenomena (B. L. Holian)

1. Introduction

There is growing interest in the complex transport behavior of cesium in graphite.^{10,11} At least two transport modes are indicated by recent experiments: 1) slow bulk diffusion and 2) fast surface diffusion. In order to study the mechanisms involved in the latter phenomenon, molecular dynamics computer simulations of the transport of a cesium atom across a graphite surface have been undertaken. The classical equations of motion need be

solved for one atom only, since the behavior at low surface coverage, where the interaction between adsorbed cesium atoms can be neglected, is of particular theoretical and practical interest. Even with this simplification of the dynamics to the motion of one particle, the force acting on the cesium atom is quite complicated. In this section structural considerations and theoretical estimates of atomic properties will be combined to give a reasonable potential energy function for use in subsequent molecular dynamics calculations. The following six subsections describe individual terms in the potential, with the results presented in the last subsection.

2. Zero of Energy

The zero of energy for a cesium atom interacting with the graphite surface will be taken to be that of the atom separated infinitely far from the graphite crystal. As the atom approaches the surface, the electronic configuration of the atom becomes more and more distorted. The outer 6s electron, being loosely bound to the core, is easily snatched from the cesium by the metal-like graphite surface plane. When an electron is donated to the conduction band of the graphite plane (chemical symbol of graphite, Gr) energy is released - the electron work function, $E_w(\text{Gr})$:

The first ionization of cesium requires energy - the ionization potential, $E_I^{(1)}(\text{Cs})$:

The overall reaction [the sum of Eqs. (7) and (8)] requires energy W:

where $W = E_I^{(1)}(\text{Cs}) - E_w(\text{Gr})$ is negative, i.e., heat is given off by the reaction. In units of kK = 1000 K, $E_I^{(1)}(\text{Cs}) = 45.18$, $E_w(\text{Gr}) = 53.62$, and $W = -8.44$.

3. Bulk Electrostatic Interaction

The ionized cesium atom interacts with its donated electron in the graphite conduction band much like a point charge over an infinite perfectly conducting plane; i.e., the classical electrostatic problem of the image charge. The principal uncertainty in this model is the location of the conducting plane. If we assume that the cesium atom is centered over a hexagon of carbon atoms at a height of $z_m = 2.97\text{\AA}$ above the graphite plane (as in the case of interlamellar cesium-graphite compounds),^{12,13} then the height of the conducting plane above the plane of the carbon nuclei z_o is simply $z_m - r(\text{Cs}^+)$, where $r(\text{Cs}^+) = 1.69\text{\AA}$ is the ionic radius of cesium.¹⁴ This is consistent with a Van der Waals' radius for a graphite carbon atom of $r(\text{C}) = 1.602\text{\AA}$ (the C-C bond length in graphite is $r_o = 1.421\text{\AA}$ and the spacing between layers is $c_o = 3.354\text{\AA}$; $r(\text{C})$ is therefore very close to $1/2 c_o = 1.677\text{\AA}$, the Van der Waals' radius in graphite. (See Figs. 5 and 6.) The values of $r(\text{C})$ for rubidium and potassium interlamellar compounds¹² are $1.682\text{\AA}$ and $1.721\text{\AA}$, giving a small but systematic deviation for the series K, Rb, and Cs of +2.6%, +0.3%, and -4.5%.

The image-charge potential energy is given by

$$V_{\text{image}}(z) = - \frac{e^2}{4(z - z_o)}. \quad (10)$$

At the equilibrium position, $V_{\text{image}} = -24.72\text{ kK}$. The image-charge force is given by

$$\begin{aligned} F_z^{(\text{image})}(z) &= - \frac{dV_{\text{image}}(z)}{dz} \\ &= - \frac{e^2}{4(z - z_o)^2}, \end{aligned} \quad (11)$$

Fig. 5. Side view of bonding geometry of adsorbed cesium atom on graphite; C_1 and C_4 are carbon atoms as shown in Fig. 6; e^- is position of image charge (other symbols defined in text).

Fig. 6. Top view of bonding geometry of adsorbed cesium atom on graphite; site A is adsorption site (minimum of potential energy), site B is above C-C bond (saddle point in potential energy surface), and site C is above carbon atom (maximum of potential energy).

which is just the coulomb force between two charges $+e$ and $-e$ separated by $2(z - z_0)$. If the surface has defects, i.e., missing carbon atoms, the above approach must be modified.¹⁵ Let us suppose that there are M defects (circular holes in the conduction plane) located at (x_m, y_m) with radii a_m ($m = 1, 2, \dots, M$); then given the following functions,

$$A(x, y) = \sum_{m=1}^M a_m^2 \exp \left\{ -[(x-x_m)^2 + (y-y_m)^2] / a_m^2 \right\}, \quad (12)$$

and

$$A_\alpha(x, y) = \sum_{m=1}^M (x_\alpha - x_{\alpha m}) \exp \left\{ -[(x-x_m)^2 + (y-y_m)^2] / a_m^2 \right\}, \quad (13)$$

where $\alpha = x$ or y , the potential energy of a charge $+e$ located at (x, y, z) in the presence of M defects in the conducting plane at $z = z_0$ can be approximated by:

$$V(x, y, z) = - \frac{e^2}{4[A(x, y) + (z-z_0)^2]^{1/2}}, \quad (14)$$

and the forces are

$$F_\alpha(x, y, z) = \frac{e^2 A_\alpha(x, y)}{4[A(x, y) + (z-z_0)^2]^{3/2}}, \quad (15)$$

for $\alpha = x$ or y and

$$F_z(x, y, z) = - \frac{e^2 z}{4[A(x, y) + (z-z_0)^2]^{3/2}}. \quad (16)$$

These expressions reduce to the image-charge expressions (Eqs. 7 and 8) far from defects, including the condition that F_x and F_y vanish. Further, from Eq. (15) it is clear that a defect is a scattering center from considerations of the bulk electrostatic interaction.

4. Induction Interaction

The charge on the cesium ion can induce an instantaneous dipole moment in the carbon atoms of the graphite crystal (and vice-versa), which leads to a potential energy contribution of the following form¹⁶

$$\phi^{(\text{ind})}(R) = -\frac{C_4}{R^4} \quad (17)$$

where $\phi^{(\text{ind})}$ is in units of $e^2/2a_0$ (e is the electronic charge and $a_0 = 0.5292 \text{ \AA}$ is the first Bohr radius), R is in units of a_0 , and C_4 is given by

$$C_4 = q_1^2 \alpha_2 + q_2^2 \alpha_1, \quad (18)$$

where q_i is the charge (in units of e) on atom i and α_i is its polarizability (in units of a_0^3). The polarizability of Cs^+ can be estimated using Slater's screening constants (Ref. 16, p. 951-ff). A better estimate is obtained by multiplying the observed value for iso-electronic xenon,¹⁷ $\alpha_{\text{Xe}} = 27.1 a_0^3$, by the ratio of α_{Cs^+} to α_{Xe} as calculated via the Slater method. The result is $\alpha_{\text{Cs}^+} = 17.4 a_0^3$. Since the polarizability of a molecule is the sum of its bond polarizabilities, the polarizability of graphite per carbon atom can be obtained from the linear interpolation of the aliphatic (single bond, bond order $n = 1$) and aromatic (benzene, $n = 1-1/2$) bond polarizabilities (carbon bond polarizability versus bond order is fairly linear). The polarizability of a graphite carbon atom is then $\frac{3}{2} \alpha_{\text{C-C}} (n = 1-1/3)$, since the graphite bond order (Ref. 14, p. 235) is $1-1/3$ and there are $1-1/2$ such bonds per atom. The result is $\alpha_{\text{C}} = 10.8 a_0^3$. The electron donated by the cesium atom is shared by at least six nearest carbon atoms, so that the charge on any carbon atom is no more than $-e/6$. Therefore, taking $q_{\text{C}} = -1/6$ as being correct for the most important nearby carbon atoms, $C_4 = 11.26 \frac{e^2}{2a_0} \cdot a_0^4$.

Define

$$A = \frac{C_4}{r_m^4}, \quad (19)$$

the induction contribution per nearest carbon atom at the equilibrium position (position A in Fig. 6); then $A = 1.188 \text{ kK}$.

5. Dispersion Interaction

Although the charge distribution in a free atom or ion is spherical, there are fluctuations due to the rapidly moving electrons that result in a net instantaneous dipole moment. This dipole can then induce an instantaneous dipole in another atom, leading to a potential energy contribution of the following form (Ref. 16, p. 963),

$$\phi^{(\text{dis})}(R) = -\frac{C_6}{R^6} \quad (20)$$

where $\phi^{(\text{dis})}$ is in units of $e^2/2a_0$, R in units of a_0 , and C_6 is given by the London-Pitzer formula¹⁷

$$C_6 = \frac{3}{2} \frac{\alpha_1 \alpha_2}{E_1^{-1} + E_2^{-1}}, \quad (21)$$

where α_i is in units of a_0^3 and E_i , the characteristic energy of atom i , is in units of $e^2/2a_0$. Pitzer has shown empirically that E_i is roughly twice the ionization potential. Since $E/E_{\text{I}} = 2.27$ for neon and 2.39 for xenon,¹⁷ let us take $E_{\text{C}} = 2.77 E_{\text{I}}^{(1)}(\text{C}) = 1.878 e^2/2a_0$ and $E_{\text{Cs}^+} = 2.39 E_{\text{I}}^{(2)}(\text{Cs}) = 4.409 e^2/2a_0$. Therefore, $C_6 = 370.8 \frac{e^2}{2a_0} \cdot a_0^6$.

Define

$$B = \frac{C_6}{r_m^6} \quad (22)$$

the dispersion contribution per nearest carbon atom at the equilibrium position; then $B = 1.010 \text{ kK}$.

6. Valence Interaction

At short range, the overlap of electron charge clouds of two atoms gives rise to a repulsive potential energy

contribution of the form (Ref. 16, p. 26)

$$\phi^{(val)}(R) = b \exp(-aR/a_0) \quad (23)$$

where R is in units of a_0 and a is given by

$$a(\frac{e^2}{2a_0})^{1/2} = E_I^{1/2}(1) + E_I^{1/2}(2), \quad (24)$$

with $E_I(i)$ in units of $e^2/2a_0$. $E_I^{(1)}(C) = 0.8273 e^2/2a_0$ and $E_I^{(2)}(Cs) = E_I^{(1)}(Cs^+) = 1.845 e^2/2a_0$; hence $a = 2.268$. Define

$$\alpha = a \frac{r_m}{a_0}; \quad (25)$$

then $\alpha = 14.11$ and

$$\phi^{(val)}(R) = Q \exp[\alpha(1 - \frac{R}{r_m})], \quad (26)$$

where Q is the valence contribution per nearest carbon atom at the equilibrium position. Q can be determined by requiring that the force on the cesium ion at position A, the adsorption site on a perfect graphite surface, be zero.

7. Integral Corrections

Because the potential energy of interaction of the cesium ion with the free-surface graphite crystal converges slowly with distance into the crystal, an integral correction must be added to the discrete sum over graphite carbon atoms. In Fig. 7, the problem is indicated schematically as a spherical sector containing discrete atoms and a continuous distribution over the remainder of the crystal (free-surface bulk minus a crater). The distance R_{max} is sufficiently large that only the induction and dispersion terms are appreciable. The integral correction for the potential term ϕ is

$$\delta\phi(R_{max}) = 2\pi\rho \int_{R_{max}}^{\infty} dR R(R-Z)\phi(R), \quad (27)$$

where ρ is the number density of graphite and Z is the height of the cesium ion over

Fig. 7. Schematic representation of lattice summation and integral correction (continuous distribution) to potential energy of cesium ion over graphite surface.

the graphite plane. Likewise, it can be shown that the z -gradient correction is

$$\begin{aligned} \delta\nabla_z\phi(R_{max}) = & -2\pi\rho[\frac{1}{2}(R_{max}^2 - Z^2)\phi(R_{max}) \\ & + \int_{R_{max}}^{\infty} dR R\phi(R)]. \end{aligned} \quad (28)$$

8. Results

As outlined above, Q was calculated by summing over 8050 graphite carbon atoms within a radius of $R_{max} = 10.29 r_m$ ($r_m = 3.292 \text{ \AA}$) and applying the integral corrections for the remainder of the graphite crystal. The resulting value of Q is 1.792 kK, which exceeds by about 0.2% the value obtained for an R_{max} half as big (approximately one-ninth the number of carbon atoms). Q was also calculated, as a check, by summing over the six nearest carbons, integrating over a uniform surface distribution for the top graphite plane minus a disk of six times the atomic surface area, and integrating over the bulk (minus the first graphite plane). The result was remarkably close to the "exact" lattice sum plus correction and was about 3% too small (likewise for the magnitude of the adsorption energy). Table VII shows results for the barriers to translational motion of a cesium ion on a perfect graphite surface. (The positions

TABLE VII

BARRIERS TO MIGRATION OF CESIUM ON A PERFECT GRAPHITE SURFACE. (POSITION A, B, AND C SHOWN IN FIGURE 6)

Position, i	z_i (Å)	ϕ_i (kK)	ϕ_i (expt.) (kK)	$\phi_i - \phi_A$ (kK)
A	2.970	-61.562	-60.5	0
B	3.046	-59.875		1.687
C	3.055	-59.679		1.883

A, B, and C are shown in Fig. 6 and are defined such that the total force on the cesium atom is zero.) The kinetic energy at a temperature of about 1000 K or more is enough for a cesium ion to surmount the barriers on a perfect graphite surface, i.e., the ion behaves essentially like a free particle. The experimental value for the adsorption energy¹⁸ was obtained from two adsorption isotherms of cesium on TS-688 graphite in the Henry's Law regime, i.e., where the Cs partial pressure is proportional to concentration. In view of the serious nature of the approximations herein employed, the close agreement with experiment should be viewed with some caution. Moreover, Zumwalt has pointed out that the true adsorption site is probably over a defect.¹⁹ The effect on the calculated adsorption energy due to a defect will be examined in future work.

With regard to adsorption behavior itself, it should be noted that the nature of the interaction changes dramatically as the cesium atom leaves the surface and the ionization reaction of Eq. (9) is reversed to give a desorbed neutral cesium atom. This essentially quantum mechanical effect can be accounted for in a semi-empirical way by multiplying the appropriate ionic quantities (polarizability, charge, etc.) by an ionic character function $\chi(z)$ shown in Fig. 8,

Fig. 8. Ionic character function $\chi(z)$ as a function of the distance z of the ion above the free surface of a crystal; λ is the characteristic length of χ .

and the corresponding atomic (neutral) quantities by $1 - \chi(z)$. Thus, a completely classical calculation, such as a molecular dynamics simulation, would include implicitly this electronic rearrangement in the potential energy terms. The characteristic length λ of the ionic character function as well as its shape could, in principle, be inferred from quantum mechanical electronic calculations.²⁰

Future work will include the molecular dynamic calculation of various

correlation functions* of a cesium ion wandering over both perfect and defective graphite surfaces. If the defect holes are either attractive or repulsive (adsorbers or scatterers), the surface transport at high temperatures should be like a random walk, or classical diffusion in two dimensions. If the surface is very smooth, however, the transport will be much like that of a free particle in a two-dimensional box. Also, a more precise calculation of the electrostatic problem of a charge over a conducting plane with a circular hole is being undertaken.²²

IV. TASK 2, PRIMARY COOLANT IMPURITIES

Efforts within this task area are directed to the analytical and experimental study of the interactions between impurities in the helium primary coolant gas and the various materials in the primary coolant circuit. The most likely impurities are steam and the products of the steam-graphite reaction: hydrogen, carbon monoxide, or carbon dioxide. Materials of interest are the core and related graphite structures, and metallic components such as steam generators, helium circulators, orifice valves, and control rod systems. Interactions between gaseous impurities and fission products, with possible formation of volatile species, are also of interest.

A. Code Development (A. Bowman)

The OXIDE-3 code received from GAC has been rewritten in a different style. The modified version, tentatively designated OXIDE-3A, is analytically equivalent to OXIDE-3, but the Fortran source code has been reduced in length by 40% and the running time has been reduced by approximately 15%. The modification consists

primarily of the elimination of unused statements, arrays, and single variables, and the combination of related groups of variables into arrays. Some of the flow paths have also been changed to eliminate unnecessary subroutines, loops, and transfers. The rounded-off atomic weights used in OXIDE-3 have been replaced by 1966 values without round-off.

The conversion to OXIDE-3A has yielded three principal benefits:

1. A cleaner, more efficient code which is easier to read;
2. a thorough understanding of the OXIDE-3 model and its computational processes; and
3. the elimination of several programming errors. Only two of the errors had any significant effect on the results. These involved the release of metallic fission products (an error already discovered and corrected by GAC) and the initialization of coolant temperatures in the core.

A meeting was held on June 16, 1975 with A. Barsell and M. Perroomian of GAC to discuss the OXIDE-3A modification and possible programming errors. This meeting increased our understanding of OXIDE-3, cleared up several points of uncertainty, and defined a few areas for further study.

The OXIDE-3A code is now operational, but some debugging is required and there are still a few sections to be modified. The results of this conversion effort suggest that there are no significant programming errors in OXIDE-3. The future work with OXIDE-3 will include a study of the validity of the model and of the simplifying assumptions used to facilitate computation. Now primary effort will be directed toward the further development of the CIMPRES code.

*The diffusion coefficient can be shown to be the time integral of the velocity autocorrelation function; see for example Ref. 21.

B. Corrosion and Mass Transport Phenomena
(R. Feber, J. Lunsford, and W. A. Stark)

In the past quarter continued effort has been expended in the area of complex equilibria calculations. Part of this effort has been devoted to the continued development of an interactive computer code, QUIL. This code features a pre-processor which accepts a chemical statement of the problem as input. The pre-processor then generates the set of non-linear equations required by the problem at execution time.

The first system solver used by QUIL relied on a combination of techniques; the Newton-Raphson, a weighted Newton-Raphson, and the method of steepest ascent. Increased use of the code in a variety of applications indicated instances for which solutions could not be obtained and consequently a more powerful technique has substituted for the method used earlier. This new method is a modification of the Levenberg-Marquardt^{23,24} algorithm. After an initial search is performed for an optimum factor by which to scale the solution vector (E search), a two-dimensional search is performed which employs both the E method and the Levenberg-Marquardt method (P search). A method of smallest least squares solutions as proposed by Osborne²⁵ which can operate with singular systems is used to extract the solution vector. This allows the system solver to operate with ill-conditioned as well as singular systems and to increase the likelihood of convergence in the wide variety of problems which occur.

Various features have been incorporated into QUIL to increase its convenience and utility. The code has been modified so as to be able to calculate equilibria in the presence of surface phases. In particular, another code, ISOT, was written which will decompose experimental sorption isotherms into a parametric model and will load these parameters into the library in

a manner identical to that in which conventional reactions have been treated. The code has been modified so that it will calculate the potential to occur for reactions which are assumed to be out of equilibrium. These "reaction potentials" are then plotted over the range of the calculation. Instances of mixed equilibria are also of interest wherein certain reactions in a system are assumed to be in equilibrium while others are not. For example, one might wish to partition equilibrium in a given system by assuming gas-gas equilibrium in the absence of gas-solid equilibrium. The code has been modified to allow for such conditions of partitioned equilibria to be imposed. QUIL has also been modified so as to allow the reactions in the library to be loaded as sums and differences.

Calculations on equilibria to be expected in the presence of cesium isotherms have only just begun. The first data so treated are those for cesium sorption on TS-688 graphite taken at GAC.²⁶ Although it is still too early to make extensive equilibrium predictions on the behavior of cesium in the reactor environment, some trends are beginning to appear of the sort indicated in Fig. 9. The ordinate of this plot is the negative log of the activity of species assumed to be present over a cesium isotherm. Here the activity is computed as the product of (concentration)(total pressure) for gas phases, the concentration for condensed phases, and as the fractional coverage relative to one mono-layer coverage for surface phases. The environment chosen for the calculation is the Peach Bottom steady state stoichiometry.²⁷ The cesium introduced corresponds to an initial coverage of 0.01% of mono-layer coverage, or about 0.01 micro-moles of cesium per mole of graphite. The temperature range indicated is from 300 to 1500 K, which is the limit to which the data in question may be extrapolated. As a matter of fact, the results should be taken

These two graphs suggest a tentative conclusion: although the cesium isotherm is insensitive to the gaseous environment over the isotherm, the distribution of cesium species that occur in the gas phase is very sensitive to the composition of that gas phase.

Reaction potentials are also computed for precipitation reactions in the system. For deposition reactions involving condensed phases at unit activity, the equilibrium constant can be computed with the condensed phases assumed to be present or absent. As an example, consider the two reactions

and

which could be solved under equilibrium assumptions to give the equilibrium distribution of species present. In this case there would be $\text{CO}_2(\text{g})$, $\text{O}_2(\text{g})$, $\text{CO}(\text{g})$, and $\text{C}(\text{s})$. The presence of solid carbon affects the resultant distribution significantly, and is equivalent to the assumption of gas-solid equilibrium. In the event that this assumption seems unwarranted, it is possible to solve for the following distribution instead. Taking the sum and difference of the two reactions presented above, one obtains

as a single reaction. The resultant distribution of species, is exactly that which would prevail if the system as assembled had no carbon in it. In effect, the system has been solved under the assumption that gas-gas equilibrium prevails while gas-solids does not.

Having excluded $\text{C}(\text{s})$ from the calculation, it is now of interest to know if the environment as calculated is predisposed

to precipitate carbon or to react with it. Consider the definition of the equilibrium constant for the first reaction written above:

$$K = P_{\text{O}_2} / P_{\text{CO}_2} \quad (32)$$

Since the reaction was not included in the system as solved in the second instance, the equality as written above is not satisfied. If instead one substitutes the identity

$$K' = P_{\text{O}_2}' / P_{\text{CO}_2}' \quad (33)$$

where K' is computed from the composition distribution solved in the absence of $\text{C}(\text{s})$, then the ratio

$$R = K/K' \quad (34)$$

is a measure of the extent to which the CO_2 reaction is out of balance and is thus a measure of the "potential" of the reaction to occur in the system as written. In this case, it is the tendency of the system to precipitate carbon from the gaseous environment assumed to be in equilibrium. The log of the ratio of these two equilibrium constants is then treated as a reaction potential. A positive reaction potential indicates a tendency for the reaction in question to run to the right as written.

Figure 11 indicates the reaction potential for the deposition of $\text{Cs}(\text{OH})$ in the liquid state in the Peach Bottom equilibrium environment in the presence of carbon. Indications are that no such precipitation would occur, since the plot is positive over the range of the calculation. Figure 12 shows the reaction potential for the deposition of cesium liquid. Again, no tendency to precipitation is indicated in the Peach Bottom environment in the presence of carbon. Calculations are yet to be made on the effect of

Fig. 11. Reaction potential for Cs(OH) (L) in the Peach Bottom steady state stoichiometry with a 0.01% cesium isotherm present. Gas phase assumed to be in equilibrium with solid carbon. Operating pressure of 2296 kPa (20 atm).

Fig. 12. Reaction potential for Cs(L) in the Peach Bottom steady state stoichiometry with a 0.01% cesium isotherm present. Gas phase assumed to be in equilibrium with solid carbon. Operating pressure of 2296 kPa (20 atm).

precipitation isotherms on heat exchanger materials in the reactor coolant loop circuit.

Actually, the trend that may be observed in the absence of carbon with increasing water is quite interesting. Since the isotherm is virtually unaffected by the gaseous environment, it effectively maintains the Cs partial pressure above the isotherm constant. In the reaction

as the (hydrogen) (oxygen) product increases, the partial pressure of the Cs(OH) goes up correspondingly. What happens in the absence of carbon at high water pressures is that the activity of the cesium hydroxide may reach the ppm level. Since

the carbon will eventually oxidize the water, it is instructive to carry out the calculation with carbon present. When one does, it is found that the reaction products of the water reduction have no such effect on the Cs(OH) activity. Thus one would expect that the Cs(OH) activity would first rise and then fall after a water ingress depending upon the rate of reduction of the water by the carbon.

Estimates of thermodynamic equilibrium compositions in the carbon-steam system have been obtained by an analytical approach which begins with material balances on hydrogen and oxygen, respectively:

where

P_i = partial pressure of component i at equilibrium

P_i^0 = initial partial pressure of component i.

On substitution of K_1 , K_3 , and K_4 , which are, respectively, the equilibrium constants for the reactions

the material balance for hydrogen yields

$$P_{\text{H}_2\text{O}} = \frac{1 + R_{\text{H}}}{4K_4 R_{\text{H}}^2} \left[\sqrt{1 + 8K_4 R_{\text{H}}^2 (P_{\text{H}_2\text{O}}^0 + P_{\text{H}_2}^0)} - 1 \right] \\ \sim \frac{P_{\text{H}_2\text{O}}^0 + P_{\text{H}_2}^0}{1 + R_{\text{H}}} \quad (41)$$

where $R_{\text{H}} = \frac{P_{\text{H}_2}}{P_{\text{H}_2\text{O}}} = \text{hydrogen-to-water ratio.}$

This approximation inserted into the oxygen material balance yields a cubic equation in R_{H} :

$$R_{\text{H}}^3 - R_{\text{H}}^2 (K + D) - R_{\text{H}} K(1 + 2K_3) - 2KK_3 = 0 \quad (42)$$

where now $K = \left(\frac{K_1}{P_{\text{H}_2\text{O}}^0 + P_{\text{CO}}^0} \right)$ and

$$D = \left[\frac{P_{\text{H}_2}^0 - P_{\text{CO}}^0}{P_{\text{CO}}^0 + P_{\text{H}_2\text{O}}^0} \right]. \quad \text{Equation (42) may}$$

be solved for R_{H} using an iteration technique; at high temperatures results are in quite good agreement with those calculated using the more sophisticated free energy minimization routines such as QUIL, as shown in Table VIII and Table IX. The discrepancies at the lower temperature are due primarily to the approximations used in the derivation of Eq. (41).

These efforts indicate that, as a first approximation, equilibria of the carbon-steam system can be treated by consideration of the major species (H_2 , H_2O , CO , CO_2 , CH_4) only. Concentrations of minor species can then be determined from suitable equilibrium constants. In principle also, the effect of additional CO or H_2 upon equilibrium compositions can be determined analytically from Eq. (42).

C. Reactions of Impurities with Graphite and Metallic Components (L. C. Michels and W. A. Stark)

A technique employing electrical resistance measurements is being evaluated for possible use in determining the kinetics of gas-metal reactions. Experimental details and the results of initial experiments were reported in the previous HTGR Safety Research Program Quarterly Progress Report, Section IV-B.²⁸ The experimental setup has since been refined to provide electrical resistance measurements with a sensitivity of $\pm 0.1\%$ (formerly $\pm 1\%$). This was accomplished through the use of a high precision digital voltmeter to measure the voltage drops across the specimens and calibrated standard resistor.

The initial experiment involving a determination of the surface oxidation kinetics of pure Ni in flowing air at 900°C was repeated with excellent results. The specimen was again 99% Ni wire of nominal 0.051 mm (0.020-in.) diam. As was reported previously an equation was derived relating the measured change in electrical resistance (R) to the thickness (T) of the metal layer lost due to surface oxidation:

$$T = kt^{1/2} \quad (43)$$

$$R = \frac{A}{(r_0 - kt^{1/2})^2} \quad (44)$$

in which k is the parabolic rate constant, $A = \frac{\rho \ell}{\pi}$, assumed constant, and r_0 is the initial specimen radius. Following the procedure previously described, values for

TABLE VIII

COMPARISON OF ANALYTICAL AND NUMERICAL COMPUTATIONS
OF EQUILIBRIUM $R = P_{H_2}/P_{H_2O}$ Ratios

Helium Pressure = 50 atm. $P_{CO}^O = P_{H_2}^O = 0$

$P_{H_2O}^O$ (vpm)	$P_{H_2O}^O$ (atm)	<u>T = 1100 K</u>		<u>T = 600 K</u>	
		<u>R_{AN}</u>	<u>R_{NUM}</u>	<u>R_{AN}</u>	<u>R_{NUM}</u>
50	2.5×10^{-3}	4419	4420	1.392	1.342
100	5.0×10^{-3}	2211	2211	1.047	0.982
500	2.5×10^{-2}	444.6	444.9	0.557	0.470
1000	5.0×10^{-2}	223.8	224.0	0.430	0.339
5000	.25	47.00	47.22	0.239	0.157
8000	.40	30.37	30.58	0.202	0.125

TABLE IX

COMPARISON OF ANALYTICAL AND NUMERICAL COMPUTATIONS,
HELIUM PRESSURE = 50 atm

$P_{H_2O}^O$ (atm)	P_{CO}^O (atm)	$P_{H_2}^O$ (atm)	<u>T = 1100 K</u>		<u>T = 600 K</u>	
			<u>R_{AN}</u>	<u>R_{NUM}</u>	<u>R_{AN}</u>	<u>R_{NUM}</u>
-0-	5.0×10^{-2}	5.0×10^{-2}	223.8	224.2	0.430	0.339
5.0×10^{-3}	7.5×10^{-3}	7.5×10^{-3}	886.2	886.2	0.728	0.647
5.0×10^{-3}	2.5×10^{-2}	2.5×10^{-2}	371.0	371.5	0.520	0.431
5.0×10^{-2}	2.5×10^{-3}	2.4×10^{-3}	213.2	213.5	0.422	0.331
5.0×10^{-2}	.25	.25	39.62	40.02	0.224	0.144
5.0×10^{-2}	5.0×10^{-3}	0.0	203.6	203.9	0.383	-
5.0×10^{-2}	0.0	5.0×10^{-3}	223.9	224.2	0.470	0.350

A and k were found to be:

$$A = 7.60 \times 10^{-3} (\Omega \cdot \text{mm}^2),$$

$$k = 4.21 \times 10^{-5} \text{ mm/s}^{1/2}.$$

Using these values of A and k in Eq. (44), the measured values of R were reproduced to within $\pm 0.25\%$; the thickness of the lost metal layer was calculated from Eq. (43) to be 7.43×10^{-3} mm. A metallographic determination of the thickness yielded a value of 7.62×10^{-3} mm showing excellent agreement between the two different techniques.

For a comparison of the parabolic rate constant to literature values, k converts to a value of $9.74 \times 10^{-6} \text{ g/cm}^2 \times \text{s}^{-1/2}$. The value of k calculated using the equation given in Ref. 29 for nickel of comparable purity (99.7% Ni) is $11.07 \times 10^{-6} \text{ g/cm}^2 \times \text{s}^{-1/2}$, about 12% higher than the measured value.

In a similar experiment 99% Ni wire was exposed to a flowing mixture of carbon monoxide and helium at atmospheric pressure in an attempt to follow the progress of carburization. The gas mixture was one to one by volume; the flow rate was $6 \times 10^{-6} \text{ m}^3/\text{s}$ ($0.76 \text{ ft}^3/\text{h}$); and the experiment was carried out at a temperature of 1173 K. The electrical resistance of the specimen increased rapidly for the first 3.6 ks (1 h) of the run, then approached a constant value. The measured resistance became essentially constant by $\sim 7.2 \text{ ks}$ (2 h).

Metallographic examination of the specimen revealed extensive precipitation in the grain boundaries near the surface of the specimen (within about 0.02 mm of the surface). This precipitate is most likely graphite, since Ni_3C is believed to be unstable under the prevailing conditions. Attempts to correlate the resistance time data with a logarithmic function derived from a simplified diffusion analysis or several power functions were unsuccessful.

It appears that the technique is not useful in a situation of this complexity without considerable additional data. A quantitative analysis of the results of this experiment would require a detailed diffusion analysis, data on the electrical resistivity of nickel as a function of carbon content, and a knowledge of the kinetics of precipitation and solution of graphite in nickel.

In a third experiment a specimen of C1095 steel was exposed to a flowing mixture of air and helium at atmospheric pressure in an attempt to follow the progress of surface oxidation plus any internal changes that might occur. The gas mixture was one to one by volume and the experiment was carried out at a temperature of 983 K.

The electrical resistance was observed to increase slowly throughout the experiment. The increase was approximately linear with time. The total observed resistance increase was 1.02%. The resistivity of the specimen decreased 2.01%. These observations indicate that in addition to an increase in resistance of the specimen due to surface oxidation and consequent geometrical changes there was a decrease in resistivity due to some other process or processes occurring simultaneously. The electrical resistance of the specimen exposed to pure helium was observed to remain constant to within the sensitivity of the measurements.

Metallographic examination of the specimens revealed no differences in microstructure to which the decrease in resistivity could be attributed. However, very accurate diameter measurements on specimens oxidized for increasing periods of time could be used for an independent determination of the kinetics of surface oxidation. This information would then allow the kinetics of the resistivity decrease to be determined from the original resistance versus time data.

It appears that the use of electrical resistance measurements to determine the kinetics of gas-metal reactions without considerable supplementary data is limited to cases in which only surface oxidation occurs (producing excellent results), and to cases in which surface oxidation plus internal changes throughout the base material occur simultaneously.

V. TASK 4, STRUCTURAL INVESTIGATION

A. Constitutive Relations of Plain and Reinforced Concrete (E. G. Endebrock and J. B. Payne)

A computer code for the plain and reinforced concrete constitutive relations of Ref. 30 has been obtained and made operational on LASL computers. This code incorporates a number of the most recent advances in the theoretical and experimental behavior of plain and reinforced concrete. Featured in the code are:

1. Plain or reinforced concrete behavior.
2. All multiaxial stress combinations in compression and tension.
3. Effects of differing amounts and directions of the reinforcing steel.
4. Orthotropic behavior after cracking in tension.
5. Crack initiation and propagation.
6. Bond-slip action between concrete and reinforcing steel under tensile stresses.
7. Rebonding effect whenever unloading and reloading occur
8. Dowel action effects.
9. Unloading and reloading capability.

This code was developed for use in general purpose finite element stress analysis programs. Since nonlinearities are inherent in plain and reinforced concrete behavior, an important feature of the code is the incremental solution of nonlinear equations. The code is limited to small deformations, stable inelastic

material behavior (i.e. the stress-strain curve must have a positive tangent modulus), and it does not include creep and temperature effects. Even so, this code appears to be the most advanced one available for representing the complex behavior of reinforced concrete.

B. Code Development for the Analysis of PCRV's

As has been reported previously the general purpose finite element code NONSAP³¹ has been selected as a basis for the development of a LASL computer code for use in the analysis of PCRV's. Important features of NONSAP are:

1. Static and dynamic analysis capability.
2. Three-dimensional isoparametric finite elements.
3. Incremental solution with time as the dependent variable.
4. Nonlinear elastic and plastic material behavior.
5. Load input as a function of time.

These features permit modification to include creep effects, tendon relaxation, and a load-history analysis.

Our present version of NONSAP is restricted by the lengthy input information required for execution of realistic problems, by limitation of output information (e.g. stresses) to the global rectangular coordinate system, by lack of a pressure loading input capability, and by lack of a thermal capability. Addition of a mesh generator and suitable transformation matrices will eliminate the first three restrictions, and these modifications to NONSAP are now underway. Addition of some sort of thermal analysis capability and programming to maximize the number of nodes and elements available for solving three-dimensional problems on LASL's computers are two efforts which we will soon undertake.

The code for the plain and reinforced concrete constitutive relations discussed in Sec. A has been incorporated into NONSAP.

C. Analytical Model Development for Core Seismic Response (J. G. Bennett, R. C. Dove, K. H. Duerre, and J. L. Merson)

1. Two-dimensional Core Seismic Analytical Model

The two-dimensional core seismic analytical model shown in Fig. 13, has been extended to include the effects of a dowel pin on the upper face of each block and a matching lower slot on the bottom of each block. The bottom row is also pinned to the lower boundary by an identical pin-slot arrangement. A free body diagram representation of the basic element that is currently in the two-dimensional model is shown in Fig. 14. The model has the capability of allowing for a different vertical contact stiffness, horizontal contact stiffness, pin stiffness, and slot stiffness.

Future applications of this model will be to study the influence of the pins in terms of the pin clearance to contact gap clearance ratios, pin stiffness and the other parameters in the light of studies conducted on the one-dimensional model that have been completed to date.

Fig. 13. Two-dimensional model.

Fig. 14. Free body diagram illustrating all effects currently in the two-dimensional model.

Preliminary indications are that the pins will serve to limit the motion of the blocks considerably, but this will probably produce rather large pin shear forces.

A computer produced movie that illustrates the pin connected model under horizontal single frequency excitation has been completed and was shown at the first annual HTGR Structural Review held at Germantown, Maryland, on June 12, 1975.

2. Core Component Stiffness Studies

As has been previously reported, studies have been undertaken to provide estimates of the stiffness for various core components. This input is needed for the core analytical model (Fig. 13).

The HTGR fuel block, locating pin, and locating pin slot are shown in Fig. 15. Two different finite element models (Figs. 16 and 17) were made of those components. The material (nuclear graphite) in all cases was assumed to be linear elastic and isotropic with values of Young's Modulus and Poisson's ratio of 13.8×10^9 N/m² (2×10^6 psi) and 0.1 respectively.

Fig. 15. Fuel block

Fig. 17. Axisymmetric model for dowel pin stiffness calculation.

Pressures were applied to a face of the component and the resulting nodal displacements were assumed to behave similarly to an array of parallel springs. The total stiffness of the component is then just the sum of nodal stiffnesses i.e.:

$$K_T = \sum_{i=1}^n K_i \quad (45)$$

where:

n = the number of nodes along the pressure face,

K_i = equivalent spring stiffness for the i th node.

The equivalent spring stiffness is defined as the slope of the force-displacement curve, $K = F/\delta$, for a given node. Values were determined for each K_i at several loadings in the linear elastic range for the finite element models of the components in Figs. 16 and 17.

Fig. 16. One model for fuel block stiffness calculation.

3. Fuel Block Horizontal and Vertical Stiffness

A special program was written to create a mesh for the plane quarter section represented in Fig. 16 for the hexagonal fuel block. Five-hundred eighty-two elements were constructed from 679 nodes. The computer program SAP-IV³² was used with the plane strain option to obtain the node deflections of the fuel block model for given applied pressures. Figure 18 shows typical force-deflection curves from which nodal stiffnesses are directly obtained. The total stiffness for the plane model was determined to be 72.9×10^6 N/m; from Eq. (45). Taking account of the length of the block then gave a total block horizontal stiffness of $K_H = 22.8 \times 10^8$ N/m.

The vertical stiffness for the graphite block was determined from $K_V = EA/l$ where E is Young's Modulus, A is the cross sectional area (excluding the voids), and l is the block length. This is the axial stiffness of a finite length bar under uniform axial loading. For the given block parameters, $K_V = 10.5 \times 10^8$ N/m.

Fig. 18. Typical nodal force-displacement curve from fuel block stiffness model.

4. Fuel Block Locating Pin Stiffness

A modified version of the SABOR/DRASTIC³³ computer code was used to analyze the locating pin under static loadings. This version of SABOR is designed to handle axisymmetric geometries under non-axisymmetric loads based on Fourier representations of the load and has been modified at LASL to handle a continuum element. A short preprocessor was written to prepare the input to SABOR based on an axisymmetric model of the hollow pin shown in Fig. 17. The half-cosine static load in Fig. 19 was built up from the five Fourier components illustrated in Fig. 20. Since the pressure distribution is an even function, only the cosine terms and constant of the Fourier series representation are non-zero. The Fourier coefficients for the first five non-zero harmonics are given in Table X. Results of these calculations are given in Fig. 21. The element stiffness based on axial height of the pin is seen to be a smoothly decreasing function.

The total effective lateral stiffness is taken to be $3 \times \sum K_i$ for one pin:

Fig. 19. Sum of Fourier components for pin loading.

Fig. 20. Fourier components used to simulate pin loading.

TABLE X

NON ZERO FOURIER COEFFICIENTS FOR
LOADING OF LOCATING PIN AND SLOT

Harmonic	Fourier Coefficient
0	+ 0.3183
1	+ 0.5
2	+ 0.2122
4	- 0.04244
6	+ 0.01818

$$K_p = 10.84 \times 10^8 \text{ N/m.}$$

Based only on shear deformation of the circular pin, a lower bound estimate of $4.7 \times 10^8 \text{ N/m}$ was obtained for this value.

5. Fuel Block Locating Pin Slot Stiffness

A similar type of finite element model is being prepared for estimating the matching lower slot stiffness for the fuel block, but results are not yet available.

Fig. 21. Typical nodal force-displacement curves from pin stiffness model.

6. Summary of Core Component Stiffness Estimates to Date

Estimates of $64 \times 10^8 \text{ N/m}$ and $19.5 \times 10^8 \text{ N/m}$ for solid fuel block lateral and vertical stiffness are reduced, due to fuel and coolant holes to the values $22.8 \times 10^8 \text{ N/m}$ and $10.5 \times 10^8 \text{ N/m}$ respectively, as obtained from finite element calculations. The lateral stiffness of the locating pin was found to be $10.8 \times 10^8 \text{ N/m}$. These are the values that are currently being used as input to the core seismic analytical models.

7. Earthquake Excitation of the One-dimensional Core Seismic Analytical Model

During the present quarter significant modifications have been made in the data output from the core block model programs. The purposes of these modifications have been to display block accelerations and contact forces versus time.

These new output forms have been used to represent the system response to earthquake excitation and in the extension of the scaling law studies which are discussed in the following section.

A program (SIMEAR) for generating simulated acceleration, velocity, and displacement versus time earthquake histories was described in the previous quarterly report. During the present quarter, motion versus time histories produced by SIMEAR have been used to drive the one-dimensional, analytical, four-block model (see Fig. 22). Because of previous testing of this model over a wide frequency range the response expected to be produced by earthquake input was anticipated. However, when the model was driven by the simulated earthquake, the response was considered incredible. As a result, the model program was rechecked by driving it with a mixed frequency consisting of five sinusoidal components (0.5, 1, 5, 10, and 25 hz) and the simulated earthquake motion-histories were investigated for consistency. The model was found to respond as expected to the analytically defined mixed frequency driving function and so attention was focused on the simulated earthquake signal. It was found that the three time histories (acceleration, velocity and displacement) furnished from the SIMEAR program are independent (i.e.,

Fig. 22. One-dimensional core seismic model.

velocities and displacements are not first and second integrals of the acceleration-time history). This is important when using the simulated earthquake to drive the model because all three motion-time signals (acceleration, velocity and displacement) are used simultaneously in model computations. As a result of this finding, SIMEAR is being used to produce only the appropriate acceleration-time history, which is then corrected as necessary to produce a velocity time history that begins and ends at zero velocity; the velocity time and the displacement-time histories are then produced by integration of the acceleration-time history. Figures 23, 24, and 25 show a SIMEAR generated and corrected acceleration-time history and the associated velocity-time and displacement-time histories. Figure 26 compares the response spectra for the acceleration-time history shown in Fig. 23 to the NRC response spectra. Motion-time histories generated in this manner are now being used successfully to drive the core block models. Figure 27 shows the

Fig. 23. Simulated earthquake-acceleration.

Fig. 24. Velocity-time history from integration of Fig. 23.

Fig. 26. Response spectra for the acceleration-time signal shown in Fig. 23.

Fig. 25. Displacement-time history from integration of Fig. 24.

Fig. 27. Acceleration response of four block model to the earthquake shown in Fig. 23.

acceleration response of block #1 (see Fig. 22), during the first 10 s, to the simulated earthquake shown in Fig. 23. Figure 28 shows the contact forces imposed by the boundary on the left side of block #1, as a result of this earthquake excitation. This information is, of course, available for all blocks in the system.

D. Physical Model Test Program for Core Seismic Response (R. C. Dove, J. G. Bennett, J. L. Merson)

In the previous quarterly progress report²⁸ and in Ref. 35 we discussed the scaling laws used to guide the development of scale models of the HTGR core and the use of the simple four-block analytical model to check these scaling laws. During the present quarter these scaling law studies have been extended. As before, the four-block analytical model (see Fig. 21) was used in making the computations; however, comparisons between the several prototype and model systems are made on the basis of accelerations and forces rather than displacements.

Fig. 28. Contact forces on four-block model.

Four different systems, having the parameter values shown in Table XI were run. All three of the "models" are designed with a length scale (N_d) of four, but differ greatly in other ways. The "true model" is designed so as to satisfy all of the scale relationships dictated by the laws of similitude. These are:

$$\text{Time Scale: } N_t = \sqrt{N_d}$$

$$\text{Acceleration Scale: } N_a = 1$$

since the gravitational constant is assumed to be the same in each system test environment.

$$\text{Force Scale: } N_Q = \frac{E_p}{E_m} \cdot N_d^2$$

that is, the force scale is the ratio of prototype modulus (E_p) to model modulus (E_m) times the length scale squared (N_d)².

The above three imply that the ratio of model modulus (E_m) to model weight (W_m) is equal to the ratio of prototype modulus (E_p) to prototype weight (W_p) times the length scale squared (N_d)².

Figure 29 shows the acceleration response of block #1 in the prototype system to a ± 1 g, 5 H_z excitation. Figure 30 shows the acceleration response of block #1 in the true model system to a ± 1 g, 10 H_z excitation (since model times are scaled by dividing by 2, i.e., $\sqrt{N_d}$, frequencies are doubled). Close inspection of these two acceleration time histories shows that when properly scaled ($N_a = 1$, $N_t = 2$) the true model is indeed predicting the prototype acceleration-time history. The prediction is most accurate during early times and as time progresses accumulating computational errors produce some divergence of results.

The next system considered is referred to in Table XI as a "distorted model". This particular model is distorted in the following way: having picked a length scale (N_d) arbitrarily, we will then use

TABLE XI

"PROTOTYPE" AND "MODEL" STUDY PARAMETERS

<u>Prototype</u>	<u>True Model</u>	<u>Distorted Model</u>	<u>Friction Corrected Distorted Model</u>
$d_p = 0.381 \text{ m (15-in.)}$	$0.381/4 \text{ m}$	$0.381/4 \text{ m}$	$0.381/4 \text{ m}$
$C_p = 0.381 \text{ cm (0.15-in.)}$	$0.381/4 \text{ cm}$	$0.381/4 \text{ cm}$	$0.381/4 \text{ cm}$
$\mu_{s_p} = 0.200$	0.200	0.200	0.2×4
$\mu_{k_p} = 0.160$	0.160	0.160	0.16×4
$E_p = 13.79 \times 10^9 \text{ N/m}^2$ $(2 \times 10^6 \text{ psi})$	$\left(\frac{E_m}{W_m} = \frac{E_p}{W_p} \times 4^2 \right)$	$13.97 \times 10^9 \text{ N/m}^2$	$13.97 \times 10^9 \text{ N/m}^2$
$W_p = 975.94 \text{ N}$ (219.4 lb)		$975.94/4^3 \text{ N}$	$975.94/4^3 \text{ N}$
$x_B = \pm 0.9944 \text{ cm}$ $(\pm 0.3915\text{-in.})$	$\pm 0.9944/4 \text{ cm}$	$\pm 0.9944/4 \text{ cm}$	$\pm 0.9944/4 \text{ cm}$
$f_B = 5 \text{ Hz}$	$5 \times \sqrt{4} = 10 \text{ Hz}$	$5 \times 4 = 20 \text{ Hz}$	$5 \times 4 = 20 \text{ Hz}$
i.e. $= \ddot{x}_B = 1g$	$1g$	$4g$	$4g$

Scales

Length - N_d	4	4	4
Time - N_T	$\sqrt{4}$	4	4
Acceleration - $N_{\ddot{x}}$	1	$1/4$	$1/4$
Force - N_Q	$E_p/E_m \times 4^2$	4^2	4^2
Stress - N_σ	$N_Q \div 4^2$	1	1

Fig. 29. Acceleration response of prototype system to $1g$, 5 Hz , excitation

the same material for the model as was used for the prototype. As a result, the material modulus of the model equals the material modulus of the prototype ($E_m = E_p$) and since, for equal material density, weight varies as the cube of the dimension, $W_m = W_p / N_d^3$. Hence, $E_m / W_m = E_p / W_p \times N_d^3$, instead of the required $E_m / W_m = E_p / W_p \times N_d^2$. The result is a model that is too light for its stiffness if it is tested in the same gravitational field as the prototype. These choices also result in a time scale equal to the length scale ($N_t = N_d$) and an acceleration scale equal to the reciprocal of the length scale ($N_a = 1/N_d$). Figure 31 shows the acceleration response of block #1 in this distorted model system to a $\pm 4g$, 20 Hz (since model times are scaled by dividing by 4, frequencies are multiplied by 4). Comparison of this record to the prototype system acceleration response (Fig. 29) indicates how this system response differs from that of the prototype. In general we note that in the distorted model the impacts are more uniformly spaced in time; however, the similarities between the two systems are more

Fig. 30. Acceleration response of true model to $1g$, 10 Hz , excitation.

surprising than the differences. In comparing Figs. 29 and 31 we note that although the peak accelerations occur at different times the distorted model predicts (when properly scaled) the peak values with reasonable success. For the

Fig. 31. Acceleration response of distorted model to $4g$, 20 Hz excitation.

prototype system:

Positive peak acc. = 437.5 g at 0.204 s

Negative peak acc. = -534.8 g at 0.623 s.

For the distorted model system:

Positive peak acc. = 1751 g at 0.196 s

which scales to

437.8 g at 0.782 s.

Negative peak acc. = -2310 g at 0.195 s

which scales to

-577.5 g at 0.779 s.

Furthermore the distorted model predicts that block #1 will receive 149 impacts in a scaled time of 2 s. The prototype test shows block #1 actually received 147 impacts. However, in Ref. 34 it was shown that this distorted model responds with a completely different displacement time history than does the prototype system.

The fourth system considered is referred to as a "friction correction distorted model" in Table XI. This system is the result of the observation that since the distorted model is too light, and hence frictional forces are too small when tested in a 1 g field, a correction should be possible and, hence, coefficients of friction (μ_s and μ_k) have been increased by a factor of four. Figure 32 shows the acceleration response of block #1 in this "corrected" system to a $\pm 4g$, 20 Hz excitation. Comparison of Fig. 32 to Fig. 29 shows that this corrected model predicts the prototype acceleration response exactly (model results must, of course, be scaled i.e., $\ddot{x}_p = \ddot{x}_m/4$, $t_p = 4 \times t_m$). This type of correction also allows this model to accurately predict prototype displacement-time histories.

Whether this simple type of correction would be physically possible or whether it would be completely effective in a three-dimensional model subjected to three orthogonal motion inputs is still unknown.*

Fig. 32. Acceleration response of friction corrected model to 4g, 20 Hz, excitation.

The results of a parameter study, which was made using the simple four-block system (see Fig. 22), were discussed in the previous quarterly report.²⁸ During the present quarter an attempt has been made to relate parameter studies of this type to the interpretation of physical model study results. The procedure for establishing a "prediction factor" which may be used with a distorted model is described in Part II of Ref. 36.

We assume that the functional equation which was developed in the previous quarterly report²⁸ can be rewritten as follows:

Equation (25) from Ref. 28 is:

$$\frac{\ddot{x}}{g} = \psi \left(\frac{x_B}{d}, \frac{c}{d}, \frac{Ed^2}{W}, \mu_k, \frac{\mu_s}{\mu_k}, \frac{E}{D}, \frac{x_B}{gt^2} \right). \quad (46)$$

By assuming the function is a product form we will rewrite Eq. (46) as

$$\frac{\ddot{x}}{g} = \psi \left(\frac{Ed^2}{W} \right) \times \psi \left(\frac{x_B}{d}, \frac{c}{d}, \mu_k, \frac{\mu_s}{\mu_k}, \frac{E}{D}, \frac{x_B}{gt^2} \right). \quad (47)$$

* Alternately, the model might be tested in an artificial, higher "g" field.

With a model distorted by using the same material for model and prototype only the term Ed^2/W need be distorted, so we write:

$$\frac{(\ddot{x}/g)_p}{(\ddot{x}/g)_m} = \frac{\psi' \cdot (Ed^2/W)_p}{\psi' \cdot (Ed^2/W)_m} \quad (48)$$

since the function ψ' is identical for both model and prototype. The "prediction factor" θ is defined as

$$\theta = \frac{\psi' \cdot (Ed^2/W)_p}{\psi' \cdot (Ed^2/W)_m} \quad (49)$$

Hence

$$(\ddot{x}/g)_p = \theta (\ddot{x}/g)_m \quad (50)$$

In the previous quarterly report it was shown that the effect of the term Ed^2/W on block acceleration $\ddot{x}$ could be expressed as

$$\ddot{x} = 425 \left(\frac{Ed^2}{W} \times 10^{-6} \right)^{0.5} \quad (51)$$

(See Eq. 30 in Ref. 28). Thus ψ' is a square root function and hence

$$\theta = \sqrt{\left(\frac{Ed^2}{W} \right)_p : \left(\frac{Ed^2}{W} \right)_m} \quad (52)$$

To test this method of approach, θ was computed from the values of E , d , and W assigned to the "prototype" and "distorted" models shown in Table XI. It can be easily shown that θ is equal to $\sqrt{N_d}$ and hence equal to 2. The "distorted model" was then tested just as if it had been a true model (i.e., $X_B = \pm 0.9944/4$ cm, $f_B = 10$ Hz) and the results are multiplied by the prediction factor, θ , to predict prototype response. Figure 33 shows the acceleration response of block #1 in the distorted model system when driven just as

Fig. 33. Acceleration response of distorted model tested for prediction factor correction.

if it were a true model. Comparison of Fig. 33 with Fig. 29 indicated that when model accelerations are multiplied by a prediction factor of 2 the prototype acceleration is predicted for homologous times ($t_p = 2t_m$).

During this quarter we have also investigated the possibility of using "compensated distortion" as discussed in Ref. 36. That is, two or more π terms may be distorted (one or more deliberately in a controlled manner) so as to produce a total, or net, prediction factor, θ , of unity. The "coefficient of friction correction of the distorted model" discussed previously is an example of this approach. Another possibility which suggests itself is to test the distorted model at an input level that will provide a prediction factor which is the reciprocal of the prediction factor associated with the distortion in term (Ed^2/W) . This is possible using the relationship between block acceleration response ($\ddot{x}$) and input acceleration ($\ddot{x}_B$) determined in the parameter study of Ref. 27 [i.e., $\ddot{x} = 670(\ddot{x}_B - u_g)^{0.451}$]. This was done by exciting the

"distorted model" system at $\ddot{x}_B = 0.372 \text{ g}$ and the resultant acceleration response of block #1 is shown in Fig. 34. Comparison of Figs. 29 and 34 indicates that although there has been some success in predicting "peak" acceleration (in Fig. 34, $\ddot{x}_{\text{peak}} = -494 \text{ g}$; in Fig. 29, $\ddot{x}_{\text{peak}} = -535 \text{ g}$), the time history and number of impacts are grossly distorted. Clearly, this is not a suitable method.

Fig. 34. Acceleration response of distorted model tested with compensating distortion.

VI. TASK 6, SAFETY INSTRUMENTATION AND CONTROL SYSTEMS

A. Impurities Monitoring (E. J. Dowdy and G. W. Taylor)

The improved version of the LASL Helium Afterglow Impurities Monitor* was completed and is shown (exclusive of the optics and electronics packages) in three views in Figs. 35-38. All piping up to the reaction chamber is stainless steel tubing, 6.35 mm OD, 0.76 mm wall thickness, with either Swagelok or hard solder

*For a discussion of the principle of operation and a block diagram of the device, refer to previous quarterly progress reports: LA-5870-PR (2/75) and LA-5975-PR (6/75)

Fig. 35. Front panel of the Helium Afterglow Impurities Monitor.

connections. All valves have brass bodies, stainless stems, teflon O-ring seals and Kel-F seats. Flows are regulated through glass tube rotameters with tantalum ball floats.

The monitor was transported to the Ft. St. Vrain plant and operated on line on May 28 and 29, 1975 for the purpose of preliminary analysis of impurities in the primary coolant. During this time, the reactor was at zero power with the helium circulators turning, the primary coolant cleanup system in operation, and

Fig. 36. Side view of the Helium After-glow Impurities Monitor. The quartz glass helium plasma tube is visible above the brass-faced reaction chamber.

Fig. 37. Side view of the Helium After-glow Impurities Monitor showing the bellows pump at lower left, the calibration volume and the LN₂ traps.

various other components being exercised. The analysis thus provided identification and quantification of the various impurities in the primary loop under cold conditions. These measurements were intended to demonstrate the suitability of the monitor for the entire range of impurities of interest.

The monitor was placed in the analytical instrument room. The primary coolant for analysis was obtained through the main sampling line external to the instrument cabinet. Clean helium for the production of the helium metastables was obtained from the carrier gas line in the instrument cabinet. The discharge helium back-pressure was regulated to approximately

10 kPa. The primary coolant pressure in the sample line was also approximately 10 kPa. The flow rates maintained for all measurements in this series were approximately 1000 $\mu\text{moles/s}$ for the metastable bearing discharge line and approximately 100 $\mu\text{moles/s}$ for the primary coolant and calibration gases.

The first scan of the emission spectrum of the primary coolant was obtained about mid-morning on May 28. The scan contained a signal for the 306.4 nm band structure of OH* corresponding to 504 ppmV H₂O in the primary coolant stream. The sample line was evacuated and repressurized for a rescan. The rescan confirmed the presence of 504 ppmV H₂O in the primary

loop. An example of these scans appears as the top trace in Fig. 38. In addition to water, we identified CO, CO₂ and N₂ as primary coolant impurities from these early scans. Characteristic lines from the helium are apparent in the scan, as well as the hydrogen Balmer series. The source of the Balmer series is at present uncertain; possibilities include free hydrogen, hydrocarbons, or the H-Atom produced by the dissociation of H₂O. This area will receive additional attention. From 11:30 a.m. until 1:30 p.m. of May 28, the 306.4 nm band signal characteristic of water was monitored. The signal strength remained at that corresponding to 504 ppmV water during this period.

At about 10:30 a.m. May 29, another scan of the primary coolant was made, and the result is shown as the middle trace of Fig. 38. The presence of CO, CO₂, N₂ and H₂O is again verified. We have also tentatively ascribed the peak at approximately 335 nm to free hydrogen. In addition, the presence of oxygen was detected by the characteristic emissions at wavelengths > 500 nm. These are not shown in the traces provided in Fig. 38. In this scan, the strength of the 306.4 nm signal corresponds to a moisture content of 25 ppmV, down roughly a factor of 20 from the previous day. Calculations show that if no additional moisture entered the primary loop after 1:30 p.m. May 28, the factor of 20 decrease in the level would be consistent with a cleanup rate of 15% per hour, the rated capacity of the Ft. St. Vrain primary coolant cleanup system.

To complete the series of measurements, the calibration gas routinely used by the Ft. St. Vrain plant operator for chromatograph calibration was scanned. The result of this scan is shown as the bottom trace of Fig. 38. With the electrometer gains as shown in the figure, we detected the H₂, N₂, CO₂, He and O₂. We have subsequently verified our ability to detect Ar and CH₄

with higher electrometer gains. The peaks characteristic of CO are also apparent in this scan. These are ascribed, in this instance, to secondary reaction processes beginning with the dissociation of CO₂. The NO β bands are also obvious in the scan and result from mixed species recombination of ionized N₂ and O₂ produced by the helium metastables. Both species are detectable separately as well.

Our analysis (using the calibration gas as standards for all but water) thus indicates that at the time of these measurements the impurities in the primary coolant at the Ft. St. Vrain plant include CO, CO₂, H₂O, N₂, O₂ and H₂ in the following quantities:

CO	- unknown due to absence in standard
CO ₂	- approximately 1.8 ppmV
H ₂ O	- varied from 25 ppmV to 504 ppmV
N ₂	- approximately 5.4 ppmV
O ₂	- << 8 ppmV
H ₂	- approximately 10 ppmV

B. Temperature Sensors (V. Starkovich)

The feasibility of using the kryptonate method for determining the peak temperature experienced by HTGR fuel has been examined. A proposal to test this method has been written and is under discussion. The test would consist of irradiation of small samples of fuel particles in the LASL Omega West Reactor. Post-irradiation reheat of the samples to the temperature for onset of release of noble gas fission products would yield peak exposure temperature. Discussions with personnel responsible for task elements which would benefit from the results of such tests will continue.

Fig. 38. Spectra obtained at the Ft. St. Vrain plant. The two upper traces are of the primary coolant, taken on different days. These show the very wide variation of moisture content observed. The bottom trace is the spectrum of the calibration gas used by the operator for gas chromatograph calibration. The composition of the gas is given in the figure.

VII. TASK 7, ACCIDENT DELINEATION

(M. G. Stevenson)

As part of the HTGR safety research effort, the accident delineation task identifies and provides descriptions of significant accident sequences. We have reviewed the recent GAC report on analyses of anticipated transients with failure of control rod motion.³⁷ Transients considered in these preliminary analyses for the Summit HTGR plant include loss of one feedwater pump, turbine trip, loss of one main circulator, and rod withdrawal from both source and full power. The HTGR design allows for control of these transients through the plant control and operating protection system and precludes the necessity for reactor trip. The assumption used in the GAC analyses was that all control and protective systems operated as designed but control rods did not move into the core and lower the reactor power. However, feedwater flow was assumed to be ramped down as the normal response to various reactor trip signals. The characteristic consequence for these anticipated transients is then high inlet helium temperatures to the steam generators. The GAC analyses have not considered consequences of possible steam generator tube failures. We are continuing further delineation of these accident conditions. This work and other initial accident delineation efforts will be presented in a report in preparation.

VIII. TASK 9, PHENOMENA MODELING AND SYSTEMS ANALYSIS

A. HTGR Neutronic Analysis (J. C. Vigil)

During the past year, we have performed extensive calculations of the safety-related neutronic characteristics of the Fulton Generating Station (FGS) initial core. These have been reported in previous quarterly reports and include the following specific calculations:

1. Isothermal temperature coefficients for one-dimensional cell and finite reactor models,³⁸
2. Separate fuel and moderator temperature coefficients,³⁴
3. Effects of burnable poison, control rods, and Xe and Sm on the isothermal temperature coefficients,³⁴
4. Effect of ^{233}U on the isothermal temperature coefficient, and
5. One- and two-dimensional power distributions.²⁸

In general, these calculations agree quite well with similar GAC analyses for the FGS initial core. We have concentrated on temperature-dependent reactivity effects since these are the most important safety-related neutronic characteristics of the large HTGR. Our calculations of the effect on the isothermal temperature coefficient of replacing ^{235}U with ^{233}U in an otherwise initial core loading were made to give a preliminary indication of the relative importance of ^{233}U in equilibrium-cycle core loadings. The FGS initial core isothermal temperature coefficient is large and negative, but becomes substantially smaller as ^{233}U is produced in the fertile (ThO_2) particles. Careful analyses, including cross-section set generation, are important in providing an independent assurance that temperature feedbacks remain negative under postulated accident conditions. The neutronics effort during FY-76 will concentrate on analyses of equilibrium cycle core loadings with emphasis on temperature coefficient effects. A detailed report of our FGS initial core neutronic calculations is in preparation.³⁹

Additional calculations of FGS initial core neutronics characteristics are reported below. We have also calculated the reactivity change due to a postulated dropping of the central refueling region in the FGS initial core. All of the calculations noted here used cross sections generated by the MICROX code⁴⁰ and

provided by GAC. We have also calculated the isothermal temperature coefficient with LASL generated cross sections and the results are reported in the next section.

1. Control-rod Worths in the FGS Initial Core

The total reactivity worths of several control-rod configurations including 1, 7, and 73 (all) rod pairs were calculated using a two-dimensional (r-z) model of the FGS initial core at design temperature. In addition to its total worth, the worth vs axial position of the central control-rod pair was calculated. Where comparison data are available, the results are in good agreement with those in the FGS PSAR⁴¹ and with those obtained previously at LASL using a one-dimensional radial model.

The calculations were performed with the TWOTRAN-II code⁴² in S_4 approximation using four energy groups including three fast and one thermal group. The four-group cross sections correspond to the FGS beginning-of-life (BOL) compositions and operating temperature. They were obtained by collapsing nine-group MICROX cross sections using one-dimensional flux spectra. Effective (self-shielded) control-rod cross sections were calculated using shielding factors obtained from auxiliary cell calculations.

Radial dimensions, axial dimensions, and material distributions for the r-z model (which includes five radial core zones or rings, three axial core zones, and reflectors at the top, bottom, and side) are the same as those reported in Ref. 28.

The calculated worths of 1, 7, and 73 control-rod pairs are summarized in Table XII below. The single rod-pair results are for the central refueling region which comprises ring 1 of the model. For this particular rod pair, calculations were also performed with the rod pair at various axial positions. The normalized

TABLE XII

CONTROL-ROD PAIR WORTH

Rod-Pairs	Worth (Δk)
1	-0.006
7	-0.036
73 (all)	-0.261

worth versus axial position curve obtained from these calculations is shown in Fig.39. Note that insertion into the bottom half of the core accounts for 60% of the total worth of the rod pair and that there is some residual worth (about 2% of the total worth) at the top of the core.

Fig. 39. Reactivity worth versus axial position for the central control-rod pair.

Previous calculations²⁸ with a one-dimensional radial model yielded a worth of $-0.037 \Delta k$ for the seven rod-pair case in good agreement with the above results. The seven rod-pair configuration includes the central rod pair and six of the 12 rod pairs in the third core ring. This configuration presumably corresponds to the hot-critical case at the beginning of the initial cycle with equilibrium xenon and samarium. The multiplication factor from the two-dimensional calculation for this configuration was 1.012.

For the all-rods-in case, Table 4.3.2-3 of the FGS PSAR gives a worth of $-0.258 \Delta k$ at operating temperature and the middle of the initial cycle. Our result ($-0.251 \Delta k$) is in good agreement with this value.

2. Reactivity Change due to Dropping of the Central Refueling Region

If the three graphite posts that support the central refueling region* in the FGS core are postulated to fail, the refueling region would drop a distance of about 2 m to the bottom of the exit plenum. This distance corresponds to the height of 2.5 fuel blocks. The reactivity change resulting from such a hypothetical geometrical rearrangement has been calculated with TWOTRAN-II.⁴² These calculations indicate that the reactivity change is only a few cents (and negative) regardless of the position of the central control-rod pair. The calculations were performed using the FGS initial core model and four energy group cross sections described above. Except for the central control-rod pair, all control rods were in their withdrawn position.

Calculations were performed with the central control-rod pair at various

axial positions. This rod pair was assumed to remain in its original position after the refueling region was dropped (control-rod support is independent of that for the refueling region). In the dropped (perturbed) configuration, that portion of the central refueling region that extended below the bottom reflector was not included in the perturbed model. This should be a good approximation because the reactivity worth of materials beyond the bottom reflector is small (two-dimensional material worth distributions have been computed for the FGS initial core and will be given in a later report).

Reactivity changes obtained from the calculated multiplication factors for the reference and perturbed configurations are summarized in Table XIII. These results show that the reactivity change is small and negative regardless of the position of the control-rod pair.

TABLE XIII

REACTIVITY CHANGE DUE TO
CENTRAL REFUELING REGION DROP

Central Rod-Pair Position	$10^{-4} \Delta k$	Cents
Completely withdrawn	-3.2	-4.9
2.5 blocks into core	-2.9	-4.5
4 blocks into core	-3.1	-4.8
6 blocks into core	-1.4	-2.2
8 blocks into core	-1.9	-2.9

Examination of the material changes that occur in each axial mesh interval as a result of the drop shows that one should expect negative reactivity effects above the core midheight and positive effects below the midheight. The results in Table XIII indicate that these effects are essentially compensatory.

*A refueling region consists of a control column and the six surrounding standard columns.

If the thermal flux is not greatly perturbed by the region drop, the worth of the control-rod pair should not change greatly (fully inserted, the worth of the central-rod pair is about 90¢). In this case the net reactivity change due to the refueling-region drop should not be strongly dependent on the axial position of the rod pair. From the results in Table XIII, this would appear to be the case. Because the net reactivity changes are small, the accuracy of the k-difference results is limited by the problem convergence. At least one of the cases will be checked out by perturbation calculations using direct and adjoint angular fluxes from TWOTRAN-II.

3. Kinetics Parameters for the FGS Initial Core

Kinetics parameters including the effective prompt-neutron generation time ($\bar{\Lambda}$), delayed-neutron fractions ($\bar{\beta}_i$, $i = 1, \dots, 6$), and decay constants ($\bar{\lambda}_i$, $i = 1, \dots, 6$) have been calculated for the FGS (BOL) core. The calculated values of these parameters are in good agreement with those reported in the FGS PSAR.⁴¹

Values for $\bar{\Lambda}$ and $\bar{\beta}_i$ ($i = 1, \dots, 6$) were computed using the DAC perturbation theory code, which is an unpublished multi-dimensional version of the one-dimensional S_n perturbation code DAC1.⁴³ Two-dimensional (r, z) four-group, S_4 , direct and adjoint angular fluxes computed with the TWOTRAN-II code⁴² were used in the DAC calculations. Compositions used in the model correspond to the BOL fuel and burnable-poison distributions with equilibrium xenon and samarium but no control rods. The geometrical model, represented by a 33 x 57 r, z mesh, includes five radial and three axial core zones surrounded by radial, top, and bottom reflectors as used in the calculations reported above.

Energy boundaries, prompt and delayed neutron spectra, and neutron velocities for the four-group energy

structure are shown in Table XIV. Cross sections for this group structure were obtained by collapsing nine-group MICROS cross sections using flux spectra from one-dimensional calculations. Prompt and delayed fission spectra were obtained from information given in Ref. 44. Velocities for the four-group structure were obtained by collapsing nine-group velocities. These nine-group velocities were in turn obtained by averaging over fine-group fast and thermal neutron spectra generated, respectively, with the MC² and the GLEN codes.^{45,46}

Calculation of the effective delayed-neutron fractions and decay constants for a given reactor requires a knowledge of the β_i and λ_i for the various fissioning isotopes present in the system. In our computations we have used the six-group delayed-neutron data given by Keepin⁴⁴ for thermal fission of ²³⁵U and fast fission of ²³²Th. In the BOL core, 99.8% of the fissions occur in ²³⁵U and the remainder (0.2%) is essentially all in ²³²Th. Because their concentrations are small compared to that of ²³²Th, fissions in ²³⁴U, ²³⁶U, and ²³⁸U are negligible.

Kinetics parameters calculated at LASL, along with those reported in the FGS PSAR, are summarized in Table XV. The LASL value of $\bar{\Lambda}$ is within 5% of that reported in Table 1.3.1-2 of the FGS PSAR. Because $\bar{\Lambda}$ is sensitive to the group velocities, particularly that in the thermal group (group four), this agreement provides an indirect verification of the detailed spectra computed with the MC² and GLEN codes.

As one would expect from the fact that most of the fissions occur in ²³⁵U and the fact that the delayed-neutron spectrum in the four-group structure does not differ greatly from the prompt-neutron spectrum, the values of $\bar{\beta}_i$ and $\bar{\lambda}_i$ are essentially those for ²³⁵U. The LASL

TABLE XIV

GROUP PARAMETERS FOR FOUR-GROUP ENERGY STRUCTURE

<u>Group</u>	<u>Lower E Boundary (eV)</u>	<u>Fission Spectrum</u>		<u>Neutron Velocity (cm/s)</u>
		<u>Prompt</u>	<u>Delayed</u>	
1	1.83×10^5	1.0	0.948	1.148×10^9
2	17.6	0.0	0.052	3.054×10^7
3	3.93	0.0	0.0	3.925×10^6
4	0.0	0.0	0.0	5.804×10^5

TABLE XV

KINETIC PARAMETERS FOR FGS BOL CORE

	<u>Prompt Generation Time (s)</u>		<u>Total Delayed Neutron Fraction</u>	
	<u>LASL</u>	<u>PSAR</u>	<u>LASL</u>	<u>PSAR</u>
	4.3×10^{-4}	4.1×10^{-4}	6.52×10^{-3}	6.55×10^{-3}
	<u>$\bar{\beta}_i$</u>		<u>$\bar{\lambda}_i (s^{-1})$</u>	
<u>i</u>	<u>LASL</u>	<u>PSAR</u>	<u>LASL</u>	<u>PSAR</u>
1	0.22×10^{-3}	0.22×10^{-3}	1.24×10^{-2}	1.24×10^{-2}
2	1.43×10^{-3}	1.47×10^{-3}	3.05×10^{-2}	3.05×10^{-2}
3	1.28×10^{-3}	1.27×10^{-3}	1.11×10^{-1}	1.11×10^{-1}
4	2.58×10^{-3}	2.57×10^{-3}	3.01×10^{-1}	3.01×10^{-1}
5	0.75×10^{-3}	0.75×10^{-3}	1.14	1.14
6	0.27×10^{-3}	0.27×10^{-3}	3.01	3.01

values for $\bar{\beta}_i$ and $\bar{\lambda}_i$ are in almost perfect agreement with those reported in Table Q4.3.2.1-2-1 of the FGS PSAR.

B. Nuclear Data Processing for HTGR Safety Research (M. G. Stamatelatos, R. J. LaEauve, and J. C. Vigil)

Development of the independent LASL cross-section processing code system has

reached a state where acceptable broad-group data can be produced for homogeneous HTGR media. Using a medium characteristic of the FGS initial core, nine-group cross sections were generated for isothermal core temperatures of 300, 1200, and 3000 K. These cross sections were used to compute multiplication factors and isothermal

temperature coefficients from a cell model which includes the effects of seven control-rod pairs, burnable poison, and equilibrium xenon and samarium. Results of these calculations are compared below with results obtained using cross sections generated from a nine-group MICROX⁴⁰ library supplied by GAC. Taking into account the expected effect of core heterogeneity on the broad-group cross sections, the results obtained with the LASL cross sections are in reasonable agreement with those obtained with the GAC cross sections.

HTGR cross sections generated previously with the LASL code system were incorrect because of problems in the MC² code.⁴⁵ Modifications required to produce satisfactory homogeneous-medium cross sections with this code are discussed below.

A single level of heterogeneity can be treated in the fast energy range with the MC² code by specifying a two-region cylindrical cell model that includes the fuel stick and surrounding moderator. The MC² calculations will be repeated using such a heterogeneous model in order to determine the effect (on the broad-group cross sections) of resonance-region self-shielding in the fuel stick.

In the future, however, the MC² code will be replaced with modified versions of the MINX and LDX codes.^{47,48} The modified MINX-LDX package, when completed, will provide treatment of both levels of heterogeneity in the fast energy range. The same procedure used to treat the fertile-particle (ThO₂) self-shielding in the fast energy range can be applied to the fissile-particle (UC) self-shielding in the thermal range. These topics are discussed below.

1. Neutronic Calculations

The seven region cell model used to calculate the multiplication factor as a function of core temperature is described in Table XVI. This model represents the control rod explicitly and the

TABLE XVI

SEVEN-REGION CELL MODEL INCLUDING CONTROL RODS

<u>Region</u>	<u>Description</u>	<u>Outer Radius (cm)</u>
1	Control Rod Spine	0.476
2	Void	2.381
3	Control Rod Inner Sleeve	2.540
4	Control Rod Absorber Compact	4.286
5	Control Rod Outer Sleeve	4.445
6	Control Rod Hole	5.080
7	Homogenized Core Medium (excluding control rods)	112.78

amount of homogenized core medium (region 7) associated with the control rod corresponds to the case in which seven control-rod pairs are present in the core. This control-rod configuration in turn corresponds to the hot-critical case with equilibrium xenon and samarium. Region 7 also contains burnable poison, which was homogenized using shielding factors obtained from auxiliary cell calculations in which the burnable poison pin was represented explicitly.

The k-calculations were performed with the DTF-IV transport theory code⁴⁹ in S₄ approximation using nine energy groups. The nine-group energy structure, shown in Table XVII, is that in use at GAC and includes five fast (> 2.38 eV) and four thermal (< 2.38 eV) groups. Generation of cross sections with this initial LASL system is time consuming and for this reason cross sections were produced for only three temperatures (300, 1200, and 3000 K) using this system. On the other hand, the generation of interpolated cross sections from an existing library of MICROX cross sections is a fast procedure.

TABLE XVII

ENERGY BOUNDARIES FOR NINE-GROUP STRUCTURE

Group	Lower Energy (eV)
1	1.83×10^5
2	961
3	17.6
4	3.93
5	2.38
6	0.414
7	0.10
8	0.04
9	0.0

Therefore GAC cross sections were generated at four additional temperatures (500, 800, 1700, and 2300 K).

Results of the k-calculations are summarized in Table XVIII and plotted in Fig. 40. Note that the multiplication factors obtained with the LASL cross sections are slightly smaller than those obtained with the GAC cross sections. The differences range between 1.2% Δk at 300 K and 2.6% Δk at 3000 K. These differences are reasonable considering the fact that heterogeneity effects have not yet been included in the LASL cross sections. Self-shielding in the fertile particle in the resonance energy range is expected to be the most important of these effects. Therefore inclusion of these effects should result principally in a smaller group three adsorption cross section for thorium. A detailed comparison of the LASL and GAC cross sections shows that this is indeed the case.

Note also from Table XVIII that the absolute reactivity change between 300 and 1200 K is almost the same with both cross-section sets while the change

TABLE XVIII

SUMMARY OF RESULTS

Core Temp (K)	Infinite Multiplication Factor	
	GAC Cross Sections	LASL Cross Sections
300	1.0920	1.0797
500	1.0678	
800	1.0461	
1200	1.0293	1.0160
1700	1.0132	
2300	0.9955	
3000	0.9765	0.9500

Temperature Interval (K)	Reactivity Change (% Δk)	
	GAC Cross Sections	LASL Cross Sections
300-1200	-6.27	-6.37
1200-3000	-5.28	-6.60

Fig. 40. Infinite multiplication factor for the FGS initial core including the effects of seven control-rod pairs, burnable poison, and equilibrium Xe and Sm.

between 1200 and 3000 K is 25% larger using the LASL cross sections. In other words, there is little difference between the average temperature coefficients in the temperature range 300-1200 K but in the range 1200-3000 K the LASL cross sections yield an average coefficient that is 25% more negative. This is also illustrated in Fig. 41 where the temperature coefficient is plotted as a function of core temperature. The curves in Fig. 41 were derived from those in Fig. 40.

Because self-shielding effects attenuate changes in broad-group cross sections with temperature, and because the Doppler effect in thorium is the principal contributor to the temperature coefficient, the inclusion of self-shielding effects in the broad-group cross sections should result in a smaller (less

Fig. 41. Isothermal temperature coefficient for the FGS initial core including the effects of seven control-rod pairs, burnable poison, and equilibrium Xe and Sm.

negative) temperature coefficient over the entire temperature range. From GAC results shown in Fig. Q4.3.2.3-2 of the FGS PSAR, one would expect the effect to be 10 - 20%. Our results shown in Fig. 41 are consistent with the GAC results above 1200 K. Below 1200 K, however, it appears that LASL cross sections could yield a slightly less negative temperature coefficient than the GAC cross sections when self-shielding effects are taken into account in the LASL sets.

2. LASL Cross-Section Generation Methods

The major source of previous disagreement with MICROX cross sections was found in the resolved resonance region where, in the case of the capture cross section of ^{232}Th , the MC² homogenized cross section was found to be lower than the MICROX cross section in which spatial heterogeneities had been accounted for. This discrepancy was initially attributed to a possible coarse energy-mesh representation in MC² for the resonance region.

"Ultra-fine" MC² runs performed with 2000 energy groups (1/120 equal lethargy mesh) between 10 MeV and 0.414 eV at 300 and 3000 K revealed negligible differences from the corresponding "all-fine" MC² result using 68 equal lethargy (0.25) groups for the same energy range.

The 68 fine-group MC² capture cross sections were then compared with MINX cross sections generated in the same energy structure. The general agreement between these two sets indicated that the MC² fine-group capture cross sections were not the main cause of discrepancy between the MC² and the MICROX broad-group capture cross sections. The broad-group collapsing method in MC² became immediately subject to inquiry.

Briefly, the MC² multigroup averaging method for the resolved-resonance capture cross section is an in-scattering source weighted collapsing process as follows:

$$\left(\frac{\sigma_{c,J}^{bg}}{\sigma_{c,J}}\right)_{\text{resolved}} = \frac{\sum_j \sum_{\epsilon} J \langle \sigma_c \rangle_j^{fg} \text{ resolved } Q_j}{\sum_j \sum_{\epsilon} J Q_j} \quad (53)$$

where

$$Q_j \equiv \int_{E_j}^{E_{j+1}} S_j^{fg} \frac{dE}{\Sigma_T(E)} \quad (54)$$

and

$$S_j^{fg} = \sum_{k \neq j} \left(\Sigma_{inel,k}^{fg} \phi_k^{fg} \frac{\langle \Sigma_{inel} \rangle_{k+j}}{\langle \Sigma_{inel} \rangle_k} + \Sigma_{n,2n,k}^{fg} \phi_k^{fg} \frac{2 \langle \Sigma_{n,2n} \rangle_{k+j}}{\langle \Sigma_{n,2n} \rangle_k} \right) + \langle \Sigma_{el} \rangle_{j-1-j} \quad (55)$$

where superscripts bg and fg indicate "broad-group" and "fine-group" respectively. J and j are subscripts referring to broad-group and fine-group respectively.

This method of multigrouping was developed for fast-spectrum systems and is not appropriate for thermal reactor systems. However, hand calculations using a straight spectrum weighting method yielded results in general agreement with the MICROX broad-group capture cross section. The larger value of the MC² resolved-resonance capture cross section was expected since spatial heterogeneity effects were not yet included in the MC² calculations. The straight spectrum weighting method was then incorporated into MC² as an alternative and the subsequent results for 300, 1200 and 3000 K were also in reasonable agreement with the MICROX cross sections as noted earlier.

In order to properly account for the double heterogeneity effects on cross sections as well as to take full advantage of the most up-to-date computational techniques employed in the MINX code system, the following course of action will be adopted in future HTGR cross-section generation work at LASL:

1. Use MINX for generating point-wise cross-sections in ENDF/B format (PENDF) over the entire energy range desired and for all materials of interest.
2. Apply particle heterogeneity corrections to the point-wise cross-sections in both the above-thermal (resonance) and thermal regions.
3. Use MINX to collapse the particle-heterogeneity corrected PENDF cross sections to the desired fine-group energy structure.
4. Calculate a fine-group neutron spectrum in the above-thermal region with the LDX code and use the same code to collapse the above-thermal fine-group cross sections applying the proper "gross" (fuel-pin/moderator) heterogeneity correction for HTGR fuel pins in a hexagonal lattice. The LDX code has been adapted to accept MINX fine-group cross sections in the Bondarenko formalism.
5. Collapse the thermal fine-group cross sections with the GLEN code.⁴⁶
6. Investigate the importance of "gross" heterogeneity effects on thermal cross sections.
7. Format final broad-group sections for input to the DTF-IV discrete-ordinates transport code.

The initial procedure to be used in applying the particle heterogeneity

corrections to the PENDF capture cross sections will be the Sauer formalism used by Wälti in the MICROX code.⁴⁰ Preliminary calculations for the two important capture resonances in ^{232}Th , at 21.78 and 23.45 eV, have given flux disadvantage factors for 400- μm ThC_2 particles of 0.7 and 0.58 respectively, in good agreement with Wälti's results. Calculations for ThO_2 particles are in progress. Comparisons of Wälti's method for treating particle heterogeneity effects on cross sections with other compatible methods and possibly with Monte Carlo calculations will be performed.

C. CHAP Code Status (P. A. Secker and J. S. Gilbert)

The Composite HTGR Analysis Program (CHAP) is an independent computer code which will simulate normal operation, anticipated transients, and postulated accidents for High Temperature Gas-Cooled Reactors (HTGR). It is generic in its description of the current GAC 2000 and 3000 Mw(t) reactor designs.

CHAP is a whole system code which will describe the thermal, fluid-flow, neutronic (including afterheat) and control response of the HTGR reactor core, primary coolant system, prestressed concrete reactor vessel (PCRV), Core Auxiliary Cooling System (CACS), and balance of plant. CHAP is designed to predict critical safety variables such as maximum fuel-rod temperatures and maximum structural-material temperatures. The output from CHAP will provide thermal-hydraulic input to descriptions of fission product release and transport and to descriptions of graphite air and/or steam reactions. Typical initiating events to be considered are reactor trip, loss of off-site power with turbine trip, loss of main loop cooling, depressurization of the primary system and reactivity insertions.

Dynamic models for reactor core, primary coolant system, steam generator, reheater and main circulator have been developed. These models are being

incorporated into CHAP after appropriate evaluation and numerical validation over a broad operating range. A steady-state, frequency response, and time response simulation program, TAF, is being utilized in these studies.^{50,28} For selected components detailed codes are being used for evaluation and verification. For example, TPROF, an auxiliary analysis code written to provide fine-mesh, two-dimensional temperature distributions in an HTGR fuel element has been used to benchmark the large-node calculations in the CHAP code.³⁴ The checkout of each component description is made to determine the simplest version for minimizing computation time, to identify the transient and frequency response limitations of the mathematical model, and to verify the accuracy of all significant variables.

TAF has also been used as a framework on which to build the CHAP code itself. TAF is a generalized simulation code providing steady-state, transient, and frequency response of a system defined by a set of first-order ordinary differential equations. The user codes this set of equations in the FORTRAN subroutine DER. In TAF a Newton-Raphson iteration scheme uses the derivatives defined in DER to obtain convergence to a steady-state solution. It then provides the time response for a user-specified transient by using a fourth-order Runge-Kutta numerical integration scheme. TAF can also be used to obtain the frequency response of the linearized system. To execute this option, TAF automatically linearizes the system equations, transforms the linearized system response matrix to the Laplace domain, and then calculates the frequency response (gain and phase angle) of any user-identified output variable with respect to any input variable. We have used this frequency response option in the numerical validation studies.

A logic schematic of CHAP is given in Fig. 42. CHAP uses much of the basic structure of TAF but does not include the frequency response option. In CHAP, as in TAF, the system variables are identified and initialization calculations are performed in subroutine INPUT. The Runge-Kutta integration in TAF has been replaced with a semi-implicit predictor-corrector numerical integration technique. This was developed for integration of the model equations used in the CHAP code and is inherently stable for any time step size. The method is based on the optimum integrating factor technique for first-order ordinary differential equations.⁵¹ Local error is controlled during a transient solution by varying the solution integration step size.

This technique has been very successful when applied to core transient studies.^{38, 34} Computer running times are short for both fast and slow transients. For example, a calculation of a 28 h real-time core heat-up transient due

to an assumed loss-of-forced-cooling required 31 s of CDC 7600 machine time. The method has also been used with good success for calculating transients due to step reactivity insertions up to one dollar.

A detailed status report describing the models developed to this point is in preparation.⁵² Progress on building CHAP into an integrated consolidated plant model will continue in FY-1976, and an initial version will be produced and released with documentation during FY-1976. This version will be comparable in scope to the GAC systems transient code TAP.⁵³ It will allow the study of many system transients and accidents, but will not include the complete balance of plant model, a containment model, nor a detailed core cooling model as given in the GAC RECA code.⁵⁴ Future versions of CHAP will include these models and other improvements reflecting analyses of accident progressions and consequences performed during FY-1976.

D. Status of HTGR Systems Analysis and Neutronics Codes (J. C. Vigil and J. S. Gilbert)

The analysis of safety-related characteristics and of postulated accidents in the HTGR requires the use of a number of computer codes. The LASL HTGR safety effort has concentrated on developing new codes or applying existing codes which have been developed independently of the HTGR vendor, the General Atomic Company (GAC). At a lower priority, we have acquired several GAC codes and begun conversion to the LASL computers. Table XIX gives the status of various codes being used or developed in the HTGR safety analysis effort.

Fig. 42. Block diagram for CHAP.

TABLE XIX

HTGR CODE STATUS

<u>Systems & Accident Analysis</u>	<u>Code</u>	<u>Originator</u>	<u>Function</u>	<u>Status</u>
	CHAP	LASL	HTGR systems transient and accident analysis	Under development with first version to be released in FY-76
	TAF	LASL	Generalized systems simulation (steady-state, transient and frequency response)	Used in numerical validation of CHAP models
	BLOOST-7	GAC	HTGR core transient analysis (point kinetics and two-dimensional heat transfer)	Has compiled and executed successfully on LASL computers
	RECA	GAC	HTGR emergency cooling analysis	A version has compiled on LASL computers, but additional information is required before execution possible
	CONTEMPT-G	GAC	HTGR containment response (temperature - pressure) analysis	Has compiled on LASL computers except for input routine
	OPUS	GAC	HTGR flow network and plant performance (steady-state) analysis	Has compiled on LASL computers but overlay structure must be modified before execution possible
<u>Neutronics</u>				
	DTF-IV	LASL	One-dimensional S_n transport calculations	Used extensively in HTGR core neutronics calculations
	TWOTRAN-II	LASL	Two-dimensional S_n transport calculations	Used extensively in HTGR core neutronics calculations
	MC ²	ANL	Multigroup cross section generation	Used at LASL to produce initial cross section sets (above-thermal)

(con't)

TABLE XIX

(con't)

<u>Code</u>	<u>Originator</u>	<u>Function</u>	<u>Status</u>
<u>Neutronics</u>			
MINX	LASL	Multigroup cross section generation	Is operable and will be used at LASL to produce above-thermal cross sections
1DX	BNWL	One-dimensional diffusion and multigroup cross section generation	Is operable and will be used in combination with MINX to produce above-thermal cross sections
TOR	LASL	Inelastic thermal-scattering matrices for crystalline materials	Used at LASL to produce inelastic scattering matrices for graphite
GLEN	LASL	Multigroup thermal spectrum and cross-section collapse	Used at LASL to produce thermal cross-section sets
HEXSCAT	GAC	Elastic thermal-scattering cross sections for crystalline materials	Used at LASL to produce elastic thermal-scattering cross sections for graphite
GGC-4	GAC	Combined fast and thermal multigroup cross-section generation for HTGR	Has compiled on LASL computers but has not been executed

REFERENCES

1. J. E. Foley, "¹³¹I Release from an HTGR During the LOFC Accident," Los Alamos Scientific Laboratory report LA-5893-MS (March 1975).
2. G. E. Cort, Los Alamos Scientific Laboratory, unpublished report, 1974.
3. R. G. Lawton, "The AYER Heat Conduction Computer Program," Los Alamos Scientific Laboratory report LA-5613-MS (May 1974).
4. O. C. Zienkiewicz, The Finite Element Method in Engineering Science (McGraw-Hill, London, 1971).
5. M. H. Schwartz, D. B. Sedgley, and M. M. Mendonca, "SORS: Computer Programs for Analyzing Fission Product Release from HTGR Cores During Transient Temperature Excursions," General Atomic Company report GA-A12462 (April 1974), Fig. 5-1.
6. Summit Power Station PSAR, Delmarva Power and Light Co., Vol. 4, Fig. 6.2-1.
7. Code of Federal Regulations, Title 10, Part 100.
8. Fulton Generating Station PSAR, Philadelphia Electric Co., Change 15, p. C.6-3 (September 1974).
9. Regulatory Guide 1.3, Directorate of Regulatory Standards, U.S. Atomic Energy Commission (June 1973).
10. "HTGR Fuels Development Quarterly Progress Report for Period Ending February 28, 1975," General Atomic report GA-A13353, p. 10.
11. C. F. Wallroth, N. L. Baldwin, C. B. Scott, and L. R. Zumwalt, "Postirradiation Examination of Peach Bottom Fuel Test Element FTE-3," General Atomic Company report GA-A13004, p. 28 ff.
12. F. R. Hennig, "Interstitial Compounds of Graphite," *Progr. Inorg. Chem.* 1, 125 (1959).
13. F. J. Salzano and S. Aronson, "On the Bonding Energy in Cesium-Graphite Compounds," *J. Chem. Phys.* 44, 4320 (1966).
14. L. Pauling, The Nature of the Chemical Bond, 3rd Ed. (Cornell, Ithaca, N.Y., 1960), 514.
15. B. L. Holian, Los Alamos Scientific Laboratory, unpublished data, 1975.
16. J. O. Hirschfelder, C. F. Curtiss, and R. B. Byrd, Molecular Theory of Gases and Liquids (Wiley, N.Y., 1954), 987.
17. K. S. Pitzer, "Inter- and Intramolecular Forces and Molecular Polarizability," *Adv. Chem. Phys.* 2, 59 (1959).
18. C. E. Milstead, "Sorption Characteristic of the Cesium-Graphite System at Elevated Temperatures and Low Cesium Pressures," *Carbon* 7, 199 (1969).
19. L. R. Zumwalt, North Carolina State University, private communication, April, 1975.
20. H. F. Schaefer III, University of California, Berkeley, private communication, March, 1975.
21. B. J. Alder, D. M. Gass, and T. E. Wainwright, "Studies in Molecular Dynamics VIII. The Transport Coefficients for a Hard-Sphere Fluid," *J. Chem. Phys.* 53, 3813 (1970).
22. A. J. Sierk, Cal Tech, private communication, May, 1975.
23. K. Levenberg, "A Method for the Solution of Certain Non-linear Problems in Least Squares," *Quarterly Appl. Math.* Vol. 2, 164-168 (1944).
24. D. W. Marquardt, "Algorithm for Least-squares Estimation on Nonlinear Parameters," *J. Soc. Indust. Anal. Ser. B*, Vol. 2, No. 2, (1965).
25. E. E. Osborne, "Smallest Least Squares Solutions of Linear Equations," *J. SIAM Numer. Anal. Ser. B*, Vol. 2, No. 2, (1965).
26. "HTGR Base Program Quarterly Progress Report, Period ending November, 1967," General Atomic Company report GA-8356.
27. J. Board, "The Effect of a Helium Environment on the High Temperature Properties of Structural Materials," *Nucl. Energy Soc. J.*, Vol 9, No. 2 101 (1970).
28. W. L. Kirk, "Quarterly Report: HTGR Safety Research Program," Los Alamos Scientific Laboratory report LA-59-75-PR (June, 1975).
29. O. Kubachewski and B. E. Hopkins, Oxidation of Metals and Alloys, (Butterworths, 1962) p. 243.
30. S. Adham, A. Bhaumik, and Jo Isenberg, "Reinforced Concrete Constitutive Relations," Air Force Weapons Laboratory, Kirtland AFB, New Mexico, Technical Report, AFWL-TR-74-72.

31. "NONSAP: A Structural Analysis Program for Static and Dynamic Response of Nonlinear Systems," University of California report UC-SESM 74-3 and UC-SESM 74-4 (February 1974).
32. "SAPIV: A Structural Analysis Program for Static and Dynamic Response of Systems," University of California report, EERC 73-11 (June 1973).
33. "SABOR/DRASTIC: A Fortran Program for Linear Elastic Analysis of Thin Shells of Revolution Under Asymmetric Loading Using the Matrix Displacement Method," MIT report, ASTRL-TR-121-6 (June 1965).
34. W. L. Kirk, "Quarterly Report: HTGR Safety Research Program," Los Alamos Scientific Laboratory report LA-5879-PR (February 1975).
35. J. G. Bennett and R. C. Dove, "Proposal for Analysis of HTGR Core Response to Seismic Input," Los Alamos Scientific Laboratory report LA-5821-MS (January 1975).
36. G. Murphy, Similitude in Engineering, (Ronald Press, New York, 1950).
37. D. D. Orvis, "Preliminary Analysis of Anticipated Transients in the HTGR with Failure of Control Rod Motion," General Atomic Company report GA-A13234 (November 1974).
38. K. D. Lathrop, "Quarterly Report: Transport Theory, Reactor Theory, and Reactor Safety," Los Alamos Scientific Laboratory report LA-5778-PR (October 1974).
39. J. C. Vigil, "Neutronics Analysis of the Fulton Generating Station Beginning-of-Life Core," Los Alamos Scientific Laboratory report, to be published.
40. P. Wälti and P. Koch, "MICROX - A Two-Region Flux Spectrum Code for the Efficient Calculation of Group Cross Sections," Gulf General Atomic report Gulf-GA-A10827 (1972).
41. Fulton Generating Station PSAR, Philadelphia Electric Company, Chapter IV.
42. K. D. Lathrop and F. W. Brinkley, "TWOTRAN-II: An Interfaced, Exportable Version of the TWOTRAN Code for Two-Dimensional Transport," Los Alamos Scientific Laboratory report LA-4848-MS (July 1973).
43. B. M. Carmichael, "DAC1, A One-Dimensional S₁ Perturbation Code," Los Alamos Scientific Laboratory report LA-4342 (April 1970).
44. G. R. Keepin, Physics of Nuclear Kinetics, (Addison-Wesley Publishing Co., Inc., 1965).
45. B. J. Toppel, D. M. O'Shea, and A. L. Rago, "MC², A Code to Calculate Multigroup Cross Sections," Argonne Nat. Laboratory report, ANL-7318 (1967).
46. W. W. Clendenin, "Calculation of Thermal Diffusion Length and Group Cross Sections: The GLEN Program," Los Alamos Scientific Laboratory report LA-3893, (1968).
47. C. R. Weisbin, P. D. Soran, D. R. Harris, R. J. LaBauve and J. S. Hendricks, "MINX, A Multigroup Interpolation of Nuclear X-Sections," Trans. Am. Nucl. Soc. 16, 127 (1973).
48. R. W. Hardie and W. W. Little, Jr., "1DX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections," Battelle-Northwest report, BNL-954 (1968).
49. K. D. Lathrop, "DTF-IV, A Fortran-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," Los Alamos Scientific Laboratory report LA-3373 (1965).
50. T. E. Springer and O. A. Farmer, "TAF-a Steady State, Frequency Response and Time Response Simulation Program," Proc. Fall Joint Computer Conference, San Francisco, 1968, Vol. 33, p. 359-370.
51. P. A. Secker, "Numerical Integration of Dynamic Nuclear Systems Equations by Optimum Integrating Factors," Los Alamos Scientific Laboratory report LA-4252.
52. P. A. Secker and J. S. Gilbert, "Status of the CHAP Composite HTGR Analysis Program," Los Alamos Scientific Laboratory report, to be published.
53. C. W. Savery, "TAP-A FORTRAN IV Program for the Transient Analysis of the HTGR Powerplant Performance," General Atomic Company report GAMD-7248 (October 1966).
54. H. W. Chi and G. J. Malek, "Description of the Reactor Emergency Cooling Analysis Code, RECA," General Atomic Company report GA-10273 (August 1970).