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ADVANCED REACTOR SAFETY RESEARCH DIVISION

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JANUARY 1 - MARCH 31, 1980

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ADVANCED REACTOR SAFETY RESEARCH DIVISION

QUARTERLY PROGRESS REPORT JANUARY 1 - MARCH 31, 1980

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FOREWORD

The Advanced Reactor Safety Research Programs Quarterly Progress Report describes current activities and technical progress in the programs at Brookhaven National Laboratory sponsored by the USNRC Division of Reactor Safety Research. The projects reported each quarter are the following: HTGR Safety Evaluation, SSC Code Development, LMFBR Safety Experiments, and Fast Reactor Safety Code Validation.

The previous reports, BNL-NUREG-50624, BNL-NUREG-50661, BNL-NUREG-50683, BNL-NUREG-50747, BNL-NUREG-50785, BNL-NUREG-50820, BNL-NUREG-50883, BNL-NUREG-50931, BNL-NUREG-50978, BNL-NUREG-51014, BNL-NUREG-51082, BNL-NUREG-51130, and BNL-NUREG-51177, have covered the periods October 1, 1976 through December 31, 1979.

ADVANCED REACTOR SAFETY RESEARCH

TABLE OF CONTENTS

	<u>Page</u>
FOREWORD	iii
I. HTGR SAFETY EVALUATION	1
Summary	1
1. Graphite	4
1.1 Oxidation-Induced Strength Loss in HTGR Graphites	4
1.2 Effect of Stress and Different Atmospheres on the Strength and Oxidation Behavior of Nuclear Graphite	24
1.3 High Temperature Mass Transport of Gases in HTGR Graphites	35
1.4 Surface Diffusion in Microporous Graphite Structures and the Langmuir-Hinshelwood Mechanism	38
Publications	48
References	48
2. Materials	50
2.1 Fatigue of Structural Materials	50
2.2 Creep Rupture Properties of Primary Circuit Structural Materials	62
2.3 Materials Test Loop	70
2.4 Helium Impurities Loop	72
3. Fuel and Fission Products	76
3.1 Molybdenum Migration in H-451 Graphite	76
3.2 Fission Product Migration Studies	78
References	79
4. Analytical	82
4.1 Conversion of HTGR Safety Codes	82

	<u>Page</u>
4.2 Application of the Available HTGR Safety Codes	88
4.3 HTGR - Gas Turbine Licensing Considerations	88
II. LMFBR SAFETY EVALUATION	89
Summary	89
1. Thermal Hydraulic LMFBR Safety Experiments	91
1.1 HCDA Bubble Energetics: Role of Taylor Instabilities	91
1.2 Heat Transfer in Internally Heated Boiling Pools	93
Nomenclature	96
References	98
2. SSC Code Development	104
2.1 SSC-L Code	104
2.2 SSC-P Code	121
2.3 SSC-W Code	125
2.4 SSC-S Code	126
Publications	127
References	127
3. SSC Code Validation	129
3.1 FFTF Acceptance Tests	129
3.2 Inter-Code Comparisons of SSC-L/FFTF to IANUS	129
3.3 Inter-Code Comparisons of SSC-L to DEMO/CRBRP	130
Publications	134
References	134

I. HTGR SAFETY EVALUATION

SUMMARY

Density profiles of H451 and PGX graphite specimens presumably oxidized in the chemical reaction control regime show that burnoff at the specimen surface is greater than burnoff in the bulk. The shapes of the burnoff profiles indicate that oxidation in the bulk is indeed controlled by chemical reaction, while at the surface a diffusion-limited reaction is occurring along with the bulk reaction. The data are explained in terms of the pore structure of graphite, which is pictured as consisting of two independent pore networks, one at the surface and the other in the bulk. The surface pore network consists of micropores, while the bulk pore network consists of the entire array of pores. The density of micropore-macropore interconnections is low enough, i.e., the surface pore network is sufficiently long, that the concentration of oxidant in surface micropores can be large for a significant distance into the specimen. Effective diffusion coefficients calculated from the high-burnoff surface regions of the burnoff profiles are of the same order as those expected for diffusion in the micropores of the as-received graphite.

Density profiles of PGX graphite specimens presumably oxidized in the diffusion-limited regime give rise to derived effective diffusion coefficients that are considerably lower than previously assumed. The worst discrepancy to date was seen with a specimen oxidized at 800°C in 0.17% H₂O + 1.7% H₂ in He to 0.3% burnoff, for which a diffusion coefficient of 4.8×10^{-4} cm²/sec was obtained; this is lower than the expected value by a factor of 7×10^{-3} . The diffusion coefficient increases with burnoff, in qualitative agreement with results obtained from General Atomic Company data. The dual network model described above was used to generate calculated burnoff profiles. It was found that curves generated with two diffusion paths (hence, two diffusion lengths) can be fitted to the data much better than those incorporating a single diffusion path. Generally, the best fitting curves utilize diffusion lengths which differ from each other by 2 to 3 orders of magnitude, which is consistent with the picture described above for the specimens oxidized presumably in the chemical reaction control regime.

The effect of different atmospheres on the strength loss of PGX graphite oxidized in 2% CO₂/He and 2% O₂/N₂ has been investigated this quarter. The specimens were oxidized at 750°C in the former mixture up to a maximum burnoff of 5.5% and at 500°C in the latter mixture up to a burnoff of 7%. The results indicate that oxidation with O₂ gives a larger loss of compressive strength than oxidation with CO₂. A variation of one order of magnitude in the O₂ concentration, as in 2% O₂/N₂ and air, does not perceptively change the effect of burnoff on strength. The effect of burnoff on strength loss for CO₂/He oxidation is almost identical to that for H₂O/He oxidation.

Experiments were carried out on the behavior of PGX graphite oxidized under stress at 440°C in 2% H₂O/He. During the experiments the stress applied to the specimens was increased in a stepwise fashion from ca. 10% to

ca. 30% of the mean tensile or compressive strength. No clear change in the reaction rate, which was monitored by means of gas chromatography, was observed during the procedure.

Burnoff dependence of the rates of oxidation of PGX and H451 graphites in $\text{H}_2\text{O}/\text{He}$ was investigated and the data thus far obtained are summarized, which indicate that for PGX graphite the reaction rate increases continuously above a burnoff of 1-1.5%, whereas for H451 graphite it increases continuously from the initiation of oxidation.

Activation energies for the reactions of H451 graphite in a 2% $\text{H}_2\text{O}/\text{He}$ mixture and PGX graphite in a 2% CO_2/He mixture were calculated from Arrhenius plots, giving 207 ± 10 kJ/mol and 229 ± 13 kJ/mol, respectively.

Photomicrography was used to determine the "true" pore size distribution (pores greater than $0.2 \mu\text{m}$ diameter) in H451 graphite. An apparent pore size distribution (pores greater than $0.12 \mu\text{m}$ diameter) was generated from Hg porosimetry measurements. The two distributions were combined to give a bivariate pore size distribution, which was incorporated into a network pore model. This model was used to calculate the room temperature gas permeability coefficient of H451 graphite, which was found to agree reasonably well with experimental values. However, some experimental inconsistencies and aberrations in the model were found; these await explanations and solutions.

The research program undertaken by workers from SUNY at Buffalo to complement the BNL High Temperature Mass Transport studies is summarized. The mechanism of catalytic oxidation of graphite is being studied by microscopy in conjunction with the gold-decoration technique. In addition, the mechanism and rate of surface migration of chemisorbed oxides is being investigated. These results will be used to test a reaction rate model currently being developed.

High cycle fatigue tests have been carried out on Incoloy 800H at 871°C (1600°F), and detailed metallographic characterizations have been made. At this relatively high temperature there is an increased tendency for intergranular cracking, which is seldom seen at lower temperatures. Oxygen is shown to be detrimental to the fatigue strength at 871°C .

Preliminary data were obtained for a new helium test environment containing 5-10 μatm . of water. For Hastelloy X tested at 871°C the strength in this environment is higher than that in air for shorter duration tests, but for extended tests the helium could be more detrimental.

All in-helium creep tests are now being conducted in the drier helium gas. Air tests are continuing as previously described. The longest air test is on Hastelloy X at 760°C and this has accumulated over 20,000 hours. The rupture lives for Incoloy 800H show no significant environment effect in the previous wet helium environment at 649°C and 760°C for up to 16,000 hours testing. Rupture lives of Hastelloy X are slightly lowered in the wet helium at 760°C and at 871°C . Preliminary data from the drier helium

environment show improvements of creep properties for both alloys at the higher temperature, but no significant changes at the lower temperature.

Concentration profiles have been obtained for the migration of Mo_2C in H451 graphite at temperatures above the melting point of the carbide (2690°C). The diffusion is consistent with the Fickian model and the diffusion coefficients which have been obtained are several orders of magnitude greater than those predicted from lower temperature thermodynamic data.

Work has been initiated to study the potential mechanisms by which semi-volatile fission products may escape from source locations in heated type H451 graphite to the ambient environment. Results from preliminary experiments with Sr indicate that a considerable fraction of the simulated fission product was transported in flowing He from the high temperature region to a filter held at ambient temperature, possibly in the form of an aerosol.

The Oak Ridge HTGR codes ORTAP, CORTAP, ORECA, and BLAST have been converted and executed successfully on the BNL 7600 computer system. Some apparently minor discrepancies in the ORTAP code remain to be resolved.

Trial runs with the ORECA code have begun. Preliminary evaluations indicate a greater than expected sensitivity of the output results to some of the model modifications that were tested. Upon completion of this evaluation its results will be communicated to Oak Ridge, including suggestions for improvements, and a summary of all applicable code limitations.

To identify areas of primary importance in safety and licensing considerations of HTGR gas turbine plants, a small exploratory systems model of such a plant is currently being developed.

1. Graphite

Investigation of strength loss mechanisms in HTGR graphites, particularly grade PGX, was directed this quarter primarily at direct thermal oxidation. Reaction rate profiles and compressive strengths of graphites oxidized under various conditions were determined. More results on the effects of prestress on oxidation rate and compressive strength are presented. In addition, some preliminary work on the permeability of graphite is discussed. This is followed, finally, with a discussion of the program undertaken by workers from SUNY at Buffalo dealing with the role of surface diffusion of oxidants in graphite.

1.1 Oxidation-Induced Strength Loss in HTGR Graphites (F. B. Growcock, J. J. Barry, M. Eto, J. H. Heiser, III, C. S. Sastre)

Axial PGX graphite specimens 3.81 cm ϕ x 7.62 cm machined from the end-piece of log 13H6-1 (designated log 3) were oxidized in the Uniform Flow Apparatus (Growcock, 1979) at 800°C and 700°C in 1 atm of He containing either 0.17% H₂O + 1.7% H₂ or 0.44% H₂O + 4.4% H₂. The flow rate was 25 SLM (24.7 cm/sec). Total burnoff of the EL-3 specimens was restricted to < 5%. Burnoff profiles in the radial direction are plotted in Figs. 1.1-1.9. The lower curves, depicting local burnoff vs. position, are obtained by differentiating the upper curves; the latter are plots of the burnoff of the residual core (bulk burnoff) left after each machining step, given by

$$B_i = \left(\frac{\rho_o - \rho_i}{\rho_o} \right),$$

where ρ_o is the density of the unoxidized material and ρ_i is the density of the residual core. Burnoff profiles of control (unoxidized) specimens were quite flat, though narrow regions of abnormal density were occasionally observed, as was the case for oxidized specimens. An analysis of the EL-3 data is given later in this section.

Specimens of H451 graphite measuring 1.91 cm ϕ x 3.81 cm were oxidized in particulate-free dried air at 550°C and 2% H₂O in He at 850°C. The gas flow rates were regulated to produce < 1% conversion of the reactant. The specimens were simply laid on the bottom of a quartz combustion tube and oxidized in that position. Burnoff profiles of these specimens are plotted in Figs. 1.10 and 1.11. Unoxidized specimens were also profiled and found to give a continuous rise in the bulk burnoff with increased penetration into the graphite. This effect arises from frictional wear of the specimen on the revolving lathe spindle; the problem has recently been eliminated by using a specimen holder of different configuration. The H451 data presented here have been corrected for this aberration.

Previous work with H451 graphite (Eto, 1979b) indicates that for specimens of this size in-pore diffusion does not limit the rate of oxidation in air below 650°C and in H₂O/He below 950°C. It is obvious from the burnoff profiles, however, that the rate of burnoff is much higher near the surface than throughout the bulk. Yet, the burnoff in the interior does not approach zero as expected for a diffusion-limited reaction. In fact,

Figure 1.1. Burnoff profiles of axial EL-3 PGX graphite specimen #65, 0.30% burnoff at 800°C.

Figure 1.2. Burnoff profiles of axial EL-3 PGX graphite specimen #109, 0.57% burnoff at 800°C.

Figure 1.5. Burnoff profiles of axial EL-3 PGX graphite specimen #96, 0.42% burnoff at 700°C.

Figure 1.6. Burnoff profiles of axial EL-3 PGX graphite specimen #29, 0.79% burnoff at 700°C.

Figure 1.7. Burnoff profiles of axial EL-3 PGX graphite specimen #11, 0.49% burnoff at 700°C.

Figure 1.8. Burnoff profiles of axial EL-3 PGX graphite specimen #60, 1.90% burnoff at 700°C.

Figure 1.9. Burnoff profiles of axial EL-3 PGX graphite specimen #7, 2.11% burnoff at 700°C.

Figure 1.10. Burnoff profiles of an axial H451 graphite specimen oxidized in air at 550°C to 4.97% burnoff.

Figure 1.11. Burnoff profiles of an axial H451 graphite specimen oxidized in 2% H₂O/He at 850°C to 4.10% burnoff.

the constant burnoff level in the interior is that expected for chemical reaction control. Similar behavior has been observed before in our group (Romano, 1977) and elsewhere (Walker, 1959). It is conceivable that in-pore diffusion-limited oxidation could manifest itself in the manner described. Since the cylinder faces were not masked, oxidation in these regions would contribute a constant total burnoff to the profile, and perhaps a little more around the edges. However, the external surface area of the faces is only 1/4 that of the cylinder wall; the mass loss contribution from the faces to the bulk burnoff is less than 10% of the measured bulk burnoff in our experiments. This was verified by repeating the experiments with longer specimens, in this case two 1.27 cm ϕ x 7.62 cm cylinders of PGX graphite oxidized in air. Density profiles were obtained after removing 1.5 cm from the ends. Burnoff profiles (one of these is shown in Fig. 1.12) similar in shape to those in Figs. 1.10 and 1.11 were obtained.

This phenomenon is being investigated in greater detail, as a result of the potential impact it may have on the measurement of oxidation kinetics of graphite.

No particulate matter was recovered after the above experiments, and, within tolerance limits ($\pm 10^{-3}$ cm), no change in the external dimensions of the specimens was noted. No measurable temperature gradient across the specimen diameters was observed using an internal shielded thermocouple; this is consistent with the calculated (see Szekely, 1976) maximum temperature gradient of 0.06°C expected for H451 oxidized in air at 550°C . Specific (B.E.T.) surface area measurements (Walker, 1959) show little difference between the inner and outer regions of machined graphite specimens. Active surface area profiles of as-received H451 and PGX graphite likewise show little difference between the inner and outer regions of the specimens; these results, however, were obtained on the powder removed from specimens during machining. Thus, some other technique must be used to profile the density of active sites in the solid as-received specimens.

Inhibition of the reaction by the products CO/CO₂ and CO/H₂ can cause non-uniform burnoff in a graphite specimen, but it cannot lead to a flat burnoff profile in the specimen interior, as observed here. To check the effect of inhibition by the reaction products, a "cocoon" experiment was run with H451 graphite in air at 500°C . An illustration of this "cocoon" is shown in Fig. 1.13. The burnoff profile obtained from one of these shielded specimens is given in Fig. 1.14. It is similar to the previous profiles, indicating that neither product inhibition of the rate nor surface washing by the carrier gas causes the observed burnoff profile. Other "cocoon" experiments with H451 graphite are underway, using longer specimens. These will be trimmed to size before obtaining their density profiles. In addition, the outer shells will be bored out after oxidation to check for the presence of a sharp density profile near those surfaces, too.

Walker, et al. (1959) speculated that the micropore-macropore structure in their material (pure carbon rods) might be responsible for the enhanced burnoff near the surface of a specimen presumably oxidized in the chemical reaction control temperature regime. However, it was believed at that time, and still is, that the micropores are so interconnected to

Figure 1.12. Burnoff profiles of an axial EL-3 PGX graphite specimen oxidized in 2% O₂/N₂ at 500°C to 0.7% burnoff.

Figure 1.13. "Cocoon" graphite specimen.

Figure 1.14. Burnoff profiles of an axial H451 graphite specimen oxidized in a "cocoon" in air at 500°C to 14.14% burnoff.

macropores that their effective lengths are too short to cause the observed behavior. The pore network of H451 graphite was examined this past quarter to check this assumption. Photomicrographs of highly polished, gold-sputtered radial and axial H451 graphite surfaces were made by R. Sabatini of the Metallurgy and Materials Science Division. Pores as small as $0.2 \mu\text{m}$ could be measured. The distribution of pores greater than $8 \mu\text{m}$ over an area 0.35 cm^2 is shown in Fig. 1.15. The pore size distribution of pores $10\text{--}400 \text{ \AA}$ in diameter was determined by Yang (1979) using N_2 desorption. Mercury porosimetry data from two H451 specimens were obtained by Micromeritics Corp.; these yield the pore size distribution curves shown in Figs. 1.16 and 1.17. The pores in H451 graphite may be divided into three groups with average pore diameters of $40 \text{ \AA}$, $0.20 \mu\text{m}$ and $20 \mu\text{m}$. The micropores ($\bar{d} = 40 \text{ \AA}$) occupy a void volume of 0.04, whereas the intermediate ($\bar{d} = 0.20 \mu\text{m}$) pores and macropores occupy a void volume of 0.14. Thus, the number of micropores per unit volume is several orders of magnitude greater than that of the larger pores, and the average distance between the large pores is large enough ($\sim 1 \mu\text{m}$ and $100 \mu\text{m}$ for the intermediate pores and macropores, respectively) that the concentration of reactant gas may be high for a significant distance into the specimen. One may postulate the existence of two independent pore networks in which oxidation is taking place, as shown schematically in Fig. 1.18: a surface network, N_{surface} consisting of micropores open at the surface and a bulk network, N_{bulk} , consisting of the entire assembly of pores. Since the accessible active surface area per unit volume of specimen is much greater in N_{surface} than in N_{bulk} , reactivity of the material near the surface may be expected to be higher than in the interior of the specimen.

Effective diffusion coefficients in N_{surface} , D_{seff} , may be approximated from the experimental burnoff profiles, using an expression after Dodson (Dodson, 1960 and Burnette, 1977):

$$\frac{B_s}{R_{O_s}} = \frac{(B - B_b)}{(B_o - B_b)} = e^{-x/L_s} \quad (1)$$

where B is the fractional mass loss at a depth x into the specimen (and B_s is B in N_{surface}), B_b is the average fractional mass loss attributed to bulk burnoff (flat profile region), B_o is the mass loss at the surface (and B_{O_s} is B_o in N_{surface}) and L_s is the diffusion length given by

$$\sqrt{\frac{D_{\text{seff}}}{K_{V_s}}}$$

where K_{V_s} is the volumetric rate coefficient in the rate expression for reaction in N_{surface} :

$$R_{T_s} = \frac{12S/V}{\rho R} \sqrt{K_{V_s} D_{\text{seff}} \eta P_i T} \quad (2)$$

Here S/V is the ratio of exposed surface area to volume, ρ is the graphite density, R is the gas constant, P_i is the pressure of oxidant, T is the temperature and η is an effectiveness factor for infinitely long cylinders (for these specimens $\eta \geq 0.89$).

Figure 1.15. Pore size distribution (pore diameter > 8 μm) in 0.35 cm^2 piece of a radial H451 graphite specimen.

Figure 1.16. Hg porosimetry-derived pore size distribution (pore diameter 0.03-1.0 μm) in H451 graphite specimen.

Figure 1.17. Hg porosimetry-derived pore size distribution (pore diameter $> 1.0 \mu\text{m}$) in H451 graphite specimen.

Figure 1.18. Schematic diagram of reactant concentration profiles in postulated graphite oxidation mechanism.

L_s is evaluated from the slope of the linearized form of equation (1) and substituted into equation (2) to obtain K_{VS} . These are then substituted into the definition of L to give D_{seff} . D_{seff} is often expressed as a function of the free binary gas diffusion coefficient: $D_{seff} = m D_{12}$. The same expression may be used for D_{seff} . Using expressions (1) and (2), one can obtain $D_{seff} = 4.52 \times 10^{-6}$ cm²/sec and $D_{seff} = 2.73 \times 10^{-5}$ cm²/sec for the H451 specimens oxidized in air at 550°C (Fig. 1.10) and in H₂O/He at 850°C (Fig. 1.11), respectively. Diffusion in the micropores of H451 graphite ($\bar{d} = 40$ Å) may be expected to be controlled by Knudsen flow. The dusty gas model (Jackson, 1976) can be used to approximate Knudsen diffusion coefficients, D_K , for $\bar{d} = 40$ Å. These are 1.73×10^{-5} cm²/sec for O₂ at 550°C and 2.70×10^{-5} cm²/sec for H₂O at 850°C. The similarity between the experimental and Knudsen diffusion coefficients suggests that the near-surface burnoff in the graphite specimens is caused by diffusion-limited oxidation in the micropores. D_{seff} calculated for the oxidized H451 "cocoon" (Fig. 1.14) is 1.66×10^{-5} cm²/sec, which compares very favorably with $D_K = 1.68 \times 10^{-5}$ cm²/sec. The outstanding agreement between these values is probably fortuitous, but it certainly lends credence to the other data and is strong evidence that the near-surface reaction is a micropore-governed phenomenon.

Burnoff profiles of PGX graphite specimens presumably oxidized in the chemical reaction control regime were presented previously (Eto, 1980b). These were analyzed in the same way as the H451 specimens. These results, along with those for the H451 specimens, are displayed in Table 1.1.

The burnoff profiles for the large PGX EL-3 specimens (Figs. 1.1-1.9) were similarly analyzed; these results, too, are included in Table 1.1. Here, however, oxidation was expected to occur in the diffusion-limited regime ($B_p=0$). Analysis of these burnoff profiles with expressions (1) and (2) is questionable, since the treatment assumes one diffusion path. Nevertheless, it is appropriate to determine D_{seff} in this manner for comparison with other results. General Atomic Company (GA, 1978) has obtained burnoff profiles for PGX graphite specimens oxidized at 790°C and 900°C. Diffusion coefficients obtained from application of equations (1) and (2) to their data are plotted alongside BNL results in Fig. 1.19. The lines drawn through the BNL results were obtained from weighted linear least squares regressions with forced ordinate intercepts at D_K . The expressions obtained are

$$\begin{aligned} D_{seff} &= \{(6.5 \pm 9.0) \times 10^{-3}\} \times \{\%BO\} + 2.64 \times 10^{-5} & \text{at } 800^\circ\text{C} \\ D_{seff} &= \{(2.6 \pm 3.0) \times 10^{-3}\} \times \{\%BO\} + 2.51 \times 10^{-5} & \text{at } 700^\circ\text{C} \end{aligned}$$

Uncertainties in the slopes are for 90% confidence limits. The functional form of D_{seff} is probably rather complex; these equations are not meant to imply a linear dependence with burnoff. Indeed, D_{seff} must approach D_{12} and some non-zero constant at the limits of 100% and 0% burnoff, respectively.

The two pore networks which are assumed to be active in the low temperature oxidation of graphite may also be expected to participate at higher temperatures. In-pore diffusion limits the oxidation rate in both networks, but to different degrees. One simple way of treating this presumed bimodality of the PGX EL-3 data is to assume that the pore networks are

Table 1.1

Data and Calculated Kinetics Parameters of Oxidized HTGR Graphites

Specimen [†]	Conditions	$R_{TS}(R_T) \times 10^8, \text{sec}^{-1}$	L_S or L, mm	K_{VS} or K_V, sec^{-1}	$D_{12}, \text{cm}^2/\text{sec}$	m_S or $m \times 10^3$
H451 Capsule	Air, 500°C	2.06 (10.3)	0.28	0.0219	1.04	0.016
H451	Air, 550°C	1.18 (21.7)	0.12	0.0312	1.16	0.0039
H451	H ₂ O/He, 850°C	0.91 (2.66)	0.07	0.374	7.00	0.0039
PGX-A	Air, 500°C	~24 (94.4)	0.30	0.24	1.04	0.21
PGX-A	Air, 500°C	9.63 (81.9)	0.13	0.22	1.04	0.036
PGX-A	H ₂ O/He, 750°C	5.36 (30.6)	0.14	1.01	6.04	0.049
PGX-107	H ₂ O/H ₂ /He, 800°C	2.43	--	--	6.51	--
PGX-65	H ₂ O/H ₂ /He, 800°C	1.28	0.075	8.6	6.51	0.074
PGX-109	H ₂ O/H ₂ /He, 800°C	6.60	0.075	44.	6.51	0.38
PGX-41	H ₂ O/H ₂ /He, 800°C	7.69	0.25	15.	6.51	1.4
PGX-66	H ₂ O/H ₂ /He, 800°C	18.67	0.50	19.	6.51	7.0
PGX-68	H ₂ O/H ₂ /He, 700°C	0.246	--	--	5.58	--
PGX-9	H ₂ O/H ₂ /He, 700°C	0.386	--	--	5.58	--
PGX-96	H ₂ O/H ₂ /He, 700°C	1.60	0.10	7.2	5.58	0.13
PGX-29	H ₂ O/H ₂ /He, 700°C	2.86	0.80	0.75	5.58	0.74
PGX-11	H ₂ O/H ₂ /He, 700°C	4.55	0.11	18.	5.58	0.42
PGX-60	H ₂ O/H ₂ /He, 700°C	2.53	0.34	3.2	5.58	0.67
PGX-7	H ₂ O/H ₂ /He, 700°C	5.19	0.90	1.6	5.58	1.4

[†]The H451 and PGX-A specimens are 1.91 cm ϕ x 3.81 cm. All other specimens are 3.81 cm ϕ x 7.62 cm.

Figure 1.19. Dependence of the effective diffusion coefficient of PGX graphite on burnoff during oxidation with H_2O in He with added H_2 ($H_2/H_2O = 10/1$).

independent and apply the Dodson expression for reaction in an infinitely long cylinder (Dodson, 1960) to the reactions in each network simultaneously. Thus,

$$\frac{B_{k1}}{B_{o1}} = \frac{I_o(r_i/L_1)}{I_o(r_o/L_1)} \quad \text{and} \quad \frac{B_{k2}}{B_{o2}} = \frac{I_o(r_i/L_2)}{I_o(r_o/L_2)} \quad (3)$$

Combining and rearranging we obtain

$$B_i r_i = 2B_{o1} L_1 \frac{I_1(r_i/L_1)}{I_o(r_o/L_1)} + 2B_{o2} L_2 \frac{I_1(r_i/L_2)}{I_o(r_o/L_2)} \quad (4)$$

Here B_k is the local burnoff, B_i is the burnoff of the residual core at a radius r_i and B_o is the local burnoff at the surface. I_1 and I_o are modified (hyperbolic) Bessel functions of the first kind, first and zero order, respectively. We have determined that one can fit expression (4) to the full burnoff profiles of PGX EL-3 specimens to obtain reasonable values of L_1 and L_2 . The curves drawn through the data in Figs. 1.1-1.9 were obtained using this simple expression. These curves fit the data much better than curves generated with single-valued L 's. Further development of the theory is needed, however, to increase its utility and properly weight the terms used in the curve-fitting routine.

The evidence gathered to date strongly suggests that oxidation of graphite in the chemical reaction control regime can lead to some burnoff near the surface. This has been interpreted as oxidation in a relatively long micropore network. This phenomenon appears to be important at higher temperatures also, where in-pore diffusion is expected to limit the reaction rate. Bimodal burnoff profiles of graphite specimens can be expected to affect their strength loss behavior as well as their oxidation kinetics, especially if the specimens are small in size.

1.2 Effect of Stress and Different Atmospheres on the Strength and Oxidation Behavior of Nuclear Graphite (M. Eto, F. B. Growcock, J. H. Heiser, III, J. J. Barry, C. C. Finfrock)

1.2.1 Loss of Compressive Strength of PGX graphite Oxidized in Different Atmospheres

The focus of experiments conducted during this quarter was the strength loss caused by oxidation in CO_2 and O_2 . PGX graphite specimens 12.7 mm ϕ x 25.4 mm were exposed to 2% CO_2/He at 600-850°C and 30% air/ N_2 (2% O_2/N_2) at 400-550°C at a flow rate of 300 sccm. The experimental method and measurement techniques were basically the same as were previously reported for other atmospheres (Eto, 1979a).

Fig. 1.20 shows the strength loss of PGX graphite oxidized in the mixtures described above to various levels of bulk burnoff. At any given burnoff level the 2% O_2/N_2 mixture caused a greater loss of strength than

Figure 1.20. Compressive strength of PGX graphite oxidized in a mixture of 2% CO_2 /He at 750°C or 2% O_2 / N_2 at 500°C as a function of bulk burnoff.

the 2% CO₂/He mixture. This result can be compared with the previously obtained result that O₂ gives rise to a greater loss of strength than H₂O. Moreover, the loss in strength caused by O₂ oxidation was found to be insensitive to the O₂ concentration. Least-squares regression analyses of the results obtained for oxidation with 2% O₂/N₂ and 20% O₂/N₂ indicate that oxidation in either environment can be expressed with the single equation

$$\frac{S}{S_o} = \left(\frac{\rho}{\rho_o} \right)^{10.6} \quad (5)$$

where S, S_o, ρ and ρ_o represent compressive strength after oxidation, mean compressive strength, density after oxidation and density before oxidation, respectively. The total bulk burnoff B (%) can be defined by

$$\frac{\rho}{\rho_o} = 1 - \frac{B}{100}$$

Equation (5) can be applied, as is shown in Fig. 1.21, at least to the specimens oxidized in 2% O₂/N₂ up to 7% burnoff at 500°C and those oxidized in air up to more than 20% burnoff at temperatures of 450 to 550°C. Experiments with 2% O₂/N₂ are being carried out at different temperatures to investigate whether the change in this parameter affects the relationship between strength and burnoff.

The data for CO₂/He and H₂O/He oxidations were least-squares fitted to the similar expressions:

$$\frac{S}{S_o} = \left(\frac{\rho}{\rho_o} \right)^{6.18} \quad \text{for} \quad 2\% \text{ H}_2\text{O/He mixture}, \quad (6)$$

and

$$\frac{S}{S_o} = \left(\frac{\rho}{\rho_o} \right)^{7.53} \quad \text{for} \quad 2\% \text{ CO}_2\text{/He mixture}. \quad (7)$$

The scatter of these data and goodness of fit are poorer than in the O₂/N₂ case. The latter can be considerably improved by including a pre-exponential factor of 1.08 for H₂O/He and 1.02 for CO₂/He, though it needs to be determined whether or not these values have any physical meaning. The modified equations are

$$\frac{S}{S_o} = 1.08 \left(\frac{\rho}{\rho_o} \right)^{4.65} \quad \text{for} \quad 2\% \text{ H}_2\text{O/He mixture}, \quad (8)$$

and

$$\frac{S}{S_o} = 1.02 \left(\frac{\rho}{\rho_o} \right)^{6.00} \quad \text{for} \quad 2\% \text{ CO}_2\text{/He mixture}. \quad (9)$$

Figure 1.21. Relationship between strength and bulk density of PGX graphite oxidized in air or 2% O₂/N₂. Here, S, S₀, ρ and ρ₀ are the compressive strength after oxidation, mean initial compressive strength, bulk density after oxidation and initial density, respectively.

The experimental values of the exponent α in the equation

$$\left(\frac{S}{S_o} \right) = \left(\frac{\rho}{\rho_o} \right)^\alpha$$

can be compared with those obtained by previous investigators. The value for O_2 oxidation, 10.6, is in good agreement with that of 11.6 obtained by Knibbs (1971) for PGA graphite oxidized in air at $470^\circ C$. Griggs (1956) obtained the value of 6.3 for CS-GBF graphite oxidized in CO_2 at $950^\circ C$. PGA graphite oxidized in CO_2 at $770^\circ C$ gave a value of 6.8 (Morgan, 1974). These values are very similar to those obtained for CO_2 and H_2O oxidations in the present experiments. However, some investigators obtained the value $\alpha \approx 6.5$ for TSX graphite oxidized in air at 600 to $750^\circ C$, and almost the same values for PGA graphite oxidized in air at $700^\circ C$ and in CO_2 at 875 to $960^\circ C$, i.e. $\alpha \approx 8$ (Morgan, 1974).

The difference in the value of α between O_2 oxidation and CO_2 or H_2O oxidation obtained in the present experiments may be attributable to the selective attack of oxygen on a particular region of polycrystalline graphite, as was suggested elsewhere (Eto, 1980a). The detailed mechanism for the strength loss will be discussed in upcoming progress reports, with consideration of the results of density profile measurements (Growcock, 1980a) and observed structural changes arising from oxidation.

1.2.2 Oxidation of PGX Graphite under Compressive or Tensile Stress

The stress rig described in a previous Quarterly Progress Report (Eto, 1979a) has been used to investigate the effect of tensile and compressive stress up to about 30% of the mean tensile or compressive strength on the reaction rate of PGX graphite oxidized in a 2% H_2O/He mixture at $440^\circ C$. This low temperature was chosen for the first runs to ensure homogeneous oxidation. Helium containing 2% H_2O at 1 atm was passed around the specimens at a flow rate of 300 sccm. Stresses were applied to three compressive specimens stacked in the center of the compression plates and three tensile specimens which surrounded the compressive specimens. The stress is applied with an air piston, the details of which have been described previously (Eto, 1979a). When the reaction rate stabilized, a stress of about 10% of the mean tensile or compressive strength was applied to the tensile and compressive specimens while monitoring the reaction products via gas chromatography. After 10 hr of operation at ca. 10% of the mean strengths, the stress was increased to ca. 20% of the mean strengths, and later to ca. 30% of the mean strengths. Despite the positive report on the effect of stress on oxidation rate (Krefeld, 1973), the experiment thus far has shown no effect of stress on reaction rate, in agreement with other studies (Growcock, 1978; Thrower, 1977).

Similar experiments will be carried out at higher temperatures and at higher stresses for PGX and other grades of graphites, including H451 graphite, to clarify the effect of stress on oxidation.

Research on the effect of prestress on the reaction rate of H451 graphite was continued during this quarter. An H451 graphite specimen was

oxidized in a 2% H₂O/He mixture at 850°C for some time and bulk burnoff was measured. Then the specimen was prestressed and reoxidized for a while, after which bulk burnoff was again measured. The experiment has been repeated in this manner, the results of which are shown in Fig. 1.22. Here solid circles represent reaction rate data after the specimen was prestressed to 75% of the estimated compressive strength of the specimen. Although the rate seems to have been affected positively by the prestress, the enhancement of the rate is small and falls within the scatter of results for unstressed specimens oxidized to similar burnoff levels (see next section).

1.2.3 Burnoff Dependence of Reaction Rate

The burnoff dependence of the reaction rates of PGX and H451 graphites has been reported previously (Eto, 1979b, 1980b). In this quarter, data for oxidation in a 2% H₂O/He mixture have been obtained for both graphites. These are summarized in Figs. 1.23 and 1.24. For PGX graphite the rate increased rapidly with burnoff up to ca. 1% and decreased with increasing burnoff until it reached a relatively constant value at ca. 8%. Similar trends have been observed before at higher temperatures (Growcock, 1977). In contrast, the reaction rate of H451 graphite increased monotonically with burnoff at 750°C and 850°C. It should be noted, however, that the change in the rate was not as great for H451 as it was for PGX graphite.

1.2.4 Activation Energy for Oxidation in a Mixture of 2% H₂O/He or 2% CO₂/He

Activation energies were determined for the following reactions: PGX graphite oxidized in a 2% CO₂/He mixture at temperatures of 750 to 850°C and H451 graphite oxidized in a 2% H₂O/He mixture at temperatures of 700 to 850°C. Experiments similar to those reported before were carried out to obtain the relationship between reaction rate and reaction temperature. In contrast to previous experiments, the temperature was decreased in a stepwise fashion, rather than increased, to minimize the effect of burnoff on the rate.

Arrhenius plots are shown in Figs. 1.25 and 1.26 for PGX graphite in CO₂/He and H451 graphite in H₂O/He, respectively. In the latter case, the value of 207 ± 10 kJ/mol was obtained, where the burnoff ranged from 0.25 to 0.45% (circles), from 0.35 to 1.70% (squares) and from 0.45 to 3.12% (triangles). As was the case for air oxidation, the energy is slightly higher than that for PGX in 2% H₂O/20% H₂/He, for which a value of 189 kJ/mol was obtained (Eto, 1979b). From the result shown in Fig. 1.25 for the reaction of PGX graphite with CO₂ over a burnoff range of 1.5% (800°C) to 3.75% (700°C), an activation energy of 229 ± 13 kJ/mol can be calculated. All of the uncertainties were calculated for 90% confidence limits. The temperature dependence of PGX graphite oxidation in O₂/N₂ will be determined next.

Figure 1.22. Reaction rate of H451 graphite with or without prestress oxidized in a 2% H₂O/He at 850°C as a function of burnoff.

Figure 1.23. Burnoff dependence of the reaction rate of PGX graphite oxidized at various temperatures in 2% H₂O/He.

Figure 1.24. Burnoff dependence of the reaction rate of H451 graphite oxidized at 750 or 850°C in 2% H₂O/He.

Figure 1.25. Arrhenius plot for PGX graphite oxidized in 2% CO₂/He.

Figure 1.26. Arrhenius plot for H451 graphite oxidized in 2% H₂O/He.

1.3 High Temperature Mass Transport of Gases in HTGR Graphites (F. B. Growcock, J. H. Heiser, III)

The permeability of HTGR graphites is of some concern since this phenomenon, i.e. flow induced by a pressure gradient, increases in importance with increasing system pressure. In an HTGR the relatively high pressures (ca. 50 atm) of the helium coolant coupled with non-negligible pressure gradients across the graphite webbing could lead to enhanced penetration of reactive impurity gases into the graphite matrix, hence a deeper oxidation profile and a greater concomitant loss in strength at a given total burn-off.

Preliminary measurements of forced flow of He through H451 and PGX graphite indicated that the permeability of PGX graphite is at least one order of magnitude greater than that of H451 graphite (Growcock, 1980b). It is of interest to model the permeabilities of HTGR graphites for the information that may be gained about their pore structure. At present no a priori theoretical models exist. A semi-empirical model which requires only that the pore size distribution of the porous medium be known, has met with success in predicting the room temperature permeabilities of sandstones (Dullien, 1974). This model is constructed using a bivariate pore size distribution, wherein macropores are completely connected with each other through necks, or pore entries, which control the flow of fluid media. Since the pores in graphite are often assumed to have a bimodal character, it is only natural that we should attempt to fit the structure of graphite to such a model.

The permeability may be calculated using the following expression (Dullien, 1974):

$$B_o = \frac{\epsilon}{96 \sum_j V_{ij}} \sum_i \frac{\left(\sum_j V_{ij} / d_j^2 \right)^2}{\sum_j V_{ij} / d_j^6} \quad (10)$$

where B_o is the permeability coefficient (Grove, 1967), ϵ is the void volume of through pores and V_{ij} is the volume of the j pores with diameter d_j and entry diameter d_i . A more exact calculation can be made in which account is taken of the excess momentum of the gas molecules which is lost due to the convergent-divergent character of the pores (Azzam, 1976). However, this is expected to change the calculated permeabilities by only 10%; for our purpose here, this is a needless complication.

A pore volume matrix has been constructed for H451 graphite using the pore size distribution curve obtained from Hg porosimetry (Figs. 1.16 and 1.17) to determine the entry diameters d_i . The overall pore size distribution was determined from photomicrographs of the graphite surface; a pore size distribution histogram, shown in Fig. 1.27, was constructed from the measured pore frequency distribution (see, for example, Fig. 1.15 for the frequency distribution of pores $> 8 \mu\text{m}$). The Hg porosimetry curve was divided into several regions of equal volume; the average pore diameter in a region was designated d_i for that region. The minimum pore diameter used, as noted in Fig. 1.16, was $0.12 \mu\text{m}$ (Hg pressure 10 MPa); the pore structure

Figure 1.27. Pore size distribution (pore diameter $> 0.2 \mu\text{m}$) of a radial specimen of H451 graphite.

appeared to change above this pressure of Hg. The overall pore size distribution was divided into regions of equal volume, too, each encompassing the entire d_j range, and each of these was subdivided into subregions with average values d_j . The percentage of the total pore volume in each subregion characterized by d_j with entry pore d_i was calculated from the overall pore size distribution curve. The pore volume matrix generated for four values of d_i is shown in Table 1.2.

Incorporation of these V_{ij} , d_j and d_i values, along with $\epsilon = 0.137$, into equation (12) gives $B_0 = 7.6 \times 10^{-11} \text{ cm}^2$. Experimental values of B_0 for radial specimens of H451 graphite fall in the range $(3-4) \times 10^{-11} \text{ cm}^2$. The agreement is reasonable. However, the calculation was found to be quite sensitive to the number of regions into which the Hg porosimetry curve was divided. Using only one region gives $B_0 \sim 7 \times 10^{-11} \text{ cm}^2$, while the calculation with two values of d_i gives $B_0 = 2.9 \times 10^{-11} \text{ cm}^2$. The reason for this sensitivity is that the terms with large d_i dominate the others. Another problem is the void volume. By using $\epsilon = 0.137$, we have assumed that the micropores ($\epsilon = 0.04$) do not contribute to the permeability and that only the intermediate and macropores are important; this assumption is probably valid. However, we have included blind pores; blind pores with diameter d_j are counted using the photomicrographic technique, but the blind pores with diameter d_i (Hg porosimetry) may or may not be counted. At any rate, both ϵ and the V_{ij} are in error; it is not yet possible to ascertain how these may be corrected. Finally, the photomicrographic technique yields a total void volume (blind + through pores) of ca. 0.03 for $d > 0.2 \text{ } \mu\text{m}$, rather than 0.137. This large discrepancy also awaits a solution.

In the meantime, the permeability of PGX graphite will be similarly calculated. Photomicrographs of a PGX graphite surface are being made to generate the overall pore size distribution, which will be coupled to that obtained from Hg porosimetry.

Table 1.2

Pore Volume Matrix for Radial Specimen of H451 Graphite

$i \backslash j$		1	2	3	4	5	6	7	8	9	10	11	12	D_i
V_{ij}	1	1.79	0.81	0	1.20	2.16	3.75	1.65	1.60	3.62	3.08	3.10	2.24	1.4
	2	0	0.41	0	0.90	2.16	4.83	2.48	3.78	4.63	2.63	1.50	1.68	6.2
	3	0	0	0	0.60	2.16	5.39	3.31	3.91	5.00	2.20	1.30	1.13	10.5
	4	0	0	0	0.30	2.16	5.79	4.14	4.38	5.25	1.76	0.66	0.56	17.4
D_j		1.4	6.2	10.5	17.4	39.9	60	80	100	120	140	160	180	

1.4 Surface Diffusion in Microporous Graphite Structures and the Langmuir-Hinshelwood Mechanism (N. J. Desai, P. J. Talarico, C. Wong, R. T. Yang, SUNY Buffalo)

The program is undertaken to assist Brookhaven National Laboratory to obtain a basic understanding of the chemical and physical phenomena taking place in the graphite reactor which result in the weakening of the strength of the graphite.

Three tasks are being performed in parallel. In the first task, the surface mobility of the chemisorbed oxide on carbon at high temperatures is being measured, and it is to be incorporated in the surface oxidation mechanism. Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) in conjunction with the gold-decoration technique are being employed in the second task to study the catalytic oxidation mechanism, as well as the surface migration phenomenon. The third task is concerned with modeling of the interplay between the pore diffusion step and the surface oxidation step during the overall reaction mechanism.

1.4.1 High-Temperature Surface Diffusion on Graphites

Gasification of carbon proceeds through chemisorbed species. For the reactions involved in graphite reactor safety problems, as well as some important processes in industry, the chemisorbed oxide on carbon is known as the intermediate species.

The chemisorbed oxide, denoted by $\text{C}(\text{O})$, is mobile on the surface at the reactor temperatures.

The objective of this task is to measure the mobility of this oxide on the surface and hence to obtain a better understanding of the gasification mechanism. To achieve this goal, two independent experiments are being conducted. One is to measure the high-temperature chemisorption, both isotherms and energetics. Measurements of surface diffusion of the chemisorbed oxide are to follow. For both experimental programs, a clean carbon surface is required. The term "clean surface" here refers to a carbon surface free of oxide. Such a clean surface can be obtained by degassing the carbon sample at 750°C (Chen, 1979) to 800°C (Laine, 1963). To accomplish these goals, three major pieces of experimental apparatus are to be used. These are: (1) a vacuum system capable of pumping to $\leq 10^{-6}$ torr; (2) a chemisorption apparatus; and (3) a modified Wicke-Kallenbach-type total flux apparatus. The first two are being constructed at SUNY at Buffalo. The total flux measurements will be conducted, as kindly agreed to by Brookhaven National Laboratory (BNL), at BNL. The following is a brief description of the apparatus and the status of their construction.

Vacuum System. The vacuum system comprises a Varian 2-inch oil diffusion pump and is a metal system. It is being constructed.

Chemisorption Apparatus. The amount of chemisorption is to be measured manometrically. The apparatus consists of a stainless steel reservoir (volume $\approx$ 600 ml), a stainless steel sample holder (volume $\approx$ 50 ml), and a pressure gauge (0 - 900 mm Hg). The two steel vessels are to be housed in a tubular furnace. The interconnecting tubing is 304 stainless steel of 1/8" diameter. All parts have been gathered, and will be set up shortly. The major problem facing us now is the sealing of the system at temperatures up to 900°C.

The major adsorbate that is to be used is CO. The carbon in CO, once chemisorbed, should be undistinguishable from the surface carbon; and the oxide should be the same as the chemisorbed oxide which functions as the intermediate in the carbon gasification reactions.

With the present design, it is expected that 1% of the chemisorbed CO on H451 graphite may be measured without any difficulty.

Total Flux Measurement. The apparatus designed by BNL (Growcock, 1980b) seems to be ideally suited for measuring the surface flux of the chemisorbed CO, or O, on graphites. The design is the best known to alleviate the leakage problem for high-temperature studies. Arrangements are being made for the diffusion measurements to be conducted at BNL. The gas phase flux of CO in the graphite sample is to be estimated from the fluxes of at least two nonadsorbable gases, e.g., He, Ar and N₂.

1.4.2 SEM and TEM Studies

The following instruments will be used for this program:

1. Scanning electron microscope (SEM), JEOL-JSM-U3, with Ortec 6200 multichannel energy dispersive x-ray analyzer. The SEM has a maximum magnification of 100,000X. The x-ray analyzer provides surface elemental analysis to the ppm level of elements heavier than Na. Three-dimensional elemental analysis of the graphite sample may also be made. The instrument is shown in Fig. 1.28a.

Several natural graphites have been purchased. Some SEM micrographs are shown in Fig. 1.29. Most of the surface is single crystal basal plane. The edges or damages as shown on the micrographs are sporadic.

2. Transmission electron microscope (TEM), JEOL-JEM-100 DC (shown in Fig. 1.28b). This model is capable of "seeing" materials (or resolution) as small as 10Å. For graphite samples, the thickness must be below 1000Å. We will use this instrument, with the gold-decoration technique, to study the expansion of edge carbon atoms after surface reaction. Gold decoration is to be accomplished with an Edward 306 Microscopy Coater (Fig. 1.28c), which is also available to us. One of us (CW) is now perfecting the technique of shearing, or splitting of the natural single crystal graphite to obtain a layer of thickness below 1000Å.

A quartz tubular reactor for surface etching of the graphite is being constructed.

Figure 1.28a. SEM with x-ray analyzer.

Figure 1.28b. TEM for thin layer graphite studies.

Figure 1.28c. Microscopy coater for gold decoration.

Figure 1.29a. Transmission micrographs of natural graphite (from Essex County, NY). Edges, damages and stacking of the basal planes are shown. Magnification 80X.

Figure 1.29b. Transmission micrographs of natural graphite (from Essex County, NY). Edges, damages and stacking of the basal planes are shown. Magnification 80X.

Figure 1.29c. Transmission micrographs of natural graphite (from Essex County, NY). Edges, damages and stacking of the basal planes are shown. Magnification 10,000X.

Figure 1.29d. Transmission micrographs of natural graphite (from Essex County, NY). Edges, damages and stacking of the basal planes are shown. Magnification 10,000X.

We are planning two basic studies using the above instruments. First, the surface diffusion mechanism will be characterized with the gold-decoration technique (and TEM). Second, the mechanism of catalysis of gasification by metal oxides, especially CaO and MgO, which has been puzzling to scientists, will be studied. These oxides are relatively abundant in all nuclear graphites. The catalysts will be deposited on the single crystal surface through contact with aqueous solutions of the salts followed by their thermal decomposition.

1.4.3 Penetration Depth of Gaseous Oxidants in H451 Graphite at High-Temperatures

In graphite reactors, the temperature can be as high as 1050°C at various locations. In this temperature range, pore diffusion can play an important role in the overall gasification rate, which creates a nonuniformity in the strength of graphite reactor. The temperature range for pore diffusion to be important is expected to be higher for H451 graphite as compared with PGX graphite, because PGX is more chemically reactive than H451 by 1-3 orders of magnitude. The interaction between pore diffusion and surface oxidation results in a "surface burning" of the graphite, and we call this surface region "penetration depth". Knowledge of the penetration depth is basic to the understanding of the high-temperature gas-carbon reaction kinetics.

A simple way of measuring the penetration depth, or the depth of the reaction zone in the surface layer, has been developed. Briefly, a disc of H451 graphite was fitted on the bottom of the diffusion cell for overall rate measurement, and Ar containing a few percent CO₂ was swept over the open end of the cell (Yang, 1977). The penetration depth was much smaller than the thickness of the disc, and therefore, a quasisteady state was reached during the reaction, as witnessed by a steady, constant overall rate. As the specimen was completely consumed, the front of the reaction zone advanced until it reached the bottom of the sample-holding cell, when the overall rate started decreasing to zero. Experiments were also performed in which the CO₂ supply was cut off at the end of the constant-rate period. The thickness of the remaining disc was measured (which was on the order of 100 μm) with a micrometer; this thickness was the penetration depth. Such measurements were done at various temperatures (1000 - 1600°C) and concentrations of CO₂. This technique is a substantial improvement over previous ones used at Penn State, in the Soviet Union and elsewhere, where the reacted graphite was shelled on the surface and the shelled materials (~10-20 μm per shell) were measured for surface area and bulk density. The penetration depth was then estimated to be at the decay point on the surface area-depth plot.

A model for the interaction of the pore diffusion step and the chemical reaction step is summarized below.

The effective diffusivity of gaseous carbon dioxide into the porous carbon is often approximated by

$$D_e = \epsilon^2 D_{\text{gas}}$$

where ϵ is the porosity.

Since the porosity varies from 1 at the surface to ϵ_0 at the reaction zone/unreacted carbon interface, the assumption of a constant porosity may not be appropriate.

As a first approximation we have assumed that the porosity varies linearly with 'x' in the reaction zone. However, in order to obtain an analytical solution we are unable to relax the assumption of constant surface area in the reaction zone.

q_A = flux of CO_2

k = rate constant cm/sec

C_A = Conc. of CO_2 cm moles/cm³

Subscripts A, B, C = CO_2 , CO, Ar

y = mole fraction

Mass balance of CO_2

$$-\frac{dq_A}{dx} = k S_v C_A$$

S_v = surface area/unit vol cm²/cm³

The flux of CO_2 (q_A) is given by

$$q_A = - \frac{C_T D_{AC}}{1+y_A} \frac{dy_A}{dx}$$

where C_T is the molar concentration of gas mixture.

Substituting gives

$$\frac{d}{dx} \frac{C_T D_{AC}}{1+y_A} \frac{dy_A}{dx} = k S_v C_A$$

$$\text{Let } D_{AC} = D_{gas} \epsilon^2$$

Substituting and simplifying

$$\epsilon^2 \frac{d^2 y^*}{dx^{*2}} + 2\epsilon \frac{d\epsilon}{dx^*} \frac{dy^*}{dx^*} - \frac{k h^2 S_v}{D_{gas}} y^* = 0 \quad (11)$$

Assuming $1+y_n \approx 1$

$$y^* = y_A / y_{Ao}$$

$$y_{Ao} = C_A / C_{Ao}$$

$$x^* = x/h$$

where subscript o indicates quantities at $x = 0$.

The boundary conditions are

$$\begin{aligned} x^* = 0 & \quad y^* = 1 \\ x^* = 1 & \quad y^* = 0 = \frac{dy^*}{dx^*} \end{aligned}$$

The overall reaction rate is given by

$$-\frac{dm}{dt} = k C_T y_{Ao} \pi R_o^2 h \bar{S}_v \int_0^1 h^* dx^* \quad (12)$$

m = mass of carbon disc

R_o = Radius of disc

Equation (11) is of the form

$$(ax^* + b)^2 \frac{d^2 y^*}{dx^{*2}} + 2a(ax^* + b) \frac{dy^*}{dx^*} + A y^* = 0$$

$$\epsilon = ax^* + b$$

$$\text{and } A = - \frac{k h^2 S_v}{D_{gas}}$$

An analytical solution exists if $\frac{A}{a^2} < 1/4$. Since A is negative, $\frac{A}{a^2} < 1/4$ and the solution is given by

$$y^* = a_+ (ax^* + b)^{n_+} + a_- (ax^* + b)^{n_-}$$

where

$$n_+, n_- = \frac{-1 \pm \sqrt{1 - 4A/a^2}}{2}$$

Substituting the appropriate values one can obtain the two constants a_+ and a_- . The measured quantities are the reaction rate, $-dm/dt$, the penetration depth, h , and physical properties of the carbon samples.

Calculation of the penetration depth

The weight of the graphite which consists of only the reaction zone was measured. Assuming no change in porosity in the reaction zone we can calculate the penetration depth by measuring the thickness of starting substance.

eg. wt at start = 241.8 mg

thickness = .0711 cm

wt at change of dm/dt = 25.85 mg

$$h = \frac{25.85 \times .0711}{241.8} = .0076 \text{ cm}$$

Assuming a linear porosity profile

$$m_p = \pi R_0^2 \rho_s h \left\{ 1 - \left(\frac{1+\epsilon_0}{2} \right) \right\}$$

m_l = wt of graphite at change.

Substituting, we obtain the penetration depth as

$$h = .0142 \text{ cm}$$

If a quadratic expression is used for porosity $h = .0106$ cm. Assuming a linear concentration profile an approximate value of the rate constant can be calculated from equation (12). Substituting the value of k in equation (11) we can get the concentration profile y^* vs. x^* as a first approximation. An iteration routine is being developed.

Experimental data on the porosity and surface area as functions of burnoff are of great importance for further modeling. Such measurements are being conducted at BNL.

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2. Materials

This program covers the evaluation of four main categories of materials: (1) metallic materials, (2) graphites, (3) PCRV, and (4) other materials. Included in (4) are control rod materials and thermal barrier insulation. At this time, however, the major emphasis is centered on metals. The objectives of the work are to critically review available materials data pertinent to HTGR safety, identify areas where information is sparse or unavailable, and to design and initiate experiments to yield data which will permit accurate assessments to be made of materials-related safety problems.

2.1 Fatigue of Structural Materials (P. Soo, R. Sabatini, J. Hare)

The current effort on fatigue is focused on the high cycle fatigue regime to evaluate the behavior of components subjected to rapidly oscillating stresses. Tests are conducted in air and a simulated HTGR helium environment under load control at a cycling rate of 40 Hz. Six Material Test Systems (MTS) closed loop electrohydraulic fatigue machines are being used in the program. At this time 5 units are being used for in-helium testing. Test gas is supplied from the Materials Test Loop (MTL).

In this reporting period the helium test gas has been changed from the usual standard which contained 2500 μ atm. H_2O , 200 μ atm. H_2 , 40 μ atm. CO , 20 μ atm. CH_4 and 10 μ atm. CO_2 , at a total pressure of 1.3 atm. The new environment is identical to the old one except that it is significantly drier, containing 5-10 μ atm. H_2O . In selecting the new water level it was intended to continue to evaluate off-normal gas chemistries which could conceivably affect the fatigue properties in a detrimental fashion. At the same time, however, we did not wish to duplicate the test environments used by General Atomic Co., General Electric Co., and Oak Ridge National Laboratory in their HTGR programs which are designed to evaluate ideally operating reactor systems in which the water levels are $\lesssim$ 2 μ atm.

In this report a description will be given of metallographic examinations of specimens tested in the old wet environment and then a brief outline of tests carried out in the drier helium gas.

Chemistries of the test materials studied in the fatigue and creep program are:

	<u>C</u>	<u>P</u>	<u>S</u>	<u>Mn</u>	<u>Si</u>	<u>Cr</u>	<u>Ni</u>	<u>Mo</u>	<u>Fe</u>	<u>Others</u>
Incoloy 800H (Ht. HH7427A)	0.05	NA	0.003	0.67	0.46	19.83	32.17	NA	Bal.	0.65 Cu 0.43 Ti 0.39 Al
Hastelloy X (Ht. 4-2809)	0.11	0.021	0.008	0.50	0.41	20.67	Bal.	8.86	18.66	2.10 Co 0.55 W
2 1/4 Cr-Mo	0.14	0.012	0.016	0.57	0.37	2.2	0.16	0.92	Bal.	

NOTE: NA = not analyzed. All concentrations in weight percent.

2.1.1 Tests on Incoloy 800H at 871°C (1600°F) in the 2500 μ atm. H₂O Environment

In the previous quarterly report it was shown that at 871°C (1600°F) there was a very large effect of test environment on the high cycle fatigue strength of Incoloy 800H. For tests in the cycles-to-failure (N_f) range less than about 10^7 the strength in the helium was much higher than in air. For longer duration tests the strength levels off and becomes essentially independent of the environment. In Fig. 2.1 scanning electron microscope/microprobe (SEMM) X-ray line scans were carried out on 4 specimens. One specimen (MNF-231) was tested in air for a short test time (low N_f , high stress) and another (MNF-232) for a long test time (high N_f , low stress). Two other specimens (MNF-238 and MNF-237) were tested for approximately similar lifetimes in helium. The data do not provide any conclusive evidence for the effect of the environment on fatigue strength, but some basic observations are apparent:

- For all 4 tests, titanium is clearly present in the surface scale regions. In earlier work it was found that titanium does not concentrate in the surface layers of specimens exposed for long times (~ 1 mo.) at 649°C (1200°F) - see Fig. 2.2 - but it is present at 760°C (1400°F) for tests of similar duration (see quarterly report for period July - September 1979). For the low N_f (high stress) air test the normal Cr/Mn scale has either not formed or it has been lost by spallation during the test.
- For air tests the scale appears to be less protective based on the larger amount of intergranular corrosion beneath the scale.
- Recrystallization of the cold worked surface layers (the specimens were left in the as-fabricated surface ground condition) readily occurs at 871°C (1600°F) as seen by the relief effect caused by etching the polished samples.

Based on the above observations a tentative model to explain the environment effect may be proposed. It seems possible that in air the rate of corrosion is much higher than for the helium tests so that spallation of the Cr/Mn scale which forms readily at most temperatures easily occurs under the action of the large cyclic stresses. In the absence of this protective scale rapid intergranular penetration is possible, which seems to be the case for specimen MNF-231. This conclusion is based on the observed width of the oxygen peak and the abnormal etching characteristics on the surface layers of the specimen. Such intergranular oxidation is likely to enhance the rate of crack nucleation and/or crack propagation, thereby reducing the strength.

In the case of the helium environment, for which the oxide scales are formed more slowly, it appears that the Cr/Mn scale can form and be resistant to spallation. Note the high integrity of the scale in specimen MNF-237 compared to that in specimen MNF-232 which is badly cracked.

Figure 2.1. Scanning electron microscope/microprobe line scans through the surface of Incoloy 800H high cycle fatigue specimens tested in air and HTGR helium at 871°C (1600°F). Magnifications 750X.

Figure 2.2. Scanning electron microscope/microprobe line scan through the surface of an Incoloy-800H specimen (MNF-166) fatigue tested in HTGR helium at 649°C (1200°F) at an alternating stress of 213.7 MPa (31.0 ksi). Cycling rate was 40 Hz and failure occurred after 1.1×10^8 cycles. Magnification 1125X.

More comprehensive metallographic data are required, however, before the environmental effect on high cycle fatigue can be determined with confidence.

2.1.2 Tests on Incoloy 800H Thermally Aged in the 2500 μ atm. H₂O Environment

In order to more fully understand the effects of long term oxidation on the high cycle fatigue of Incoloy 800H, two series of specimens were preaged in the 2500 μ atm. water environment. Aging times of 3000 and 6000 h were used for specimens in the unstressed condition. During aging it is anticipated that surface recrystallization will occur during the aging period. All specimens were subsequently tested in the same helium environment.

The data obtained are shown in Fig. 2.3. Although there is some scatter in the data it does appear that the specimens aged for 3000 h are slightly weaker than those aged for 6000 h prior to testing. However, the difference in strength is small. An interesting point to note is that the strength of the aged specimens is close to that found for unaged air tested specimens (see previous quarterly report).

Fractographs of preaged specimens are given in Fig. 2.4. For the 3000 h aged specimens (MNF-214, MNF-219) the fracture surfaces are atypical. For the high stress specimen (MNF-214) the scalloped surface indicates that several cracks initiated independently and joined to form a common crack. This is indicative of embrittlement because of the relative ease of crack nucleation. For the low stress specimen (MNF-219) the surface is highly "rumpled" and devoid of the usual "river line" patterns seen in failed fatigue samples.

In the case of the 6000 h specimen (MNF-207, MNF-212) the river lines are clearly seen and emanate from the bottom edge of the failed surface where the fatigue crack initiated. There appears to be more ductility associated with these samples since the cracks propagated across the width of the sample and a "chisel edge" is formed in the region where final separation occurred. Figs. 2.5 through 2.8 show comparisons between the 3000 h and 6000 h aged specimens in selected regions of the fracture surface. There is not a completely consistent pattern since intergranular crack propagation characteristics are observed in both types of aged specimen. However, it seems that the 6000 h specimens show this to a lesser extent, which is consistent with their higher strength (Fig. 2.3).

Fig. 2.9 shows enlarged views of the fracture surfaces of failed samples. Fine dispersions of oxidation products are seen in all cases. These particles and whiskers are very similar to those previously observed for tests at 760°C (1400°F), and may be connected with localized oxidation during the crack propagation procedure.

Figure 2.3. Effect of thermal aging in helium on the high cycle fatigue strength of Incoloy 800H at 871°C (1600°F).

Figure 2.4. Fractographs of thermally aged Incoloy 800H High cycle fatigue specimens tested at 871°C (1600°F) at low and high stress levels. Magnifications approximately 10X.

Figure 2.5. Crack initiation points in thermally aged Incoloy 800H high cycle fatigue specimens tested at 871°C (1600°F) for low and high stress levels. Magnifications 100X.

Figure 2.6. Crack propagation characteristics in thermally aged Incoloy 800H high cycle fatigue specimens tested at 871°C (1600°F) at low and high stress levels. Cracks propagated from left to right. Magnifications 240X.

Figure 2.7. Appearance of edges of fracture surfaces in thermally aged Incoloy 800H high cycle fatigue specimens tested at 871°C (1600°F) at low and high stress levels. Cracks propagated from left to right. Magnifications 120X.

Figure 2.8. Fracture surfaces in thermally aged Incoloy 800H specimens tested at 871°C (1600°F) at low and high stress levels. Regions close to final separation point. Cracks propagated from left to right. Magnifications 240X.

Figure 2.9. Oxidation products in fracture surfaces of Incoloy 800H high cycle fatigue specimens tested at 871°C (1600°F) at low and high stress levels. Magnifications 2400X.

2.1.3 Preliminary Fatigue Test Results for the New 5-10 μ atm. H_2 Environment

Some preliminary data have been obtained for Hastelloy X tested at 871°C (1600°F) in the new drier helium environment. Fig. 2.10 shows these results and compares them with data for the previous wet helium and the standard air condition. Both helium environments give a higher fatigue strength than air to cycles-to-failure below about 5×10^7 . For longer duration tests there appears to be a tendency for air to be more beneficial than helium. There does not seem to be a significant difference between the fatigue strengths in the wet and the drier helium environments. These observations will be more comprehensively evaluated as additional results become available.

2.2 Creep Rupture Properties of Primary Circuit Structural Materials (K. S. Lee, J. Chow, P. Soo, L. Gerlach)

The study of interactions of primary circuit structural metals with impurities in the helium coolant is an important safety consideration because these interactions may cause the degradation of mechanical properties of these metals. The objectives of our current program are to investigate the long term creep behavior of the primary circuit metals in an HTGR helium environment and to evaluate the possible changes in relations to a standard air environment.

The compositions of impurities in helium gas supplied from Material Test Loop (MTL) and the chemistries of test alloys are given in Section 2.1. The creep testing has been concentrated on Hastelloy X and Incoloy 800H.

With the commencement of testing in the new drier atmosphere, as described in Section 2.1, three tests accumulations over 16,000 hours in the old wet helium environment have been aborted, while nine air tests are still in operation. The longest test under way is in air for Hastelloy X at 760°C which has been running for 20,000 hours. Five Hastelloy and six Incoloy 800H specimens are set up in eleven units and tests are being conducted in the drier helium environment. 1/2" diameter x 1/4" thick round coupons are attached in the retort with the specimen to study the oxidation characteristics in the new test gas. The weight changes of the coupons will be measured after completion of the creep tests.

2.2.1 Incoloy 800H

Effects of the wet helium environment on the stress rupture life and on the minimum creep rates of Incoloy 800H at 649°C (1200°F) and 760°C (1400°F) are described in the previous quarterly report.

Fig. 2.11 is the stress-time plot for 1%, 2%, and 5% total elongation for Incoloy 800H at 649°C and 760°C. Points have been obtained from individual creep curves. The temperature effect on elongation is obvious. It seems that specimens in the wet helium environment deform faster than in air up to 5% total elongation. However, almost negligible effects of the

Figure 2.10. Effect of test environment on the high cycle fatigue of Hastelloy-X at 871°C (1600°F).

Figure 2.11. Stress-time plot for various amount of total deformation for Incoloy 800H.

helium environment on the stress rupture life and the minimum creep rates have been reported. The higher 5% strain to rupture time in the low stress range may indicate that environmental effects on the microstructural stability play a major role in determining the creep behavior in long term tests.

Preliminary results obtained to date from the drier helium environment are shown in Fig. 2.12 along with creep curves from air and the wet helium environment. At 649°C (1200°F) up to 600 hours, no significantly different creep behavior was observed in the drier helium atmosphere. However, the drier atmosphere improves the creep behavior at 760°C (1400°F) at the 7 ksi stress level. This effect will be more clearly understood as additional results become available.

2.2.2 Hastelloy X

Stress-time plots for 1%, 2%, and 5% total elongation for Hastelloy X at 760°C (1400°F) and 871°C (1600°F) are shown in Fig. 2.13. Each point has been obtained from individual creep curves. At 760°C (1400°F), specimens tested in the wet helium environment elongated faster than for air, but this effect was reversed at 871°C (1600°F). A slight lowering of stress rupture life and almost no effect on minimum creep rates by the wet helium environment have been reported previously in this study.

To date, one Hastelloy X specimen being tested at 16 ksi and 760°C (1400°F) has ruptured in the drier helium environment. Its creep curve is shown in Fig. 2.14 along with tests from air and the wet helium environment. Although its creep curve looks different, its rupture time of 762 hours, total elongation of 57% and minimum creep rate of 3.5×10^{-4} in/in/hour are very close to that for air or the wet helium environment. Significant improvement of creep property has been observed at 1600°F in the drier helium. However, detailed information will be obtained when the long duration tests are completed.

Metallographic studies were made on specimens fractured in the drier helium to determine the effects on microstructural changes. As shown in Fig. 2.15, the overall structures are similar to those for the wet helium environment, except there is a thinner oxide layer. Air tested specimens show dissolution of small carbides close to the surface.

Scanning electron microscope/microprobe analyses were carried out to investigate the changes of chemical composition of carbide phases in specimens fractured in the wet helium environment. The primary carbide is an M_6C type, which has a variable composition of Mo, Ni, Cr, Fe. Very small amounts of Cr rich $M_{23}C_6$ type carbides have been observed. The chemical changes in the carbides of specimens tested in air or helium can be attributed to diffusion controlled processes, resulting from oxidation. No definitive conclusions can be drawn concerning the effects of the helium environment on the changes of chemical composition of carbide phases. No significant changes of carbide chemistry through the specimens width have been noted in spite of the different carbide sizes and distributions in specimens tested over a range of temperatures and times.

Figure 2.12. Creep curves of Incoloy 800H.

Figure 2.14. Creep curves of Hastelloy X.

Figure 2.15. Microstructure of Hastelloy X rupture tested at 16 ksi at 760°C. Magnifications 500X.

2.3 Materials Test Loop (K. S. Lee, L. Gerlach, J. Hare)

Owing to the change of the helium chemistry from 2500 ppm water to 5-10 ppm water, some modifications have been made to the Materials Test Loop. These are as follows:

- 1) Installation of an automatic H₂ injection and venting system.
- 2) Replacement of Parametrics moisture monitor by Beckman Trace Moisture Analyzer (TMA).
- 3) Installation of an automatic water injection system.
- 4) Installation of an activated charcoal filter between the helium supply and the main helium loop.

In the past, the major reaction in the loop was

With high concentration of H₂O and CO, excess H₂ and CO₂ have always been produced in the loop. Therefore, H₂ content was controlled by venting the loop whenever the accumulation of H₂ exceeded the predetermined level. However, in the current drier environment in which insufficient H₂O is available to produce H₂, an external H₂ injection device became necessary to keep the H₂ level constant.

The inability to measure water content by the Parametrics moisture monitor has been described previously. The degradation of the aluminum oxide probe was probably the reason for the inaccurate water control. Accordingly, a new device, Beckman Trace Moisture Analyzer (TMA), has been installed. This instrument uses a detector cell made of thin coatings of P₂O₅ between the two rhodium electrodes. The moisture renders the P₂O₅ electrically conductive allowing the current to flow between the electrodes. This current dissociates the absorbed moisture into H₂ and O₂ regenerating dry P₂O₅. The current passing between the electrodes is directly proportional to the concentration of water in the sample.

The Beckman TMA installed was calibrated against an EG&G dew point meter. The results are shown in Fig. 2.16. Between the 10 and 60 ppm of water range, two readings are in good agreement. This instrument has functioned well during the last two months, but the detection cell can be deteriorated with time as with any other instruments working under the same principles.

At the beginning of the tests in the new drier environment, several anomalies were observed in the loop. Specifically, fast buildup of CO was noted. Without graphite to react with water, the origin of CO buildup has not been determined. In routine operation, the chemistry of the MTL is summarized in Table 2.1.

Figure 2.16. Calibration curve of Beckman Trace Moisture Analyzer against EG&G dew point meter for measurement of water vapor concentration.

Table 2.1

Impurity Levels in MTL (ppm)

	<u>Design</u>	<u>Average</u>
CO	40	45
CO ₂	10	4
H ₂	200	190
CH ₄	20	20
H ₂ O	5-10	7.6

2.4 Helium Impurities Loop (C. Sastre)

The analysis of previous experiments has continued for the purpose of developing a numerical model. The loop has been modified to improve its performance.

2.4.1 Stoichiometry of the CO/CO₂ Conversion

To study the reaction of CO and CO₂ in the loop, several experiments were performed in previous quarters. In these experiments, the hot sections of the loop were maintained at 1000°K, no graphite samples were present. The concentrations of either CO or CO₂ were changed by injection of a measured amount of gas and the composition of the gas in the loop was followed as the gases equilibrate.

The results of 21 experimental runs are shown in Figure 2.17. The plot displays CO concentration vs. CO₂ concentration, both in units of parts per thousand volume fraction. Each point represents a pair of gas concentration measurements, and each experiment results on a trajectory on this CO, CO₂ plane. For such plots a reaction in which one mole of CO₂ changes to one mole of CO would result on straight lines at a slope of -45 degree.

The figure shows two groups of trajectories. One group moves left and the other mainly down and slightly right. All trajectories appear to converge to a central region.

The trajectories starting from (5.5), (5.0), (3.0) and (1.0) follow a clear -45 degree slope, indicating a conservation of carbon in the gas phase. This is interpreted as a wall reaction

which conserves carbon on the gas phase.

The trajectories starting with CO rich mixtures, show a more complicated behavior. The excess CO could adjust by

resulting in slopes of -45 degree, -63 degree and -90 degree, respectively. The trajectories observed show some initial portions at about -63 degree slope followed by a steeper drop, indicating that no reaction clearly dominates the kinetics. The cluster of trajectories starting at 6.5 CO corresponds to a series of runs starting after the loop was hydrogen fixed to reduce the walls. The first trajectory is the one that drops rapidly. As the walls become more oxidized the trajectories show that more of the CO is converted to CO₂.

STOICHIOMETRY OF CO CO₂ CHANGES

Figure 2.17

2.4.2 Model for Gas Kinetics

A simple model is being developed for the correlation of the kinetics of the loop. The assumptions used in the model reflect the observations in experiments conducted to date. The reactions are all of the gas-solid form. The oxidation and reduction of carbon and hydrogen involve the oxidation and reduction of iron, which is consistent with the observed equilibria of CO-CO₂ and H₂-H₂O. The activities of iron and iron oxide are less than one and change during the course of an experimental run. Reaction rates for a reaction of the form

are

$$\frac{dA}{dt} = K_1 A \cdot B - K_2 C \cdot D$$

with the condition that K_1 and K_2 satisfy the thermodynamic equilibrium constant. The activity of a solid is of the form

$$a_A = \frac{A}{b + A}$$

where b is an arbitrary constant.

At present the reactions being considered are:

The reaction

has not been included, it can be entered into the model if the need arises as more data is analyzed. Similarly, the reaction

known to occur in the loop has not been modeled yet to control the initial complexity of the model.

A term for the diffusion of H₂ out of the loop will have to be included since the changes in its concentration are dominated by this loss mechanism.

2.4.3 Hydrogen Diffusion

A series of runs were made to investigate the loss of hydrogen from the system. The rate of loss of hydrogen was found to be approximately

proportional to the partial pressure, with a half-life of about 200 hours. The loss of hydrogen was followed at 920°K, 970°K and 1020°K (at room temperature the rate could not be measured) and the rate was found to vary with temperature with an apparent activation energy of about 30 Kcal/mole.

While performing these experiments it was found that a dead end volume existed in the loop and this introduced a "memory" that complicated the observed transients and confused the interpretation. The loop has been modified to insure adequate circulation and mixing everywhere.

2.4.4 Loop Improvements

The loop has been shut-down for changes. A better temperature control of the hot zone has been installed. A vacuum gage has been added to aid in leak and outgassing control. An EG&G water analyzer was installed to supplement the infrared analyzer. The piping to the main manometer has been rerouted to avoid dead end volumes.

3. Fuel and Fission Products

3.1 Molybdenum Migration in H-451 Graphite (G. Uneberg, C. Sastre, D. G. Schweitzer)

In a hypothetical worst case scenario the complete loss of cooling of the core of a High Temperature Gas Cooled Reactor (HTGR) could ultimately result in core temperatures as high as 3600°C. The prediction of migration of radioactive materials through the graphite is necessary for the analysis of such hypothetical accidents.

Since extrapolation from models formulated for lower temperatures is uncertain, experimental determinations of diffusion coefficients were initiated.

In our initial work on this problem, molybdenum, in the form of Mo₂C, has been chosen as the migrating species. This is because molybdenum is a fission product, is chemically stable as a carbide, and has non-decaying isotopes that can be used to simulate the active isotopes.

The experiments are performed by loading a thin layer of Mo₂C into a flat bottomed cavity in a H451 graphite (Great Lakes Carbon Corp.) cylinder used as the susceptor of a 30 kw induction furnace.

After heating the sample to temperatures spanning the melting point of Mo₂C (2690°C), the graphite is machined to separate the cylindrical portion lying directly below the plane of the Mo₂C melt. This cylinder is then sliced along planes parallel to the plane of the melt and these slices are ashed and assayed for molybdenum. This results in values of concentration averaged over the volume of the slice for various distances from the Mo₂C source.

To check the possibility that molybdenum was diffusing into the sample susceptors from the surrounding environment (e.g. the insulating medium), a blank graphite susceptor containing no molybdenum was heated to a temperature of 3000°C for 4 hours and then assayed. No molybdenum other than an approximate 0.5 ppm background was found.

It is noteworthy that the family of curves (Figure 3.3) generated by this series of experiments seem to extrapolate back to a virtual source of about 30 ppm concentration. This would seem to indicate that there is more than one phenomenon involved in the diffusion process, since the real source has a molybdenum concentration orders of magnitude greater. Interestingly, 30 ppm molybdenum corresponds to less than monolayer coverage of the graphite. Accordingly, the "apparent" diffusion coefficients, D, have been calculated using the assumption that the molybdenum is drawn from a non-depletable source of 30 ppm concentration. Under these circumstances, the diffusion very closely resembles Fickian diffusion in the geometry of the experiment.

The geometry of the sample had been selected originally to approach a constant infinite plane source to simplify the analysis. However, the

region in which the molybdenum concentration is non-negligible was found to have dimensions comparable with the lateral dimensions of the source and of the diffusion volume. Therefore, the fitting of the data for the inference of an effective diffusion coefficient required a two dimensional time dependent analysis. The heat conduction computer code, TAC-2D was used to solve the time dependent-two dimensional analog. The geometrical dimensions were retained in the calculation and the diffusivity was set to 1 cm²/sec. Adiabatic boundary conditions were assumed for the outer surfaces of the volume. Since the time scales inversely proportional to the diffusion coefficients, if the distribution observed after T seconds matches the distribution computed for t seconds;

$$D = \frac{t}{T} \text{ cm}^2/\text{sec} .$$

The computed diffusion equation solutions were averaged over the cross section of the cylinder sliced for samples for analysis. The average concentration as a function of distance from the source was plotted as a function of distance from the source with time as a parameter. This set of curves was used to match the results and determine the time t, and thereby infer D.

The experimentally obtained diffusion coefficients are;

$$D = 5.6 \times 10^{-4} \text{ cm}^2/\text{sec} \quad @ 3200^\circ\text{C for 1 hour}$$

$$D = 4.0 \times 10^{-4} \text{ cm}^2/\text{sec} \quad @ 3100^\circ\text{C for 33 minutes}$$

$$D = 2.4 \times 10^{-4} \text{ cm}^2/\text{sec} \quad @ 3000^\circ\text{C for 8 hours}$$

$$D = 2.8 \times 10^{-4} \text{ cm}^2/\text{sec} \quad @ 3000^\circ\text{C for 4 hours}$$

$$D = 8.3 \times 10^{-5} \text{ cm}^2/\text{sec} \quad @ 2900^\circ\text{C for 1 hour.}$$

The results appear to be internally self-consistent, with two independently obtained coefficients at 3000°C agreeing to within 16%. Noteworthy is the fact that the experimentally observed results give a diffusion coefficient which is several orders of magnitude greater than that calculated using the correlation used in the SORS code:

$$-\log_{10} D = A + \frac{B \times 10^3}{T}$$

where, for MO: A = 1.0, B = 19.2 and T in in °K. This has been discussed in a previous progress report.

An Arrhenius plot of the diffusion coefficient, shown in Figure 3.2, yields an activation energy of 132 kcal per mole for the diffusion of Mo₂C in H451 graphite. Since the 90% confidence interval is rather large (60 to 204 kcal/mole) this value must be considered preliminary, until more data can be obtained.

Although several experiments were performed at temperatures below the melting point of Mo₂C (2690°C), diffusion coefficients for these have not been obtained. At these lower temperatures the diffusion is so slow that the molybdenum present as background in the graphite (0.1-0.5 ppm) masks any due to diffusion. In any case, the sub-ppm region is at the lower limits of detectability for the wet chemical method used for analysis.

3.2 Fission Product Migration Studies (I. N. Tang and H. R. Munkelwitz)

An experimental program was initiated during the report period to study the migration of semi-volatile fission products from source locations in heated type H451 graphite to the ambient environment. One of the mechanisms under investigation is the transport of Sr associated with or adsorbed on the airborne condensation nuclei evolved when graphite is heated to high temperatures.

A high temperature flow system capable of temperatures in excess of 2400°C was constructed and tested. Basically it consists of an inductively heated temperature gradient tube through which the volatilized species are passed in flowing helium. The removal of the condensibles is effected by diffusion to and deposition on the cold walls following the high temperature section. Particles carrying the species of interest (in this case Sr) pass through and are collected on 0.2 µm floropore filters which are subsequently analyzed for Sr by atomic absorption.

A typical experiment is conducted in the following manner. Thin (2 mm x 2 cm) wafers of H451 graphite are placed in a vacuum oven and outgassed under vacuum at about 150°C until a constant weight is attained. The pre-weighed wafers are then placed in a glass vessel which is first evacuated and then backfilled with Sr(NO₃)₂ aqueous solution of a predetermined concentration. After an overnight soak the wafers are removed from the vessel, dried in the vacuum oven to a constant weight and the final weight is noted. The amount of Sr(NO₃)₂ salt absorbed in the pore structure of the graphite is then calculated from the weights before and after impregnation for each wafer.

Both the impregnated and some unimpregnated wafers are then alternately spaced on an H451 graphite pedestal and placed in the temperature gradient apparatus. The assembled source is then inductively heated in flowing helium with the floropore filters bypassed to a temperature of about 1100°C where the Sr(NO₃)₂ is converted to SrO:

After allowing a sufficient time for conversion (about 30 min) the filter is exposed to the flowing gas stream and the temperature of the specimen is slowly increased. At a predetermined level the temperature is held constant for the run duration. At the conclusion of the run the filters are removed and analyzed for Sr by atomic absorption. From the analytical result and the measured initial amount of strontium in Sr(NO₃)₂ the percent of strontium on the filter is calculated.

The results of three preliminary experiments at various initial concentrations of SrO are shown in Table 3.1. These experiments were conducted with the same source geometry with identical heating rates for the same time period and temperature (1500°C). The results indicate that a considerable portion of the starting Sr reached the filter presumably as an aerosol. Since SrO may be reduced to metallic Sr by graphite at high temperatures, the vaporized Sr is likely to be in the metallic state condensed on particle surfaces. More work is in progress to elucidate the transport mechanism and to determine the parameters governing fission product migration under conditions postulated for HTGR accidents.

Table 3.1 (1500°C)

<u>Initial SrO</u>	<u>Initial Sr</u>	<u>Filter Sr</u>	<u>Percent Sr Transported</u>
0.0887 g	0.0750	0.0032	4.27
0.0612 g	0.0518	0.0043	8.30
0.0091 g	0.0077	0.0003	3.90

REFERENCES

- PETERSON, J. F., "TAC2D. A General Purpose Two-Dimensional Heat Transfer Computer Code," GA-8868, Sept. 1969.
- SCHWARTZ, M. H., SEDGLEY, D. B. and MENDONCA, M. M., "SORS: Computer Programs for Analyzing Fission Product Release From HTGR Core During Transient Temperature Excursions," GA-A 12462, April 1974.
- UNEBERG, G., SASTRE, C. and SCHWEITZER, D. G., "Molybdenum Migration in H451 Graphite," in Reactor Safety Research Quarterly Progress Report, April 1 - June 30, 1979, Brookhaven National Laboratory, BNL-NUREG-51082.

Figure 3.1. One half of a susceptor showing that region directly under the plane of the melt which is subjected to wet chemical analysis. Slices of thickness .125"-.500" are taken in the plane parallel to the melt.

ACTIVATION ENERGY.. = 131.824 kcal/mol
 90% CONFIDENCE INTERVAL... 59.677 to 203.970
 Temperature deg K

Figure 3.2. Arrhenius plot of data from Figure 3.3.

Figure 3.3. Experimentally obtained diffusion profiles for the migration of molybdenum in H451 graphite.

Figure 3.4. Solutions, in the experimental geometry, generated by the computer code TAC2D.

4. Analytical

4.1 Conversion of HTGR Safety Codes (J. Colman)

The Oak Ridge codes ORTAP, CORTAP, ORECA, and BLAST have been converted to run on the BNL CDC 7600, except for their plotting capabilities. The sample test cases for CORTAP, ORECA, and BLAST were matched with satisfactory accuracy. The code appears to be running satisfactorily with no major problems; however, in some areas, the results of the sample test case do not match the Oak Ridge results as closely as expected. These differences appear to come primarily from the turbine section of the code and Oak Ridge is giving some assistance in attempting to locate the origin of the differences.

Table 4 is a listing of our HTGR Safety Code Library to date.

Table 4

HTGR Safety Code Library

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
CRECT	OP	NP	Corrects data on ENDF/B tape.
LISTFC	OP	NP	Lists data from ENDF/B tape.
RIGEL	OP	NP	Manipulates data on ENDF/B tape.
ENDFB2	OP	NP	Converts data on ENDF/B tape to binary.
FLANGE	OP	NP	Prepares thermal cross section transfer arrays.
GAND2	OP	NP	Prepares fine group fast, resonance, and thermal cross sections from ENDFB2 binary tapes.

C = In the process of being converted to the CDC 7600.
 OP = Operational on the BNL CDC 7600 system under Scope 2.
 R = Recently received from General Atomic Co. or Argonne Code Center.
 P = General Atomic Co. proprietary code.
 NP = Not considered to be a proprietary code.
 B = In the process of development at Brookhaven National Laboratory.
 L = Recently received from Los Alamos Scientific Laboratory.
 I = Inactive.
 O = Recently received from Oak Ridge National Laboratory.

Table 4 Cont'd.

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
GFE2	OP	NP	Prepares fine group fast cross sections from ENDFB2 binary tapes.
MAKE	OP	NP	Prepares fine group fast cross section tape from GFE2 for spectrum codes.
WTFG	OP	NP	Prepares fine group thermal cross section tape from GAND2 or FLANGE for spectrum codes.
PRINT	OP	NP	Reads the fast cross section tape produced by MAKE.
SPRINT	OP	NP	Reads the thermal cross section tape produced by WTFG.
GGC4	OP	NP	Prepares broad group cross sections from MAKE and WTFG tapes.
INTERP	OP	NP	Prepares broad group cross sections from MICROX output data tapes.
1-DX	OP	NP	Performs one-dimensional, diffusion theory, steady state calculations.
FEVER-7	OP	NP	Performs one-dimensional, diffusion theory, burnup and reload calculations.
TEMCO-7	OP	NP	Computes reactor temperature coefficients from input cross section data.
BLOOST-7	OP	NP	Performs zero-dimensional reactor kinetics calculations.
GAKIT	OP	NP	Performs one-dimensional reactor kinetics calculations.
TWICL	OP	NP	Performs two-dimensional light water reactor kinetics calculations.
TAC-2D	OP	NP	Performs two-dimensional, transient conduction analyses.

Table 4 Cont'd.

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
FLAC	OP	NP	Calculates steady state flow distributions in arbitrary networks with heat addition.
POKE	OP	P	Calculates steady state flow distributions and fuel and coolant temperatures in a gas cooled reactor.
PREPRO	OP	P	Prepares input data and source code revisions for RECA code.
RECA	I	P	Calculates time dependent flow distributions and fuel and coolant temperatures in the primary system.
CORCON	OP	P	Computes the temperature history and fission product redistribution following a loss of all convective cooling of the core.
SORS	OP	P	Computes the release of volatile fission products from an HTGR core during thermal transients.
GOPTWO	OP	NP	Analyzes the steady state graphite burn-off and the primary circuit levels of impurities.
OXIDE-3	OP	P	Analyzes the transient response of the HTGR fuel and moderator to an oxidizing environment.
SAMPLE	OP	NP	Propagates uncertainties in probability distributions by Monte Carlo technique.
TAP	OP	P	Calculates the transient behavior of the integrated HTGR power plant.
SORSG	OP	P	Computes the release of non-volatile gaseous fission products from an HTGR core during thermal transients.
DIFFTA	OP	NP	Solves the steady state, two-dimensional diffusion equation by finite element method.

Table 4 Cont'd.

Program	Status	Proprietary	Function
DIFFT1	OP	NP	Solves the time dependent, 2-D diffusion equation by the finite element method.
PDQ-7	OP	NP	Analyzes reactors in up to three space dimensions via diffusion theory.
SOSNCC	OP	NP	Calculates steady state natural convection flow rates during long term loss of power.
OSCIL	OP	NP	Simulates one-dimensional spring mass system for seismic analysis of HTGR core.
H-CON1	OP	NP	Calculates one-dimensional heat conduction for an HTGR fuel pin by finite difference method.
HYDRA-1	OP	NP	Computes thermal/hydraulic parameters for single phase liquid due to external heat source.
CONTEMPT-G	OP	P	Simulates temperature-pressure response of an HTGR containment atmosphere to postulated coolant circuit depressurization.
SOSSME	OP	NP	Solves the steady state one-dimensional momentum equation.
HAZARD	OP	NP	Analyzes gas layering and flammability in an HTGR containment vessel following a depressurization accident.
CIRC (formerly JETS)	OP	NP	Calculates fluid dynamics in an HTGR containment vessel following a depressurization accident.
ORIGEN	OP	NP	Solves the equation of radioactive growth and decay for large numbers of isotopes with arbitrary coupling.
MOSBDA	OP	NP	Analyzes experimental data from Mossbauer spectrometer.
INREM	OP	NP	Calculates internal radiation doses.

Table 4 Cont'd.

Program	Status	Proprietary	Function
EXREM	OP	NP	Calculates external radiation doses.
SODEMME	OP	NP	Calculates transient thermal hydraulic aspects of circulating gas systems.
KACHINA	OP	NP	Calculates fully interpenetrating fluid flows using Implicit Multifield (IMF) method, for handling different material fields.
SWIRL-S	OP	NP	Calculates fluid dynamics for two-dimensional steady state recirculating flows.
SWIRL-T	B-I	NP	Calculates fluid dynamics for two-dimensional time-dependent recirculating flows.
CHAP-1 (Jan. 1978)	OP	NP	Simulates the overall HTGR plant with both steady state and transient solution capabilities.
EVAP	OP	NP	Calculates evaporation and redistribution of fission products during a temperature transient.
BAAL	OP	NP	Calculates three-dimensional fluid flows at all speeds with an Eulerian-Lagrangian computing mesh.
LEAF	I	NP	Calculates fission product release from a reactor containment building.
SUVIUS	I	NP	Solves the behavior of fission gases in the primary coolant of a gas-cooled reactor.
FYSMOD	I	NP	Calculates the two-dimensional solution of HTGR core blocks subjected to external motion.
NONSAP-C	I	NP	Calculates static and dynamic response of three-dimensional reinforced concrete structures, in addition to creep behavior.

Table 4 Cont'd.

Program	Status	Proprietary	Function
LARC-1	I	NP	Calculates fission product release from BISO and TRISO fuel particles of an HTGR during the LOFC accident for single isotopes.
LARC-2	I	NP	Similar to LARC-1; in addition, handles release from isotope chains.
QUIL/QUIC	OP	NP	Solves complex equilibrium distribution in chemical environments.
FENG, RATE and SURF	OP	NP	Three codes which create or add to the reactions data library for QUIL and QUIC codes. Reactions added are of types Free Energy, Rate and Surface, respectively.
RICE	OP	NP	Solves transient Navier-Stokes equations in chemically reactive flows.
THGRAF	OP	NP	Calculates position and velocity of the thermo-chromatograph as a function of time for various models.
FPPROD	OP	NP	Performs simplified fission product production analysis.
LASAN-LASL	I	NP	A general systems analysis code consisting of a model independent systems analysis framework with steady state, transient and frequency response solution capabilities. There are two versions of the code available - the original LASL version and the converted BNL version.
LASAN-BNL	OP	NP	
CHAP-2 (dec. 1978)	I	NP	Simulates the overall HTGR plant with both steady state and transient solution capabilities.
ORECAL	OP	NP	Simulates the dynamics of HTGR cores for emergency cooling analyses.
CORTAP	OP	NP	A coupled neutron kinetics - heat transfer program for the dynamics simulation of the HTGR core.

Table 4 Cont'd.

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
BLAST	OP	NP	A dynamic simulation of the HTGR reheater - steam generator module.
ORTAP	O/C	NP	A nuclear steam supply system simulation for the dynamic analysis of HTGR transients.

4.2 Application of the Available HTGR Safety Codes (P. G. Kroeger)

Following successful implementation of the Oak Ridge HTGR codes ORECA, CORTAP and BLAST, familiarization with these codes through trial runs has begun, with the ultimate objective, to enhance the confidence in these codes and to outline any inherent limitations, thus increasing the utility of these codes for licensing computations.

The ORECA code was executed with several variations of input parameters and with some modification of the model, to assess the sensitivity of the resulting core and coolant temperatures to study changes. Preliminary indications are that some of the variations, for instance modifications of the temperatures used in some of the pressure drop terms, resulted in significant changes of the core and coolant temperature histories, indicating that the sensitivity of the output data to such model variations would be greater than expected. This result and other variations are currently being investigated in more detail.

During these preliminary evaluations and trial runs several questions regarding some details of the code have arisen. Upon completion of this sensitivity evaluation the results and any remaining questions will be taken up with Oak Ridge personnel, with suggestions for code improvements and/or a summary stating limitations of these codes.

4.3 HTGR - Gas Turbine Plant Licensing Considerations (P. G. Kroeger)

To identify areas of primary importance in safety and licensing considerations of HTGR gas turbine plants, as well as HTGR process heat or cogeneration plants, a small exploratory systems model of the thermohydraulics of such cycles has been outlined and is currently being programmed. This program uses simple first-order models of the various system components and employs a modular structure, permitting later refinement of individual components, as desired. A computations framework including steady state and transient capabilities has been programmed and debugged, and is executing with recuperator and precooler modules. Preliminary modules of the core and of the turbo-machinery have been programmed, and will be added to the system program shortly.

II. LMFBR SAFETY EVALUATION

SUMMARY

The effect of a dispersed condensed phase on Rayleigh-Taylor stability of the gas-liquid interface in an expanding post-disassembly bubble was investigated numerically. Growth constants for the two-phase bubble expanding against the liquid sodium pool are calculated from both Taylor and porous media models for various interface accelerations. Both theories predict a critical disturbance wave number at which the growth constant becomes maximum, the fastest growing disturbance. Decreasing the permeability of the bubble is shown to have a stabilizing effect on interfacial disturbance growth. For a UO_2 bubble with 90% void fraction and droplet radius approximately $1\text{ }\mu\text{m}$ or less, the potential for entrainment by Taylor instability is shown to be vanishingly small, whereas for particles of radius approximately $100\text{ }\mu\text{m}$, the heavy phase has no effect on the development of instabilities and entrainment of sodium is possible.

The problem of natural convection heat transfer along a vertical flat plate with uniform volumetric heat source in the fluid was investigated. The transport equations were non-dimensionalized and the Rayleigh number based upon $\dot{q}'''$ was identified as

$$\text{Ra}^* (\dot{q}''') = \frac{g\beta \dot{q}''' x^5}{\rho c v^3}$$

Experimental data were taken at wall angles of 90° (vertical), 75° , and 60° . The average and local heat transfer data were correlated similarly to conventional natural convection and the exponent for the Rayleigh number was assumed equal to 0.25. The preliminary results for the local and average correlations are listed below:

$$\text{LOCAL: } \text{Nu}(x) \simeq (.188 \pm .026) \text{Ra}^* (\dot{q}''', x)^{0.25}$$

$$\text{AVERAGE: } \overline{\text{Nu}} \simeq (.158 \pm .013) \text{Ra}^* (\dot{q}''', L)^{0.25}$$

These correlations are useful for calculating heat losses from volume-heated pools and for computing pool growth into melting media. These correlations are preliminary and subject to change.

The Super System Code (SSC) development program encompasses a series of four computer codes: (1) SSC-L for system transients in loop-type LMFBRs; (2) SSC-P for system transients in pool-type LMFBRs; (3) SSC-W for system transients in LWRs and (4) SSC-S for long term shutdown transients in reactor systems.

During this quarter, under SSC-L code development, investigations of localized thermal buoyancy effects in LMFBR piping systems were done. It was found for a very severe transient, that the one-dimensional treatment used in SSC-L is sufficient to adequately predict the thermal response in the piping. Hypothetical loss-of-heat-sink analyses were conducted to study in-vessel natural convection in homogeneous and heterogeneous core designs. It was found that the homogeneous core design led to higher in-vessel recirculation flow rates than the heterogeneous design. Work on LMFBR accident progression analysis is continuing. A simple correlation to predict the steady-state natural circulation behavior of LMFBR plants was developed. Modifications and extensions are being implemented in the fuel heat conduction and steam generator modules. User support is continuing.

Under the SSC-P development effort, the SSC-P code was applied to analyze protected and unprotected loss-of-electric-power events. Substantial new data was derived, particularly for the Phenix core, from related information uncovered in the literature.

A major milestone was met under the SSC-W development effort when the first version of the SSC-W code became operational at BNL in late March. This version is applicable to PWR system designs utilizing once-through steam generators. Extensive testing and applications work are being initiated.

Work on the SSC-S code was resumed in the area of intra-assembly effects.

During this quarter, primary attention under the SSC code validation effort continued to focus on the prediction of the FFTF acceptance tests, with SSC-L. A report covering these analyses has been written. Additionally, inter-code comparisons for specific transients are being accomplished using SSC-L/DEMO for CRBRP transients and SSC-L/IANUS for FFTF transients.

1. Thermal Hydraulic LMFBR Safety Experiments

1.1 HCDA Bubble Energetics: Role of Taylor Instabilities (J. Moszynski, U. of Delaware; T. Ginsberg)

The objective of this task is to characterize the mechanisms of entrainment of liquid sodium into the post-disassembly multi-phase bubble during a hypothetical core disruptive accident in an LMFBR. The present effort is directed primarily toward analysis of the influence of the heavy liquid phase of the bubble on the growth rate of Taylor instabilities.

1.1.1 Effect of a Dispersed Condensed Phase on the Rayleigh-Taylor Stability of a Gas-Liquid Interface.

In a previous quarterly report (Ginsberg, et al., 1980) a porous matrix model was described, which provides a bounding estimate of the effect of a heavy entrained phase in an expanding post-disassembly bubble on the development of Rayleigh-Taylor instabilities. The basic model assumption is that the entrained phase is characterized by infinite inertia and acts simply to exert a drag force on the fluid flowing past it. The drag force is modeled using Darcy's law. Calculations were presented for systems which have been studied experimentally, e.g., water-nitrogen. The objective of the following discussion is to present additional calculations for conditions prototypic of post-disassembly bubble circumstances.

A multi-phase bubble, composed of UO_2 vapor and UO_2 liquid and solid is assumed expanding against a pool of liquid sodium, as represented schematically in Fig. 1.1. Table 1.1 presents the material property values used in the calculations. Permeabilities of the porous matrix medium (multi-phase bubble) were computed using Brinkman's theory (Scheidegger, 1957) for a bubble void fraction of 0.9, and for various particle sizes. The permeabilities are shown in Table 1.2.

Results are presented in Figs. 1.2(a)-1.2(d) for the exponential growth constants, as a function of disturbance wave number. These were computed using the relationship (Ginsberg, et al., 1980)

$$\bar{n} = -\frac{\mu_2}{2\rho_1 k} \pm \sqrt{\left(\frac{\mu_2}{2\rho_1 k}\right)^2 + \left(1 - \frac{\rho_2}{\rho_1}\right) \bar{a} \kappa} \quad (1.1)$$

The classical Taylor theory gives the relationship (Taylor, 1950)

$$n = \sqrt{a \kappa \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2}} \quad (1.2)$$

Figure 1.2 presents the growth constant results for both the Taylor and porous medium models, for accelerations of 10 , 10^2 , 10^3 and 10^4 m/s^2 . Note that both theories predict a cutoff wave number, beyond which disturbances do not grow. This is due to the surface tension effect. A strong influence of permeability is observed, especially for small accelerations. The smaller the permeability, the greater is the influence of the entrained heavy phase on the instability growth. The drag between the particles (or droplets) and the accelerating vapor provides a stabilizing effect on the interface. For large permeability, the porous medium model results approach that of the Taylor model. This is especially true for the larger accelerations, where the influence of the permeability is not as strong as for the smaller accelerations.

Both the Taylor and porous medium theories predict that at some critical wave number, K_{CRIT} , the growth constant is a maximum. These constants represent the growth rate of the fastest growing instability for a given set of conditions (permeability and acceleration). The magnitude of K_{CRIT} is, for a given acceleration, independent of the permeability. The growth constants corresponding to the critical wave numbers are presented in Fig. 1.3 as a function of permeability. They are presented in dimensionless form, using the Taylor result as the scale factor.

The results display the strong stabilizing effect of the permeability on the disturbance growth rate, especially for small and intermediate accelerations. For bubble void fractions of approximately 0.9, if the heavy entrained phase particle radius is $100 \mu\text{m}$ (corresponding to $k \approx 10^{-8} \text{ m}^2$), then the stabilizing influence of the porous medium drag disappears. The presence of particles does not influence the interfacial disturbance growth rate. On the other hand, if the particle size is $1 \mu\text{m}$, the growth constant is affected by at least one order of magnitude for all accelerations up to 10^4 m/s^2 . This effectively means that the disturbance growth rate would become vanishingly small.

The porous medium (infinite particle/droplet inertia) model of multi-phase bubble dynamics represents one limit of particle-vapor interaction under acceleration. The model predicts that the medium permeability limits instability growth.

1.1.2 Implications with Respect to Sodium Entrainment.

The basic issue to which this work is addressed is that of the potential for entrainment of liquid sodium into an expanding HCDA bubble. Whether the entrained sodium acts to amplify the work potential of the bubble, or whether it acts as a heat sink, depends upon the rate and quantity of sodium entrained. The work presented here is directed specifically to evaluation of the potential for entrainment by the mechanism of growth of Rayleigh-Taylor instabilities.

The porous medium instability growth model described here suggests

- (1) If the HCDA bubble is characterized by a void fraction of approximately 0.9, and if the heavy entrained phase droplet or particle radius is approximately $1 \mu\text{m}$ or less, then the potential for

entrainment by Taylor instabilities is small for accelerations up to 10^4 m/s^2 . Since the potential for entrainment is small, then sodium entrainment by Taylor instability growth would have little influence on the work potential of the HCDA bubble.

- (ii) If the heavy particle radius is approximately $100 \mu\text{m}$ or greater, then the presence of the heavy phase has no influence on the development of Taylor instabilities, and entrainment by the growth of these instabilities is possible. The rate of early (linear) growth of the disturbances may be computed using the Taylor theory, neglecting the presence of the heavy phase. The rate of entrainment cannot be predicted using the linear theory. The influence of sodium entrainment, by growth of Taylor instabilities, on the work potential of the HCDA bubble cannot be predicted using the methods described here.

The above conclusion with respect to sodium entrainment via growth of Taylor instabilities must be evaluated against a model which accounts for the finite inertia of the entrained discrete phase. Such a model has been developed and will be reported in future work.

1.2 Heat Transfer in Internally Heated Boiling Pools (G.A. Greene)

The purpose of this task is to study and characterize local boundary heat transfer and void distributions in volume-heated pools. Experiments have been performed for boiling pools with vertical and inclined boundaries and models have been developed for local and average heat transfer correlations and void fraction distributions.

This quarterly report presents the preliminary correlation of local and average heat transfer data from volume-heated non-boiling pools to vertical and inclined surfaces.

1.2.1 Analytical Development

Consider the problem of natural convection along a vertical flat plate with uniformly distributed volumetric heat source in the fluid. Adopting the usual boundary layer convention and neglecting terms of order less than one, the governing equations become

$$\text{MASS:} \quad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (1.3)$$

$$\text{MOMENTUM:} \quad \frac{Du}{Dt} = \nu \frac{\partial^2 u}{\partial y^2} + g_{\text{eff}} \beta (T - T_{\infty}) \quad (1.4)$$

$$\text{ENERGY:} \quad \rho c \frac{DT}{Dt} = k \frac{\partial^2 T}{\partial y^2} + \dot{q}''' \quad (1.5)$$

Define the following dimensionless variables

$$u^* = u/u_{\text{ref}} \quad (1.6a)$$

$$v^* = v/u_{\text{ref}} \quad (1.6b)$$

$$x^* = x/L \quad (1.6c)$$

$$y^* = y/L \quad (1.6d)$$

$$\theta = \frac{(T - T_{\infty})}{\dot{q}''' L^2 / \rho c v} \quad (1.6e)$$

where $u_{\text{ref}} = v/L$. Then substituting into Eqs. (1.3-1.5), the governing equations become transformed into dimensionless form as shown below in Eqs. (1.7-1.9), respectively:

$$\frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*} = 0 \quad (1.7)$$

$$u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*} = \frac{\partial^2 u^*}{\partial y^{*2}} + Ra^* \theta \quad (1.8)$$

$$u^* \frac{\partial \theta}{\partial x^*} + v^* \frac{\partial \theta}{\partial y^*} = \frac{1}{Pr} \frac{\partial^2 \theta}{\partial y^{*2}} + 1 \quad (1.9)$$

The boundary conditions are

$$u^* = v^* = 0, \theta = \theta_w ; y^* = 0 \quad (1.10a)$$

$$u^* = \theta = 0 ; y^* \rightarrow \infty \quad (1.10b)$$

Note the appearance of the Rayleigh number, Ra^* , which is defined on the basis of the uniform volumetric heat source, $\dot{q}'''$, and not in the usual fashion based upon a film temperature difference or uniform wall heat flux. The form of the Rayleigh number is

$$Ra^* = \frac{g_{\text{eff}} \beta \dot{q}''' x^5}{\rho c v^3} \quad (1.11)$$

The local and average heat transfer data from volume-heated non-boiling pools will be correlated to this parameter as

$$Nu = K Ra^{*n} \quad (1.12)$$

where K and n will be determined from log-log-linear least square fit to the data.

1.2.2 Experimental Procedure

The experiments performed with volume-heated non-boiling pools were identical to the procedure for the boiling heat transfer experiments previously performed with the obvious difference that the pool was not boiling and the void fraction was zero (Greene et al, 1980a). The local heat transfer coefficient, $h(x)$, was calculated from the experimental data as previously reported (Greene et al, 1979),

$$h(x) = \frac{k_{BN} (T_F(x) - T_B(x))}{a \cdot (T_{pool} - T_F(x))} \quad (1.13)$$

Since, in non-boiling pools, T_{pool} is not constant along the vertical axis of the pool, a characteristic reference temperature was chosen. T_{pool} was measured outside the wall boundary layer at a point along the vertical axis midway between the pool bottom and the free surface.

The average heat transfer coefficient was calculated as reported previously (Greene, 1980a) by integrating the local heat transfer coefficient along the heat transfer surface as

$$h_{av} = \frac{1}{L} \int_0^L h(\eta) d\eta \quad (1.14)$$

Experiments were performed for wall angles of 90° (vertical), 75°, and 60°. The effective gravitational component (Greene et al, 1980b) parallel to the surface was used in Eq. (1.11).

1.2.3 Preliminary Data Correlation: Local and Average Boundary Heat Transfer

For the local and average heat transfer data, the local and average Nusselt number and Rayleigh number were calculated. The local data for all wall angles (90°, 75°, and 60° wall inclination from horizontal) tested are plotted without statistical culling in Figure 1.3.

For the purpose of this report, the exponent n in Eq. (1.12) was assigned a value of 1/4 for all the experimental data. The coefficient K was calculated as follows,

$$K_{av} = \frac{1}{N} \sum_{i=1}^N \frac{Nu_i}{Ra_i^{1/4}} = \frac{1}{N} \sum_{i=1}^N K_i \quad (1.15)$$

The standard deviation, σ_K , in the correlation coefficient, K_{av} , was calculated as follows,

$$\sigma_K = \left[\frac{1}{N} \sum_{i=1}^N (K_i - K_{av})^2 \right]^{1/2} \quad (1.16)$$

All points outside the range $\pm 1 \sigma$ were disregarded in the correlation. Due to

the condition that the exponent n was assigned a value of $1/4$, these correlations are to be treated as preliminary and subject to change.

For the local non-boiling heat transfer data, the correlation was of the form,

$$Nu(x) \simeq (.188 + .026) Ra^*(x)^{1/4} \quad (1.17a)$$

and for the average non-boiling heat transfer data, the correlation was of the form,

$$\overline{Nu} \simeq (.158 + .013) Ra^*(x)^{1/4} \quad (1.17b)$$

NOMENCLATURE

a	Test wall thickness
$\overline{a}$	Acceleration of interface
c	Specific heat
g_{eff}	Effective gravity
h	Heat transfer coefficient
K	Coefficient (see Eq. 1.12)
k	permeability
k_{BN}	Thermal conductivity of Boron Nitride
L	Length of boundary layer
n	Exponent (see Eq. 1.12)
$\bar{n}$	Exponential growth constant
N	Total population
Nu	Nusselt number
Pr	Prandtl number
$\dot{q}'''$	Volumetric heat source
Ra^*	Rayleigh number
T	Temperature

u	X-component velocity
v	Y-component velocity
x	Coordinate parallel to surface
y	Coordinate normal to surface

Greek Symbols

α	Thermal diffusivity
β	Coefficient of thermal expansion
η	Variable of integration
θ	Dimensionless temperature
κ	Disturbance wave number
μ_2	Viscosity of vapor
ν	Kinematic viscosity
ρ	Density
ρ_1	Liquid density
ρ_2	Vapor density
σ	Standard deviation

Subscripts

av	Average
B	Back-side
F	Front-side
local	Local
i	Iteration counter
pool	Pool value (at $y \rightarrow \infty$)
ref	Reference
∞	Infinity

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Figure 1.1. Schematic of HCDA Bubble in Reactor Vessel.
(BNL Neg. No. 3-1296-80)

Table 1.1
PROPERTY VALUES

Density Upper Liquid (Sodium), $\rho_1 = 823.3 \text{ kg/m}^3$
 Density Vapor in Bubble (UO_2), $\rho_2 = 1.1 \text{ kg/m}^3$
 Surface Tension (Sodium), $\sigma = 0.1529 \text{ N/m}$
 Viscosity Vapor in Bubble (UO_2), $\mu_2 = 8.4 \times 10^{-5} \text{ N s/m}^2$
 Density Entrained Heavy Phase in Bubble (UO_2), $\rho_E = 8700 \text{ kg/m}^3$

Table 1.2
POROUS MEDIUM PERMEABILITIES

$\bar{\alpha}$	$r \text{ (}\mu\text{m)}$	$k \text{ (m}^2\text{)}$
0.9	1	0.93×10^{-12}
0.9	10	0.93×10^{-10}
0.9	100	0.93×10^{-8}

Figure 1.2(a)

Growth Constants from Taylor and Porous Medium Instability Analyses.
(BNL Neg. No. 3-1291-80)

Figure 1.2(b).

Growth Constants from Taylor and Porous Medium Instability Analyses.
(BNL Neg. No. 3-1289-80)

Figure 1.2(c).

Growth Constants from Taylor and Porous Medium Instability Analyses.
(BNL Neg. No. 3-1290-80)

Figure 1.2(d).

Growth Constants from Taylor and Porous Medium Instability Analyses.
(BNL Neg. No. 3-1288-80)

Figure 1.3. Experimental Data For Local Boundary Heat Transfer From Volume-Heated Non-Boiling Pools: $Nu(x)$ vs $Ra^*(x)$.
(BNL Neg. No. 4-382-80).

2. SSC Code Development (J. G. Guppy)

The Super System Code (SSC) Development program deals with the development of an advanced thermohydraulic code to simulate transients in LMFBRs and LWRs. During this reporting period, work on four codes in the SSC series was performed. These codes are: (1) SSC-L for simulating short-term transients in loop-type LMFBRs, (2) SSC-P is analogous to SSC-L except that it is applicable to pool-type designs, (3) SSC-W for simulating short-term transients in LWRs, and (4) SSC-S for long-term (shutdown) transients occurring in either loop- or pool-type LMFBRs or LWRs. Reference is made to the previous quarterly progress report (Guppy, 1980) for a summary of accomplishments prior to the start of the current period.

2.1 SSC-L Code (J. G. Guppy)

2.1.1 Prediction of Localized Thermal Buoyancy Effects in LMFBR Piping Systems (M. Khatib-Rahbar)

Most of the existing system simulation codes represent the thermal transport processes in LMFBR piping systems by one-dimensional models. Inherent in these models is the assumption that the influence of radial temperature variations is insignificant. However, under extreme circumstances, distortions in the radial temperature profile may develop leading to local, density driven recirculation and redistribution. For example, cold sodium entering a warm pipe may tend to slide under the warm sodium rather than advance in the plug-like, perfectly-mixed manner as assumed by the one-dimensional models.

The influence of local thermal buoyancy and flow redistribution in a horizontal pipe section has been examined (Khatib-Rahbar, 1980a) by comparing the one-dimensional results for a very severe flow and temperature transient with parallel three-dimensional calculations (Trent, 1979 and Chen, 1980). Further investigation shows that an indication of the relative magnitude of the free-and forced convection effects may be obtained from the magnitudes of the flow transport numbers. For turbulent flow inside long tubes, (Jackson and Fewster, (1977) derived an expression for mixed convection region which is based on equating the total buoyancy force acting on a thin thermal sublayer to the net shear force. They obtained the following dimensionless parameter:

$$\lambda = \overline{Gr}/Re^{2.625} \sqrt{Pr} = \overline{Ri}/Re^{0.625} \sqrt{Pr}$$

The available experimental data, obtained from water experiments, show that the effect of buoyancy can be as high as 10% or more if:

$$\lambda > 10^{-4}$$

Using one-dimensional calculations, the value of λ was determined as a function of time into the transient, and comparisons with 3-D predictions showed that this semi-quantitative approach may be used to predict the time period of significant thermal buoyancy effects (Khatib-Rahbar, 1980a). Furthermore, inclusion of thermal buoyancy effects into the forced convection Nusselt number can improve the 1-D predictions.

(Jackson and Fewster, 1977) suggest that, the mixed convection Nusselt number can be evaluated as:

$$\frac{Nu}{Nu_f} = (1 + K\lambda)^n$$

where Nu_f is the forced convection Nusselt number evaluated at the mixed convection condition, K and n are experimentally determined constants ($K = 4500$; $n = 0.31$); and Gr is defined as:

$$Gr \equiv \frac{g(\rho_b - \bar{\rho})\rho_b D^3}{\mu_b^2}$$

where ρ_b is the sodium density evaluated at the bulk temperature, and $\bar{\rho}$ is the temperature averaged sodium density defined as:

$$\bar{\rho} = \frac{\int_{T_b}^{T_w} \rho dT}{\int_{T_b}^{T_w} dT}$$

where T_b is the bulk temperature and T_w is the wall temperature.

The influence of localized force convection effects on system natural circulation conditions is currently being studied.

2.1.2 Hypothetical Loss-of-Heat-Sink and In-Vessel Natural Convection: Homogeneous sub Heterogeneous Core Design (M. Khatib-Rahbar)

The pre-boiling response of homogeneous and heterogeneous LMFBR core designs to hypothetical loss-of-heat-sink (LOHS) accidents leading to in-vessel natural convection cooling was studied with a detailed system representation using the SSC-L code (Khatib-Rahbar, 1980b).

Figure 2.1 Schematic of the Flow Patterns Inside the Reactor Vessel

Following the LOHS accident the reactor vessel is essentially isolated (see Figure 2.1) and therefore relying solely on in-vessel circulation for cooling. The results summarized below indicate that considerable flow reversal can occur in the reactor core leading to substantial sodium flow redistribution. This recirculation rate is shown to be much lower for the heterogeneous as compared to the homogeneous core design.

To improve the safety features of LMFBRs, use of reactor cores with low positive sodium void reactivity effect has been considered for large power reactor designs. A number of alternative designs have recently been examined as substitutes to the conventional cylindrical core with two zones of fuel enrichment and surrounded by breeder material. Among those core designs, the introduction of internal blanket layers into the fissile fuel regions is often foreseen according to various patterns. These designs are termed heterogeneous or parfait as compared with the homogeneous concept.

The parfait designs are generally more advantageous from the point of view of breeding and doubling time. Another intrinsic characteristic of this type of core is the presence of internal blanket assemblies which have relatively slow thermal response characteristic and produce an incoherency in the time and sequence of thermal excursions.

Therefore, from the safety point of view it is important to understand the core dynamics behavior under accident conditions in order to determine the merits of each concept. For example, the impact of radial temperature distribution coupled with widely different time response characteristic can alter the nature of flow redistribution phenomenon at low flow conditions.

For the purpose of this analysis the recently completed Alternative Fuel Management Scheme (AFMS-M) of CRBRP will be compared to the Reference Fuel Management Scheme (RFMS) based on a homogeneous design. Detailed descriptions of the two designs are given in (CRBRP, 1979a, b).

The CRBRP-RFMS design consists of 198 fuel and 150 blanket assemblies arranged in a homogeneous configuration. The fuel assemblies are serviced by five orifice zones; the blanket assemblies by four orifice zones; in addition there are 19 control assemblies in the reactor core.

The CRBRP-AFMS-M design consists of 156 (odd cycle) or 162 (even cycle) fuel and 214 (odd cycle or 208 (even cycle) blanket assemblies arranged in a heterogeneous configuration. The fuel and blanket assemblies are serviced by twelve orifice zones (six each); in addition, there are 15 control assemblies in the reactor core.

For an SSC-L simulation, assemblies can be grouped together. The grouping can proceed according to either similar hydraulic characteristics, similar power characteristics or similar power and flow characteristics. In this study, the assemblies were grouped based on similar power and flow characteristics. This assures preservation of possible core wide incoherencies which influence the core transient response characteristics.

Figure 2.2 shows various orifice zones and the SSC-L channel number for a 30° sector of the RFMS design and a 60° sector of the AFMS-M design. The steady state power and flow fractions assigned to the twenty channel representation are noted in Table 2.1 for the homogeneous core and in Table 2.2 for the heterogeneous core design. It should be pointed out that only one fuel assembly in the entire core was used to represent the hot fuel channel. Similarly, the hot blanket channel represents only one blanket assembly in the reactor. Note that the power fraction values are expressed in terms of fraction of core-generated heat of 967.4 MW(t). When heat generated by sodium pumps (six of them) are included, the total power becomes 975 MW(t). Heat losses through insulation and other components are small and, hence, neglected. Total in-vessel flow of sodium is 5224 kg/s. A steady-state plant characterization is performed by the code from the above information and other design data, including power shapes. All conditions here are representative of end-of-life equilibrium cycle (EOEC7 for RFMS and EOEC4 for AFMS-M); except, the fuel hot channel in the RFMS is assumed to be at the beginning-of-life equilibrium core. The AFMS-M hot channel temperatures include the 3 uncertainty factors only. The decay heat values were taken to be 125% of the nominal values for the fission product heating and 110% of the nominal values for the decay of the transuranic elements. It should be noted that there are 217, 61, and 37 pins in each of the fuel, blanket and control assemblies, respectively.

The LOHS simulations were performed for two different cases; namely (1) LOHS occurring at 90 seconds following reactor shutdown, and (2) LOHS occurring at 10 hours following reactor shutdown.

Figure 2.2 Orificing Scheme and SSC-L Channels for CRBRP
(a) Homogeneous Core, and (b) Heterogeneous Core

Table 2.1 RFMS Steady State Data (EOEC7)

Channel	Orificing Zone	Type	No. of Assemblies	Flow Fraction	Power Fraction	Temperature Rise $\Delta T^*(K)$
1	1	Fuel	1	0.0044	0.0096	315
2	9	Blanket	1	0.0004	0.0008	289
3	1	Fuel	29	0.1290	0.1569	175
4	1	Fuel	18	0.0800	0.0769	138
5	1	Fuel	18	0.0800	0.0890	160
6	2	Fuel	18	0.0718	0.0865	173
7	2	Fuel	24	0.0958	0.1003	150
8	2	Fuel	18	0.0718	0.0890	178
9	3	Fuel	36	0.1352	0.1496	159
10	2	Fuel	18	0.0718	0.0717	143
11	4	Fuel	12	0.0419	0.0402	138
12	5	Fuel	6	0.0183	0.0185	145
13	7	Blanket	18	0.0214	0.0112	75
14	7	Blanket	12	0.0142	0.0100	101
15	6	Blanket	24	0.0308	0.0255	119
16	8	Blanket	30	0.0211	0.0162	110
17	8	Blanket	24	0.0168	0.0171	146
18	9	Blanket	41	0.0154	0.0174	163
19	-	Control	19	0.0383	0.0136	51
20	-	Bypass	--	0.0416	0	0

*Inlet Temperature = 655 K

Table 2.2 AFMS-M Steady State Data (EOEC4)

Channel	Orificing Zone	Type	No. of Assemblies	Flow Fraction	Power Fraction	Temperature Rise $\Delta T^*(K)$
1	6	Fuel**	1	0.0043	0.0062	208
2	7	Blanket [†]	1	0.0021	0.0025	171
3	8	Blanket	1	0.0019	0.0019	144
4	8	Blanket	18	0.0333	0.0358	155
5	7	Fuel	36	0.1512	0.1730	165
6	3	Fuel	9	0.0357	0.0428	172
7	7	Blanket	33	0.0596	0.0748	154
8	7	Blanket	23	0.0485	0.0540	160
9	6	Fuel	5	0.0213	0.0264	178
10	1	Fuel	39	0.1760	0.1863	152
11	2	Fuel	18	0.0756	0.0766	146
12	3	Fuel	12	0.0476	0.0566	171
13	4	Fuel	18	0.0656	0.0665	146
14	10	Blanket	36	0.0417	0.0390	134
15	9	Blanket	12	0.0179	0.0164	132
16	5	Fuel	24	0.0852	0.0252	144
17	11	Blanket	48	0.0403	0.0327	116
18	12	Blanket	36	0.0222	0.0150	97
19	--	Control	15	0.0260	0.0083	46
20	--	Bypass	--	0.0340	0	0

*Inlet Temperature = 655 K

**162 Fuel Assemblies

[†]208 Blanket Assemblies

LOHS At High Decay Heat Level

Figure 2.3 shows the primary loop sodium flow rate as a function of time after scram. It is observed that the flow rate goes to zero at 90 seconds following reactor scram, causing the LOHS. At this time the reactor vessel is totally isolated from the heat transport loops and can rely only on in-vessel natural circulation caused by nonuniform radial temperature gradients. The effect of interchannel flow redistribution is displayed in Figure 2.4. Here, the coolant flow fractions, $W_j(t)/W_j(0)$, are shown as a function of time after LOHS for various channels. Immediately following the accident, the flow fractions are seen to drop to nearly zero flow and as inter-channel buoyancy starts the circulation, the warmer channels draw more fluid at the expense of the cooler channels. Channels 1 and 2 (hot channels) draw a substantial portion of the coolant, and channel 1 tends to draw coolant as the sodium temperature in this channel is rising (see Fig. 2.5) much faster compared to the hot blanket channel. This incoherency effect is caused by the difference in the characteristic times of the two subassemblies. Also shown in Figure 2.4 are the flow fractions in channels 6, 8, 10, 13, 14, and 19 (control assemblies). In general, all of the blanket and control and cooler fuel assembly channels undergo flow reversal; and the reversal is more severe in the blanket and control channels as compared to the cool fuel channels. The most interesting effect is observed in channel 10 (a fuel channel), where the sodium flow rate is essentially zero for an extended period of time leading to an exponential rise in temperature as observed from Figure 2.5. This figure reveals a very interesting phenomenon which is in contrast to the common belief that the worst conditions are normally reached in the hot channel; as in this case, sodium flow stagnation causes boiling to occur in channel 10 about 2.5 minutes earlier than in channel 1 (the fuel hot channel).

Figure 2.3 Normalized Primary Loop Sodium Flow Rate

Figure 2.4 Flow Fractions in Various Channels of the Homogeneous Core Following LOHS (6% Power)

Figure 2.5 Maximum Sodium Temperature in Channels 1 and 10 of the Homogeneous Core Following LOHS (6% Power)

The results also showed no significant temperature rise in the channels with substantial flow reversal, indicating sufficient heat removal capability. It is important to note that the current version of SSC-L is limited to single phase flow only, therefore the oscillations observed in the channel flow rates following boiling initiation are not physical, but only indicative of variations in sodium temperatures in those channels.

Figure 2.6 shows the typical sodium flow fractions in the heterogeneous core design. It is seen that the behavior of the core is nearly the same as the homogeneous core, except the more radial uniformity of temperature gradient has reduced the magnitude of the flow fractions, therefore, an enhancement in the rate at which the coolant temperatures increase as observed from Figure 2.7. The sodium temperatures reach boiling in channels 1 and 9 almost simultaneously. In this case some of the radial blanket channels achieved positive flow; and a higher number of fuel channels underwent flow reversal as expected.

Figures 2.8 and 2.9 illustrate the transient behavior of the sodium temperature in the reactor inlet and outlet plena for homogeneous and heterogeneous designs, respectively. It is seen that the rate at which the sodium temperature in the plena increases is very small, since the heat capacities of the coolant as well as the plena structural material are quite high, leading to a considerable mitigation of the transient.

Figure 2.6 Flow Fractions in Various Channels of the Heterogeneous Core Following LOHS (6% Power)

Figure 2.7 Maximum Sodium Temperature in Channels 1 and 8 of the Heterogeneous Core Following LOHS (6% Power)

Figure 2.8 Sodium Temperatures in the Inlet and Outlet Plena of the Reactor Vessel for Homogeneous Core

Figure 2.9 Sodium Temperatures in the Inlet and Outlet Plena of the Reactor Vessel for Heterogeneous Core

The total recirculation rate within the vessel is calculated as the sum of all positive or negative flow rates in the reactor, that is:

$$W_{Ric} = \sum_J \text{positive } (W_J) = \sum_J \text{negative } (W_J)$$

Figure 2.10 illustrates the natural circulation rate as a function of time after LOHS for both homogeneous and heterogeneous core design concepts. Immediately following the loss-of-heat-sink the recirculation rate starts from about 7 kg/s which is just the negative flow through the bypass channel (note bypass channel flow reverses prior to the LOHS event, during the initial flow coastdown, since there is no heat produced within the bypass region). As the natural convection flow is established, the recirculation rate should reach a maximum after which it would start to decrease due to continuous reduction in decay-heat. The total recirculation rate for the homogeneous core is about 20% higher than its heterogeneous counterpart. This is due to smaller radial temperature gradient in the latter case.

Figure 2.10 Total Recirculation Rate in the Vessel Following LOHS (6% Power)

LOHS At Low Decay Heat Level

The decay heat for CRBRP is estimated to decrease to about 1% of the total reactor power (10 MW(t)) in about 10 hours after reactor scram. It was argued earlier that the natural circulation rate within the vessel is higher if the radial temperature gradient is larger; therefore, a delayed loss-of-heat-sink occurring several hours following the reactor shutdown was also studied to determine the impact of isothermality on the establishment of in-vessel natural convection cooling.

The sequence of events leading to the LOHS consists of (1) reactor scram at time zero, followed by trip to pony motor level; (2) decay heat removal for 10 hours, and (3) LOHS at 10 hours following scram.

Table 2.3 summarizes the reactor vessel thermal condition prior to the LOHS at 1% power level, 10 hours after reactor shutdown. Comparisons of these values to those at 100% full power condition of Tables 2.1 and 2.2 show a considerable reduction in the radial temperature gradient for both design concepts.

Figure 2.11 illustrates the flow fractions in several typical channels for the RFMS design. It is evident that a small radial temperature gradient produces a period of oscillation before natural convection cooling is established. Also evident is the incoherency effect between the hot fuel and blanket channels caused by the substantial difference in their corresponding characteristic times.

The bypass channel flow fraction shown in Figure 2.11 is seen to be the first to reverse and then, as the natural circulation starts to stabilize it tends to increase and approach stagnation.

A similar behavior was observed for the heterogeneous core; with the exception of greater oscillation for the first 2 minutes following the accident as seen in Figure 2.12.

Figure 2.13 shows the maximum sodium temperature for both homogeneous and heterogeneous core designs. It is seen that the initial excursion causes a sharp increase in sodium temperatures in the hot channel. The temperature and flow behaviors are also seen to be similar, and these variations are expected to continue until the initiation of boiling. It was also observed that all blanket and control assemblies and the five cooler fuel assemblies experienced flow reversal and/or stagnation. The total recirculation rate within the vessel is shown in Figure 2.14. It is seen that it takes approximately 2 minutes before the natural circulation flow is established. As expected, the flow rate is much higher for homogeneous cores as compared to its heterogeneous counterpart.

2.1.3 LMFBR Accident Progression Analysis (K. M. Jamali)

A computer program has been written for the event lumping procedure as described earlier (Guppy, 1980). For the rest of the analysis, the lumped events will be treated in the same manner as the original primary events. All primary event probabilities are represented by n-vectors, where n is the number of random deviates generated by Monte Carlo techniques. These arrays will be used in subsequent analysis for the probabilistic determination of the dominant minimal cut sets (MCS) (Guppy, 1980).

Probabilistic Determination of the Dominant MCS

Each minimal cut set is the product of one or more primary events. The total number of MCS generated in a fault tree analysis can become extremely large, but practical considerations of MCS size and probability enables the analyst to limit their number to a manageable

Figure 2.11 Flow Fractions in Various Channels of the Homogeneous Core Following LOHS (1% Power)

Table 2.3 Reactor Temperature Rise at 1% Power

Channel No.	Temperature Rise, $\Delta T^*(K)$	
	RFMS	AFMS-M
1	46	31
2	45	23
3	26	20
4	20	21
5	23	24
6	26	25
7	22	21
8	26	22
9	24	26
10	21	22
11	20	21
12	21	25
13	12	25
14	16	23
15	19	22
16	19	25
17	26	22
18	31	21
19	4	3
20	0	0

*Inlet Temperature = 557 K

Figure 2.12 Flow Fractions in Various Channels of the Heterogeneous Core Following LOHS (1% Power)

Figure 2.13 Maximum Sodium Temperatures in the Hot Channel of the Homogeneous and Heterogeneous Core Designs Following LOHS (1% Power)

Figure 2.14 Total Recirculation Rate in the Reactor Vessel Following LOHS (1% Power)

amount, say 2000 as a maximum. If the primary (independent) events of the fault tree are represented by n -vectors, the MCS probability can be obtained from the product of the constitutive n -vectors. Thus, each MCS probability will also be represented by an n -vector. Each random sampling of these vectors can be used to obtain a new ordering of the MCS (Guppy, 1980). The results can be represented by an ordering matrix O as follows:

$$O = \begin{bmatrix} \text{MCS}_1 & \cdot & \text{MCS}_I & \cdot & \cdot & \cdot \\ \text{MCS}_2 & \cdot & \text{MCS}_J & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \text{MCS}_m & \cdot & \text{MCS}_K & \cdot & \cdot & \cdot \end{bmatrix} \quad \begin{array}{l} m = \text{number of retained} \\ \text{cut sets} \end{array}$$

$n = \text{number of Monte Carlo trials}$

Matrix O can be collapsed by a row-wise summation of all of the occurrences of each cut set:

$$O_{\text{Coll.}} = \left[\begin{array}{ccccccc} N_1 \cdot (\text{MCS}_1) & \cdot & \cdot & N_p \cdot (\text{MCS}_I) & \cdot & \cdot & 0 \\ L_1 \cdot (\text{MCS}_2) & \cdot & \cdot & L_p \cdot (\text{MCS}_J) & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ K_1 \cdot (\text{MCS}_M) & \cdot & \cdot & K_p \cdot (\text{MCS}_M) & \cdot & \cdot & 0 \end{array} \right] \Bigg\}^M$$

$\hat{n}$

N_1 = number of times MCS #1 has appeared in the first position

K_1 = number of times MCS #M has appeared in the last position

Each MCS can now be represented in terms of an $(n,2)$ array:

$$\text{MCS}(I) = \begin{bmatrix} p_{1,I} & N_I(1) \\ p_{2,I} & N_I(2) \\ \cdot & \cdot \\ \cdot & N_I(M) \\ \cdot & 0 \\ p_{n,I} & 0 \end{bmatrix}, \quad N_I(K) = \text{number of times the } I\text{-th MCS has appeared in the } K\text{-th position}$$

We can now define a (discrete) random variable p_I for I -th MCS describing its position with pdf of f_I

It is reasonable to believe that the density function f_I will be symmetric and falling off asymptotically at the extremes. Also, the shape of the f_I 's is controlled by the interplay of a large number of different distributions (log normal and multiple convolutions of several log normals). Thus, it is expected that the analytical fit to the discrete f_I 's will be nearly a normal distribution with an improving fit as the number of Monte Carlo deviates are increased.

This procedure yields a sequence of probability distribution functions as follows:

Thus, the following information can be obtained:

1. The dominant minimal cut sets.
2. The for each MCS as a measure of the top event sensitivity to the uncertainty in the MCS position in the neighborhood of that position.
3. The most probable ordering obtained from the maxima of the f_I 's.
4. An ordering of significant primary events.

Construction of the (Lumped) SHRS Fault Tree

Work is progressing towards a reconstruction of the Shutdown Heat Removal System (SHRS) fault tree (Trainer, 1979) in a lumped form. A study of potential accident initiating events was also undertaken to assess whether a linking needs to be established between particular initiators and the applicable form of the fault tree.

2.1.4 Radial Temperature Profiles in Fuel Pins (W. C. Horak)

In order to provide improved modeling capability and also to yield adequate fuel pin temperature information even when as few as one radial node is utilized, a revised fuel temperature computational scheme has been developed for SSC. This numerical scheme is based on a nodal method which directly yields the spatially averaged temperature within a node.

In the steady state case, the average nodal temperature is solved analytically using nodal interfaces. The gap conductivity equation is used to relate the temperatures across the fuel-clad gap.

For transient problems, the temperatures are approximated over a node using a local expansion. Using this local expansion for the nodal temperatures, a set of coupled o.d.e.'s for the time-dependent behavior of the average nodal temperatures is developed. This set of coupled o.d.e.'s is then solved using a standard Runge-Kutta method.

The steady-state formalism has been tested in SSC and yielded answers which were in good agreement with the present finite difference method, at a significant reduction in computing time. Comparisons between the new formulation and standard "benchmark" methods have not been done. The transient formalism is still undergoing development, specifically in ways to reduce the time required to evaluate the expansion coefficients.

2.1.5 Analysis of Steady-State Natural Circulation in LMFBR Plants (A. K. Agrawal, L. G. Epel, M. Khatib-Rahbar, and I. K. Madni)

The steady-state natural circulation behavior of LMFBR plants can be predicted by developing a simple correlation which relates the mixed-mean core temperature rise to the reactor power level under decay heat natural

convection conditions.

Solution of steady-state energy and momentum balance equations can be used to relate the reactor ΔT to the reactor power as follows:

$$\Delta T = \zeta \cdot P^{\left(\frac{2-n}{3-n}\right)} \quad (2.1)$$

where n is the exponent in the overall friction factor correlation. For fully developed turbulent flow $n=0.2$, while for laminar flow $n=1$. Since the coolant flow in the entire circuit is between turbulent and laminar, an average value of 0.60 may be used. Therefore:

$$\Delta T = \zeta P^{0.58} \quad (2.2)$$

where $\bar{P}$ is the power normalized to its 100% value.

The constant of proportionality, ζ , can be evaluated when all design data are used. Alternately it can be determined by matching experimental results or detailed calculations with Equation 2.2 for a given power level.

The validity of Equation (2.2) has been verified both experimentally and by using detailed calculations with SSC-L. Table 2.4 summarizes the results as obtained from the correlation and comparisons to experiment or detailed calculations for various LMFBR plants. Agreement is seen to be excellent for both loop and pool plant concepts, except of Phenix.

The deviations between SSC-P calculations and Equation (2.2) can be attributed to the lack of steady-state conditions in the former. This can be explained as follows. During the first few minutes of the transient, the IHX primary outlet temperature drops about a hundred degrees from its steady-state value. Thereafter, the very large thermal inertia of the cold pool causes its temperature to respond very slowly to this change. Thus, 0.5 hour into the transient, the temperatures are changing about a degree every 100 seconds and the system is still far from steady state.

Calculations are currently being extended to longer times, with lower secondary flow rates (closer to expected Phenix flow rates, as observed from the results of a low-power test). The new results will be reported soon.

2.1.6 Plant Protection and Control Systems (M. Khatib-Rahbar, R. J. Kennett, S. Dang)

The steam generator control systems are nearing completion. The work during this quarter focused on debugging and code modifications for incorporation of control valves and feedwater pump speed controller.

Table 2.4 Comparison of Plant Data to Correlation

$\Delta T(K)$ $\bar{P}$	CRBRP =1248.43		FFTF =1282.71		Phenix =948.81		PFR =1155.48	
	SSC-L	Eq.2.2	SSC-L	Eq.2.2	SSC-P	Eq.2.2	Exp.	Eq.2.2
0.01	91	86.4	81.9	88.7	44.8	65.64	78	79.94
0.02	126	129.1	131	133	84	98.12	117.33	119.5
0.03	162	163.3	167	168	117.72	124.14	151.18	151.18*
0.04*	193	193	198	198	146.68	146.68	--	178.63

*The 4% power point was used to match the detailed calculations to Equation (2.2) for each of the first three reactors. For PFR, the 3% power point was used.

A revised part load profile calculation is also proceeding in order to resolve some convergence problems at low operation power conditions.

PPS-PCS documentation is also in progress. A draft report describing the PPS-PCS model is nearing completion.

2.1.7 Steam Generator Modeling (G. J. Van Tuyle, W. C. Horak, S. F. Carter, R. J. Kennett, and T. Nepsee)

Since all steam generator changes presently being modeled as part of the SSC-W development effort are being incorporated into the SSC program library on a generic basis, please refer also to the appropriate section under SSC-W Development.

The extensive modifications to the steam generator modules of the SSC program library have now been coded and debugged. A new cycle of SSC-L containing these modifications has been created and is undergoing extensive testing. Models are available in the feedwater, turbine, turbine bypass and relief valve areas. Additionally, improvements in the FORTRAN coding of several transient segment subroutines have been accomplished.

As part of the effort to complete the first version of SSC-W, several relatively minor errors in the generic steam generator model were discovered and corrected. The most notable modification was in the solution of the time-dependent wall heat conduction equation, the heat flux terms were altered to

contain current values, rather than advanced time values. This change makes the solution of this equation consistent with the energy equation solution for the fluids on either side of the tube.

2.1.8 User Support (J. G. Guppy, R. J. Kennett)

The German user of SSC-L (GRS) was given a set of the latest update corrections recently made to the SSC program library. GRS is nearing a point where SSC-L will be applied to verify certain SNR-300 licensing calculations. An input deck for the SNR-300, generated by GRS, will be sent to BNL shortly.

2.2 SSC-P Code (I. K. Madni)

During this reporting period, the code was applied to analyze protected and unprotected loss-of-electric-power events, it is currently being extended to long-time simulations, in order to analyze the steady-state, low power thermal response of the Phenix reactor core under natural convection cooling conditions. Substantial new data were derived, particularly for the Phenix core, from related information uncovered in the literature. These include power and flow fractions for fuel and blanket channels, as well as axial power fractions in the fuel. Furthermore, a hot channel has been added in the fuel region. Details are presented below.

2.2.1 Input Data (I. K. Madni)

Flow fractions:

From (Agrawal, 1979), the average flow per fuel assembly is 22.7 kg/s. Thus, flow through 103 fuel assemblies is 2338 kg/s. With a core flow rate at rated power of 2760 kg/s, this gives the flow fractions as 84.5% for the fuel channel and 15.5% for blankets, etc.

Power fractions:

From CRBRP natural circulation runs we see, at 400 seconds into the transient, that

$$\frac{\text{normalized power in blanket}}{\text{normalized power in fuel}} = 1.4839$$

At full power conditions (i.e., $t=0$ sec.), this ratio is 1.0. Also, at 400 sec. following scram, the power generation is due exclusively to decay power. Therefore, we can write

$$\frac{(P_b)_b}{P_{bo}} \bigg/ \frac{(P_f)_d}{P_{fo}} = 1.4839$$

or

$$\frac{P_{bo}}{P_{fo}} = \frac{1}{1.4839} \frac{(P_b)_d}{(P_f)_d}$$

(2.3)

where $(P_f)_d$, $(P_b)_d$ are the decay power in fuel and blanket assemblies, respectively, and P_{fo} , P_{bo} are the respective powers corresponding to full-power conditions.

We assume that Equation 2.3 also applies to Phenix. From (Phenix, 1970), during refueling, 17 fuel assemblies produce 40kW of decay heat, and 11 blanket assemblies produce 7kW of decay heat (assuming the power due to control assemblies is lumped in with the blankets). Using this information, and using $(P_f)_d$ as power per respective assembly, we derive the ratio of full power conditions per assembly as:

$$\frac{P_{bo}}{P_{fo}} = 0.182 \quad (2.4)$$

now,

$$90 P_{bo} + 103 P_{fo} = 563 \text{ MW} \quad (2.5)$$

Combining Eqs. (2.4) and (2.5) gives:

$$P_{fo} = 4.728 \text{ MW}$$

$$P_{bo} = 0.8445 \text{ MW}$$

Or, the total power generated in fuel assemblies is 485.75 MW and in the blanket assemblies, etc. is 76.05 MW.

This gives the power fractions in fuel and blanket regions respectively, as 86.5% and 13.5%.

Hot channel:

The radial peaking factor for Phenix is 1.3, (Wolfe, 1973). The power generated in the hot channel is therefore 6.1464 MW, corresponding to a power fraction in the hot channel of 1.092%, with a power fraction of 85.408% for the remaining 102 fuel assemblies.

From the analytical results reported in (Freston, 1979) we obtain a temperature rise (ΔT_{HC}) of 235.24 °C in the nominal fuel hot channel.

Energy balance for the coolant in the hot channel can be written as:

$$W_{HC} \overline{C_p} \Delta T_{HC} = 6.1464 \times 10^6 \text{ W} \quad (2.6)$$

where C_p is the average heat capacity of coolant. From Eq. (2.6), the flow through the hot channel (W_{HC}) is determined to be 20.701 kg/s. The flow fraction is 0.75% in the hot channel, and 83.75% in the average channel (comprising the remaining 102 fuel assemblies).

Axial power profile in fuel:

Since the heat flux on fuel element surface, (Phenix, 1971), is 143 W/cm² (avg.) or 208 W/cm² (max.),

$$\frac{q_{\max}}{\overline{q}} = 1.4545 \quad (2.7)$$

where $\overline{q}$ is the average power fraction in the fuel element. To obtain an axial power profile one could construct a parabolic profile:

$$q' = \frac{q}{\overline{q}} = A z^2 + B z + C \quad (2.8)$$

where A, B and C are constants and z is the axial distance along the fuel element.

Boundary conditions on Eq. (2.8) are:

- (i) $q' = 0$ at $z = 0$
- (ii) $q' = 0$ at $z = L$ ($L = .85\text{m}$).
- (iii) $q' = 1.4545$ at $z = \frac{L}{2}$ ($L = 0.85\text{m}$)

Applying (i), (ii) and (iii) to Eq. (2.8), we obtain the coefficients A, B, C and the profile, given by:

$$q' = -8.053z^2 + 6.845z. \quad (2.9)$$

The nodes are equidistant and we can construct a table of q' corresponding to midpoints in each nodal volume as shown below in Table 2.5.

Table 2.5 Normalized Nodal Axial Power Profile

N	q'
1	0.2764
2	0.7418
3	1.0909
4	1.3236
5	1.4400
6	1.4400
7	1.3236
8	1.0909
9	0.7418
10	0.2764

These can be read in for the 10 axial nodes of the fuel region.

Primary pump friction:

From (Appleby, 1975), it is known that the pump reaches approximately 10% speed in 60 seconds. The coefficients in the frictional torque correlation, (Madni, 1979), have been altered to represent this condition. Thus, in the equation

$$\tau_{fr} = \tau_R (c_o + c_1 \alpha + c_2 d^2) \quad (2.10)$$

the altered coefficients are

$$c_o = 0.001, c_1 = 0.034, c_2 = 0.0 \quad \text{for } 0.0117 < \alpha \leq 1.0 \quad (2.11)$$

To assure continuity, we redefine

$$c_o = 0.117, c_1 = -0.458, c_2 = 0.0 \quad \text{for } \alpha \leq 0.0117 \quad (2.12)$$

$$c_o = 0.005, c_1 = 12.942, c_2 = 0.0 \quad \text{for } 0 \leq \alpha \leq 0.005$$

2.2.2 Transient Analysis (I. K. Madni, e. G. Cazzoli)

LOEP event with scram: The LOEP calculations for Phenix show adequate cooling by natural convection. The maximum coolant temperature in the hot channel exhibits a wide margin ($\sim 300^\circ\text{C}$) to boiling.

LOEP event without scram: An unprotected loss-of-electric-power event in the Phenix plant was simulated using the current input deck for Phenix. The aim was to exercise the code and make some trend comparisons with analytical results reported by NOVATOME in (Frestion, 1979). The transient power history shown in the literature for this transient was fitted by a sixth order polynomial. The dynamic behavior of the plant was analyzed for 70 seconds following accident initiation. Computed results of primary flow decay and hot channel outlet temperatures in the core were compared with the results reported in (Frestion, 1979), and show good agreement. Both calculations predict the occurrence of boiling in the hot channel within one minute of pump trip.

Steady-state natural circulation at 4 MW: The code is being used to simulate the steady-state, low power thermal response of the Phenix reactor core under natural convection cooling conditions. Currently, with rather high intermediate flows, the IHX becomes overcooled, and the results would take longer to reach steady-state due to the large thermal inertia of the cold pool in the primary tank. The steam generator elevation with respect to the IHX is being adjusted to yield the expected natural circulation flow in the intermediate circuit corresponding to a reactor power of 4 MWth (i.e. $< 1\%$).

2.3 SSC-W Code (J. G. Guppy)

2.3.1 Initial Operational Version (S. F. Carter, J. G. Guppy, W. C. Horak, R. J. Kennett, T. Nepsee, G. J. Van Tuyle)

The initial version of SSC-W was made operational at BNL in late March. This version is applicable to pressurized water reactor (PWR) system designs utilizing once-through steam generators (OTSGs).

SSC-W has been constructed essentially by rearranging and extending the basic SSC program library. Important features that were utilized from the existing program library include: 1) neutron kinetics package, 2) fuel heat conduction package, 3) multi-channel core representation capability, 4) pump models, 5) piping models, 6) steam generator solution method, 7) steady-state initialization package, and 8) input processing scheme. Important features which had to be added/modified include 1) pressurizer model, 2) changing all sodium properties to water, 3) deletion of the intermediate heat exchanger and cover gas linkages, 4) overall code solution logic and 5) steam generator models.

System-wide transients have now begun to be run on a routine basis. The longest test case to date has been a coastdown to natural circulation run, which was simulated out to 180 seconds. Extensive testing and applications work are being initiated.

2.3.2 Steam Generator Modeling (G. J. Van Tuyle, W. C. Horak, S. F. Carter,

Since all steam generator changes presently being modeled as part of the SSC-W development effort are being incorporated into the SSC program library on a generic basis, please refer also to the appropriate section under SSC-L Development.

The modifications made in converting the generic steam generator to represent B&W once-through steam generators have been debugged to a level where transients can be run. The correction set used to modify Cycle 31 of the SSC-L program library was altered to make equivalent modification to Cycle 32. Several of the changes made in going from Cycle 31 to Cycle 32 were done in order to improve the flexibility of representing some of the peculiarities of the B&W once-through steam generator. Many of the parallel efforts made over the last several months have therefore come together.

2.3.3 SSC-W Future Plans

In order to better plan the future work for the SSC-W development effort, a meeting was held at BNL between BNL staff members and SSC consultants. The main focus of the meeting was to discuss the potential for, and ramifications of including a drift flux model in the steam generator. Professor John C. Lee (Michigan) discussed his experiences and preliminary results gained through application of various formulations of the drift flux model in the TRANSG code. Professor John E. Meyer (MIT) contributed thoughts concerning the potential for the application of drift flux to the SSC momentum integral model, as well as to the analysis of certain transient conditions.

2.4 SSC-S Code (J. G. Guppy)

2.4.1 Inter- and Intra-assembly Effects (B. Chan)

Work on the SPAC code (Steady-state Porous-body Assembly Code) has been resumed. SPAC, developed at BNL from the ENERGY-III code, is being used to formulate the methodology to account for intra-assembly effects within the framework of SSC. This work encompasses a portion of the overall effort to account for inter-assembly effects in SSC.

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3. SSC Validation (J. G. Guppy)

3.1 FFTF Acceptance Tests (L. G. Epel)

At the request of HEDL personnel (Nutt, 1980), the FFTF version of SSC-L has been used to simulate a variant of the Loss of Electric Power transient from 5% full power, steady-state conditions. In this variation, the reactor is scrammed, all primary and secondary pumps are tripped, and all of the DHX fan motors are also de-energized. However, although power is not restored to the primary pump pony motors, it is restored to the secondary pump pony motors. Thus, when the secondary pumps coast down to 10% rated speed, they are maintained at this level.

The results of this case indicate that the maximum core exit temperature for the hottest channel is somewhat less (5K) than when the secondary pump pony motors are not reactivated. In general, there was good agreement between the results of this run and a corresponding one done at HEDL utilizing IANUS (Nutt, 1980). The one significant disagreement concerns the timing of the peak exit temperature; SSC-L predicts the time of the peak considerably later than does IANUS. This matter is being investigated jointly by HEDL and BNL personnel and the cause of the disagreement will hopefully be resolved in the near future.

3.2 Inter-Code Comparisons of SSC-L/FFTF to IANUS (L. G. Epel)

A number of transients that have been run at BNL utilizing the IANUS code (Perkins, 1979) have been selected to be studied with the FFTF version of SSC-L. During this quarter, the class of scenarios ensuing from pipe ruptures in various parts of the primary loop have been simulated using SSC-L/FFTF and the results have been compared to the analogous IANUS results. Any significant differences in predictions from the two codes are traceable to the combined effects of differences in modeling of the flow from a pipe break, differences in modeling check valve characteristics, and to a small extent, differences in primary pump response to the loss in back pressure at the pump outlet.

Specifically, the four simulations done are (in ascending order of severity):

- double ended break at check valve inlet
- 0.048 m² break at reactor vessel inlet (RVI)
- double ended break at check valve outlet
- double ended break at RVI

The first two simulations illustrate the effects of check valve behavior and break flow modeling, respectively. The discussion here will therefore be limited to these two cases.

3.2.1 Double Ended Break at Check Valve Inlet

In SSC-L the check valve is modeled as having no mass. Thus as soon as a back pressure sufficient to close the check valve is reached, (input variable) the check valve can shut instantaneously. By contrast, in IANUS

there are two options available to the user who wishes to include a check valve in his simulation (IANUS, 1976). There is a "perfect" check valve modeled, much like the one in SSC-L, which has no inertia; however, a representation which is dynamically modeled is also available. This representation was used in the IANUS reference runs; the effect of differences in check valve behavior on break flow, as computed by the two codes is shown in Figure 3.1. In the figure, a positive flow represents flow back through the check valve from the reactor vessel. The larger back flow computed by IANUS during the first second or two results in a greater depletion of core flow when compared to the SSC-L calculations for this time interval. This causes the temperature of the sodium leaving the active portion of the core to be higher when calculated by IANUS than in SSC-L; the comparison for this case is 908 K versus 886 K.

3.2.2 Break at Reactor Vessel Inlet

When the rupture occurs downstream of the check valve, the effect of the check valve is minimal. For this transient, the core flow, and hence the temperature of the sodium leaving the core, depends strongly on the manner in which the flow from the break is modeled. IANUS contains a simple model which uses the assumption that the pressure in the fluid emanating from the break is equal to the outside ambient pressure. SSC-L utilized a more sophisticated model (Quan and Agrawal, 1977) which results in relatively smaller flow through the rupture. Figure 3.2 shows a comparison of the break flow behavior for the first three seconds of the transient as calculated by the two codes. The discrepancy in break flow causes a significant difference in the peak core exit temperature; SSC-L/FFTF predicts a first peak of 893 K at about 3/4 seconds while IANUS predicts a 948 K peak.

According to both codes, flow reversal in the core occurs about 40 seconds after the rupture, which causes a second temperature peak just as flow reversal is initiated. Since the second peak temperatures obtained by both codes agree quite well (7 K difference), it is evident that the SSC-L/FFTF core heat transfer modeling at low coolant flow rates is similar to that in IANUS.

3.3 Inter-Code Comparisons of SSC-L to DEMO/CRBRP (R. Pyare)

In order to better investigate the differences between SSC-L and DEMO, a case with detailed DEMO output was sought. The case selected involves a pump coastdown transient to pony motor speed. In SSC-L, the reactor was simulated by four channels: average fuel assembly, average radial blanket, hot fuel assembly and bypass. The simulation included the entire plant. A 300 second transient was run and the results were carefully reviewed. Areas where differences were found are discussed below:

(1) Reactor Power

The worths of the primary and secondary control rods were adjusted and the transient decay power was changed to match the DEMO input.

Figure 3.1
Normalized Backflow Through Checkvalve
Following Double Ended Pipe Rupture

(2) Primary Flow and Pump

The rated primary pump conditions for SSC-L were changed to match the DEMO input. During the transient, the pump speed response as used in both codes were in close agreement. There was a slight difference in the primary flow after the pump reached pony motor speed.

(3) Intermediate Flow and Pump

After a coding error in SSC-L was discovered and corrected,, excellent agreement was obtained between the pump speeds. However, the intermediate flow differs by 4.5%. The cause of this difference in being investigated.

(4) Reactor Coolant Temperature

There are various items which affect the coolant temperature in the channels, such as flow redistribution, gap conductance, heat transfer coefficient, number of radial nodes etc. The optimum numbers of radial nodes for SSC-L were found to be 4 for the fuel pins and 8 for the radial blankets. A smaller number of nodes could be used for lesser accuracy.

With constant gap conductance and flow fractions (same as in DEMO), the coolant exit temperature in the average channels deviated less than 5°K before pump reached pony motor speed. Thereafter, a maximum deviation of 10°K occurred (see item 2 above) before the reactor inlet temperature started deviating at about 100 seconds because of difference in item (3) above.

The effects of flow redistribution and variable gap conductance were found to be significant. In the hot channel, the uncertainties in the properties and heat transfer coefficients were not included. The deviation in the coolant exit temperature followed the same pattern as for the average channel.

(5) Tertiary Loop

The recirculating pump provided forced circulation in the evaporator throughout the transient. The feedwater was specified as a function of time in tabular form. The steam generator output will be compared after resolving the cause of difference in item (3).

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