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Compiled by

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HTGR SAFETY RESEARCH PROGRAM

QUARTERLY PROGRESS REPORT

for

OCTOBER - DECEMBER 1974

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 Atomic Energy 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 first of a series of quarterly progress reports, and as such, includes some background of previously reported information.

II. SUMMARY

Information is being gathered and correlated on the failure and release of fission products from coated fuel particles at abnormal HTGR operating temperatures.

As a first step in the analysis of fission product release from HTGR's, the release of ^{131}I from the HTGR core and containment building has been studied for the

loss-of-forced-cooling (LOFC) accident. Core release has been calculated using both a very simplified and a more sophisticated model. These results have been compared to General Atomic results. Similarly, the release from the containment building and the resultant thyroid dose have been calculated and the results examined. This work shows that for the LOFC accident, the governing factor for total dose from ^{131}I is the total amount of the isotope released into the containment building.

The core release model has been modified to apply to the more general case of isotopes with long-lived precursors.

A model of the metallic fission product release to the helium coolant under normal operating conditions has been developed for the multi-species case accounting for both diffusion through and adsorption in the fuel block graphite. The current model using a constant fission product source will be generalized to account for the time-varying release of fission products from the fuel during temperature transients.

The development of a computer code for modeling the chemical reactions between graphite and flowing gases is continuing. This code, named CIMPRES(Coolant IMPurity REactions), is now operational for the two-dimensional steady-state heat transfer problem, but quantitative agreement with the analytic solution of a test problem has

not yet been achieved. We have started to add time-dependence and three-dimensional capability to the code.

Experiments are being planned to study reactions between primary coolant impurities and the primary circuit structural materials. Design of the experimental arrangement is well underway.

An equilibrium thermodynamics approach is being used to study the chemistry of the impurities in the primary circuit. While this technique does not account for the kinetics of the reactions, we feel that this approach is useful in representing the limits of reaction. An interactive computer code, QUIL, for the computation of chemical equilibria has been written and preliminary investigations made into the reactions resulting from water inleakage.

Except for final editing, a report reviewing PCRV technology has been completed during this quarter. Areas in which additional research would be helpful have been outlined.

The computer program CONC, used to determine the stress-strain relationship of concrete subjected to multi-axial stress, has been modified to make it compatible with NONSAP, a general purpose finite-element code. Refinement and generalization of CONC will continue.

The effort to establish the scaling laws which govern the physical modeling of the HTGR core was completed and the results published in a LASL report, LA-5821-MS.

The basic analytical method under development for HTGR core motion has been applied to simple models to develop and evaluate the computer techniques. Visual displays of the model motion are being generated as part of the output.

Construction of a moisture detection system based on the helium afterglow technique has been completed. This test unit is now being prepared for calibration and

performance measurements. Investigation of other techniques for moisture measurements is continuing.

The effects of gas permeation and helium embrittlement on the integrity of the core exit thermocouple sheath materials were examined. Effects at operating temperature are expected to be negligible.

We have reviewed the accident analysis included in the Fulton Plant PSAR and prepared a compilation of accident summaries for this system as a first step in our accident delineation effort.

We have continued parametric studies of the temperature coefficient for the Fulton Station HTGR initial core. During the quarter the fuel and moderator components of the temperature coefficient and the separate effects of burnable poison, control rods, and fission-product poisons have been studied. Further definition of a set of independent codes to generate multigroup cross sections for HTGR cores is in progress.

We have evaluated and checked the core model for the CHAP systems analysis code. Modeling of the balance-of-plant dynamic behavior has been started.

III. TASK 1, FISSION PRODUCT TECHNOLOGY

A. Coated Fuel Particle Failure and Release Rates (G. A. Whan)

The release rate of fission products from coated fuel particles is a complex function of irradiation conditions and fabrication parameters, but the most important factor is the percent of coating failures. In HTGR safety studies to date,¹ the release rate from fuel particles with failed coatings has been predicted to be orders of magnitude higher than that from particles with intact coatings. The basis of such predictions, especially under conditions leading to fuel temperatures above 1700 K, is not well established.

The factors controlling fuel coating failure can be categorized as mechanical effects and thermochemical effects.

Mechanical models for fracture of coating layers, taking into account internal pressure, irradiation-induced creep, and anisotropic dimensional changes, are used primarily to guide experimental research.² Failure fractions of less than one percent at irradiation conditions of 1523 K, 75% FIMA, and 8×10^{21} n/cm² ($E > 0.18$ MeV) have been reported for TRISO particles.³ Similar results have been obtained at 1373 K for BISO particles whose pyrocarbon layer had relatively low anisotropy.⁴

Fuel particle coating failure from thermochemical effects is dominated by the amoeba phenomenon, the diffusion of buffer layer carbon from the hot side to the cold side of the particle, at operating temperatures below 1700 K. The mechanism and extent of amoeba migration is well understood at temperatures between 1500 K and 2300 K for carbide fuel particles and with less understanding is predictable from empirical data for oxide particles.⁵ At temperatures above 1700 K, chemical attack of fission products on the silicon carbide coating begins to be the dominant thermochemical effect in carbide fuel particles.⁴

The vast majority of fuel-coating failure research has purposely aimed at the design of particles to perform well at normal HTGR operating temperatures below 1700 K. At temperatures above 1700 K, however, less information is available upon which to base predictions of fuel particle failure rates. Our current program is therefore gathering and correlating experimental data on fuel failure rates at temperatures above 1700 K. The correlation of these data will be used to develop analytical expressions for coated particle failure rates at abnormal HTGR operating conditions involving temperature transients.

B. ¹³¹I Release From an HTGR During the LOFC Accident (J. E. Foley, G. E. Cort)

1. Introduction

The release of ¹³¹I from an HTGR during the loss-of-forced coolant (LOFC) accident was studied. The release from both the core and the containment building was investigated so that the total amount released to the environment during the accident can be determined.

The time-dependent release of fission products from the HTGR core is calculated by General Atomic Company (GAC) with a computer program called SORS.¹ The basic techniques used in the SORS program to calculate the release are simple; however, the bookkeeping required to keep track of all the isotopes, temperatures, release rates, etc., is complicated. In the SORS model, the core is divided into many small regions and the total fission product release is obtained by summing the release from each region. The temperature of each region is calculated with a computer program called CORCON.⁶

We have developed two additional core release models: a simplified uniform core temperature model and a more sophisticated AYER heat conduction model.

2. Core Release Models

a. Simplified Core Release Model

A simplified model was developed so that fission product release from the core during the LOFC accident could be studied easily with hand calculations. The following assumptions were made:

- The entire core is at a uniform temperature,
- All the coated particles fail at the same time,
- Fission products are released only from failed particles (no release from intact particles),
- The release rate of an isotope from the failed particles is given by the release constant

from the SORS report (Ref. 1, Fig. 5-3), and

- There is no buildup of the isotope from precursor decay.

The amount of the isotope released from the core (R_i) during any time interval of width Δt is given by

$$R_i = N_{i-1} \left(\frac{r_i}{r_i + \lambda} \right) [1 - e^{-(r_i + \lambda) \Delta t}] \quad (1)$$

where

N_{i-1} is the amount of the isotope in the core at the end of the $(i-1)^{st}$ time interval,

r_i is the release constant of the isotope from fuel particles for i^{th} time interval,

λ is the radioactive decay constant.

The amount of the isotope in the core at the end of the i^{th} time interval is

$$N_i = N_{i-1} e^{-(r_i + \lambda) \Delta t} \quad (2)$$

These two equations are used to calculate the release of the isotope from the core for all time intervals.

b. AYER Core Release Model for Iodine

Because iodine is not strongly adsorbed on graphite at the temperatures experienced in the LOFC accident, and because the release rate from failed particles is several orders of magnitude greater than the release rate from intact particles, the release to the coolant is simply determined as the release from the failed particles. Particle failure is assumed to occur at 1573 K corresponding to the approximate 50% failure probability after 2.5 years of irradiation life.

The active core and reflector regions are subdivided into concentric rings for the finite element program AYER.⁷ The finite elements correspond approximately in cross section to a fuel block. The heat generation rate in each finite element at a given time during the

transient is the product of the decay power and the radial and axial factors. The outer boundaries of the model are assumed to be adiabatic. This is a good assumption for up to 6 h and can probably be used for up to 20 h.

As an initial condition, it is assumed that none of the fuel particles have failed prior to the LOFC, and no iodine has escaped from the intact particles.

The iodine concentration in a small core volume, representing the i^{th} finite element is $N_i(t)$. The rate of change is:

$$\frac{dN_i}{dt} = -N_i r_i \quad (3)$$

where r_i is evaluated at the local temperature, T_i , and $r_i = 0$ for $T_i < 1573$ K. Therefore,

$$\frac{N_i(t+\Delta t)}{N_i(t)} = \exp [r_i(t) t - r_i(t+\Delta t) (t+\Delta t)] \quad (4)$$

For temperatures increasing with time, the release rate will be increased by setting $r_i(t) = r_i(t+\Delta t)$. The iodine released from the small volume v_i at T_i during the increment is:

$$\begin{aligned} V_i [N_i(t) - N_i(t+\Delta t)] \\ = N_i(t) V_i \{1 - \exp[-\Delta t r_i(t+\Delta t)]\} \end{aligned} \quad (5)$$

Since iodine should approach its equilibrium concentration in the fuel within a few weeks, the initial local concentration is proportional to the local power density and $N_i(0) = AF_i \cdot RF_i$, where AF_i and RF_i are the radial and axial power factors. The total release for the core is the summation of Eq. (5) over all finite elements, normalized to the active core volume.

c. ^{131}I Release From the Core for LOFC Accident

The core release models were used to estimate the time-dependent release of ^{131}I from the HTGR core during the LOFC accident. This isotope was selected because it is probably the most important one in accident situations (also, there is no significant buildup of ^{131}I from precursor decay after the reactor trip).

The amount of ^{131}I in the coolant normalized to the initial core inventory is shown in Fig. 1; results of the GAC SORS model (Ref. 1, Table 6-1) and the LASL models are shown. The agreement between the simple, uniform temperature model and the more sophisticated models is good.

From Fig. 1 (using any of the release models) it is seen that there is little release of ^{131}I to the coolant during the first 4 h after the onset of the accident. Most of the release to the coolant occurs during the 4-12 h time period; the release is essentially complete 12 h after the onset of the accident.

Fig. 1. Calculated ^{131}I release from HTGR core during the LOFC accident.

d. Effects of the Time of Fuel Failure

The effects of the time at which the fuel particles fail on the time-dependent release to the coolant was investigated by varying the time of fuel failure after the onset of the accident. Figure 2 illustrates the amount released calculated using the AYER model for fuel failure temperature of 1573 K (~ 2 h after the onset of the accident) and 2073 K (~ 5 h after the onset). The 3 h delay in fuel failure results in only $\sim 1/2$ h delay in the release of 50% of the iodine core inventory. Thus, the time-dependent release of ^{131}I to the coolant is nearly independent of the fuel failure model. The reason for this is that the fuel particles fail when the release constants (r_i) for failed particles are small. The release is governed by the release constants, not by the integrity of the fuel particles. Thus, for the LOFC accident, the fuel failure model is not important.

3. Fission Product Release From Containment Building

a. Containment Building Model

The release of the volatile fission products from the containment building involves two steps: 1) leakage of

Fig. 2. Calculated ^{131}I release from HTGR core during the LOFC accident for two fuel failure temperatures.

the isotope from the PCRV (into the containment building), and 2) release of the isotope from the containment building.

Fission products released from the PCRV become the time-dependent source of the isotope in the containment building. To simplify the analysis, it is assumed that this source is constant over a short time interval; the source strength is the average value in the time interval. The rate of change of the number of atoms of the isotope $N'(t)$ in the containment building during the i^{th} time interval (ignoring buildup from precursor decay) is given by

$$\frac{dN'_i(t)}{dt} = S_i - (\lambda + V_i + L_i) N'_i(t) \quad (6)$$

where

- λ is the radioactive decay constant of the isotope.
- V_i is the containment cleanup system removal rate during the i^{th} interval.
- L_i is the containment building leak rate during the i^{th} time interval.
- S_i is the constant source strength during the i^{th} time interval.

If the same time intervals that are used for calculating the release from the containment building are used for calculating the release from the core, then, during any time interval, the source strength S_i is equal to the core release R_i (given by Eq. 1).

The assumption is made that all of the iodine released to the coolant during any time interval gets into the containment building; that is, there is no time delay in the transfer of the isotope from the coolant to the containment building and there is no deposition of the isotope along the flow path. Regulatory Guides 1.3 and 1.4^{8,9} for light-water cooled reactors (LWR) suggest that only 25% of the iodine in the core is released during a core meltdown (the remaining 75% adheres firmly to

surfaces). GAC applies this same reduction factor to the iodine released in the HTGR LOFC accident; however, it is not obvious that this reduction should be used for the HTGR. No reduction will be used for the calculations presented here. The reduction could be included by simply multiplying the source term S_i by 0.25.

The amount of the isotope released R'_i from the containment building during the i^{th} time interval is:

$$R'_i = \frac{L_i}{\lambda_i^*} \left(N'_{i-1} - \frac{S_i}{\lambda_i^*} \right) \left(1 - e^{-\lambda_i^* \Delta t} \right) + L_i \frac{S_i}{\lambda_i^*} \Delta t, \quad (7)$$

where

- N'_{i-1} is the number of atoms of the isotope present in the containment building at the end of the $(i-1)^{\text{st}}$ time interval (at time t_{i-1}).
- $\lambda_i^* = \lambda + V_i + L_i$ is the total "decay" constant for the i^{th} time interval.

The total release from the containment building during the entire duration of the accident is obtained by summing the individual releases during each time interval.

b. Calculated ^{131}I Release From the Containment Building for LOFC Accident

The release of ^{131}I from the containment building was calculated for the LOFC accident. The containment building leak rates used for the calculation were obtained from the Fulton Plant PSAR;¹⁰ 0.1%/day for the first 24 h after the onset of the accident, and 0.05%/day thereafter. The actual leak rate of the HTGR containment building may be significantly greater than these values because of the high internal pressure (~15 psig) in the containment building after a PCRV depressurization.¹¹ These above values were used here for lack of better ones.

The containment cleanup system removal rate for ^{131}I was chosen to be 0.9 h^{-1} ; this value is consistent with that given in the Fulton Plant PSAR for the removal of elemental iodine.¹⁰ The three chemical forms of ^{131}I - elemental, organic, particulate - are removed by the containment cleanup system at different rates because of the different collection efficiencies of these forms in the filters. Each chemical form should be treated separately in the containment building by applying the appropriate source terms and the proper containment cleanup rates. However, since 91% of the iodine release is considered to be elemental,¹⁰ the cleanup constant for elemental iodine was used. This simplification introduces some error into the calculations, but not enough to be of concern here (we are in effect calculating the release of elemental ^{131}I from the containment building).

c. Atmosphere Conditions

Regulatory Guides 1.3 and 1.4 imply that the 8 h time period for the worst atmospheric transport of the fission products (the period of least dilution) should coincide with the period of the maximum release of fission products from the containment building. The period used in the Fulton Plant PSAR for the worst atmospheric conditions is 4 to 12 h after the onset of the accident. The metallic fission products are released from the core at a much slower rate and the period of maximum release of Sr, for example, does not occur until ~30 h after the onset of the accident (Ref. 1, Fig. 6.4). Because the release rates of the various fission products from the HTGR core are different, it is difficult to apply the procedures of Regulatory Guides 1.3 and 1.4 (which were developed for LWR's) to HTGR's in a satisfactory manner.

d. Dose Calculations for ^{131}I

The thyroid dose (D) from inhalation of the released ^{131}I to an individual located at the LPZ boundary during

the 4 to 12 h time interval is given by

$$D = CB \left(\frac{X}{Q} \right) \sum_{i=4}^{12} \frac{R_i}{h} \quad (8)$$

where

$\frac{X}{Q}$ is the atmospheric dilution factor.

C is the dose conversion factor.

B is the breathing rate.

The sum of the releases in Eq. (8) is equal to the total amount of the iodine released during the time interval. Thus, the dose received by an individual during the 4 to 12 h time interval (or any time interval) is proportional to the total amount of the isotope released during the time interval; it is not a function of the time-dependency of the release. This assertion is true if the breathing rate and the atmospheric dilution factor are constant during the time interval.

Figure 3 shows the time-dependent release of ^{131}I from the containment building calculated using the uniform core temperature and the AYER core release models. It is seen from Fig. 3 that the

Fig. 3. Calculated ^{131}I release from the containment building following the LOFC accident.

total amount of ^{131}I released during the 4 to 12 h time period is relatively independent of the core release model; for example, the cumulated amount released from the containment building 12 h after the onset of the accident (very little release occurs before 4 h) is calculated to be ~ 3400 Ci using the uniform temperature model and ~ 2800 Ci using the AYER release model. Since the dose to the individual is proportional to the total amount released during the interval, the calculated dose is relatively insensitive to the core release model. The dose received during the 4 to 12 h interval calculated using the AYER model is $\sim 80\%$ of that calculated using the simplified model. Thus, the governing factor in the dose calculations is the total amount of the isotope released into the atmosphere of the containment building.

C. Release of Isotopes With Long-Lived Precursors - AYER Calculations

(G. E. Cort)

1. Introduction

The calculations of ^{131}I release using volumetric summation of the local release fraction was described in the previous section. These calculations were greatly simplified by the fact that ^{131}I has no long-lived precursors.

The AYER⁷ model was modified to include a generalized six-element decay chain where decay constants, release rates, and branching ratios may be arbitrarily specified for each element in the chain.

2. Model

The equations for the concentration of each isotope in the fuel particles are solved analytically by means of an integrating factor. For example, the rate of change in the number of atoms in the fuel for the third isotope in the chain is

$$\frac{dN_3}{dt} = -(\lambda+r)_3 N_3 + B_{21} \lambda_2 N_2 + B_{12} \lambda_1 N_1 \quad (9)$$

where

N_i = number of atoms of isotope i .

λ_i = decay constant.

r_i = release rate = $a_i e^{-k_i/T}$. a_i and k_i are release rate constants, and T is the local temperature.

B_{ij} = branching ratio of element i in either one of two (j) directions.

The solution at time t for a time step, Δt is:

$$N_3(t) = [N_3(t-\Delta t) - A_2 N_2(t-\Delta t) - A_4 N_1(t-\Delta t)] e^{-(\lambda+r)_3 \Delta t} + A_2 N_2(t) + [A_3 - A_1 A_2] N_1(t) \quad (10)$$

where

$$A_1 = \frac{\lambda_1 B_{11}}{(\lambda+r)_2 - (\lambda+r)_1}$$

$$A_2 = \frac{\lambda_2 B_{21}}{(\lambda+r)_3 - (\lambda+r)_2}$$

$$A_3 = \frac{\lambda_1 B_{12}}{(\lambda+r)_3 - (\lambda+r)_1}$$

$$A_4 = A_3 + A_1 A_2 \frac{(\lambda+r)_3 - (\lambda+r)_2}{(\lambda+r)_3 - (\lambda+r)_1}$$

The series of equations for each isotope in the chain is solved at each time step for each finite element in the AYER model of the core.

Since iodine and noble gases are not strongly adsorbed on graphite, the total release to the coolant is simply the summation of the release from the fuel for all finite elements. For metallic elements which are adsorbed, the calculations described will provide a time and space-dependent source term within the core to replace the constant source use to date.

3. Results

Figure 4 compares the calculated release for the chain with mass number 85 (^{85}Kr and ^{85m}Kr) with results from SORS.¹

Fig. 4. Calculated ^{85}Kr and $^{85\text{m}}\text{Kr}$ release from HTGR core during the LOFC accident.

A three-element chain, starting with Barium-85, was modeled. The branching ratios, decay constants, and release rate constants, a_i and k_i , were taken from Ref. 1. The initial concentrations were taken from Ref. 12.

D. Containment Building Leak Rate Versus Internal Pressure (G. A. Baca)

Calculations of the release of fission products from the containment building have been made using an assumed leak rate of 0.1%/day for the first 24 h and 0.05%/day for the remainder of the accident. Because the internal pressure in the containment building of an HTGR following a depressurization of the PCRV is high (>15 psig), a search of the literature was made to obtain estimates of the leak rate as a function of internal pressure. Leak rate tests were performed on the Carolinas Virginia Tube Reactor (CVTR)¹³ containment building, a building with a design similar (but with a smaller volume) to those proposed for HTGR's.

A third-order quadratic equation was fitted to the leak rate versus pressure data from the CVTR containment building. Selected values are shown in Table I. These data imply that the leak rate in a reinforced concrete, steel-lined containment

building may be $\sim 0.3\%$ /day at 15 psig, rather than 0.1%/day.

The ^{131}I release from the LOFC accident was calculated using the leak rate data from the CVTR containment building rather than the leak rate normally assumed (0.1%/day and 0.05%/day); the amount of iodine released increased by a factor of ~ 3.0 when the pressure dependent leak rate was used. The thyroid dose increased by a similar amount.

This discussion is not intended to imply that the leak rate from an HTGR containment building will be 0.3%/day rather than 0.1%/day, but it does point out the fact that since the internal pressure in the containment building after an HTGR depressurization accident is high, the leak rates normally assumed in reactor safety ($\sim 0.1\%$ /day) may not be correct. Certainly more information and experience is needed.

E. Release of Metallic Fission Products From A Reference 300 MW HTGR Under Normal Operation (B. L. Holian)

A model of the metallic fission product release to the helium coolant for a reference 300 MW(t) HTGR (or 1/10th of the release from a 3000 MW(t) HTGR) under normal operating conditions (without coolant cleanup) has been developed. The diffusion through the graphite core has been solved analytically, and the evaporation and condensation between internal adsorption sites in the graphite and the helium coolant are treated as a completely time-dependent problem. The calculation proceeds under the following conditions and assumptions:

TABLE I

LEAK RATE VERSUS PRESSURE IN CVTR CONTAINMENT BUILDING

Leak rate(%/day)	0.00	0.231	0.297	0.371
Pressure(psig)	0	6	13	21

1. All fuel particles are identical and uncoated, or, equivalently, all fuel particles are BISO (pyrolytic carbon-coated) particles which have been in operation for about 100 days, thereby having reached steady-state saturation with metallic fission products. Thus, the release rate is roughly twice that of a true HTGR with TRISO (silicon carbide-coated) particles, which effectively contain all metallic fission products at normal fuel temperatures. The rate of generation (atoms per unit time) of the i^{th} fission product species ($i = 1, 2, \dots, n$) is assumed to be

$$Q_{oi}(t) = PFY_i, \quad (11)$$

where P is the average power of the reactor, F is the number of fissions per unit time per unit power, and Y_i is the fractional fission yield of species i . In reality, the rate of generation at any given time varies widely at different parts of the core, depending on the refueling history, and widely with time at any given point in the core, depending on the age of the fuel. Nevertheless, the full core average at any time is given by Eq. (11).

2. The diffusion coefficients of all metallic fission products in the charcoal matrix of the fuel stick are assumed to be infinite, so that the charcoal is instantly saturated. In reality, the diffusion coefficient in charcoal is indeed much larger than that in graphite, although charcoal is about 100 times more adsorptive of metal atoms (1000 times the internal surface area with 1/10th the

monolayer capacity for adsorption¹⁴). Full saturation is probably achieved within 100 to 200 days, given the rate of generation of atoms of various metallic species relative to the monolayer coverage in the charcoal, and given that the fuel particle coatings are saturated by about 100 days.¹⁵ Consequently, by about one year the steady-state flux is equal to that from the bare fuel particles. The concentration profile in the fuel region is virtually flat because of the high diffusion coefficient.

3. In the graphite near the fuel hole boundary, the concentration drops by a factor of about 100 from the fuel stick value.^{14,15} Because the diffusion coefficient is lower in graphite than in the fuel stick, the concentration profile in graphite is steeply sloped. At the fuel stick-graphite block boundary, the mass flux just inside the fuel region is, by conservation of mass, equal to the mass flux just inside the graphite. This assumes, of course, that the two materials are both continuous media with a perfectly sharp boundary between them, thereby ignoring any fuel-hole gap effect. The graphite block geometry, represented by a coolant hole surrounded by six fuel holes, can be approximated by a hollow cylinder of graphite of inner radius a , the coolant hole radius, and outer radius b , corresponding to the shortest distance from the center of the coolant hole to a fuel-hole boundary. The diffusional flux J_{oi} of atoms of species i entering radially into the outer wall of the cylinder times the area of the wall is given by Eq. (11),

following the previously stated assumptions. The graphite is assumed to be at a constant temperature, so that the diffusion coefficient D_i is constant throughout. Actually, the temperature drops, as does the diffusion coefficient, from the outer wall of the cylinder to the coolant hole. To a good approximation, the hollow cylinder geometry can be replaced by an infinite slab of thickness $L = b - a$ (roughly 15% overestimation for times $t \leq 4L^2/\pi^2 D_i$, or about 80 days; for larger times, the error becomes negligible). This speeds the calculation considerably, since the concentration as a function of position x ($0 \leq x \leq L$) and time is a infinite series of trigonometric functions (rather than Bessel functions whose arguments must be determined iteratively):

$$C_i(x, t) = \frac{J_{oi}}{D_i} x - \frac{8LJ_{oi}}{\pi^2 D_i} \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2} \sin \frac{(2k+1)\pi x}{2L} \cdot \frac{\lambda_i + \frac{(2k+1)^2 \pi^2 D_i}{4L^2} \exp \left[- \left(\lambda_i + \frac{(2k+1)^2 \pi^2 D_i}{4L^2} \right) t \right]}{\lambda_i + \frac{(2k+1)^2 \pi^2 D_i}{4L^2}}, \quad (12)$$

where λ_i is the radioactive decay constant for species i and Danckwerts' method¹⁶ for diffusion with first-order chemical reaction has been applied.

4. Sink boundary conditions are applied at the coolant hole, i.e., the bulk concentration of metal atoms drops to zero. The surface concentration of metal atoms at the coolant hole is obtained by depositing all atoms in the

diffusional flux at sites in the bulk graphite, which are assumed to be in contact with the circulating (turbulent) helium coolant. Consequently, this surface concentration is depleted by evaporation to the coolant and is fed by the diffusional flux from the bulk graphite and by condensation from the coolant. The mass transfer rate of species i as a function of time t from the graphite to the coolant is proportional to the difference of the partial pressure at the graphite internal surface, $P_{gi}(t)$, and the partial pressure in the coolant, $P_{ci}(t)$:

$$R_i(t) = R_{oi} [P_{gi}(t) - P_{ci}(t)], \quad (13)$$

where the constant R_{oi} depends on the product of the mass transfer coefficient and flow rate of the helium coolant. (See Ref. 17 for

discussion of similar treatment.) The partial pressure in the coolant is proportional to the number of atoms released into the coolant, provided that the mole fraction of species i is small. At the graphite internal surface, the partial pressure of species i depends on the fractional surface area covered by species i atoms. At low coverage, the heat of adsorption at any occupied adsorption site is a

constant (Langmuir adsorption isotherm), while at some critical coverage, much less than a monolayer, the adsorption behavior is characterized by the Freundlich isotherm, corresponding to an exponentially-decaying distribution of heat of adsorption over occupied adsorption sites. In other words, in the Langmuir regime, each occupied adsorption site behaves independently from all others and contributes a constant to the total heat of adsorption, while in the Freundlich regime 63% of the occupied adsorption sites contribute less than the average to the total heat of adsorption. Thus, the partial pressure in the Langmuir regime is linear with the number of adsorbed atoms, while in the Freundlich regime it follows a power law. Based on the Freundlich adsorption isotherm,

$$P_i = P_{mi} (C_i/C_{mi})^{u_i}, \quad (14)$$

and Glueckauf's treatment of binary adsorption,¹⁸ Zumwalt has obtained the following empirical expression¹⁹ for multispecies adsorption in the Freundlich regime ($\theta_L < \theta < 1$):

$$P_i = P_{mi} (C_i/C_{mi})^{\theta_L^{u_i-1}}, \quad (15)$$

and in the Langmuir regime ($\theta < \theta_L < 1$)

$$P_i = P_{mi} (C_i/C_{mi})^{\theta_L^{u_i-1}}; \quad (16)$$

where

- P_i = vapor pressure of species i in the helium boundary layer near the graphite surface,
- P_{mi} = vapor pressure of species i at monolayer coverage,
- C_i = surface concentration of species i ,
- C_{mi} = surface concentration of species i at monolayer coverage,
- u_i = $\bar{E}_i/RT$ = Freundlich adsorption isotherm exponent ($\bar{E}_i$ is average adsorption energy per mole),
- $\theta = \sum_{i=1}^n C_i/C_{mi}$ = fraction of monolayer coverage, and
- θ_L = fraction of monolayer coverage at which transition from Langmuir to Freundlich regime occurs.

The overall release rate of species i to internal surface adsorption sites in the bulk graphite, as well as to the helium coolant is given by

$$\frac{dN_i(t)}{dt} = Q_i(t) - \lambda_i N_i(t), \quad (17)$$

where N_i is the overall release, Q_i is the diffusional flux at the coolant hole boundary of the graphite times the area of the graphite-coolant interface, and λ_i is the radioactive decay constant of species i . The release rate to the coolant alone is given by

$$\frac{dN_{ci}(t)}{dt} = R_i(t) - \lambda_i N_{ci}(t), \quad (18)$$

where N_{ci} is the release to the coolant (the coolant "inventory" of species i) and $R_i(t)$ is given by Eq. (13). These two coupled first-order differential equations are easily decoupled in the linear Langmuir

regime, but must be iteratively decoupled in the nonlinear Freundlich regime. Since R_i , the mass transfer rate, is negatively proportional to N_{ci} , the effective decay constant for the release to the coolant is equal to the condensation rate constant plus the radioactive decay constant. Therefore, an integration scheme, such as the trapezoidal rule, which may be applicable to the total release rate equation for a given size time step, may not be at all appropriate to the release to the coolant, which has a much larger effective decay constant. In order to remedy this difficulty, the following algorithm has been developed for the integration of

$$A(t) = \int_0^t dt' B(t') e^{-k(t-t')}, \quad (19)$$

which is the solution of the first-order differential equation

$$\frac{dA(t)}{dt} = B(t) - kA(t), \quad (20)$$

where A is the release (either N or N_c), B is the source (either Q or the evaporation rate), and k is the decay constant (either the radioactive decay constant λ or λ plus the condensation rate constant). Let $\Delta t = t_{n+1} - t_n$, with the notation $f_n \equiv f(t_n)$, and $\tau = k\Delta t$; then there are the following two cases:

$$1. \quad 0 < \tau < \varepsilon \ll 1$$

$$(x = 1 - \tau + \frac{1}{2} \tau^2 \approx e^{-\tau}),$$

$$A_{n+1} = A_n x + \frac{1}{2} \Delta t (B_n x + B_{n+1}), \quad (21)$$

the usual trapezoidal rule.

$$2. \quad \tau > \varepsilon [D = (B_{n+1} - B_n)/\tau],$$

$$A_{n+1} = [B_{n+1} - D + (kA_n - B_n + D)e^{-\tau}]/k \quad (22)$$

which is based on the assumption (usually satisfactory or, at least, unavoidable) that B is a linear function of time over the interval Δt .

The release of the n metallic fission product species to the coolant is thus calculated as a dynamic function of time, i.e., both diffusion and adsorption are accounted for, in a reasonable approximation to the actual phenomena. A significant effect on release, namely, competition among various metallic fission product species for adsorption sites, is taken into account. The only important restriction is that the source from the fuel is assumed to be constant in time. This restriction will be removed in future work on accidental heatup of the core.

The results of the above model for release of ^{90}Sr with $n = 1, 3$, and 8 species can be seen in Fig. 5, where the model is compared with the more complicated finite difference solution of the diffusion equation by Appel and Roos¹⁵ for $n = 1$, and 3 . A break in the release curve for the above model as a function of time occurs where the adsorption isotherm undergoes a transition from Langmuir to Freundlich behavior. The precise time at which the critical coverage is achieved is determined by a self-consistent iterative calculation. Note that the breaks for $n = 1, 3$, and 8 occur along a common curve, as is required by the independent adsorption phenomenon of the Langmuir regime. By including two species in addition to ^{90}Sr , the release of ^{90}Sr is increased by a factor of 10; with seven additional species, the release increases by a factor of 100. Although the agreement between this model and the calculation of Appel and Roos is excellent, two principal differences are apparent: 1) the release in the above calculation is higher for the first half year than Appel and Roos' since a constant source from the fuel has been assumed, while Appel and Roos consider the more realistic case of a buildup to the steady

Fig. 5 ^{90}Sr release to the coolant.

state by about 100 days; and 2) the release rate in the above calculation is lower than that of Appel and Roos for the first four years, because in order to calculate the rate of ^{90}Sr generation, the average power is used in the above work, while Appel and Roos account for a decline in the fuel power density from a maximum at zero time to a minimum at six years. More recent measurements of the diffusion coefficients of metallic fission products in graphite,¹⁷ as well as the more recent HTGR design characteristics (most notably, the moderator temperature), give a calculated release lower by a factor of 10,000 after four years. Increasing the graphite temperature to that of the fuel region still gives a release lower by a factor of 100 after four years.

IV. PRIMARY COOLANT IMPURITIES

Efforts within this task area are directed to 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 and carbon monoxide. Materials of interest are the core and related graphite structures, and the metallic components comprising, for example, the steam generators, helium circulators, orifice valves, and control rod systems. Interactions between gaseous impurities and fission products with subsequent formation of volatile species are also of interest.

A. Code Development (A. Bowman)

We are continuing the development of a computer code for modeling the chemical reactions between graphite and flowing gases. This code has been named CIMPRES (Coolant IMPurity REactions). The code is operational now for the two-dimensional steady-state heat transfer problems, but quantitative agreement with the analytic solution of a test problem has not yet been achieved. We have started to add the

time-dependence capability and to expand to the three-dimensional problem.

Validation of CIMPRES will proceed concurrently with the development of the code, and will proceed from comparison to simple analytical problems to comparison to small scale experiments and thence to much larger scale experiments. This validation procedure will give confidence when advanced forms of CIMPRES are compared with such complex codes as OXIDE-3.

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

Experiments are being planned to study reactions between contaminant gases present in the primary coolant helium gas and the alloy structural materials used for the HTGR primary coolant circuit boundaries. The experiments will be carried out under conditions that closely simulate the conditions prevailing in operating and proposed HTGR's. The reactions of interest include but will not be limited to both surface and internal oxidation, carburization, and decarburization. The environmental variables concerned are temperature, pressure, flow rate, and impurity concentrations in the helium gas. The materials variables involved are alloy composition, condition of heat treatment and/or cold work, grain size, and surface condition. Initially the experiments will focus on the alloys composing the steam generator tubing, since the integrity of this structure is crucial from the point of view of reactor safety. Specifically, the alloys to be studied are medium carbon steel, 2-1/4 Cr-1Mo ferritic steel, and Incoloy 800.

The alloys will be exposed to flowing, impure helium gas at temperatures ranging from 573 K (572°F) to 1033 K (1400°F) at a pressure of 5.0 MPa (~ 720 psi) and a flow rate of $1-16 \times 10^{-6} \text{ m}^3(\text{STP})/\text{s}$ (1.14-2 ft³/h). High flow rate experiments will be deferred until more experience is gained with high pressure gas system control. The

helium gas will contain controlled amounts of H_2O , H_2 , CO , CO_2 , and CH_4 in the ppmv ranges. These levels are comparable to those existing in an HTGR under steady-state operating conditions with an inleakage of small quantities of steam.²⁰ Much higher levels of contaminants will be introduced into the helium gas to simulate operation under accident conditions, and initially short term exposure experiments will be run with high levels of selected contaminants present in the helium gas. Later, experiments will be run in which exposure times will range from about 360 ks (100 hours) to several thousand ks (several thousand hours) and in which lower contaminant levels are present in the helium gas (corresponding to normal HTGR operating conditions).

The proposed experimental arrangement can be broken down as follows:

1. Pure Helium Source

Liquid helium will be used as the source of pure helium. The liquid helium will be vaporized to gas and brought to room temperature and pressure by flowing it through an air-warmed coil of tubing. The flow rate will be measured, and controlled by regulation of the gas pressure over the liquid helium in the cryostat. The liquid helium will be filtered through a sintered, porous stainless steel filter prior to vaporization to remove any contaminant ice particles that may be present. The flow rate of the helium gas will be about $1.6 \times 10^{-5} \text{ m}^3 (\text{STP})/\text{s}$ ($\sim 2 \text{ ft}^3/\text{h}$) for each experiment being run. The maximum total flow rate of the helium gas will be about $7.9 \times 10^{-5} \text{ m}^3/\text{s}$ ($10 \text{ ft}^3/\text{h}$) at STP (corresponding to a maximum of five experiments running simultaneously). These flow rates correspond to liquid helium usage rates of $2.3 \times 10^{-8} \text{ m}^3/\text{s}$ (2 liters per day) and $1.2 \times 10^{-7} \text{ m}^3/\text{s}$ (10 liters per day) not counting losses of about $2.3 \times 10^{-8} \text{ m}^3/\text{s}$ (2 liters per day). The flowing gas will be analyzed periodically to check the purity level.

2. Helium Delivery System

The helium delivery system will consist of a pump to pressurize the helium gas to 5 MPa ($\sim 720 \text{ psi}$), a means for introducing the contaminant gases into the pressurized, flowing helium in controlled amounts, and a means for heating the system to at least 373 K downstream of the contaminant gas injection. The heating has a twofold purpose. The first is to help bring to completion the reaction $2\text{H}_2 + \text{O}_2 = 2\text{H}_2\text{O}$ as the hydrogen and oxygen contaminants that have been introduced upstream pass over a platinum gauze catalyst. The second is to reduce adsorption of the contaminant gases on the tubing walls. The gas will be analyzed periodically downstream of the contaminant injection to check the impurity levels.

3. Helium Heating and Specimen Reaction System

The proposed helium heating and specimen reaction system will consist of a vertically mounted Inconel 625 tube approximately 0.5 m (18 inches) long with a hot zone 0.3 m (12 inches) long. A series of platinum baffles in the lower two-thirds of the hot zone will help insure turbulence of the flowing gas. This will enhance mixing and heat transfer to the gas. The alloy specimens will be located in the top end of the hot zone. The cylindrical specimens will be 1.6 mm ($\approx 0.0625 \text{ inch}$) in diameter and 10 mm ($\approx 0.39 \text{ inch}$) long. The specimens will be stacked vertically in the Inconel 625 tube. There will be six to ten layers of specimens with six to ten specimens per layer. The specimens will be separated from the Inconel 625 tube wall and from one another by an inert spacer material (e.g., platinum gauze). The Inconel 625 tube will be heated with a multi-zone resistance furnace, since it may be necessary under some experimental conditions to employ two-zone heating to heat the helium gas and specimens separately in order to gain better control of the gas composition.

For circumferential stress the ASME Boiler and Pressure Vessel Code²¹ gives the maximum allowable operating pressure for a cylindrical pressure vessel as:

$$P = \frac{SEt}{R + 0.6t}$$

P = design pressure
S = maximum allowable stress value
E = joint efficiency (in this case E = 1, no joints)
t = wall thickness
R = inside radius

For 11.11 mm (7/16-in) o.d. x 1.65 mm (0.065-in) wall Inconel 625 solution annealed tubing and a design temperature of 1033 K (1400°F)

S = 51.7 MPa (7500 psi)²²
t = 1.65 mm (0.065-in)
R = 3.9052 mm (0.15375-in)
P = 17.43 MPa (2529 psi)

Assuming a loss in load bearing wall thickness of 0.0025 mm (0.010-in) over the duration of the experiment

$$P = 14.45 \text{ MPa (2096 psi)}.$$

The expression for the maximum allowable operating pressure for longitudinal stress, $P = \frac{2SEt}{R - 0.4t}$, would yield a considerably higher design pressure. Thus, there is considerable margin for safety, since the operating pressure will be ~ 5 MPa (720 psi). If two-zone heating is used, it may be necessary to incorporate into the design pressure calculation an allowance for thermal stresses set up by the axial temperature gradients at the ends of the hot zone and also between the zones.

The tubing used through the system (except for the Inconel 625 heater tube) will be type 316 stainless steel tubing. All fittings will be type 316 stainless steel swage-lock type.

The system as designed has sufficient flexibility to allow a wide range of temperatures and gas compositions to

be employed. The large specimen capacity will allow specimens of all three alloys in all conditions to be loaded for each set of experimental conditions chosen, thereby reducing the number of runs necessary. Experiments to study graphite steam/air reactions can also be performed using this system as designed or with only slight modifications. Several experiments can be run simultaneously by adding tube and furnace assemblies and increasing the total flow rate.

The alloy specimens will be weighed before and after exposure to the impure helium to determine weight gain/loss. In addition duplicate specimens will be descaled and weighed following exposure to determine the amount of metal reacted for comparison with the weight-gain/weight-loss measurements. The specimens that have not been descaled will be mounted for metallographic and electron microprobe analysis to determine film thicknesses and film compositions, and, compositions and microstructural changes in the base metal. The extent to which internal reactions have occurred will be investigated. The primary purpose of these examinations and measurements is to determine which of several possible reactions occur, the mechanisms and kinetics, and the conditions under which they occur.

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

An equilibrium thermodynamics approach is being used to study the chemistry of the impurities in the primary coolant. Basically, free energy minimization techniques are used to determine equilibrium concentrations of multi-component mixtures of interfacing chemical species. While this technique does not account for kinetics of reactions, it is felt that the results obtained do represent limits of reaction. These limits can provide guidelines for the study of the primary coolant chemistry; the technique may also supply insight into possible reaction paths.

An interactive code, QUIL, for the calculation of complex chemical equilibria has been written. The code features a preprocessor which allows the input to the code to be in the form of a chemical statement of the problem to be solved. The preprocessor then writes the nonlinear system solver required by that chemical statement of the problem.

The system solver utilizes a multiple approach to solving the set of equations. The method of steepest ascent, the Newtonian method, a weighted Newtonian method, and the damped method of Levinberg are all available to the system solver during any particular interaction. Depending upon the difficulty of solution, different combinations of the four methods are called upon as convergence progresses. The present version of the code has been able to handle as many as 13 species successfully.

A plotting subroutine has been written which allows the results of the code to be presented graphically.

Preliminary investigations have been made into the primary coolant loop impurities resulting from water leakage. All results represent equilibrium distributions at constant temperature and pressure. Water concentrations are reported in parts per million (ppm) by volume before reaction. Cesium levels are reported as parts per billion (ppb) by volume before reaction. Distributions have been calculated as a function of temperature and pressure from 400 K to 3000 K and from 0.1 to 5.0 MPa. Water impurities from 1 to 10,000 ppm and cesium impurities at 1 ppb were used for starting stoichiometries. The species present are labelled as such in the distribution plots.

Reaction kinetics are not accounted for in these calculations. Instead, the results are calculated with and without carbon present. Such an approach is thought to represent a realistic bound on the distribution of the species present.

Figure 6 is a plot of the water reaction from 400 K to 3000 K with 100 ppm H_2O in helium. Dissociation at 5.0 MPa is not appreciable until the upper end of the temperature scale. Figure 7 indicates the water reaction with carbon present. Here the carbon is seen to oxidize the water at high temperatures and the dominant species at higher temperatures are seen to be CO and H_2 . Oxygen levels are decreased over the entire temperature range and CH_4 , H_2O , and CO_2 are seen to group in a band that falls some six orders of magnitude with the temperature variations as indicated.

Fig. 6. Temperature equilibrium plot - water system, 100 ppm H_2O in helium.

Fig. 7. Temperature equilibrium plot -
water/carbon system 100 ppm H₂O
in helium with carbon present.

Figure 8 is a plot of the water re-action with 1 ppb cesium at the reactor design pressure. Three regimes are indicated. At the lower end of the temperature scale, the dimeric hydroxide, $\text{Cs}_2(\text{OH})_2$, is the dominant specie. At the high end, elemental cesium vapor dominates. In the center, the monomeric hydroxide, $\text{Cs}(\text{OH})$, is seen to be the important specie. The transition temperatures between the two regimes are around 600 K and 2200 K. The species CsO , Cs_2 , and Cs_2O are seen to be unimportant. Preliminary results suggest

that the hydride and the Cs ion are similarly unimportant.

Figure 9 shows the water reaction in the presence of carbon with 1 ppb cesium present. The dominant species of cesium are still $\text{Cs}_2(\text{OH})_2$, $\text{Cs}(\text{OH})$, and Cs . Also, the order of occurrence is unchanged from the distribution without carbon present. The lower temperature transition is still of the order of 600 K, while the second transition temperature has moved down to some 900 K.

Fig. 8. Temperature equilibrium plot -
water/cesium system. 100 ppm H_2O ,
1 ppb Cs in helium.

Fig. 9. Temperature equilibrium plot - water/carbon/cesium system. 100 ppm H_2O , 1 ppb Cs in helium with carbon present.

Figure 10 and Fig. 11 are plots of the water-cesium and of the water-carbon-cesium systems at 600 K as a function of pressure. From Fig. 10 it can be deduced that, in the absence of carbon, both the monomeric and the dimeric hydroxides of cesium are some 8 orders of magnitude more abundant than is elemental cesium at the inlet core temperature (600 K) at 100 ppm initial H_2O . Figure 11 indicates that, with carbon present, the hydroxides are some 4 orders of magnitude more abundant than is elemental cesium, again at 100 ppm H_2O .

Fig. 10. Pressure equilibrium plot - water/cesium system. $T = 600$ K. 100 ppm H_2O , 1 ppb Cs in helium.

Figures 12 and 13 are plots of the species distributions at the core exit temperature (1100 K) without and with carbon present. In Fig. 12, with carbon absent, the monomeric hydroxide is of the order of 4 orders of magnitude more abundant than is elemental cesium at 100 ppm H_2O . Figure 13 indicates that when carbon equilibrium is assumed at the core exit temperatures with 100 ppm H_2O present, elemental cesium is the most abundant species of cesium present by some 3 orders of magnitude.

Fig. 11. Pressure equilibrium plot - water/carbon/cesium system. T = 600 K. 100 ppm H₂O, 1 ppb Cs in helium with carbon present.

These results may have important implications with regard to fission product release, but some future effort must be directed toward modifying the code to allow the inclusion of adsorbed species. It is also intended that the code shall be modified to allow the calculation of potentials for reactions not assumed to be at equilibrium in the reactor environment.

For applications in the complex equilibria codes and for other estimates of fission product release in HTGR safety

Fig. 12. Pressure equilibrium plot - water/cesium system. T = 1100 K. 100 ppm H₂O, 1 ppb Cs in helium.

applications, the vapor pressure of elemental cesium over cesium adsorbed on nuclear graphite is commonly described by the Freundlich adsorption isotherm:

$$\ln P = \alpha + \beta \frac{10^3}{T} + [\zeta + \gamma \frac{10^3}{T}] \ln C \quad (23)$$

where P is vapor pressure, atmospheres

T is temperature, K

C is concentration of the adsorbed cesium

Fig. 13. Pressure equilibrium plot - water/carbon/cesium system. $T = 1100$ K. 100 ppm H_2O , 1 ppb Cs in helium with carbon present.

α , β , ζ , γ are the Freundlich constants. The concentration units of C are variously reported as $\mu\text{mol}/\text{m}^2$, $\mu\text{mol}/\text{gm}$, and $\mu\text{mol}/\text{cm}^3$. For this report data have been reduced to $\mu\text{mol}/\text{gm}$. Thus, for example, if data are reported with C (denoted by C_A) in units of $\mu\text{mol}/\text{m}^2$, the Freundlich constants may be recalculated to a $\mu\text{mol}/\text{gm}$ basis (denoted C_m) provided the specific surface area, S , m^2/gm is known

$$C_m = C_A \cdot S \quad (24)$$

$$\ln C_A = \ln C_m - \ln S$$

On insertion into the Freundlich equation it is found that

$$\alpha_m = \alpha_a - \zeta_a \ln S$$

$$\beta_m = \beta_a - \gamma_a \ln S \quad (25)$$

$$\zeta_m = \zeta_A$$

$$\gamma_m = \gamma_A$$

where the m and a subscripts refer to mass and area basis for concentration, respectively. A similar correction may be made for volume concentration ($\mu\text{mol}/\text{cm}^3$) provided the density, ρ , gm/cm^3 is known.

Several sets of data were examined and reduced to common concentration units ($\mu\text{mol}/\text{gm}$). The Freundlich parameters derived are shown in Table II.

Two graphites were unspecified; the SP-1C is a natural graphite flake not typical of nuclear graphite. The data from Ref. 15 were quoted as being "experimental"; however, no details were given. It has been assumed that the data of Ref. 15 are for a nuclear graphite and therefore they were included in the calculated average of line 3.

The constants of line 6 of Table II are those used in the SORS Code of GAC. It is of interest to compare cesium pressures calculated using the SORS Freundlich parameters with those calculated using the average parameters developed earlier. The results are shown in Table III.

In general it is seen that the SORS expression overestimates the cesium pressures, at least for coverages up to ~ 1.0 $\mu\text{mol}/\text{gm}$. Above this coverage the Cs pressures are underestimated.

TABLE II
FREUNDLICH PARAMETERS FOR
CESIUM ADSORPTION ON GRAPHITE

<u>Graphite</u>	<u>α</u>	<u>β</u>	<u>γ</u>	<u>ζ</u>	<u>Ref</u>
HLM-85	28.11	-56.20	-15.28	24.67	14
TS-688	22.53	-52.50	- 7.32	15.26	19
?	26.6	-55.7	-14.5	24.2	15
Average	25.69	-54.72	-12.32	21.33	*
SP-1C	9.93	-29.46	- 8.39	14.47	19
?	7.8	-29.84	0.2351	1.873	23

* This average is not the arithmetic mean of the Freundlich coefficients. Rather, the equilibrium Cs pressures were calculated using each of the three expressions, and the average pressure at each temperature and composition obtained. A new fit to the Freundlich equation then yielded these new constants.

It is felt that the concentration of CsH(g) would be comparable to those of other gaseous cesium species at equilibrium. Since the ideal gas thermodynamic functions were not available for CsH(g), the necessary functions were calculated using a modification of the usual approximation to numerical summation of vibrational-rotational levels given by Mayer and Mayer.²⁴ For that purpose spectroscopic constants for the $1\Sigma^+$ ground state as listed by Bartky²⁵ were used. The dissociation energy of the ground state (D_0^0) has been estimated as 1.81 ± 0.04 eV.²⁶

Two other electronic states with relatively low dissociation energies are known for CsH.^{25,26} Because the approximation using the Euler-Maclaurin summation formula is not satisfactory for electronic states with low dissociation energies,²⁴ these states were not included in the calculation. The approximation method sums to infinite vibrational number, and for low dissociation numbers this is a bad approximation. For such states it is preferable to perform a direct summation of vibrational-rotational states and

take account of the cut-off of rotational-vibrational quantum numbers as limited by pre-dissociation at the dissociation limit. This more complicated calculation has been described elsewhere.²⁷ The results of these calculations are presented in Table IV.

The simplified method used for the thermodynamic functions is considered satisfactory to 3000 K. By ignoring the excited electronic states at that temperature the entropy and free energy function may be low by approximately 1% and 0.1%, respectively.

V. STRUCTURAL INVESTIGATIONS

A. Review and Evaluation of Concrete Failure Prediction Techniques (E. G. Endebroek)

Two non-proprietary general purpose finite element codes which have the capability of treating material non-linearities in three-dimensional structures are known to exist at the present time. They are NONSAP (a Structural Analysis Program for Static and Dynamic Response of Non-Linear Systems) and NEPSAP (Non-Linear

TABLE III
COMPARISON OF EQUILIBRIUM CESIUM PRESSURES

<u>C, $\mu\text{moles/g}$</u>	<u>T, K</u>	<u>P_{Cs}, atm</u>	
		<u>Average</u>	<u>SORS</u>
0.1	1000	2.4×10^{-22}	2.1×10^{-12}
	1100	3.0×10^{-18}	4.7×10^{-11}
	1200	7.9×10^{-15}	6.2×10^{-10}
	1300	6.2×10^{-12}	5.5×10^{-9}
	1400	1.8×10^{-9}	3.6×10^{-8}
0.5	1000	4.8×10^{-16}	6.2×10^{-11}
	1100	2.7×10^{-13}	1.1×10^{-9}
	1200	5.1×10^{-11}	1.1×10^{-8}
	1300	4.4×10^{-9}	8.2×10^{-8}
	1400	2.0×10^{-7}	4.5×10^{-7}
1.0	1000	2.5×10^{-13}	2.7×10^{-10}
	1100	3.6×10^{-11}	4.0×10^{-9}
	1200	2.3×10^{-9}	3.9×10^{-8}
	1300	7.5×10^{-8}	2.6×10^{-7}
	1400	1.5×10^{-6}	1.4×10^{-6}
5	1000	4.9×10^{-7}	8.0×10^{-9}
	1100	3.1×10^{-6}	9.1×10^{-8}
	1200	1.5×10^{-5}	7.0×10^{-7}
	1300	5.4×10^{-5}	3.9×10^{-6}
	1400	1.7×10^{-4}	1.7×10^{-5}

TABLE IV

IDEAL GAS THERMODYNAMIC FUNCTIONS FOR CESIUM HYDRIDE (CsH) FW = 133.913

T, K	J/mol·K			kJ/mol			Log ₁₀ Kp
	C _p ^o	S ^o	-(G _T ^o - H ₂₉₈ ^o)/T	(H _T ^o - H ₂₉₈ ^o)	ΔH _F ^o	ΔG _F ^o	
0.0	0.0	0.0	Infinite	- 8.851	119.652	119.652	Infinite
298.15	31.58	215.22	215.22	0.000	116.545	97.260	-17.027
300	31.62	215.42	215.22	0.059	116.516	97.143	-16.902
301.55	31.64	215.56	215.24	0.109	116.491	97.046	-16.798
301.55	31.64	215.56	215.24	0.109	114.401	97.046	-16.798
400	33.32	224.75	216.48	3.308	113.032	91.582	-11.951
500	34.61	232.34	218.92	6.708	111.831	86.365	- 9.016
600	35.53	238.73	221.70	10.216	110.725	81.370	- 7.079
700	36.21	244.26	224.54	13.809	109.792	76.547	- 5.708
800	36.74	249.14	227.31	17.456	108.862	71.861	- 4.689
900	37.15	253.48	229.98	21.149	107.970	67.293	- 3.903
951.6	37.33	255.52	231.30	23.075	107.522	64.936	- 3.562
951.6	37.33	255.52	231.30	23.075	39.701	64.936	- 3.562
1000	37.49	257.42	232.53	24.883	39.772	66.259	- 3.459
1100	37.78	261.00	234.96	28.647	39.940	68.897	- 3.269
1200	38.04	264.30	237.27	32.441	40.116	71.522	- 3.111
1300	38.28	267.36	239.47	36.255	40.292	74.131	- 2.976
1400	38.50	270.20	241.56	40.095	40.467	76.731	- 2.861
1500	38.70	272.87	243.56	43.955	40.643	79.314	- 2.760
1600	38.89	275.37	245.48	47.832	40.802	81.885	- 2.671
1700	39.08	277.73	247.30	51.730	40.957	84.456	- 2.593
1800	39.26	279.97	249.06	55.649	41.108	87.002	- 2.523
1900	39.44	282.10	250.74	59.585	41.246	89.552	- 2.460
2000	39.62	284.13	252.36	63.538	41.368	92.085	- 2.403
2100	39.80	286.06	253.92	67.507	41.460	94.626	- 2.352
2200	39.97	287.92	255.42	71.497	41.535	97.147	- 2.305
2300	40.14	289.70	256.87	75.504	41.589	99.684	- 2.262
2400	40.32	291.42	258.28	79.528	41.606	102.205	- 2.223
2500	40.50	293.06	259.64	83.568	41.577	104.725	- 2.187
2600	40.68	294.66	260.95	87.626	41.510	107.258	- 2.153
2700	40.86	296.19	262.23	91.704	41.393	109.796	- 2.123
2800	41.04	297.68	263.47	95.799	41.221	112.325	- 2.094
2900	41.22	299.12	264.67	99.910	40.987	114.870	- 2.068
3000	41.40	300.53	265.84	104.039	40.681	117.424	- 2.043

Elastic Plastic Structural Analysis Program). NONSAP is currently available at LASL whereas NEPSAP is not. NEPSAP treats static loads only but does handle thermal loading and temperature-dependent material properties (creep). NONSAP handles static or dynamic loads but does not have capabilities for including creep or thermal effects.

Except for final editing, a report on "Review of PCRV Technology" has been completed this quarter. This report lists the areas in which the present technology is lacking and the areas in which sufficient technology presently exists. Areas in which additional research would be helpful include:

1. More efficient methods for predicting concrete fracture and the direction of the fracture.
2. An efficient method for predicting fracture propagation.
3. Stress-strain relations of concrete subjected to multiaxial stress states.
4. Long-term temperature effects on materials.
5. More efficient solution methods for non-linear equations.
6. Constitutive relations of reinforced concrete.

B. Analytical Model Development for Prestressed Concrete (E. G. Endebrock, J. B. Payne)

The modification of the computer program CONC has been completed. CONC is used to determine the stress-strain relationship of concrete subjected to multiaxial stress states. CONC was modified to make it compatible with NONSAP. NONSAP utilizes the elements of a constitutive matrix. CONC originally yielded the total stresses as its output. Modification of CONC was therefore necessary to change its output to the constitutive matrix. The constitutive relations contained in CONC are given in principal coordinates. The transformation of the constitutive matrix

from principal to global coordinates was therefore necessary.

The transformation relationship is based upon the conservation of energy. The strain energy of a material element is the same in all coordinate systems. For an elastic system, the transformation relationship is:

$$C_G = R^T C_P R \quad (26)$$

where

C_G = constitutive matrix in global coordinates

C_P = constitutive matrix in principal coordinates

R^T = transformation matrix

The program CONC yields non-linear stress-strain relationships. Both CONC and NONSAP utilize an incremental solution. The transformation of the constitutive matrix for the non-linear case must therefore be based upon an energy expression that admits non-linear stress-strain relationships. Either complementary or strain energy may be used to determine the constitutive matrix transformation relationship. The use of complementary and strain energy expressions yield results which appear different; however, both yield the same final results. A more direct and simple derivation occurs with the use of complementary energy. The constitutive matrix transformation relationship for non-linear cases is developed below based on complementary energy.

The notation used is as follows:

- ϵ_P = total strains in principal coordinates at time $t + \Delta t$,
- ϵ_G = total strains in global coordinates at time $t + \Delta t$,
- ϵ_P^o = total strains in principal coordinates at time t ,
- ϵ_G^o = total strains in global coordinates at time t ,
- $d\sigma_P, d\epsilon_P$ = incremental stresses and strains in principal coordinates,

$d\sigma_G, d\epsilon_G$ = incremental stresses and strains in global coordinates,

C_p = constitutive matrix in principal coordinates,

C_G = constitutive matrix in global coordinates,

D = strain transformation matrix.

The expression for the conservation of complementary energy in matrix form is

$$\epsilon_p^T d\sigma_p = \epsilon_G^T d\sigma_G \quad (27)$$

The incremental stress-strain relationships are

$$d\sigma_p = C_p d\epsilon_p$$

and

(28)

$$d\sigma_G = C_G d\epsilon_G$$

The total strains are

$$\epsilon_p = \epsilon_p^o + d\epsilon_p$$

and

(29)

$$\epsilon_G = \epsilon_G^o + d\epsilon_G$$

The strain transformation relationship is

$$\epsilon_p = D \epsilon_G$$

or

(30)

$$\epsilon_p^o + d\epsilon_p = D(\epsilon_G^o + d\epsilon_G)$$

Now, assuming that the principal directions do not change during a stress and strain increment, then

$$\epsilon_p^o = D \epsilon_G^o \quad (31)$$

and

$$d\epsilon_p = D d\epsilon_G$$

Substitution into the complementary energy expression yields

$$\epsilon_G^T D^T C_p D d\epsilon_G = \epsilon_G^T C_G d\epsilon_G \quad (32)$$

Now $d\epsilon_G$ and ϵ_G can be assigned arbitrary values; therefore,

$$C_G = D^T C_p D, \quad (33)$$

which is the desired constitutive matrix transformation relationship. Note that it takes the same form as the transformation relationship for the elastic case. It should be noted that in the use of tensor notation, the stress transformation matrices are not the same. The transformation matrix D used above is the strain transformation matrix.

C_G , C_p , and D are 6 x 6 matrices in the general three-dimensional case. The transformation relationship

$$C_G = D^T C_p D$$

is valid for transformation from any coordinate system to another. Computational reduction is possible if one coordinate system is the principal stress and strain coordinate system. In principal coordinates, the matrix C_p can be reduced to a 3 x 3 nonzero matrix. Because of the many zeros of the principal constitutive matrix C_p , the matrix D can be reduced to a 3 x 6 matrix. C_G remains a 6 x 6 matrix. The result is a simplification from

$$C_G = D^T C_p D \quad (34)$$

6x6 6x6 6x6 6x6

to

$$\begin{matrix} C_G & = & D^T & C_P & D & . \\ 6 \times 6 & & 6 \times 3 & 6 \times 3 & 3 \times 6 & \end{matrix} \quad (35)$$

For the directional cosines arranged in columns as shown below

$$\begin{matrix} C_1 & C_4 & C_7 \\ C_2 & C_5 & C_8 \\ C_3 & C_6 & C_9 , \end{matrix}$$

the simplified matrix D is

$$D = \begin{matrix} C_1^2 & C_2^2 & C_3^2 & C_1C_3 & C_1C_2 & C_2C_3 \\ C_4^2 & C_5^2 & C_6^2 & C_4C_6 & C_4C_5 & C_5C_6 \\ C_7^2 & C_8^2 & C_9^2 & C_7C_9 & C_7C_8 & C_8C_9 . \end{matrix} \quad (36)$$

The computer program CONC has been incorporated into the computer program NONSAP as a subroutine. The combination is not yet operational. Difficulties in the formation of the finite element stiffness matrix within NONSAP have been encountered.

Refinements in the computer program CONC are being continued. The goal is to find a convenient and systematic manner for utilizing concrete data obtained from specific tests such that the behavior of any concrete can be mathematically described. Due to the many variables associated with concrete, progress in this area has been slow.

During the next quarter there will be a continued effort directed toward refining and generalizing the computer program CONC. In addition, an effort will be directed toward the debugging of the three-dimensional nonlinear part of the computer program NONSAP.

The design of the proposed concrete triaxial testing machine for concrete and graphite is expected to be initiated.

The review and evaluation of structural techniques as related to PCRVs will continue.

C. Core Physical Model Test Program

(R. C. Dove)

The effort to establish the scaling laws which govern the physical modeling of the HTGR core was completed during this quarter. The results of this study have been presented in a LAMS informal report (LA-5821-MS) and therefore will only be briefly summarized here. We conclude that it is not feasible to consider the construction of an exact scale model, i.e., a model in which all characteristics of the prototype are faithfully reproduced to scale. This conclusion results from the fact that the only way to exactly scale material properties is to use the same material for the model as is used in the prototype (i.e., graphite), and if this is done other constraints which are present, if all possible variables are considered, force the length scale to unity.

Initially, it appears much more feasible to consider using scale models in the following two ways: First, simplified models might be constructed to determine the relative importance of the various parameters that govern the HTGR core response to seismic excitation. These models would contain one-, two- and three-dimensional arrays of blocks but not necessarily in the same pattern, number, or shape as the HTGR core. Properties and design features, the relative effect of which must be much better understood, include effect of the frictional forces between blocks, effect of internal energy losses that may accompany block deformation, effect of block stiffness and the possible importance of graphite's known nonlinearities, effect of block clearance, effect of block locating techniques, etc. Second, physical models might be constructed to simulate simplified mathematical models that will be developed to analyze core response. Verification of mathematical models at

early and intermediate steps as they are progressively extended to represent the HTGR core seems especially desirable. The numerical values for many of the parameters that will be used in later analytical models may be obtained from these physical models.

As a result of our study of physical modeling we have concluded that physical models already constructed by others should not be used to finally demonstrate actual core behavior until these models have been verified. Verification, as used here, means that it should be demonstrated that all pertinent variables have been properly scaled and that some type of check has been made.

Proposals for specific physical models and the required test facilities will be completed during the next quarter.

D. Analytical Model Development for Core Seismic Response (J. G. Bennett, R. J. Bartholomew, W. A. Bradley, B. J. Donham, G. A. Reynolds, J. L. Merson, A. J. Webb)

During the present quarter the program to develop an analytical model for the HTGR core has reached several significant milestones. The basic method under development (the component element method combined with an equilibrium iteration procedure) has been described in the LAMS informal report previously mentioned. As a "proof of method," the program developed has been applied to the simple one-dimensional system shown in Fig. 14. Several computer runs on this system have been made to demonstrate the program's ability to handle wide variations in such important parameters as block clearance, block stiffness, static and kinetic coefficients of friction, and amplitude and frequency of applied motion. The LAMS report mentioned above contains the details of these program runs.

Fig. 14. First Model.

As a second step in the development of progressively more realistic mathematical models the original program has been modified to apply to the system shown in Fig. 15. In this system the entire block support system is driven in a prescribed oscillatory manner. Runs made on this program indicate that the program can handle a realistic range of variables without serious difficulty; however, care is required in the presentation of the data. With low-frequency, large-amplitude driving motion (i.e., the low-frequency end of the earthquake spectrum) the relative displacement between the blocks and the base is so small compared to the total motion that there is insufficient resolution in the position versus time plots for the individual blocks to give information about the collision process. In this region it will be necessary to print and plot block accelerations to obtain the desired information. With high-frequency, small-amplitude driving motion (i.e., the high-frequency end of the earthquake spectrum) the absolute velocity of the blocks

Fig. 15. Second Model.

is so small that relatively long times are required before the blocks impact the boundary. For example, with an input motion of 0.00508 cm (0.002 in.) and frictional values of 0.2 (μ_s) and 0.16 (μ_k), 3.76 sec (real time) elapse before the first collision takes place. Obviously, driving motions simulating earthquakes will contain a wide band of frequencies and the best method (or methods) of data presentation will have to be carefully considered.

The effect of varying block stiffness (K_B) has been considered using the program just discussed. From previous studies it was known that for a single impact the displacement of a given block was insensitive to the block stiffness (K_B). This of course, is the basis for using an impulse-momentum solution to the core block problem. However, in the actual multiple collision problem the contact time (which is not negligible compared to the time interval between contacts) must vary with block stiffness and this must have a cumulative effect on displacement over many impacts. To test this effect the system shown in Fig. 15 was run with various values of block stiffness. Figures 16 and 17 show the displacement-time histories for block No. 1 assuming two different values for K_B [$K_B = 1.051 \times 10^9$ n/m (6×10^6 lb/in.) in Fig. 16, and $K_B = 1.051 \times 10^7$ n/m (6×10^4 lb/in.) in Fig. 17]. As expected, the effect of block stiffness on the displacement-time history increases with time. The effect of variations in block stiffness on accelerations, forces, and stresses is expected to be more pronounced.

This program has also been used to check the scaling laws developed for use with future physical models. The prototype was arbitrarily selected as a system having the parameter values shown in Table V. This prototype was forced to 10 Hz with

an amplitude of 0.1-in. The resultant response motion of block No. 1 is shown in Fig. 18.

Fig. 16. Response with block stiffness of 1.051×10^9 newtons/meter (6×10^6 lb/in.).

Fig. 17. Response with block stiffness of 1.051×10^7 newtons/meter (6×10^4 lb/in.).

TABLE V
PARAMETERS FOR SCALING LAW STUDIES

	<u>Prototype</u>	<u>True¹ Model</u>	<u>Distorted² Model</u>
Size of Block (m ³)	0.381 ³	0.0762 ³	0.0762 ³
Weight of Block (N)	975.94	7.807	7.807
Stiffness of Block (N/m)	5.254 x 10 ⁶	0.2101 x 10 ⁹	1.0508 x 10 ⁹
Clearance Gap (cm)	0.381	0.0762	0.0762
Static Coefficient of Friction (-)	0.20	0.20	0.20
Kinetic Coefficient of Friction (-)	0.16	0.16	0.16

¹ With the gravitational constant (g) included as an independent variable, similitude dictates that the time scale (N_t) must be equal to the square root of the length scale (N_d); i.e. $N_t = \sqrt{N_d}$. Furthermore, having selected the density scale as unity (which makes the weight scale as N_d³) the block stiffness must be scaled as the square of the length scale.

² With the gravitational constant (g) neglected, and assuming the same material is used for both the model and the prototype, similitude dictates that the time scale (N_t) must be equal to the length scale (N_d); i.e., $N_t = N_d$. Furthermore, the block stiffness must be scaled as the length scale.

Fig. 18. Prototype Test.

A one-fifth (1/5) scale model was then programmed with the parameter values shown in the second column of Table V, and it was forced at 22.36 Hz (10.Hz x 5) with an amplitude of ± 0.051 -cm ($*0.254\text{-cm} \div 5$). The resultant response motion of block No. 1 is shown in Fig. 19.

The similarity is obvious and, indeed, if the response motion of the model is scaled by x 5 and homologous times are computed by multiplying the model times by $\sqrt{5}$ the results are identical.

The model just described was scaled in such a way as to include the force of gravity (g) as an independent variable. It is possible to scale a model neglecting (g), and if this is done the parameter values for a 1/5 scale model are as given in the third column of Table V. This "distorted" model was forced at 50 Hz

Fig. 19. True Model Test.

(10 Hz x 5) with an amplitude of $\pm 0.051\text{-cm} (*0.254\text{-cm} \div 5)$. The resultant response motion of block No. 1 is shown in Fig. 20. The lack of similarity to prototype motion is immediately apparent, and there is no way to predict prototype motion from this model.

Studies to determine the effect of parameter variations on accelerations, forces, stresses, and relative motions are currently being conducted. These parametric studies are being run on this same one-dimensional analytical model. For this study the independent variables have been grouped to give the greatest possible physical insight. For example, the relative importance of the various forces which act are being investigated by computing response (displacement and acceleration) for various ratios of (1) inertia forces to contact forces and (2) inertia forces to friction forces.

Fig. 20. Distorted Model Test.

Because it is believed that visual presentation of core motion will eventually be required, the techniques for generating computer movies to display program solutions have also been developed and checked. A movie produced to display the motion of the simple four-block system shown in Fig. 15 shows the power of this method for displaying future results on more complicated systems.

During the present quarter the mathematical model has also been extended to handle the two-dimensional system shown in Fig. 21. In this system slippage can occur on either or both surfaces of each block. Parameter studies will be conducted using this model; however, it is anticipated that the guidance of the results obtained on the one-dimensional model will significantly reduce the runs required for the parameter study.

Fig. 21. Two-Dimensional Model.

VI. SAFETY INSTRUMENTATION AND CONTROL SYSTEMS

A. Primary Coolant Moisture Monitors (E. J. Dowdy, G. W. Taylor, V. S. Starkovich)

1. Helium Afterglow Monitor

Construction of a moisture detection system based on the helium afterglow technique²⁸ has been completed. The technique is based on the detection of the characteristic radiation resulting from Penning type ionization reactions between metastable helium atoms and impurities. Specifically, for water molecules, the reaction set is presumed to be:

(37)

In this case the OH^* emission line at 306.4 nm indicates the presence of moisture, and the intensity of the line is a measure of the quantity of water.

Figure 22 is a schematic of the system as built. The metastable helium atoms are produced by a cold cathode discharge (14)[†] between tantalum electrodes in a tube above the reaction chamber. The pressure differential produced by the action of the vacuum pump (9) carries these into the reaction chamber (13) where they are mixed with the gas under analysis which is metered into the reaction chamber with one of the flowmeters (12). The reactions which occur are monitored by a scanning monochromator (2) and attached photomultiplier tube (3). The current from the photomultiplier tube is measured with an electrometer and displayed on a strip chart recorder (5). The "pure" helium from which the metastables are produced consists of twice-LN₂-trapped (16) (23) research grade helium (26). Components between valves (10) and (27) constitute the calibration system. Water is injected through the septum (20) into the standard volume (19) and mixing is accomplished by circulating the moist gas by use of the pump (18). The calibration gas is then metered into the reaction chamber. Reactor gas for analysis would be introduced at the flowmeter (12). This test unit is now being baked out and pumped down prior to calibration tests and performance measurements.

2. Radiation Based Monitors

We have continued our examination of the possibility of detecting moisture through nuclear techniques. These have included two active techniques based on neutron irradiation of a primary coolant sample and the passive technique of measuring the 6.13 MeV γ -ray emitted by ¹⁶N in the ¹⁶O(n,p)¹⁶N reaction as water passes through the core.

[†] Numbers refer to corresponding numbered portions of the figure.

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The two active techniques consist of detecting either the neutrons scattered by hydrogen or the 2.226 MeV γ -ray emitted in neutron capture in hydrogen. The former of the active techniques requires a favorable competition between neutron scatter from hydrogen and neutron scatter from helium. Without resorting to the use of cold neutrons, the cross section for thermal neutron scatter from hydrogen is only 50 times as large as from helium so that a moisture content of 20,000 ppmV would be required for signals of equal strength from hydrogen and helium scatter. An enhancement of a factor of ~ 20 can be realized by making extra cold neutrons to reduce the moisture content to 1,000 ppmV for equal signals for scatter from hydrogen and helium. The technique for monitoring the 2.225-MeV hydrogen-capture gamma radiation has a limiting count rate of 1.1×10^{-8} γ -rays per cm^3 of coolant per second per unit thermal neutron flux per ppmV water, e.g., for a flux of 10^6 $\text{n}/\text{cm}^2/\text{s}$ and 100 ppmV water, the emission rate of 2.226-MeV γ -rays is 1.1 per cm^3 per second. Accounting for backgrounds and detector efficiencies would reduce the effective sensitivity accordingly.

The earlier technique investigated, the measurement of the 6.13-MeV gamma ray from ^{16}N , appears most favorable of those examined. We earlier had calculated a count rate of 2 s^{-1} for 1 ppmV water content using what we consider to be conservative estimates of detector efficiencies and sample extraction times. Further examination of this technique is planned.

3. Crystal-Controlled Oscillators

Special quartz crystals, capable of controlling frequencies to 1 part in 10^9 have been commercially available for a number of years, and have been used in a wide variety of applications including moisture detection.^{29,30} Under carefully controlled conditions, the sensitivity to mass change can be as low as 10^{-12} g .

The technique generally used is to select two quartz crystals with almost identical frequency-temperature characteristics, with resonant frequencies of about 8 MHz. Two crystal-controlled oscillators are then made, the outputs of which (f_1 and f_2) are mixed, giving a difference frequency $f_2 - f_1$. For moisture detection a difference frequency of $\sim 1 \text{ kHz}$ can be used. An $\sim 300\text{-nm}$ -thick film of hygroscopic material is evaporated onto one of the crystals, and this crystal is placed within the gas containing the water vapor. When this hygroscopic film absorbs or adsorbs water vapor, the effective mass of the acoustic resonator increases, and hence the frequency of oscillation decreases. The relationship between the change in weight and the change in frequency is³¹

$$\Delta f = 2.3 \times 10^6 f^2 \Delta w / A \quad (38)$$

where Δf is the change in frequency in Hz, f is the frequency of the unloaded crystal in MHz, Δw the change in weight in grams, and A the area of the hygroscopic material in cm^2 . For a 8 MHz-crystal of area 1 cm^2 we have a frequency shift

$$\frac{\Delta f}{\Delta w} = 2.3 \times 10^6 \times 64 = 147.2 \frac{\text{MHz}}{\text{g}}$$

or (39)

$$\sim 1.5 \frac{\text{Hz}}{10^{-8} \text{ g}} .$$

Frequency shift detectability is in the range of $\sim 0.1 \text{ Hz}$ so that 10^{-9} grams could be detected.

In summary, the suitability of the quartz crystal resonator technique for moisture detection in HTGR's is dependent upon the proper choice of hygroscopic material. At present, no single material is known which will meet all of the necessary conditions, although it might be possible

to build a pressurized system with a re-purification network and employ certain liquids such as alcohol as the hygroscopic coating.

B. Temperature Sensors (V. S. Starkovich)

The effects of gas permeation and helium embrittlement on the integrity of the core exit gas thermocouple sheath materials were examined. The solubility of helium in either Inconel or tantalum was found to be negligible at the expected operating temperature with no information available about the possible increased solubility with elevated temperatures expected for off-normal or accident conditions. However, experience with thermocouples qualified for the ROVER Program would indicate that the penetration of gases in metals of this class would be quite limited up to the temperatures at which thermal failure of the thermocouples would be expected.

An incident in which the temperatures in the vicinity of the core exit gas thermocouples exceed 2000°F would cause failure of many of the thermocouples, precluding adequate post-incident monitoring of this variable. We are consequently beginning a study of suitable alternate or supplementary sensors for the purpose of postincident temperature measurements.

VII. ACCIDENT DELINEATION

(M. G. Stevenson)

The primary object of accident delineation is to identify accident sequences having potential impact on public safety and to provide detailed descriptions of these sequences for use in probabilistic analyses, phenomena modeling, and systems analyses. As part of this effort, we are reviewing various HTGR accident analyses and cataloging summaries of the analyses in the format shown in Table VI. This example includes analyses performed for the Fulton Generating Station and included in the PSAR for that plant.³² The summaries provide a convenient reference for the faults

involved in a given sequence and for the results of the analyses, i.e., consequence estimates. In addition to the summaries of accidents analyzed by the reactor vendor, we will catalog summaries of our independent accident calculations as they are performed.

VIII. PHENOMENA MODELING AND SYSTEMS ANALYSIS

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

We have continued parametric studies of the temperature coefficient for the 3000-MW(t) Fulton Generating Station (FGS) HTGR initial core using the methods described in a previous report.³³ During the quarter the fuel and moderator components of the temperature coefficient have been analyzed, and the separate effects of burnable poison, control rods, and fission-product poisons Xc and Sm on the net isothermal coefficient have been studied.

1. Fuel and Moderator Components of Temperature Coefficient

The GAC method³⁴ for calculating the fuel or "prompt" coefficient assumes that it is due entirely to changes in the fast cross sections (Doppler effect). Thus the same thermal cross sections are used for all the fuel temperatures specified. Furthermore the moderator coefficient is assumed by GAC to be given by the difference between the net isothermal coefficient and the fuel coefficient. This implies that the fuel and moderator coefficients are separable and that the moderator coefficient includes the moderator contained within the fuel pins (fuel moderator) as well as that external to the fuel pins (bulk moderator).

Fuel and bulk moderators comprise 20% and 80%, respectively, of the total moderator in the HTGR core. During a reactor transient the temperature response of the fuel moderator will be prompt compared to that of the bulk moderator because of the relatively large thermal resistance presented by the gap between

TABLE VI

FULTON GENERATING STATION ACCIDENT SUMMARIES

Initial Event	Initial Effects	Expected Protective Actions	Postulated Secondary Faults	Ultimate Consequences
Loss of single main helium circulator (several possible causes)	Total helium flow decreases, helium temperatures increase, steam temperatures increase. If no protective action, then core power would equilibrate at higher level.	(1) PPS (Plant Protective System) initiates trip of affected loop, <u>and</u> (2) OPS (Operating Protective System) initiates power setback (six shim rod pairs inserted) until core power/flow or steam generator inlet temperature returns to nominal, <u>or</u> (3) PPS initiates reactor trip on high power/flow or steam generator inlet temperature, <u>or</u> (4) Operator has several minutes to initiate trip before fuel damage reached.	No power setback (failure of OPS).	PPS initiates reactor trip on steam generator inlet temperature (41.7 K above normal) at 140 s. Peak core power/flow reaches 1.3 . <u>No damage expected.</u>
<u>Partial loss of steam generator feedwater flow</u> (loss of one or two feedwater pumps, feedwater pipe rupture). Analysis assumes loss of two (on same side) pumps.	Loss of about 50% of flow to steam generators. This reduces heat removal from helium which begins to heat up. Loss of flow to circulators reduces helium flow which increases rate of temperature rise.	(1) Affected turbine-generator unit is tripped. (2) PCS (Plant Control System) brings power down to about 50%.	(1) Failure of PCS to reduce power. (2) Failure to trip on high core power/flow at 10 s.	Reactor trip (PPS) on high steam generator inlet helium temperature at 100 s. Core temperatures heat up, maximum outlet temperature is 1158 K. Maximum average fuel temperature is about 1680F. <u>No damage</u> to system and no release noted.
<u>Secondary coolant leakage into containment</u> (steam pipe ruptures, etc.)	Loss-of-coolant from ruptured pipe. Partial loss of flow in steam system.	(1) Detection of rupture and shutdown of affected loop with cooling continued on remaining loops. (2) If leakage continues, high containment pressure leads to reactor trip. Core auxiliary cooling system (CACS) is used for cooling in this case.	None.	Blowdown from ruptured pipe releases from 1360 kg to 10,000 kg of coolant (depending on location) prior to loop shutdown. Maximum release to containment is 0.2 Ci of tritium assumed to be contained in steam system.

the fuel pins and the bulk moderator. Furthermore, in the initial core, the effect of fuel moderator heating will be more prompt than the Doppler effect in the thorium because the fuel moderator must be heated first in order to transfer heat from the fissile (UC_2) and to the fertile (ThO_2) fuel kernels. For these reasons we believe that the effect of the fuel moderator temperature on the thermal neutron spectrum should be included in the fuel coefficient rather than in the moderator coefficient.

The fuel and moderator components of the net temperature coefficient were computed for the initial unpoisoned FGS using both the GAC definitions of these components (Case A) and the definitions which we believe to be more appropriate (Case B). Results of the calculations are shown in Figs. 23 and 24. These results show that inclusion of the fuel moderator temperature effect in the fuel coefficient (Case B) rather than in the moderator coefficient (Case A) results in a more negative moderator coefficient. The reason for this is that the moderator coefficient is negative in the initial core. Thus for this case the GAC method (Case A) yields a conservative (less negative) fuel coefficient. At the end of the equilibrium cycle, however, the moderator coefficient may become positive due to the buildup of fission products and ^{233}U , depletion of the burnable poison, and withdrawal of the seven control-rod pairs that control the excess reactivity at the beginning of the cycle. In this case the GAC method would not yield a conservative value for the fuel coefficient.

By comparing the sum of the fuel and moderator components with the net isothermal coefficient computed previously, we have verified that these components are indeed separable over the entire temperature range for Case A. These results also verify the consistency among the calculated values of fuel, moderator, and net

temperature coefficients. For Case B, however, the fuel and moderator components are not separable if there is a large temperature difference between the fuel pins and the bulk moderator.

Fig. 23. Fuel temperature coefficient for the initial unpoisoned FGS core.

Fig. 24. Moderator temperature coefficient for the initial unpoisoned FGS core.

2. Effect of Burnable Poison on Isothermal Coefficient

Burnable poison pins containing B_4C are used in the HTGR design to reduce the excess reactivity that must be compensated with control rods. A three-region cylindrical cell model, in which the poison pin is represented explicitly, was used to study the effect of this component on the isothermal temperature coefficient. As shown in Fig. 25, the effect of burnable poison is to make the temperature coefficient more negative.

The negative effect of burnable poison on the temperature coefficient results from an increase in the fraction of neutrons absorbed in the poison pins with increasing core temperature. The reason for this is that thermal self-shielding in the poison pins is significant and decreases with core temperature, whereas self-shielding in the fuel pins is negligible. Thus, although unshielded thermal cross sections are affected in approximately the same manner (i.e., $\sim 1/v$) in both the pin and the fuel by a shift in the thermal neutron spectrum, this effect is offset to some extent in the poison pin by the increasing thermal disadvantage factor.

Fig. 25. Effect of burnable poison on the isothermal temperature coefficient.

3. Effect of Control Rods on Isothermal Coefficient

Calculations have been performed with various numbers of control-rod pairs inserted including 73 (all), 37, 19, and 13 rod pairs. The associated control-rod configurations are based on the rod-withdrawal sequence specified for the Fulton Generating Station, and result in all cases in a uniform distribution of control-rod pairs in the core. A 7-region, one-dimensional, cylindrical cell model that includes details of the control-rod design was used in the calculations. In this model the size of the fueled region surrounding the control rod depends on the number of control rods that are present in the core. Obviously the model cannot take into account the interaction between the two rods in a pair nor that between adjacent rod pairs. The minimum separation between rod pairs is four times greater than the separation between the two rods in a pair. Thus the interaction between rod pairs should be small compared to that between the two rods in a pair. Assuming that the intra-rod-pair interaction effect does not change significantly with core temperature, the one-dimensional model should be adequate for determining the effect of control rods on the temperature coefficient.

As shown in Fig. 26 the effect of control rods is to make the isothermal temperature coefficient more negative. The magnitude of the effect depends on both the core temperature and the number of control rods inserted. Results for the 73 and 37 rod-pair cases are only of academic interest in that the reactor cannot be made critical with these configurations. According to the vendor, the 19 rod-pair case corresponds to the cold-critical configuration and the 13 rod-pair case corresponds to the hot-critical configuration before equilibrium Xe is established.

Fig. 26. Isothermal Temperature Coefficient for various control-rod configurations.

The negative effect of the control rods on the temperature coefficient is due to the same mechanism as that from the burnable-poison pins. However, because of a higher boron loading the control-rod absorber is much more heavily self-shielded than was the case for the burnable-poison pins. Because of self-shielding the effective (shielded) thermal absorption cross section for the boron in the control-rod absorber is essentially independent of temperature, whereas that for ^{235}U in the fuel varies approximately as $1/T$ (i.e., $\sim 1/v$). This behavior is shown in Table VII for the 37 rod-pair case. As a result of this behavior, the fraction of neutrons absorbed in the control rod increases with core temperature.

The interaction between the two rods in a pair has been found by the vendor to reduce the worth of a single rod by 15% at room temperature. If we apply this correction factor (which we intend to verify in future studies) to our results, we find that at room temperature the worth of all

TABLE VII
EFFECTIVE THERMAL ABSORPTION CROSS
SECTION FOR B IN CONTROL-ROD ABSORBER
AND ^{235}U IN FUELED REGION
(37 CONTROL-ROD PAIRS INSERTED)

T (K)	Cross Section (barns)	
	B	^{235}U
300	2.326	292.3
500	2.359	269.2
800	2.340	240.9
1200	2.307	212.1
1700	2.285	184.6
2300	2.278	158.4
3000	2.272	136.5

control-rod pairs is $0.280 \Delta k$. This value is 11% larger than that ($0.253 \Delta k$) quoted in the FGS PSAR.³² The agreement is reasonable considering the simple model used in our calculations.

4. Effect of Xe and Sm on the Isothermal Coefficient

Cell calculations have been performed to determine the effect of ^{135}Xe and ^{149}Sm on the isothermal temperature coefficient. In a thermal reactor such as the HTGR, these two fission products are the most significant with respect to their effect on both reactivity and the temperature coefficient of reactivity. Calculations were performed for five different cases including equilibrium and peak Xe with no Sm, equilibrium and peak Sm with no Xe, and equilibrium Xe and Sm. Peak values are based on the assumption of a rapid shutdown from full power after equilibrium has been established.

The effects of Xe and Sm on the temperature coefficient are summarized in Fig. 27. Except for Sm at 300 K, these results indicate that both Xe and Sm make a positive contribution to the temperature coefficient over the entire temperature range studied. For the equilibrium Xe and Sm case, the effect is nominal at 300 K, but increases rapidly with temperature. At the design temperature (1100 K) of the

Fig. 27. Effect of Xe and Sm on the isothermal temperature coefficient.

HTGR, equilibrium Xe and Sm reduce the temperature coefficient by almost a factor of two (from -4.2×10^{-5} to $-2.4 \times 10^{-5}/K$).

The contributions of various nuclides to the temperature coefficient with equilibrium Xe and Sm are given in Table VIII. Both Xe and Sm are primarily thermal neutron absorbers and their absorption cross sections exhibit strong non- $1/v$ variations in the thermal energy range. The effect of these nuclides on the temperature coefficient arises from the shift in the thermal neutron spectrum to higher energies with increasing core temperature. Thus these nuclides affect primarily the moderator component of the net isothermal coefficient. Because most of the absorptions in ^{232}Th occur above the thermal energy range, its contribution to the isothermal temperature coefficient is not greatly affected by the presence of Xe and Sm. On the other hand the contribution from ^{235}U , which is principally a thermal absorber, is affected by the presence of Xe and Sm. This is particularly true above about 500 K where the contributions from Xe and Sm become increasingly important compared to that from ^{235}U .

The positive contribution of ^{135}Xe to the isothermal coefficient increases with temperature up to about 800 K, and then decreases beyond this temperature. This behavior is consistent with the absorption cross section of ^{135}Xe which is almost constant up to about 0.1 eV and then falls sharply between 0.1 and 1.0 eV. The contribution from ^{149}Sm is negative at 300 K, zero at 500 K, and positive beyond 500 K with the largest positive contribution occurring at 1200 K. This behavior is also consistent with the absorption cross section of ^{149}Sm which has a resonance at ~ 0.1 eV ($\sim 15\,000$ b peak) and another at ~ 0.9 eV (~ 2000 b peak) with a deep valley (~ 100 b floor) between the two resonances.

5. Work in Progress

The effects of burnable poison, control rods, and Xe and Sm on the temperature coefficient have been studied separately in order to obtain a detailed understanding of these effects and to evaluate their relative importance. We are now in the process of calculating the temperature coefficient for the beginning-of-life (BOL) core in which all of these effects are included. These calculations will conclude our work on the BOL temperature coefficient. Calculation of the power profile for the BOL core is also in progress. Other work in progress is a study of the effect of ^{233}U on the temperature coefficient. This study is pertinent to the end-of-life core in which significant amounts of ^{233}U will be present.

B. Nuclear Data Processing for HTGR Safety Research (M. G. Stamatelatos and R. J. LaBauve)

The present route for generating multigroup cross sections for comparison with cross sections generated by the General Atomic Company at all necessary temperatures is shown in Fig. 28. We have used the MC² code³⁵ for generating above-thermal fine-group cross sections and for

TABLE VIII

CONTRIBUTION OF VARIOUS NUCLIDES TO THE TEMPERATURE
COEFFICIENT WITH EQUILIBRIUM Xe AND Sm ($10^{-5}/K$)

T (K)	^{232}Th	^{235}U	^{135}Xe	^{149}Sm	Other ^a	Total
300	-6.06	-5.02	+0.44	-0.17	+0.21	-10.60
500	-4.75	-3.96	+0.94	0.0	+0.23	- 7.54
800	-3.28	-2.38	+1.33	+0.17	+0.13	- 4.03
1200	-2.41	-1.15	+1.19	+0.20	+0.03	- 2.14
1700	-1.95	-0.57	+0.84	+0.15	-0.05	- 1.58
2300	-1.62	-0.44	+0.58	+0.10	-0.07	- 1.45
3000	-1.26	-0.47	+0.34	+0.05	-0.07	-1.41

^aFrom total minus contributions from nuclides listed.

Fig. 28. Data flow for HTGR cross-section generation.

calculating an above-thermal neutron spectrum to be further used for collapsing the fine-group set to a broad-group set.

In the thermal region we have used MC² for calculating fine-group absorber cross sections. The fine-group graphite scattering cross sections are generated from physics parameters (e.g. Bragg edges, phonon distributions, etc.) by use of the HEXSCAT code³⁶ and the LASL TOR code.³⁷ HEXSCAT calculates coherent elastic

scattering cross sections in hexagonal lattices and TOR calculates the inelastic scattering cross sections in the incoherent approximation. The direct use of these codes rather than the processing of the graphite ENDF thermal files by codes like FLANGE³⁸ is motivated by the fact that the data on the ENDF files are currently incomplete for the required energy range and must be complemented by additional calculations. Also, the energy grid for which the available graphite thermal data are tabulated on ENDF files does not necessarily correspond to the desired fine-energy grid and therefore the data on these files require interpolation.

The fine-group thermal cross sections are used by the GLEN code³⁹ to calculate a thermal-neutron spectrum which is further used to collapse the fine-group cross sections to the desired broad-group set. The above thermal and the thermal broad-group cross sections are then merged and formatted for use in the DTF code⁴⁰ by JMBLFAT, a small code we have written for this specific purpose. This procedure will

be used to generate initial multigroup cross-section sets. Future plans include the use of the LASL MINX code⁴¹ to generate cross sections for the entire energy range.

C. CHAP Code Development - Primary System Modeling (P. A. Secker)

We have continued development of the Composite HTGR Analysis Program (CHAP), which will provide an independent evaluation of HTGR performance during normal or anticipated transients and accident sequences requiring analysis of the overall plant response. Presently the simulation model includes the thermal, fluid-flow, neutronic, and afterheat description of the HTGR reactor core, reflector, support blocks, upper and lower plena, and flow orifice valves.

A significant effort has been spent in parametrically evaluating the reactor core model. We began with an average (radial power factor equals unity) coolant channel core region description and obtained both transient and steady-state core responses to various modes of operation. The auxiliary code, TPRØF, was used to supplement the reactor core thermal analysis in the CHAP code. TPRØF provides detailed steady-state temperature distributions and is useful for performing parametric studies of core thermal diffusion. The temperature maps provide a method of obtaining geometric shape factors and initial conditions for the simpler CHAP model. TPRØF was added as a subroutine to the CHAP code to provide consistent data transfer and interfacing. For the beginning of life power distribution for the Fulton Generating Station, the axial temperature distribution of Fig. 29 and the incremental temperature histogram at mid-channel given in Fig. 30, were computed using TPRØF for an average channel. Fig. 29 also indicates how well an 8-section axial representation matches a 30-section axial representation along the fuel rod centerline. The agreement is good and for this reason we have

selected a simplified core model in CHAP based on 8-axial nodes.

Fig. 29. Axial temperature distributions.

Fig. 30. Temperature contributions to fuel centerline.

We have developed two afterheat models for transient analyses. For HTGR's, the afterheat transient profile, when direct fission power ceases, is presented in the GAC report by Sund⁴². From these data we have derived a model valid from 0 to 1 day and a model valid from 0 to 1000 days. Two sets of constants for each case were computed; (1) a_i - the fraction of decay power produced by fissioning per unit time, and (2) b_i - the decay constant for each group in the model. The first model contains

five groups; the latter contains ten groups. These data are presented in Tables IX and X.

The form of the models is

$$\frac{dQ_i}{dt} = a_i n - b_i Q_i; \quad i = 1, NG \quad (40)$$

where Q_i is the afterheat contribution, n is the prompt neutron power, and NG is the representative number of afterheat groups.

The total afterheat power is

$$Q_{AH} = \sum_{i=1}^{NG} Q_i \quad (41)$$

The profile given by Sund has been extrapolated back to steady state (time = 0) to provide data to derive the constants given here. The results overpredict the actual decay power for a negligibly short initial time period.

D. CHAP Code Development - Balance of Plant Modeling (J. S. Gilbert)

We have begun work on a dynamic model of the steam generator reheater as part of the balance-of-plant (BOP) modeling for the CHAP code. The reheater analysis is an essential part of the modeling of the

tightly coupled water/steam flow system in the HTGR BPO. In this system superheated steam produced in the main steam heat exchanger bundle goes to the high-pressure turbines. The steam exiting from the high-pressure turbines drives the main helium circulators and then enters the reheater coils in the steam generator. The reheater steam receives energy from the helium exiting the core, which, after heating the reheat steam, enters the main steam heat exchanger bundle. The hot reheat steam is used to drive the intermediate and low-pressure turbines. In the reheater, energy is transferred to the reheat steam at different temperatures as the reheater coils reverse the direction of the steam flow relative to the helium flow; thus, two reheater nodes are required for each primary coolant node. The tightly coupled nature of this system requires an integrated model to calculate the system dynamics.

The basic equations utilized in the reheater model are grouped according to the material under study. The mass, momentum, and energy balance equations for the reheat steam at fixed volume segment i are, respectively,

TABLE IX
PRODUCTION AND DECAY
RATES FOR 5 GROUP TRANSIENT AFTERHEAT MODEL
(Valid For Time After Shutdown $\leq$ 80 000 Seconds)

Group	Steady-State Yield (% of full power)	Production Rate (sec ⁻¹)	Decay Rate (sec ⁻¹)
1	6.59	0.05953	0.7877
2	2.75	5.661×10^{-4}	0.01795
3	1.60	2.240×10^{-5}	1.221×10^{-3}
4	0.94	1.450×10^{-6}	1.345×10^{-4}
5	0.92	4.084×10^{-8}	3.871×10^{-6}
Total	12.80		

TABLE X
PRODUCTION AND DECAY
RATES FOR 10 GROUP TRANSIENT AFTERHEAT MODEL
(Valid For Time After Shutdown $\leq$ 1000 Days)

Group	Steady-State Yield (% of full power)	Production Rate (sec ⁻¹)	Decay Rate (sec ⁻¹)
1	6.5825	0.04171	0.5526
2	2.65	5.938×10^{-4}	0.01954
3	1.60	2.527×10^{-5}	1.377×10^{-3}
4	0.80	1.823×10^{-6}	1.987×10^{-4}
5	0.42	1.851×10^{-7}	3.843×10^{-5}
6	0.19	1.223×10^{-8}	5.615×10^{-6}
7	0.28	2.694×10^{-9}	8.391×10^{-7}
8	0.15	4.388×10^{-10}	2.551×10^{-7}
9	0.10	9.162×10^{-11}	7.989×10^{-8}
10	<u>0.0275</u>	3.057×10^{-12}	9.695×10^{-9}
Total	12.80		

$$\frac{d\rho_i}{dt} = \frac{2}{V_i} (w_i^{\text{in}} - w_i), \quad (42)$$

$$\frac{dw_i}{dt} = \frac{A_i}{L_i} (P_i^{\text{in}} - P_i^{\text{out}} - \frac{K w_i^2}{\rho_i}),$$

and

$$\begin{aligned} \frac{d(M_i H_i)}{dt} &= 2W_i (H_i^{\text{in}} - H_i) \\ &+ h_{s,i} A_i (\phi_i - T_i). \end{aligned} \quad (43)$$

The quantities ρ , P , and M represent the steam density, pressure, and mass, respectively, with geometric relations defined by L , A , and V . The reheater tube wall segment temperature is ϕ_i .

The enthalpy of the steam entering and leaving each segment, H_i^{in} , is averaged when calculating the segment enthalpy, H_i . The same procedure is used for the steam flow rate, W_i . In determining the heat transfer coefficient from the tube to the steam, $h_{s,i}$, allowance is made for the curvature of the tube bundle.⁴³

$$Nu_{\text{curved}} = Nu_{\text{straight}} \{0.962$$

$$\times [Re(\frac{d}{D})^2]^{0.25}\}, \quad (44)$$

where the tube diameter is d and the coil diameter is D , with Nu and Re the Nusselt and Reynolds numbers, respectively.

The primary coolant temperature, θ_i , for each segment is determined by the quasi steady-state primary coolant energy balance given the inlet helium temperature, θ_i^{in} , and the tube wall temperature.

$$\theta_i^{\text{in}} = 2\theta_i - \theta_{i-1}^{\text{in}} \quad (45)$$

and

$$\theta_i = \frac{h_{g,i} A \phi_i + W_g C_p \theta_i^{\text{in}}}{W_g C_p + h_{g,i} A} \quad (46)$$

with W_g the helium flow rate and C_p the specific heat.

The gas side heat transfer coefficient, $h_{g,i}$, is based on a modified form of the correlation proposed by Grimison⁴⁴ from the data of Huge and Pierson. This

correlation, having the form

$$Nu = 0.245 Re^{0.618} \left(\frac{Pr}{0.69} \right)^{1/3}, \quad (47)$$

where Pr is the Prandtl number, accounts for moderate changes in the fluid Prandtl number with thermal properties evaluated at the film temperature; hence, an interactive procedure is required.

The energy equation for tube wall segments is

$$\begin{aligned} \frac{M d\phi_i}{dt} = & h_{s,i} A(\theta_i - T_i) \\ & + h_{g,i} A(\phi_i - \theta_i). \end{aligned} \quad (48)$$

The above expressions have been coded, and, with the addition of a steam property routine, code debugging will begin.

The model will be evaluated for sensitivity to number of equal surface area nodes, e.g., 8, 4, or 2. After model checkout and model sensitivity evaluation, the model will be included in CHAP as the first step in the balance-of-plant modeling.

E. CHAP Applications (P. A. Secker)

Two different problems have been investigated with CHAP using the average core model. Transient studies of open loop step reactivity insertions have been performed. We have also looked at loss-of-forced-cooling from 3000 MW with failure to scram.

Previously, we presented calculations of beginning-of-life isothermal coefficients, and earlier in this report (see Sec. VIII.A) we showed calculations of separate fuel and moderator coefficients. The parametric studies performed with CHAP used these reactivity coefficients, which were given as a function of temperature.

These studies provided a check on the steady-state accuracy of the core simulation model at several arbitrary open reactivity insertions (both positive and

negative). We are also evaluating the accuracy, stability, and efficiency of a number of numerical integration techniques. These reactivity studies have provided an understanding of the dynamic response and range of core variables following large reactivity insertions. They also indicate the dynamic differences in the two reactivity feedback formulations.

To check the steady-state accuracy of the model, several reactivity steps of various magnitudes were used as input, and the model equations were numerically integrated until a new steady state was achieved as the temperature reactivity feedback compensated for the input step. In these studies, the core inlet plenum helium temperature, pressure, and flow rate were held constant. The resultant steady-state power level was then used as input to the TPRØF code to obtain a check on temperatures throughout the simpler CHAP core model. Table XI presents a comparison of several key temperatures obtained from CHAP and TPRØF with reactivity steps of +20 cents and +1.0 dollar from 3000 MW.

In these studies, we used the isothermal reactivity coefficients. The more realistic reactivity transients result, of course, from the separate fuel/moderator description of reactivity feedback. The faster prompt feedback effect (compared to the isothermal reactivity description) arising from utilization of the fuel reactivity coefficient reduces the peak power by as much as 22% for a +1.0 dollar step insertion. Figures 31 and 32 show the response of core thermal power in each case to a +1.0 dollar reactivity insertion. Figures 33 and 34 show the maximum fuel rod temperature and the average core temperature vs time for a one dollar step. The maximum temperatures in both cases are lower than obtained from the isothermal reactivity description because the peak power is lower. At 3000 MW the core exhibits only

TABLE XI
COMPARISON OF KEY TEMPERATURES
AT SEVERAL STEADY-STATE POWER LEVELS

	a. 3000 MW			b. 3166 MW			c. 3921 MW	
Temperature	CHAP	TPRØF		CHAP	TPRØF		CHAP	TPRØF
Average Moderator Temperature in 4th axial core section. (K)	1089	1073		1117	1116		1240	1233
Average Fuel Temperature in 4th axial core section. (K)	1290	1300		1323	1334		1480	1500
Maximum Fuel Center-line Temperature (K)	1310	1322		1344	1367		1504	1531
Coolant Core Exit Temperature (K)	873	866		1115	1104		1233	1223

- a. Reactivity Step = 0. dollars
b. Reactivity Step = 20 cents
c. Reactivity step = 1.00 dollar

- HTGR Reactivity Study -
Fig. 31. Isothermal reactivity coefficient with a one dollar step.

- HTGR Reactivity Study -
Fig. 32. Separate fuel/moderator coefficients with a one dollar step.

- HTGR Reactivity Study -
(Separate fuel/moderator)

Fig. 33. Maximum fuel rod temperature vs elapsed time for a one dollar step.

- HTGR Reactivity Study -
(Separate fuel/moderator)

Fig. 34. Average core temperature vs elapsed time for a one dollar step.

a 1.45°C temperature rise for each cent of reactivity.

The second set of core studies concerned the loss-of-forced cooling with failure to scram. In this situation neutronic power is reduced as the uncooled core heats up because of the negative feedback effect of the temperature coefficients (fuel/moderator). After the neutronic power becomes negligible, temperatures continue to increase slowly because of residual decay heat and the absence of forced cooling. The core is treated adiabatically with no heat loss to the surroundings and no heat loss to the helium. We added axial heat conduction to the CHAP model, utilizing the composite axial conductivity description given by GAC. Later we intend to perform these studies with natural convection added to study the effects of reversed flow. We also plan to use several more coolant channels radially coupled to the present description.

Figure 35 shows the core thermal power response to loss of core flow for 3000 seconds. The shutdown mechanism is the negative temperature feedback effect. Feedback reactivity is presented in Fig. 36, and exceeds minus one dollar ($\beta=0.0065$) at 300 seconds. The volume averaged core temperature and maximum fuel element temperature vs time are presented in Figs. 37 and 38. The rate of temperature rise for the average core is approximately 0.17°C per second at 300 seconds and decreases to about 0.08°C per second after one hour. After one hour axial heat conduction begins to become quite important as the core materials seek a uniform isothermal condition.

Fig. 35. HTGR loss of forced cooling with failure to scram from 3000 MW.

Fig. 36. HTGR loss of forced cooling with failure to scram from 3000 MW.

Fig. 37. HTGR loss of forced cooling with failure to scram from 3000 MW. Core average temperature vs time.

Fig. 38. HTGR loss of forced cooling with failure to scram from 3000 MW. Maximum fuel temperature vs time.

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