MASTER

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QUARTERLY PROGRESS REPORT

JULY 1 - SEPTEMBER 31, 1977

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REACTOR SAFETY RESEARCH PROGRAMS

QUARTERLY PROGRESS REPORT

JULY 1 - SEPTEMBER 30, 1977

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DEPARTMENT OF NUCLEAR ENERGY

BROOKHAVEN NATIONAL LABORATORY, ASSOCIATED UNIVERSITIES, INC.

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FOREWORD

The Reactor Safety Research Programs Quarterly Progress Report describes current activities and technical progress in the programs at Brookhaven National Laboratory sponsored by the USNRC Reactor Safety Research Division. The projects reported each quarter are the following: Gas Reactor Safety Evaluation, THOR Code Development, SSC Code Development, LMFBF and LWR Safety Experiments, Fast Reactor Safety Code Validation and Technical Coordination of Structural Integrity.

This report is the fourth of a series of quarterly reports which combines the reports of the individual projects mentioned above. The previous reports, BNL-NUREG-50624, BNL-NUREG-50661 and BNL-NUREG-50683, have covered the periods October 1, 1976 through June 30, 1977.

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TABLE OF CONTENTS

	<u>Page</u>
FOREWARD	
I. HTGR SAFETY EVALUATION	1
Summary	1
1. Fission Product Release and Transport	3
1.1 Interaction of CsI with HTGR Materials	3
1.2 Thermochromatographic Study of the Interaction of Elemental Iodine with HTGR Materials	5
1.3 Simple Theoretical Models for the Process of Thermochromatographic Separation	13
1.4 Interaction of Cesium with Fused Silica	15
1.5 Fission Product Release from Irradiated Fuel Kernels	18
1.6 The Permeability and Retentivity of Stressed Concrete Relative to Fission Product Iodine	18
References	30
Appendix I	33
References	42
2. Materials, Chemistry, and Instrumentation	43
2.1 Materials	43
2.2 Materials Test Loop	66
2.3 Characterization and Oxidation Kinetics of PGX Graphite	67
2.4 Helium Impurities Loop	75
2.5 Safety Instrumentation and Control Systems	78
References	78
3. Structural Evaluation	79
3.1 Core Seismic	79
3.2 Steam Generator Tube Weld Evaluation	79

	<u>Page</u>
References	89
4. Analytical	90
4.1 Gas Dynamics in the Containment Vessel	90
4.2 HTGR Code Library	93
4.3 Preliminary Investigation of Turbulent Reactive Mixing in PCRV/CV Gas Mixtures	99
References	123
II. LMFBR SAFETY EVALUATION	124
Summary	124
1. Fast Reactor Assessment -- Accident Sequence Studies	125
1.1 Hydrodynamic Characteristics of Two-Phase Dispersal Systems	125
1.2 Dispersion and Heat Transfer in Two-Phase Boiling Systems	128
1.3 Boiling Pools with Internal Heat Generation	132
1.4 Two-Phase Solidification Dynamics of Flowing Core Debris	139
References	146
2. Technical Coordination of Structural Integrity	147
3. SSC Code Development	148
3.1 Transient Fuel Heat Transfer and Coolant Flow Computation	148
3.2 Heat Transport System	148
3.3 Steam Generating System	155
3.4 System Integration Method	156
3.5 Code Development	156
References	157
4. SSC Code Validation	159
4.1 Analysis of Integral Thermohydraulic Experiments	159
4.2 SSC-L Needs	159

	<u>Page</u>
4.3 Sensitivity Analysis Methods	159
4.4 Critical Experiments	165
References	166
III. LIGHT WATER REACTOR SAFETY	167
Summary	167
1. Light Water Reactor Thermal/Hydraulic Development Program	169
1.1 Development of Constitutive Relations	169
1.2 Design, Construction and Checkout of Experimental Equipment	173
1.3 Development of Instrumentation Techniques	175
References	192
2. THOR Code Development	193
2.1 General Program Objectives and Approach	193
2.2 Status and Current Goals	193
2.3 Current Achievements	194
2.4 Component Modeling for Two-Loop PWR	197
2.5 System Modeling	204
References	207
3. Appraisal of Analysis Development in Foreign Countries	208
3.1 NICKY	208
3.2 NORCOOL	208
3.3 BRUCH-S	209
3.4 BRUCH-D	211
3.5 RISQUE	212
References	212

I. HTGR SAFETY EVALUATION

SUMMARY

The thermochromatographic data on CsI volatilization indicate that partial dissociation of CsI occurs upon heating to 1500°C in helium containing 2% water vapor. The dissociation product iodine is collected in a cold trap while cesium interacts with quartz at the hot end of the gradient tube. Whereas CsI deposited on stainless steel was found to decompose readily at 550°C in helium containing 10% O₂, CsI deposited on quartz at 550°C did not decompose even in helium containing 30% O₂ or in air containing 2% water vapor.

Experiments performed on bulk CsI samples indicate that replacing He by air or N₂ environments does not strongly affect the stability of CsI at 650°C. Preliminary results indicate that a uranium iodide is formed upon heating UO₂.10 together with CsI at 1000°C.

Thermochromatographic data on deposition of elemental iodine on steels indicate that iron iodide can be formed at a temperature >430°C but deposits in the range 150-300°C. Formation of iron iodide appears to be kinetically favorable at lower temperatures, too. Deposition of iodine may occur in several temperature regions; at least two of these deposits exhibit long-term stability, even in the presence of an oxidizing environment.

Three simple models have been proposed as an aid in interpreting the results of thermochromatographic experiments. The models correctly predict the deposition temperatures for CsI and I₂.

An investigation of the interaction of cesium with fused silica has been initiated at Brooklyn College. Fused silica is the HTGR material which will be exposed to the gaseous helium environment at the highest temperatures during normal operation.

The gamma spectrum of short-term irradiated TRISO fuel kernels indicates the presence of ¹³¹I, ¹³³Xe and ¹⁴⁰Ba. The kernels will be thermally failed in a graphite matrix and the liberated fission products will be examined thermochromatographically.

The work on the project "Permeability and Retentivity of Stressed Concrete Relative to Fission Product Iodine" has principally involved: (1) Inert gas permeability experiments on 3-inch cube samples subsequently used for ¹³¹I-tagged iodine vapor Permeability Experiments 3 and 4. (2) ¹³¹I-tagged iodine vapor Permeability Experiments 3 and 4. The samples exposed to the ¹³¹I-tagged iodine vapors were subsequently sectioned at predetermined points for concentration profiles. A comparison of the concentration profile fit parameters from the two permeability experiments with those from the Sorption Experiment 4 (April-June 1977 quarter) is also included. (3) Study of inert-carrier gas (helium) saturation with respect to tagged iodine vapors as a function of flow rate through the source tube. (4) High-temperature Sorption Experiment 5 still in progress.

Sixteen creep-rupture test units are being used for the testing program. Tests of Incoloy-800H and Hastelloy-X are under way in air and in an impure helium environment from the MTL loop.

Mean tensile stresses are shown to be detrimental to high-cycle fatigue strength for Incoloy-800H, annealed 2½Cr-1Mo steel and Type 422 stainless steel. In the case of the latter material, for which the 900°F test temperature was low enough to minimize creep deformation, Goodman's analysis for estimating the magnitude of the mean-stress effect is probably adequate.

Work continued on the fractography of oxidized graphite. In particular, the mechanism of failure was studied in PGX graphite tensile specimens which had been oxidized in the HIL loop at BNL.

The Materials Test Loop began operation this reporting period, supplying controlled helium to 4 creep testing machines and 1 high-cycle fatigue machine. The control of all of the impurity levels, except for hydrogen, has been accomplished to a satisfactory degree. The hardware and electrical wiring for 4 aging retorts have been completed and the retorts are virtually ready to be connected to the MTL.

Oxidation kinetics experiments with a PGX graphite specimen containing >1000 ppm Fe yielded a reaction order with respect to H₂O of ~0.76 at 820°C over a concentration range of 10-9000 ppmv. Activation energy measurements indicate possible changes in the reaction mechanism over the temperature range 640-905°C. The effect of burnoff up to several percent on the reaction rate was also investigated and found to enhance the rate by at least an order of magnitude; this suggests, as expected, quite rapid surface development during H₂O oxidation of PGX graphite.

A series of chemistry experiments has been completed in the Helium Impurities Loop. In one set of tests CO was injected into the HIL and allowed to circulate while the decline in CO level and increase in CO₂ concentration were observed. In another set of tests CO₂ was injected and allowed to circulate, but there were no significant changes in molecular species.

The mass spectrometer for monitoring the coolant composition at Fort St. Vrain is still under construction.

Fine mesh studies using the CIRC code confirm the lack of circulation found previously with a coarse mesh. Changes have been made in the code which allow a variably-dimensioned spatial mesh; this will allow details to be analyzed where necessary. An experimental program to justify analytical calculations of the depressurization has been initiated.

Analytical/numerical work has been initiated on diffusive mixing/finite-rate chemical kinetics in PCR/V/CV gas mixtures. Preliminary results indicate that such fluid mechanic phenomena should be pursued further.

The vertical array test rig was further modified to extend the range of coupled vertical and horizontal excitation inputs. Only weak coupling between the two excitations has been noted to date. Efforts to develop a three-dimensional test rig and to compile a three-dimensional array analysis code continue. The elastic analysis of steam generator weldments was repeated using tube geometry and loading parameters consistent with General Atomic's latest design practice. The LEFM computer code validation studies and the results of the code applications are reported.

1. Fission Product Release and Transport

1.1 Interaction of CsI with HTGR Materials

Based on fission yields and thermodynamic considerations, CsI has often been inferred as the compound likely to form in high burnup oxide and carbide fuels. Recent electron microprobe work (Kleykamp, 1975) has indicated the possible presence of CsI in the pyrocarbon coatings of uranium carbide fuel particles. CsI has also been identified (Aitken, 1974) as a product formed from a synthetic mixture of $(U,Pu)O_{2+x}$, Cs_2O and PdI_2 heated to $1150^\circ C$ in the hot end of a sealed stainless steel (s.s.) temperature gradient capsule. A knowledge of the stability and reactivity of CsI is needed for calculating the distribution of fission product cesium and iodine released into the environment from a potential accident.

1.1.1 Thermochromatographic Study of CsI with HTGR Materials (I. Tang, H. Munkelwitz, F. Growcock)

The results of all the thermochromatographic experiments on CsI completed to date are summarized in Table 1.1 (Tang, 1977). The data on samples 1 through 4 have previously been discussed (Aronson, 1977). Although the data in Table 1.1 are of a preliminary nature, some interesting conclusions can be drawn from the experimental observations.

(1) The presence of up to 1% water vapor in helium did not affect the stability of CsI upon release at $800^\circ C$; however, partial dissociation of CsI occurred when it was heated to $1500^\circ C$ in helium containing 2% water vapor. The dissociation product iodine was carried by the gas flow to the charcoal trap located at the cold end of the temperature gradient tube, while cesium was found to have reacted with quartz surfaces on the hot end of the gradient tube where it was collected.

(2) CsI deposited on quartz surfaces at $550^\circ C$ was not oxidized by passing over it helium containing 2% water vapor, 15% CO_2 + 15% CO , 30% O_2 or air containing 2% water vapor. However, CsI deposited on Type 304 s.s. surfaces, although resistant to water vapor oxidation, was found to decompose quickly and completely in a helium stream containing 10% oxygen. A large fraction of the Cs residue (possibly Cs_2O) from the oxidation of CsI deposited on s.s. surfaces could be revaporized by heating it to $800^\circ C$ (Aronson, 1977).

Additional experiments will be performed to investigate the stability of CsI in helium and oxidizing environments at a temperature of $2000^\circ C$. The interaction of CsI with stainless steel and other HTGR metals in an oxidizing atmosphere will also be further investigated.

1.1.2 The Reactivity of Bulk CsI Samples (S. Nicolosi)

The thermochromatographic experiments deal primarily with milligram quantities of material spread over a fairly large physical surface. Enough material is generally not available so that the chemical compounds deposited on surfaces can be readily identified by such techniques as X-ray diffraction. Some experiments utilizing gram quantities of CsI are, therefore, under way.

Table 1.1

Summary of Results from CsI Deposition Experiments

Sample Description	Atmosphere	Deposition Surface	Deposition Temperature	Comments
1. 15 mg CsI in graphite crucible at 800°C	He at 50 ml/min	s.s. 304	570-630°C	Molecular CsI was released.
2. 15 mg CsI in Al ₂ O ₃ crucible at 800°C	He+0.6% H ₂ O at 50 ml/min	s.s. 304	540-610°C	CsI was not oxidized by water vapor.
3. 15 mg CsI in graphite crucible at 800°C	He+0.6% H ₂ O at 50 ml/min	s.s. 304	560-610°C	CsI was not oxidized by water vapor.
4. CsI deposited on s.s. surfaces at 550°C	He+10% O ₂ at 50 ml/min	s.s. 304	Cs: 490-560°C I: charcoal trap at ambient	CsI was oxidized by O ₂ .
5. 10 mg CsI in graphite crucible at 1550°C	He at 140 ml/min	quartz	520-570°C	CsI was stable up to 1550°C.
6. 10 mg CsI in graphite crucible at 1500°C	He+2% H ₂ O at 140 ml/min	quartz	CsI: 460-500°C Cs: 850-900°C I: charcoal trap at ambient	CsI was partially oxidized by water vapor.
7. CsI deposited on quartz surfaces at 550°C	He+2% H ₂ O He+30% O ₂ He+15% CO+15% CO ₂ Air+2% H ₂ O	quartz	CsI peak position moved from 550°C to 475°C in 9 hours at 140 ml/min	CsI remained on surfaces.

A simple flow system is being used to study the reaction between CsI and various gases. The gas flows through an 8 millimeter diameter tube which passes through a furnace and is connected to a cold trap maintained at -77°C by a refrigeration unit. A CsI pellet, which is pressed in an argon atmosphere dry box, is placed in the high temperature region ($620-670^{\circ}\text{C}$) of the furnace. As the furnace is heating to temperature (typically 2 1/2 hours) the reactant gas is passed first through a $\text{Mg}(\text{ClO}_4)_2$ tube to remove water vapor, then through the heated reaction tube containing the CsI pellet and then through two cold traps maintained at -77°C . Typical flow rates are 0.5-1 SCFH. The sample is maintained at temperature for 5-20 hours. Most experiments were performed using Cerac/Pure, Inc. CsI (99.9%). Several experiments were performed with Alfa Ventron ultrapure CsI (lot analysis of less than 35 ppm impurities for 18 elements and sulfate). The CsI source produced no difference in results.

It was observed that free elemental iodine is slowly liberated from the reaction tube when a 10% O_2 in He gas mixture is passed over the molten CsI at 650°C . This reaction appears to proceed very cleanly with no other reaction products collecting in the cold trap. When the experiment is performed with compressed air or N_2 (99.996%) as the reactant gas, a yellow material is collected in addition to some elemental iodine. Repetition of the experiment several times yielded enough material in the cold trap to enable powder X-ray diffraction to be performed. The analysis indicated the presence of cesium iodide in addition to other components which were not readily identifiable from ASTM cards. Additional experiments were performed to determine if the yellow reaction product resulted from reaction with the quartz reaction tube. CsI was exposed to flowing air at 650°C in a Type 304 stainless steel tube. The same reaction products and similar yield were observed. When the experiment was performed using argon no deposit was observed. With CO_2 , the material was observed in highly reduced yield. Work on this problem is currently being completed.

A general conclusion that can be drawn from the data is that the quantity of material volatilized from the CsI samples in any of the gaseous atmospheres is quite small relative to the quantity of CsI present in the hot zone.

Work has been initiated on the interaction of CsI with non-stoichiometric UO_2 . CsI was heated at 1000°C with $\text{UO}_{2.10}$ (40 mole percent CsI) for 24 hours in an evacuated, sealed, quartz ampule. To facilitate chemical analysis, a large quantity (30 grams) of mixture was used. During the experiment material deposited in the cold portion of the ampule. The material contained some crystals which were similar in appearance to uranium iodide. Analysis by X-ray fluorescence indicated the presence of uranium, iodine, arsenic, iron, nickel, copper and zinc. The latter 4 elements are typically seen as impurities distilled from the CsI reagent which is used.

1.2 Thermochromatographic Study of the Interaction of Elemental Iodine with HTGR Materials (F. B. Growcock, A. Hosseini)

Iodine from irradiated fuel may be liberated during normal operating conditions as I atoms and chemisorb and/or react with coolant loop materials as it flows through the reactor. During a core heatup accident the entire core in-

ventory of iodine may be liberated; the chemical state of the iodine is unknown under these conditions, but it appears likely that a significant fraction of the iodine is present as an equilibrium $I_2 \rightleftharpoons 2I$ mixture. Consequently, it is imperative that we understand the sorption behavior of elemental and atomic iodine on HTGR materials; this is the subject of the current study.

The thermochromatographic apparatus was modified slightly to accommodate gaseous samples, as well as solids. A pyrex sample trap packed with pyrex wool and maintained at a constant temperature was attached to the inlet of the quartz reaction tube. A charcoal trap followed by a bubbler filled with mineral oil were attached to the tube exit. Total gas flow was maintained, in general, at 50 cc/min. Helium at ~ 1.0 atm. was purified by passing it through a 5X molecular sieve trap kept at -196°C and copper turnings maintained at 550°C . The previously used NaI(Tl) detector and pre-amplifier were replaced with newer, more efficient ones, and an amplifier/oscilloscope system attached for better viewing. Most counting measurements were made with the furnace closed; this attenuated the counting rate by $\sim 50\%$ and produced apparently broader deposition peaks. Counting was generally done at intervals of 1 inch for 1 minute. In the first two experiments, however, activities were too low for good precision, so counting times of 4 minutes were employed. Oxidized steel tubing was used as the substrate material; prior to use it was scrub-cleaned with trichloroethane, Alconox, distilled water and finally methanol, and then air-dried for 1 hour.

For the first 2 experiments I_2 was prepared by the oxidation of NaI (with tracer ^{131}I) solution by HNO_3 and extracted into CCl_4 . To remove the latter, the solution was allowed to set in the sample trap for 14 hours over activated coconut charcoal and then heated to $\sim 100^\circ\text{C}$ under a dry stream of helium. To liberate the tagged I_2 into the carrier stream of the thermochromatograph the charcoal was heated slowly, increasing the temperature up to $< 600^\circ\text{C}$. A 5-foot long tube of Incoloy 800H was positioned in the quartz tube so that 1 foot extended from the furnace entrance. In the first experiment a very high flow rate (~ 10 l/min) gave rise to negligible deposition in the reaction tube; all of the activity was confined to the charcoal trap. The second experiment, run at the usual flow rate, gave the result shown in Figure 1.1; no activity was found in the charcoal trap. The deposition peak maximum occurred at $\sim 270^\circ\text{C}$ initially, but shifted to $\sim 260^\circ\text{C}$ within 2 1/2 hours. During that time interval 3% H_2O and 3% $\text{H}_2\text{O} + 8.5\% \text{H}_2$ were successively injected into the He stream. The peak activity decreased rapidly during this procedure in exponential fashion (the lost activity was found in the trap).

For the rest of the experiments I_2 was prepared by decomposition of tagged PdI_2 in vacuo at $300\text{--}400^\circ\text{C}$. PdI_2 was synthesized from an acid solution of PdCl_2 (pH ~ 1.2) to which NaI containing ^{131}I tracer was added; the solution was filtered and the precipitate washed with doubly-distilled H_2O to rid it of the H^+ , Na^+ and excess PdCl_2 , and flushed with acetone into a trap. Mild heating in vacuo removed all traces of acetone and water.

Carbon steel tubing, in 1-foot lengths, was used to investigate the effect of temperature on the deposition of iodine. In experiment No. 3 the steel ran the length of the furnace, 0-48 inches. Deposition occurred as a wide multi-peak band as shown in Figure 1.2. The apparent peak maxima occurred at 300, 340 and 375°C , but some activity was also found up to $\sim 630^\circ\text{C}$. After quenching and

Figure 1.1 Deposition of iodine on oxidized Incoloy-800H tubing: (a) deposition in helium stream, followed immediately by (b) passage of H₂O-He mixture over deposit and (c) passage of H₂O-H₂-He mixture over residual deposit.

Figure 1.2 Deposition of iodine on carbon steel tubing positioned at 0-48 inches along reaction tube.

removing the steel tubes, the quartz tube was counted: no activity was observed.

In experiment No. 4 carbon steel was positioned at 0-24 inches. Again, some activity was found in the high-temperature region; most of the activity occurred in a narrow region with a sharp maximum at $\sim 270^{\circ}\text{C}$, as shown in Figure 1.3.

In experiment No. 5 the steel tubes were positioned at 24-48 inches. The activity curve obtained possessed only one distinct peak with a maximum at $\sim 430^{\circ}\text{C}$, as shown in Figure 1.4(a) for time = 0. The effects of time and gaseous environment on the deposition profile were of interest. In Figure 1.5 the decrease in activity of the 430°C peak as a function of time is depicted; in 1 hour the activity had decreased by more than 50% (a rate of loss of $\sim 1.47 \times 10^{-4} \text{ sec}^{-1}$ is obtained). The apparent linear decrease was suddenly halted at that time, and decreased very slowly thereafter, so that after a total of 3 hours the total activity was down to $\sim 40\%$ of that observed initially. No ^{131}I activity was found in the charcoal trap at this time, but 2 peaks of similar size appeared at $\sim 340^{\circ}\text{C}$ and 260°C . At this time $\sim 0.7\% \text{ H}_2\text{O}$ was added to the He stream for 2 hours, but no unusual effects were observed. The curve obtained at 5 hours is shown in Figure 1.4(a). The charcoal trap still showed no activity.

Experiment No. 5 was continued with the addition of $\sim 5\% \text{ O}_2$ to the He stream. Counting measurements during this interval showed no change in the peak at 430°C , but the other 2 peaks did exhibit strange behavior. The 340°C peak gradually shifted to 360°C and decreased in size, while the 260°C peak increased and then decreased to its original level. When $0.9\% \text{ H}_2\text{O}$ was substituted for the O_2 , the 340°C (360°C) peak continued to decrease while the 260°C peak shifted up and down but eventually stabilized at the original level again. During these operations activity began to accumulate in the charcoal trap. The result after a total heating time of 22 hours is shown in the third curve of Figure 1.4(a).

The experiment was continued with pure helium, so that after a total time of 27 hours the first curve of Figure 1.4(b) was generated. Again, the activity of the central peak decreased significantly, with a concomitant rise in the charcoal trap activity. Further heating produced no significant changes, as shown in the second and third curves of Figure 1.4(b) for 48 and 91 hours total heating times. The peak at 260°C did, however, shift to a slightly lower temperature ($\sim 240^{\circ}\text{C}$). As a final check on the stability of the deposition toward oxidants, $2\% \text{ H}_2\text{O}$ was injected into the He stream for 0.5 hour; a slight decrease in the activity of the central region was noted, as shown in the 91.5-hour curve of Figure 1.4(b), but it may not be significant. After quenching the system and removing the steel tubes, the quartz tube was counted: no activity was observed.

Detailed analysis of the results will not be possible until further experimental work is done. Suffice it to say that the effects observed above are indicative of the deposition of different iodine species, whose behavior may be explained by surface saturation effects; oxidation of these deposited species may not be important. The formation of iron iodide is favorable at temperatures $> 430^{\circ}\text{C}$, but its deposition appears to occur in the low-temperature region ($150\text{--}300^{\circ}\text{C}$). Likewise, its formation appears to be kinetically favorable at temperatures $< 430^{\circ}\text{C}$.

Figure 1.3 Deposition of iodine on carbon steel tubing positioned at 0-24 inches along reaction tube.

Figure 1.4 Deposition of iodine on carbon steel tubing positioned at 24-48 inches along reaction tube: (a) initial deposition (curve at 0 hr); 0.7% H_2O added after 3 hours for 2 hours (curve at 5 hr); passage of ~5% O_2 in He for 1 hour, followed by 0.9% H_2O in He for 1 hour, followed by 15 hours of pure He (curve at 22 hr). (b) Passage of pure He over iodine deposit (curves at 27, 48 and 91 hr); passage of 2% H_2O in He for 0.5 hour (91.5 hr curve).

Figure 1.5 Time dependence of activity of iodine deposit at 430°C in Experiment #5 (Figure 1.4).

1.3 Simple Theoretical Models for the Process of Thermochromatographic Separation (J. M. Dickey, I. Tang)

The thermochromatograph separates different chemical components because of their different mobilities through a tube along which is maintained a temperature gradient. He flows slowly down the tube. The substance under consideration is vaporized at the hot end of the tube. A molecule of the impurity then travels along the tube, alternately condensing on the surface and re-evaporating into the vapor phase. The impurity as a whole forms a narrow band on the surface of the tube and this band moves toward the lower temperatures with a velocity which decreases very sharply as the temperature of the band falls. After about half an hour the band is essentially stationary as the velocity has fallen to the order of 1 inch per hour. The dimensions of the apparatus, flow rates, etc. are such that several physical processes play a role in determining the mobility of a species. Thus no single simple model can accurately describe the thermochromatograph. However, for a first approach it is useful to consider 3 different simple models, each of which emphasizes certain aspects of the problem and so is an oversimplification, for then the correct solution must contain features from all the models.

We can write the total current in the vapor phase, J , as the sum of 2 terms, a convective term and a diffusive term:

$$\vec{J} = c\vec{V} - D\vec{\nabla}c$$

The relative magnitude of the 2 terms depends on the ratio $V/(D\nabla c/c)$. Two relatively simple extreme cases would be to completely neglect one of these terms, i.e. to assume that the impurity is carried along by the He carrier and that diffusion is relatively unimportant (giving a small correction) - this is the usual assumption in chromatography - or to assume that the He flow rate is so slow that the motion is due to diffusion down the concentration gradient which is created by the temperature fall along the tube. For the experiments under consideration the ratio of the 2 currents is of the order of 1:3 so in practice there is a complex interplay of both processes; thus, a detailed analysis is required. However, some insight can be gained by considering the 2 extreme models mentioned above. A third simple model is to consider the progress of a narrow uniform band along the tube. The vapor density of the impurity and also the velocity of the gas will vary from the wall of the tube to the center. In the simple models, it is assumed that both these quantities are independent of r at any cross section. In 2 models, the "diffusion" and "convection" models, it is assumed that the partial pressure at any point in the tube is equal to the equilibrium vapor pressure. The diffusion model corresponds to a zero flow rate and is an approximate lower limit for slow flow rates. In the convection model, diffusion is neglected and the impurity atoms are swept downstream by the helium atoms. The "band" model is intermediate between these 2 extremes as the partial pressure is taken to be constant within a narrow band.

In Figure 1.6 are shown the results of calculations based on these 3 models for CsI using the experimental data. The location of the experimental peak is also shown and it can be seen that the peak does fall at a temperature at which all the models would predict that further motion of the deposit along the tube should be very slow. Similar calculations were performed for the 3 chemical

Figure 1.6 Time taken for the deposit to travel along the tube.
a) convection model, b) band model, c) diffusion model.
The location of the observed deposit is shaded.

species CsI, I₂ and Cs using the convection model, and the experimental peaks are indicated. It can be seen that even these simple models can predict the widely different temperatures at which different compounds should be deposited (Figure 1.7).

1.4 Interaction of Cesium with Fused Silica (S. Aronson, J. Mittelman - Brooklyn College)

The HTGR primary coolant, helium, circulates through the reactor system at relatively high temperatures, 400°C to 900°C, with transient temperatures of 1200°C possible at certain locations. Both metallic and ceramic thermal insulating materials are used to keep the PCRV at a reasonably cool temperature. The principal metallic high temperature materials are Incoloy-800, Hastelloy-X and special composition steels (Roberts, 1974). The principal ceramic high-temperature materials are fused silica block, fused silica fiber and alumino-silicate fiber (Roberts, 1974). There is relatively little information in the literature on interactions with metallic materials and almost no information on interactions with non-metallic materials.

We plan to investigate plate-out, lift-off and penetration of cesium, strontium and iodine-base substances with fused silica which is the material that will be exposed to the gaseous helium environment at the highest temperatures during normal operation, 1200°C. The chemical interactions will be studied as a function of temperature and fission product concentration in vacuo and in gaseous environments of either helium or mixtures of helium and water vapor.

The apparatus shown in Figure 1.8 will be used to study the interaction of elemental cesium with fused silica in vacuo. This system is similar to that used by Milstead and Zumwalt (Milstead, 1966) to study cesium interactions with steels. Elemental cesium tagged with ¹³⁴Cs will be vaporized by the furnace at the left of Figure 1.8 to achieve cesium vapor pressures of 10⁻² to 10⁻⁶ torr. The cesium vapor will interact with fine quartz rods (√2 mm diameter) positioned in a second furnace at a temperature of interest in the range of 600°C to 1100°C. Absorption of cesium by the quartz in cesium vapor and desorption of cesium from the quartz in vacuo will be followed with a γ-scintillation detector focused on the quartz rods. Construction of the apparatus is now under way.

A study which is under way of the release of cesium from graphite in mixed adsorbates containing cesium and strontium has been temporarily suspended. This investigation requires the doping of graphite with cesium and strontium salts (e.g., CsNO₃, Sr(OH)₂) which would presumably decompose at elevated temperatures to yield elemental cesium and strontium co-adsorbed on graphite. Some preliminary experiments on the volatilization of CsNO₃ performed in the thermochromatographic apparatus at BNL have indicated that the decomposition of CsNO₃ in the presence and absence of graphite is more complex than expected. The decomposition processes for other cesium and strontium salts are equally obscure. Experimental work will, therefore, be deferred until a reliable method is found to co-adsorb cesium and strontium on graphite.

Figure 1.7 Time taken to travel along the tube for 3 chemical species.
Observed deposits are indicated by an arrow.

Figure 1.8 Apparatus for studying the absorption of cesium by silica in vacuo.

1.5 Fission Product Release from Irradiated Fuel Kernels (F. B. Growcock, A. Hosseini)

Twenty-five TRISO fuel particles were vacuum sealed in a quartz ampoule and irradiated for 15 minutes in the HFBR facility ($\Phi \sim 10^{14}$ neutrons/cm²-sec). After allowing 2 days for the quartz to cool, energy scans of the intact particles were made at intervals of 1-2 days with a NaI(Tl) scintillation counter. Typical of the results obtained is the spectrum shown in Figure 1.9. From the available information we can only be certain of the presence of 3 radionuclides: ¹³¹I, ¹³³Xe and ¹⁴⁰Ba.

A high-resolution Ge(Li) detector is due to arrive soon; it will be coupled to the TN-11 computer previously utilized in the graphite oxidation effort. Isotope analysis of the fission products liberated from fuel kernels will become possible.

Fuel kernel heatup experiments are under way. At the entrance to the thermochromatographic apparatus, an H451 graphite crucible is suspended inside a refractory insulating tube lying in the quartz flow tube; the crucible serves as the susceptor for a 5 kW Lepel induction heater, which can potentially heat the graphite to $\sim 2000^\circ\text{C}$. Initial measurements of the coating failure rate of unirradiated fuel kernels as a function of temperature should furnish a working temperature range within which the short-term irradiated fuel particles can be studied.

1.6 The Permeability and Retentivity of Stressed Concrete Relative to Fission Product Iodine (L. R. Zumwalt, J. F. Mirza - North Carolina State Univ.)

1.6.1 Inert Gas Permeability

In this part of the experiment helium gas was forced across a 3-inch concrete cube with a through-crack at different external applied pressures, (P_a), for closing the crack. The helium gas flow pressure drop, (P_f), across the cube was measured for various flow rates using a water manometer (see Appendix I).

The data obtained were plotted showing the variation of flow rate as a function of P_f for various isobars of given P_a .

Figure 1.10 is such a plot obtained for Sample No. 4 (which was subsequently used for Permeability Experiment 4). From Figure 1.10 it can be concluded that the resistance to flow increases with P_a (applied pressure to close through-crack). The rate of increase of P_f was found to be linear over a flow rate range of 100 ml/min to 1700 ml/min for P_a values of 518 psi and above.

For lower P_a values in the range of 345 psi to 460 psi, the relationship between P_f and flow rate was found to be linear for flow rates of 480 ml/min and higher.

For the crack geometry of Sample No. 4, the P_f range was found to be 0.1 cm of water to 4 cm of water for P_a and flow rate ranges of 345 psi to 806 psi and 6 ml/min to 1700 ml/min, respectively.

Figure 1.9 Gamma spectrum, at 0-0.7 MeV, of TRISO fuel kernels exposed to $\sim 10^{17}$ n/cm².

Figure 1.10 Helium Flow-rate vs. Flow Pressure Drop Isobars (for Indicated P_a)

The data obtained lead us to believe that even at pressures up to 800 psi the through-crack in the concrete cube was not fully closed and provided a path of least resistance to gas flow.

The data from inert gas Permeability Experiment 3 were not conclusive but the trends noticed were similar to those from Experiment 4. It might be expected that a difference in through-crack geometry (i.e., its width and surface roughness) and the amount of material lost from the faces of the crack during crack induction would yield different results (P_f vs. flow rate) as was observed. Unfortunately, it is not possible to characterize the cracks in a quantitative manner.

1.6.2 Tagged-Iodine Vapor Permeability Through Concrete

In this quarter, two ^{131}I -tagged iodine vapor permeability experiments were completed. In these experiments, helium gas was used to transport iodine across through-cracked concrete cubes at a flow rate of 34 ml/min and P_a (applied pressure to close crack) of 460 and 806 psi for Experiments 3 and 4, respectively.

The procedure followed to obtain sections, and the theory of the observed diffusion profiles have been described in the quarterly report for the period April through June 1977 (see Appendix I).

The result of the "fit" of parameters is given in Table 1.2 where the symbols used are defined as:

C_f^0 = concentration of fast component at the surface of the concrete due to in-pore gas and surface diffusion and sorption into the bulk.

D_f = diffusion co-efficient of the fast process.

K_f = rate constant for transfer of atoms in fast path to a more or less immobile sorbed state in the bulk of the concrete which is taken as corresponding to the state of the flow component.

D_s = diffusion coefficient for the slow process in the bulk.

C_s^0 = the slow component concentration of ^{131}I -tagged iodine at the surface.

The average concentrations of ^{131}I -tagged iodine in the concrete cubes at the end of exposure periods are listed in Table 1.3.

A bulk calibration procedure was used to determine the average concentration. The procedure involves dispersion of ^{131}I -tagged iodine solution with a known specific activity over a through-cracked concrete cube equivalent to the one used in the experiment. Using this cube and the same setup as for the experiment, the count rate is obtained. The count rates of this sample and of the experiment are compared to estimate the amount of tagged iodine in the cube used in the experiment.

Comparing the data from the permeability experiments to that from the sorption experiments (see Appendix I) it can be seen that:

Table 1.2

Diffusion Parameters and Boundary Concentrations Obtained from Concentration Profiles

Exp. No.	P_a (psi)	Profile No.	P_{I_2} (atm.)	Exposure Time	C_f^0 mg I_2 /g Concrete	C_s^0 mg I_2 /g Concrete	C_T^0 mg I_2 /g Concrete	D_s cm ² /sec.	K_f/D_f (cm ⁻²)	Profile given in Fig. No.
3	460	1	3.95×10^{-5}	2.322×10^6	2.207	10.07	12.28	7.52×10^{-10}	4.23	1.11
4	806	1	3.95×10^{-5}	2.159×10^6	1.2	6.18	7.38	6.44×10^{-9}	5.0	1.12
4	806	2	3.95×10^{-5}	2.159×10^6	1.73	5.45	7.18	6.31×10^{-9}	2.7	1.13

Figure 1.11 Experimental Data and Theoretical Fit for Profile from Permeability Experiment 3.

Figure 1.12 Experimental Data and Theoretical fit for Profile 1 from Permeability Experiment 4.

Figure 1.13 Experimental Data and Theoretical fit for Profile 2 from Permeability Experiment 4.

Table 1.3

Average Concentration of Iodine in Concrete Cube

Experiment No.	P_{I_2} (atm.)	Exposure Time (sec.)	$\bar{C}$
			Average Concentration (mg I_2 /g Concrete)
3	3.95×10^{-5}	2.32188×10^6	0.340
4	3.95×10^{-5}	2.15904×10^6	0.393

(1) C_f^0 , C_T^0 and C_S^0 values for the permeability experiments are higher by factors of 5 to 10.

(2) The D_s values for Permeability Experiment 4 are of the same order as those for the sorption experiments. However, the D_s value for Permeability Experiment 3 is lower by a factor of 10.

(3) The K_f/D_f values for the sorption experiments are higher by factors of 2 to 5.

(4) The exposure times for the permeability experiments were higher by factors of 2 to 10.

(5) The partial pressure of ^{131}I -tagged iodine vapor was in the range of 3.95×10^{-5} to 5.0×10^{-4} atm. compared to 3.95×10^{-5} atm. for the permeability experiments.

(6) The values of average concentration for the sorption experiments are higher by factors of 1.5 to 2.

It is believed that these differences can be attributed to the following:

(1) A difference in the geometry of the experiments.

(2) A difference in gas phase diffusion in the experiments due to forced flow conditions in the permeability experiments.

(3) The size (thickness) of the samples for the sorption experiments was 1/6 of those used for the permeability experiments.

(4) A difference in exposure times.

Figures 1.11, 1.12 and 1.13 show the experimental data and the theoretical profile fit corresponding to the concrete sample sections listed in Table 1.2. Figure 1.14 shows one of the profiles for Permeability Experiment 4 which gave the following data:

$$D_s^0 = 9.49 \times 10^{-9} \text{ cm}^2/\text{sec}$$

$$C_T^0 = 6.5 \text{ mg I/g concrete}$$

Figure 1.14 Experimental Data and Tentative (Eyeball) Fit for Profile 3 from Permeability Experiment 4.

$$C_f^o = 12 \text{ mg I/g concrete}$$

$$C_s^o = 4.85 \text{ mg I/g concrete}$$

$$K_f/D_f = 5.0 \text{ (cm}^{-2}\text{)}$$

In this case, the "fit" of the fast component is poor, though the values of D_s^o , C_T^o , C_f^o , C_s^o and K_f/D_f are in reasonable agreement with the data from the other profiles (Figures 1.12 and 1.13) of Permeability Experiment 4.

Table 1.4 lists the time taken by the ^{131}I -tagged iodine vapor to "break-through" the crack in the cube to the other side in the cases of Permeability Experiments 3 and 4.

Table 1.4

Time Taken to Break-through

<u>Permeability Experiment</u>	<u>P_a (psi)</u>	<u>P_f (cm H₂O)</u>	<u>Break-through Time (sec.)</u>
3	460	1.5	1.013×10^6
4	806	0.1	7.2×10^4

Break-through time is defined as the time elapsed from the start of the experiment to the time first traces of ^{131}I -tagged iodine are detected in the activated carbon trap. Helium sweep gas flows past the rear face of the cube to transport any tagged iodine coming through the crack to the activated carbon trap.

The break-through time for Experiment 3 was found to be higher by an order of 14 than that of Experiment 4. The break-through time correlates with the P_f value in the sense that with a higher P_f there is more holdup (sorption) of iodine in the concrete. This seems reasonable in that a higher P_f implies a greater crack closure (more flow resistance) and hence a larger ratio of diffusive flow of iodine into the concrete crack face relative to convective transport of iodine through the crack.

1.6.3 Study of Inert Carrier Gas Saturation

The aim of this experiment was to determine the range of inert carrier gas flow rates wherewith inert gas (He) will be saturated upon flowing through the source tube employed in our experiments (see Figure 1.15).

The experiment consisted of passing helium over tagged iodine crystals held at 0°C in the source tube ($P_{\text{I}_2} = 3.95 \times 10^{-5} \text{ atm.}$). The tagged mixture was then passed through a liquid nitrogen trap where the tagged iodine deposited. The liquid nitrogen trap was monitored for ^{131}I activity, using a NaI(Tl) scintillation detector with a single channel analyzer counting system. The flow rate of helium monitored, using a flowmeter, was held at various values for prolonged

Figure 1.15 Schematic Drawing of Source Tube

periods (~ 2 to 3 days) to allow the transport phenomenon to reach a steady state. The count rates obtained were plotted as a function of time (Figure 1.16). From this plot, the slope for the linear-most sections corresponding to a given flow rate was obtained.

A plot of the slope as a function of flow rate is shown in Figure 1.17. The plot shows a linear behavior up to a helium flow rate of 950 ml/min. Beyond this flow rate there is a large deviation from linearity. This leads us to conclude that helium passed over the tagged iodine crystals is saturated with iodine for flow rates up to about 950 ml/min. Lower flow rates were employed in all of our sorption and permeability experiments; accordingly, saturation can be assumed in estimating the vapor pressure of iodine to which concrete samples were exposed.

1.6.4 High Temperature Sorption Experiment

The high temperature sorption experiment was started in the second week of September. For sorption experiment procedures refer to Quarterly Reports January through June 1977. The only difference in this experiment is that the concrete samples are being held at 100°C instead of room temperature ($\sim 20^{\circ}\text{C}$).

To date, two samples have been exposed to ^{131}I -tagged iodine vapor for 9 days and 3 days, respectively. These samples were subsequently sectioned to obtain iodine concentration profiles. The data from these samples are being analyzed.

Currently, a third sample is being exposed. The planned exposure period for this sample is 27 days.

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Figure 1.16 Count Rate as a Function of Time for Helium Carrier Gas Saturation Experiment

Figure 1.17 Slope of Count Rate from Fig. 1.16 as a Function of Flow Rate in Helium Carrier Gas Saturation Experiment.

APPENDIX I

Quarterly Progress Report for Period April-June, 1977

This report was inadvertently omitted from the Reactor Safety Research Programs Quarterly Progress Report, April 1-June 30, 1977, BNL-NUREG-50683.

The Permeability and Retentivity of Stress Concrete Relative to Fission Product Iodine (L. R. Zumwalt and J. F. Mirza - North Carolina State University)

Summary

The April through June 1977 work on the project "Permeability and Retentivity of Stress Concrete Relative to Fission Product Iodine" has principally involved the completion of Sorption Experiment 4 which began last quarter, and Permeability Experiment 3 described below. Sectioning experiments were carried out on each of the samples exposed in the sorption experiment and profiles were obtained. These profiles were analyzed using a computer. Permeability experiments were carried out using inert gas on a sample cube with a through-crack. A tagged iodine vapor permeability experiment (No. 3) is in progress on the same concrete sample.

Sorption Experiments

Iodine Sorption Experiment 4 was completed in June. The sample holder had been modified so that parallel-piped samples could be removed and sectioned. Successive exposures were made whereby a fresh concrete sample was placed in the sample holder upon removal of an exposed sample. Several equilibrium concentration values as well as corresponding concentration profiles could be obtained by this procedure since the boundary (near-the-surface) concentration of the exposed samples corresponds to the equilibrium concentration. Four samples were exposed to constant partial pressures of iodine for different exposure times. Particulars regarding the partial pressures and exposure times of the samples are given below:

Sectioning of Samples and Concentration Profile Analysis

Samples exposed in Sorption Experiment 4 were sectioned to obtain concentration profiles. A portable drill press utilizing a solid carbide fluted spiral end mill bit was used to drill a core out of the cube in very thin sections. The concrete dust was collected on a filter paper using a suction device after each section was drilled. A calibrated NaI(Tl) well-type detector was used to count the samples. Samples were then weighed and profiles obtained.

After examining the profiles, it was evident that the diffusion-sorption model proposed in the January through March 1977 Quarterly Progress Report could not completely describe the total profile. The profiles were more complex than was expected from a single diffusing component obeying Fick's law. All iodine profiles appear to be composed of a slow diffusion path and a fast diffusion path.

This type of multi-path diffusion has been analyzed by Zumwalt, et al,¹ in studies of the diffusion of fission products in graphite. In this treatment it

is assumed the fast and slow components are not coupled, at least as a first approximation. Accordingly, the slow component of concentration, C_s , is fit to the classical Fick's Law equation:

$$D_s \nabla^2 C_s = \frac{\partial C_s}{\partial t} \quad (1)$$

In our case, using an infinite slab approximation, the solution for the concentration of the slow component is:

$$C_s(x) = C_s^0 \operatorname{erfc} \left(\frac{x}{2 \sqrt{D_s t}} \right) \quad (2)$$

where

- C_s^0 = the slow component concentration at the boundary
- x = depth of penetration
- D_s = diffusion coefficient for the slow process
- t = time period of the diffusion

The diffusion of the fast process is taken to be rapid enough so a steady state for diffusion has been substantially reached. However, this is only a quasi-steady state in that sorption into the bulk of the concrete is assumed to occur. Furthermore, the sorption process (to a first approximation) is assumed to occur as a first-order rate process. Thus, the diffusion and sorption of the fast component is given by the following equations:

$$D_f \nabla^2 C_f - K_f C_f = \frac{\partial C_f}{\partial t} = 0 \quad (3)$$

$$\frac{dC_s}{dt} = K_f C_f \quad (4)$$

$$C_s = K_f t C_f \quad (5)$$

where

- D_f = fast diffusion coefficient
- C_f = concentration of the fast component
- K_f = rate constant for transfer of atoms in fast path to a more or less immobile sorbed state - which is taken as corresponding to the state of the slow component

It is noted that in this treatment the transfer of atoms from the fast paths (or fast component state) to the slow paths (or slow component state) is assumed to be irreversible -- i.e., the reverse process has a rate which approaches zero. A more general treatment is appropriate for some systems (such as in the diffusion of cesium in graphite) where the reverse process has a finite rate. In this

case coupled diffusion equations must be solved.² Eq. (5) exhibits the buildup of the slow component with time. The total concentration due to fast diffusion in the region beyond which there is no contribution due to slow diffusion from the boundary of the sample is given by:

$$C_T = (1 + K_f) C_f \quad (6)$$

The total concentration at any position is:

$$C_T = C_f + C_s \quad (7)$$

The fast component concentration rate change with position can be written as (corresponding to a quasi-steady state):

$$D_f \frac{d^2 C_f}{dx^2} - K_f C_f = 0 \quad (8)$$

The solution of Eq. (7) is found to be:

$$C_f = C_f^0 \frac{\cosh \gamma(a-x)}{\cosh \gamma a} \quad (9)$$

where

a = half-width of the sample

x = depth of penetration

$\gamma = \sqrt{K_f/D_f}$

C_f^0 = concentration of fast component at the surface

In regard to the nature of the slow component of iodine in concrete we are not certain of its nature but believe it is likely that it involves the penetration of iodine into the inner pore structure of the concrete, i.e., into the cement gel structure discussed by Mikhail and Selim.³

The fast component is very likely to be due to in-pore gas and surface diffusion of iodine, which is accompanied by a process whereby iodine molecules are fixed to inner pore sorption sites. A quasi-steady state is reached, and assuming the adsorption rate coefficient remains constant, a concentration profile is established whose shape does not change with time although its magnitude continues to rise.

Computations Using Uncoupled Model

A 370 IBM model 165 computer was used in conjunction with a computer program written to perform a non-weighted least-squares to minimize the error of fit with respect to each parameter. The program utilizes a modified version of a grid search subroutine in Bevington⁴ to search for the minimum X^2 . The program requires the user to choose a break-point between the predominantly slow diffusion concentration region near the surface and the fast diffusion concentration region further in the sample. The break-point position was changed until the optimum

fit was obtained for each profile. Fast component data were first fit using Eq. (9). This solution was extrapolated to the predominantly slow component region and the values of the total concentration due to the fast component were subtracted from the experimentally determined concentration in the region. This remainder was fit using the solution of the classical slow diffusion equation (Eq. (2)). The results of the fit of parameters are given in Table 1.

The large value obtained from Sample 2 is thought to be because of the large initial partial pressure of iodine to which the sample was exposed, and also the strong sorption properties of concrete with respect to iodine. It should be noted that the C_0 's are much larger than the average saturation concentration found in earlier experiments shown below:

Exp. No.	P_{I_2} (atm.)	$\bar{C}$
		Average Conc. (mg I_2 /g concrete)
2	3.14×10^{-4}	0.704
2	3.95×10^{-5}	0.489
3	3.95×10^{-5}	0.711

These results suggest that there is a practical limit to the amount of iodine that can be absorbed by concrete that is smaller than the surface concentration. The samples in earlier work apparently were not saturated, i.e., had not reached a true equilibrium.

The slow diffusion coefficient D_s is quite small as can be seen in Table 1. Values for K_f/D_f are scattered. This was because of the small number of data points and also the spread in the experimental data in the fast component region. However, from this data we can conclude that the ratio of K_f (the adsorption rate constant) to D_f (the fast path diffusion coefficient) is about 10 cm^{-2} . These correspond to a diffusion length of:

$$\sqrt{D_f/K_f} = 0.3 \text{ cm.}$$

Figure 1 shows the profile from Sample 2. A computer fit was not done for this data because the sample was exposed to 2 vapor pressures of iodine. The fitted theoretical curve and experimental profile points, for Samples 3 through 5 are shown in Figures 2 through 4. It is evident that the slow path component is very much dominant over the fast path component in terms of iodine concentration. This appears to be the reason for the great length of time required for samples to reach a true equilibrium.

Permeability Experiments

Permeability Experiment 3 started in this quarter consists of two parts:

a) Study of the inert gas permeability response of the through-crack in the concrete cube to external pressure (P_a) applied for closing the crack.

Table 1

Diffusion Parameters and Boundary Concentrations Obtained from Concentration Profiles

<u>Sample No.</u>	<u>Exposure Time (sec.)</u>	<u>P_{I₂} (atm.)</u>	<u>C_f^o mg I₂/g Concrete</u>	<u>C_s^o mg I₂/g Concrete</u>	<u>C_T^o mg I₂/g Concrete</u>	<u>D_s cm²/sec.</u>	<u>K_f/D_f cm⁻²</u>
2*	$\frac{6.87 \times 10^4}{7.081 \times 10^5}$	$\frac{5.00 \times 10^{-4}}{1.76 \times 10^{-5}}$	-----	-----	2.66*	-----	-----
3	1.150×10^6	1.76×10^{-5}	0.095	1.37	1.44	8.5×10^{-9}	6.3
4	1.211×10^6	1.76×10^{-5}	0.106	1.53	1.64	4.1×10^{-9}	14.9
5	1.377×10^6	3.95×10^{-5}	0.55	2.16	2.71	8.1×10^{-9}	22.5

*Sample 2 was exposed at two different partial pressures. Therefore, it could not be analyzed by the above method. C_T^o is estimated by extrapolation of the profile by the experimenters.

Figure 1. Experimental Data for Sample 2 (See Table 1)

Figure 2. Theoretical Model Fit to Sample 3 Experimental Data (See Table 1)

Figure 3. Theoretical Model Fit to Sample 4 Experimental Data (See Table 1)

Figure 4. Theoretical Model Fit to Sample 5 Experimental Data (See Table. 1)

b) Forced flow of tagged iodine vapor across a through-crack concrete cube. Helium is used as a carrier gas. The cube was kept under a constant external pressure (P_a) of approximately 460 psi for closing the crack.

Inert Gas Permeability

In this part of the experiment helium gas was forced across the through-crack concrete cube at different P_a 's. The helium gas flow pressure drop (P_f) across the cube was measured for different flow rates using a water manometer. This procedure was repeated for various applied P_a 's. The results are being analyzed.

Tagged Iodine Vapor Permeability

In this experiment, which is still in progress, helium gas is being used as a carrier to transport iodine across the concrete cube at a P_f of 1.5 cm of water and a P_a of approximately 460 psi. Helium sweep gas flows past the opposite face of the cube to transport any tagged iodine coming across, to an activated carbon trap. The concrete cube and the activated carbon trap are being monitored for tagged iodine content.

To date (28 days), the increase of tagged iodine content in the concrete cube has been linear with time. No activity has been observed in the activated carbon trap.

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2. Materials, Chemistry, and Instrumentation

2.1 Materials (J. Chow, P. Soo, J. E. Zimmer)

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.

A Materials Test Loop (MTL) has been constructed for supplying prototypic HTGR helium environments to selected creep and fatigue test machines and also for thermally aging specimens prior to creep and fatigue testing.

Subcontracted work at the Aerospace Corporation is concerned with the development of an analytical model which will predict the fracture strength and fracture mechanisms of oxidized graphites.

2.1.1 Mechanical Properties of Materials

The 5 MTS fatigue units are operating routinely and the first in-helium, high-cycle tests have been initiated. A new MTS fatigue unit and 8 new ATS creep units have been delivered to enhance testing capability. Creep testing in air and in helium is proceeding normally.

(a) Mean Stress Effects on the High-Cycle Fatigue of Steam Generator Materials

The data being reported here supplement those reported during the last quarter for Type 304 stainless steels. The materials being evaluated are annealed $2\frac{1}{2}\text{Cr-1Mo}$ steel and Incoloy-800H; their chemistries are given in Table 2.1. Owing to the limited numbers of Incoloy-800H specimens 2 additional tests on a second heat of material (Heat HH 7427A) were conducted. Table 2.2 shows the data obtained at the time of writing.

For the Incoloy-800H there is a very significant decrease in high-cycle fatigue resistance for mean-stress levels of 10 and 20 ksi (Figure 2.1). Note that the fatigue curves for these mean-stress values must extrapolate through the stress-rupture times when the alternating stress, σ_a , is zero. In the case of the $2\frac{1}{2}\text{Cr-1Mo}$ steel (Figure 2.2) the mean stress appears to be beneficial for alternating stresses in the region 25-30 ksi which is in contrast to the Incoloy-800H. The broken lines in Figure 2.2 indicate the uncertainty in the behavior of the mean-load curves in the region of low alternating stress. However, it does seem that for the 20 ksi mean-stress case, the application of a small cyclic stress will increase the failure time compared to a specimen which is rupture tested at a constant stress of 20 ksi.

This work is reported more fully by Soo (1977).

Table 2.1

Chemistries and Heat Treatments of Starting Materials

Material	Chemical Composition, %										
	C	Mn	Si	Cr	Mo	Ni	S	P	Ti	Al	Fe
2½Cr-1Mo ⁽¹⁾	0.145	0.53	0.40	2.2	0.94	0.30	0.019	0.014	-	-	Bal.
Incoloy 800H ⁽²⁾ (Ht. HH 3113A)	0.06	0.90	0.38	20.35	-	32.11	0.007	-	0.39	0.36	Bal.
Incoloy 800H ⁽²⁾ (Ht. HH 7427A)	0.05	0.67	0.46	19.83	-	32.17	0.003	-	0.43	0.39	Bal.

Notes: 1. Annealed 1700°F/2 h, furnace cooled at 50°F/h to 1100°F, then air cooled to room temperature.

2. Solution annealed at 2100°F followed by water quench.

Table 2.2

High-Cycle Mean-Stress Fatigue Data for Incoloy-800H and 2½Cr-1Mo Steel

Spec. No.	Test Temp. (°F)	Stress (ksi)		Cycles to Failure (N _f) (1)	Final Spec. Length (in) (2)	Final Spec. Diam. (in)	Orig. Spec. Diam. (in)
		Mean	Cyclic				
Heat HH 3113A (0.06% C)							
MN1-23	1100	10.0	26.0	6.4 x 10 ⁶	2.749		
MN1-22	1100	10.0	27.0	1.2 x 10 ⁶	2.710		
MN1-19	1100	10.0	30.0	9.0 x 10 ⁵	2.705		
MN1-21	1100	10.0	32.0	1.4 x 10 ⁶			
MN1-17	1100	20.0	25.0	4.2 x 10 ⁶	2.719		
MN1-20	1100	20.0	28.0	3.8 x 10 ⁶	2.725		
Heat HH 7427A (0.05% C)							
MNF-137	1100	10.0	22.0	>1.2 x 10 ⁸	3.978	0.248	0.251
MNF-133	1100	20.0	20.0	>1.2 x 10 ⁸	3.945	0.239	0.253
2½Cr-1Mo							
MC1-68	1000	10.0	25.0	>1.0 x 10 ⁸	2.656	0.112	
MC1-85	1000	10.0	28.0	7.7 x 10 ⁷	2.703		
MC1-67	1000	10.0	30.0	1.2 x 10 ⁶	2.669		
MC1-69	1000	10.0	35.0	1.5 x 10 ⁴	2.693		
MC1-72	1000	20.0	20.0	>1.1 x 10 ⁸	(3)	(3)	
MC1-73	1000	20.0	25.0	>6.2 x 10 ⁶ (4)			
MC1-77	1000	20.0	28.0	>1.2 x 10 ⁸	2.635	0.120	
MC1-84	1000	20.0	29.0	1.2 x 10 ⁵	2.677		
MC1-83	1000	20.0	31.0	1.1 x 10 ⁴	2.694		
MC1-81	1000	20.0	35.0	<2.0 x 10 ³ (5)	2.714		

Table 2.2 Cont'd.

- Notes:
1. The cyclic frequency is 40 Hz.
 2. Nominal original specimen length and diameter for Incoloy-800H Heat HH 7427A specimens are 3.938 and 0.250 inches, respectively, and for the other specimens are 2.625 and 0.125 inches.
 3. Not measured since specimen bent on removing from machine.
 4. Prematurely failed during machine malfunction.
 5. Fractured very soon after attaining required load.

Figure 2.1 EFFECT OF MEAN STRESS ON THE FATIGUE OF INCOLOY-800H AT 1100°F.

Figure 2.2 EFFECT OF A MEAN TENSILE STRESS ON THE HIGH-CYCLE FATIGUE OF ANNEALED 2-1/4 Cr-1 Mo STEEL AT 1000 °F

(b) Mean-Stress Effects on Helium Circulator Materials

A batch of Type 422 stainless steel specimens has been tested in air to evaluate the effects of mean-tensile stresses on helium circulator components. Since the maximum operating temperature component is about 900°F, creep deformation is probably negligible, hence it was an important part of this work to evaluate the adequacy of Goodman's approximation for estimating mean-stress effects in creep-free materials. Table 2.3 shows the data obtained to date.

A few tests are being run at 1000°F to cover the possibility that hot spots may exist in the circulator.

For fully-reversible deformation the temperature dependence of the fatigue strength is quite marked as shown in Figure 2.3. An endurance limit appears to become established after about 10^7 cycles. Figures 2.4(a) and 2.4(b) show that mean-tensile stresses cause a significant decrease in the fatigue life for test temperatures of 600 and 900°F. A preliminary evaluation of Goodman's analysis is given in Figure 2.5. According to this analysis the maximum and minimum stress lines are drawn so that they pass through the ultimate tensile strength value for the material and the fatigue limit for fully-reversible deformation ($\sigma_m = 0$); the triangular area between the two lines is postulated to represent a region in which failure will not occur. To a first approximation the analysis seems to be justified but more comprehensive data will be generated to establish this more firmly.

(c) In-Helium Fatigue Testing

A test was recently initiated on high-cycle fatigue testing of Hastelloy-X in a helium environment; Figure 2.6 shows the Inconel-600 test capsule which was used. It incorporates a stainless steel bellows to accommodate the axial strains applied. The test was conducted at 1600°F in a helium environment supplied by the Materials Test Loop (MTL). Impurities were controlled at the following levels: 200 μ atm. H_2 , 40 μ atm. H_2O , 40 μ atm. CO , 20 μ atm. CH_4 and 10 μ atm. CO_2 . This represents an environment which is essentially intermediate between the dry low-impurity condition being studied by ORNL in their mechanical properties program and the wet, impure condition being evaluated by General Atomic in their work. At the time of writing the Hastelloy-X specimen has accumulated 2.0×10^7 cycles without failure at a fully-reversible stress level of 20 ksi.

A second in-helium test on a Hastelloy-X specimen is also being prepared for initiation.

(d) Creep-Rupture of Primary Circuit Structural Materials in Helium

The safety of an HTGR depends on the maintenance of structural integrity in the primary circuit materials throughout the life of the reactor system. In this phase of our program an elevated-temperature creep testing effort has been established to study the long-term mechanical behavior of alloys in prototypic HTGR helium environments.

The possible degradation of mechanical properties is an important safety consideration in all types of reactors. However, it is particularly important

Table 2.3

High-Cycle Mean-Stress Fatigue Data for Type 422 Stainless Steel⁽¹⁾

Spec. No.	Test Temp. (°F)	Stress (ksi)		Cycles to Failure (N_f)	
		Cyclic	Mean		
MFF-20	600	85.0	0	2.0×10^5	
MFF-21	600	80.0	0	2.2×10^5	
MFF-28	600	75.0	0	2.8×10^6	
MFF-29	600	70.0	0	7.5×10^6	
MFF-31	600	68.0	0	3.8×10^6	
MFF-33	600	66.0	0	$>1.1 \times 10^8$	
MFF-25	600	65.0	0	$>4.0 \times 10^7$	
MFF-23	600	60.0	0	$>1.3 \times 10^7$	
MFF-34	600	65.0	50.0	3.0×10^5	
MFF-35	600	60.0	50.0	2.5×10^5	
MFF-38	600	58.0	50.0	6.8×10^5	
MFF-42	600	57.0	50.0	2.4×10^6	
MFF-37	600	56.0	50.0	$>1.1 \times 10^8$	
MFF-36	600	50.0	50.0	$>1.1 \times 10^8$	
MFF-30	600	40.0	50.0	1.0×10^8	
MFF-04	900	100.0	0	3.0×10^3	Just reached full load before failure.
MFF-03	900	75.0	0	3.0×10^4	
MFF-05	900	70.0	0	1.5×10^5	
MFF-06	900	67.0	0	7.6×10^5	
MFF-07	900	63.0	0	4.6×10^6	
MFF-11	900	58.0	0	1.2×10^6	
MFF-27	900	54.0	0	$>1.0 \times 10^8$	
MFF-17	900	52.0	0	3.3×10^6	
MFF-24	900	52.0	0	$>1.3 \times 10^7$	Furnace overheated causing specimen to fail.
MFF-19	900	48.0	0	$>1.0 \times 10^8$	
MFF-08	900	50.0	40.0	4.6×10^5	
MFF-10	900	44.0	40.0	2.4×10^5	
MFF-12	900	40.0	40.0	1.1×10^6	
MFF-14	900	34.0	40.0	5.3×10^6	Failed at internal location.
MFF-32	900	31.0	40.0	$>1.2 \times 10^8$	
MFF-18	900	28.0	40.0	$>1.1 \times 10^8$	
MFF-41	1000	65.0	0	8.9×10^4	
MFF-15	1000	52.0	0	5.6×10^5	
MFF-39	1000	48.0	0	9.5×10^5	
MFF-40	1000	45.0	0	$>9.0 \times 10^7$	Test in progress.

Note: 1. Material austenitized at 1900°F and tempered at 1050°F.

Figure 2.3 EFFECT OF TEMPERATURE ON THE HIGH-CYCLE FATIGUE OF TYPE 422 STAINLESS STEEL

Figure 2.4(a) THE EFFECT OF A MEAN TENSILE STRESS ON THE HIGH-CYCLE FATIGUE OF TYPE 422 STAINLESS STEEL AT 600 °F

Figure 2.4(b) THE EFFECT OF A MEAN TENSILE STRESS ON THE HIGH-CYCLE FATIGUE OF TYPE 422 STAINLESS STEEL AT 900 °F

GOODMAN DIAGRAM FOR TYPE 422 STAINLESS STEEL
AT 900 °F

Figure 2.5

Figure 2.6 In-helium test facility for high-cycle fatigue at elevated temperatures.

in an HTGR because most of the critical components cannot be readily inspected or repaired.

In our testing program, the effect of helium environments expected in an HTGR on creep and rupture properties of Hastelloy-X, Incoloy-800H, and $2\frac{1}{4}\text{Cr-1Mo}$ steel are being studied. The objectives of the work are to quantify the effect of the environment, and to study the mode of fracture in various helium environments.

Sixteen lever arm testing units made by Applied Test Company are being used for this study. Eight units equipped with retorts for environmental testing have been set up and are in use. Eight new units have been delivered and are now being commissioned.

The helium environment for the mechanical testing is being supplied from the MTL loop. The environmental creep tests are being performed in helium with 40 $\mu\text{atm.}$ of H_2O , 200 $\mu\text{atm.}$ H_2 , 40 $\mu\text{atm.}$ CO , 10 $\mu\text{atm.}$ CO_2 and 20 $\mu\text{atm.}$ CH_4 . It is believed that this "wet" environment simulates that which could exist in an HTGR with some leaking steam-generator tubes.

At the present, tests on Hastelloy-X and Incoloy-800H are being run. The compositions of the alloys are shown below:

	<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>
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
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

Note: NA - not analyzed

The Incoloy-800H alloy was solution treated by heating to 2100°F and water quenched. The Hastelloy-X alloy was heated to 2150°F for one-half hour and water quenched.

The results obtained to date on these alloys are tabulated in Table 2.4. The minimum creep rates are plotted in Figure 2.7. In order to eliminate heat-to-heat variations, the in-air and in-helium test specimens are taken from a single reference heat. Also, the preparation of the specimens was duplicated as closely as possible.

The stress-rupture time and creep rate of the in-air tests for both the Incoloy-800H and Hastelloy-X agree very well with published data for these two alloys. This indicates that the heat of material selected for test is a representative of each material.

Only two in-helium tests have been completed so far and four others are in progress. Figure 2.7 shows that the secondary creep rates of the in-helium tests are somewhat higher than those tested in air for Incoloy-800H at 1200°F and Hastelloy-X at 1400°F . However, these preliminary data are inadequate to formulate any conclusions.

Table 2.4

Creep-Rupture Properties of Incoloy 800H and Hastelloy X⁽¹⁾

<u>Material</u>	<u>Specimen</u>	<u>Temp.</u> (°F)	<u>Envirmt.</u>	<u>Stress</u> (psi)	<u>Time to</u> <u>Rupture (h)</u>	<u>Elong.</u> (%)	<u>Red. of</u> <u>Area (%)</u>	<u>Minimum</u> <u>Creep Rate</u> (in/in/h)	<u>Comments</u>
Incoloy 800H Heat HH7427A	MNT-179	1200	Air	26,000	132.7	26.3	41	2.5×10^{-5}	
	MNT-182	1200	Air	25,000	648.5	28.0	53	3.4×10^{-5}	
	MNT-185	1200	Air	22,000	-	-	-	4.0×10^{-6}	4100 h ⁽²⁾
	MNT-184	1200	Air	20,000	-	-	-	3.3×10^{-6}	4050 h
	MNT-165	1400	Air	12,000	(144.9) ⁽³⁾	54.0	-	1.7×10^{-3}	
	MNT-163	1400	Air	10,000	790.2	55.0	53	4.8×10^{-4}	
	MNT-164	1400	Air	8,000	2604.0	72.0	42	8.2×10^{-5}	
	MNT-166	1200	Helium	22,000	-	-	-	2.5×10^{-5}	650 h
	MNT-167	1400	Helium	8,000	-	-	-	-	100 h
Hastelloy X Heat 4-2809	MHT-19	1400	Air	19,000	(224.0) ⁽³⁾	71.5	-	5.0×10^{-4}	
	MHT-02	1400	Air	16,000	-	-	-	4.0×10^{-5} ⁽⁴⁾	
	MHT-18	1400	Air	14,000	2225.8	49.5	61	8.5×10^{-5}	
	MHT-01	1400	Air	13,000	-	-	-	3.3×10^{-5}	3600 h
	MHT-17	1400	Helium	19,000	(223.0) ⁽³⁾	81.0	-	6.6×10^{-4}	
	MHT-04	1400	Helium	16,000	814.8	115.0	82.5	6.6×10^{-4}	
	MHT-03	1400	Helium	14,000	-	-	-	-	250 h

- Notes:
1. Incoloy 800H - solution annealed - 2100°F. Hastelloy X - solution annealed - 2150°F.
 2. Test in progress.
 3. Test stopped. Specimen exceeded extensometer range without fracture.
 4. Test stopped. Malfunction of proximity switch before fracture.

Figure 2.7

SECONDARY CREEP RATE PERCENT PER hr

(e) Microstructure and Fracture of HTGR Graphites

The behavior of graphitic materials in high-temperature, gas-cooled nuclear reactors is dependent on their unique microstructures. This program is directed toward the study of the relation between microstructure and the fracture of graphites exposed to various reactor environments. This information will be used to provide improved bases for the evaluation of reactor safety.

Tension specimens that have been oxidized in the BNL Helium Impurities Loop (HIL) and tested are to be observed with the use of optical microscopy. This analysis is aimed at relating the fracture surface features to the level of oxidation burnoff and changes in the graphite microstructure. PGX graphite specimens were exposed in the HIL to helium containing 100 ppmv water at temperatures to 750°C and times to 1974 hours. The fractured tensile specimens were sectioned radially and one half polished to observe the trace of the fracture edge and the underlying microstructure. A mounting medium that may obscure some microstructural features was not used. Optical micrographs were taken with partially crossed polarized light to give the microstructure some shading representing the orientation of small regions of preferred orientation.

The analysis of the fracture behavior of the oxidized PGX tension specimens tested in the against-grain direction has been reported (Chow, 1977). The reduction in tensile strength with burnoff is more pronounced for the PGX tension specimens tested in the with-grain direction (Romano, 1977) and thus, the fracture behavior of these specimens has been investigated.

Montages of the entire width of the tension specimens are presented in Figures 2.8 and 2.9. The tensile strengths of these four specimens are listed here:

<u>Specimen</u>	<u>Weight Loss, %</u>	<u>Tensile Strength, psi</u>	<u>Percent Reduction</u>
G-6	0	1010	0
1-4-B	1.0	906	10
3-3-E	2.9	815	19
G-34	6.5	565	44

Evident in these figures is the increase in porosity with increasing burnoff and a change in the appearance of the fracture surface with burnoff. For the unoxidized specimen, the fracture surface tends to outline the large grain agglomerates characteristic of PGX graphite. As burnoff is increased, the fracture surface tends to be somewhat flatter and the fracturing appears to be controlled by the porosity and weak boundaries between individual filler coke grains within the large agglomerates. This fracture behavior is similar to that for the against-grain tension specimens.

Optical micrographs at higher magnification of these same tension specimens are shown in Figures 2.10 through 2.13. For the unoxidized PGX graphite, the mode of fracture may be described as interagglomerate, that is, the fracture path lies between agglomerates in the microstructure. The fracturing in the oxidized specimens may be described as intraagglomerate and intergranular. Evident in the upper right of Figure 2.12 is a large filler coke grain that is partially outlined by pores where the binder has been selectively oxidized. The

Figure 2.8 Optical micrographs of fracture edge of PGX graphite tension specimens, with grain, unoxidized (top) and 1.0 w/o burnoff

Figure 2.9 Optical micrographs of fracture edge of PGX graphite tension specimens, with grain, 2.9 w/o (top) and 6.5 w/o burnoff

Figure 2.10 Optical micrograph of fracture edge of PGX graphite, unoxidized

Figure 2.11 Optical micrograph of fracture edge of PGX graphite, 1.0 w/o burnoff

Figure 2.12 Optical micrograph of fracture edge of PGX graphite, 2.9 w/o burnoff

Figure 2.13 Optical micrograph of fracture edge of PGX graphite, 6.5 w/o burnoff

fractured edge of this grain appears intact, indicating that failure occurred at its boundary.

The fracture behavior for oxidized PGX graphite is similar for tension specimens tested in the against-grain and with-grain directions. This does not account for the difference in strength reduction versus burnoff for the two directions. A possible explanation involves the amount of grain boundaries in the two directions. Because of the slight preferred orientation of the PGX graphite introduced during manufacturing, the filler coke grains that have the anisotropic needle microstructure and are needle-like in shape, tend to have their long axes aligned perpendicular to the molding direction or the against-grain direction (BNL notation). Thus, in the with-grain direction, more grain boundary surface is generally perpendicular to the stress direction and the weakened, oxidized binder would play a more crucial role.

2.2 Materials Test Loop (L. G. Epel)

The Materials Test Loop (MTL) began its history as a source of controlled helium for mechanical testing machines during this quarter. There is a small amount of leakage from the system due to the seals in the retorts of the testing machines but the automatic helium makeup system maintains the operating pressure at the desired 3 to 4 psig. The behavior of the loop during the run-in period necessitated the occasional addition of CO, CH₄, and H₂O. An automatic sensing and injection system was devised that accomplishes this with minimum operator supervision. The CO₂ level had a tendency to increase with time and is being controlled by having a small bypass stream flow through the Ascarite tank in the purification system. Hydrogen exhibited the most perverse behavior, sometimes declining and other times rising in concentration. Hydrogen is added directly to the helium when needed; it is removed most easily by venting the loop to the room and allowing the makeup helium to dilute the remaining hydrogen in the loop. Some thought is being given to replacing one of the CuO tanks in the purification system with a tank containing titanium chips to remove hydrogen.

The concentrations of impurities decided upon for the first set of metallurgical tests in the MTL are listed in Table 2.5 below:

Table 2.5

Concentrations of Impurities in MTL (ppmv)

	<u>Desired</u>	<u>Average</u>
Carbon Dioxide	10	7
Carbon Monoxide	40	38
Hydrogen	200	301
Methane	20	19
Water Vapor	40	42

The data acquisition system (DAS) records the signals from the CO₂, CO, CH₂, and H₂O detectors once an hour. The H₂ concentration must be determined and recorded manually. During the month of September (up until this writing) the average concentrations recorded by the DAS compared quite favorably with the desired levels

of impurities, as shown in the last column of Table 2.5, except for hydrogen; the H_2 level was, on the average, about 50% too high. This is largely a result of the fact that there was no operator-initiated correction possible during weekends, holidays, and vacations. The impurities of greatest concern for the tests now in progress are H_2O and H_2 . Thus, this first month's experience indicates that the problem of water vapor control has been solved (the standard deviation of the water-vapor concentration was 3.5 ppmv), the less important impurities are being controlled reasonably well, and the control of hydrogen should receive further attention.

During this quarter work began on the aging retorts which will be connected to the MTL. The work on plumbing, valves, and flowmeters as well as on electrical connections, temperature controllers, and heaters has been completed for 4 retorts. Only minor adjustments need to be made before the retorts are placed into service. At the end of this reporting period 4 of the 8 creep machines and 1 of the 3 fatigue machines were incorporated into the MTL.

2.3 Characterization and Oxidation Kinetics of PGX Graphite (F. B. Growcock)

The effort on characterization of PGX graphite was continued; however, it was limited to a few experiments on the kinetics of rapid oxidation, due to a shift in emphasis to studies of fission product behavior.

Two untreated 0.9 gram cylindrical samples, 2 cm distant, were cut from the PGX log endpiece used in all our previous studies. The samples were chosen so as to obtain very different Fe impurity concentrations. The reactions were undertaken in the Flow-through System described in previous progress reports (Growcock, 1977) utilizing a constant total flow rate of 167 cc/min. Both samples were subjected to various concentrations of H_2O and $H_2O + H_2$ in helium at 1 atm at temperatures of 640-905°C.

Data presentation and calculations have been modified somewhat, for the sake of consistency and usefulness, as follows. The rate of graphite weight loss may be expressed by:

$$-\frac{dm_c}{dt} = k a P_{H_2O}^n \quad (2.1)$$

where k is defined as the overall rate coefficient, a is the macroscopic surface area, P_i the partial pressure of species i and n the reaction order with respect to H_2O .¹ The gas chromatographic data may be related to the rate of graphite weight loss by:

$$-\frac{dm_c}{dt} = \frac{(P_{CO} + P_{CO_2} + P_{CH_4})}{RT} q \times 12 \text{ g/mol} \quad (2.2)$$

where q is the total gas flow rate at temperature T and total pressure P . Combining Eqs. (2.1) and (2.2) we obtain:

$$k \sim \frac{(P_{CO} + P_{CO_2} + P_{CH_4})}{P_{H_2O}^n} \times \frac{12 q}{aRT} \quad (2.3)$$

in units of g/min-cm²- atmⁿ.

The reaction order with respect to H₂O may be determined from the gas chromatographic data by rearranging Eq. (2.3) to give:

$$\log \left\{ \frac{12 q (P_{\text{CO}} + P_{\text{CO}_2} + P_{\text{CH}_4})}{RT} \right\} \approx \log k_a + n \log P_{\text{H}_2\text{O}} \quad (2.4)$$

Data obtained at 818°C for PGX-5A, a sample containing >1000 ppm Fe, were normalized to 0.24% burnoff and are plotted in Figure 2.14 according to Eq. (2.4). The slope so obtained is $n \approx 0.76 \pm 0.10$ and the ordinate intercept at $\log P_{\text{H}_2\text{O}} = 0$ is $\log k_a \approx -3.1 \pm 0.25$.

The ratio $P_{\text{CO}_2}/P_{\text{CO}}$ was found to be independent of $P_{\text{H}_2\text{O}}$ in the range 10^{-5} - 10^{-3} atm at low burnoffs, where production of H₂ is low. However, as burnoff was increased, the resulting increase in the rate of formation of H₂ led to suppression of CO₂ while the CO yield continued to increase.

In using Eq. (2.4) we have assumed that the same reaction mechanism is operative over the range of H₂O pressures employed and that, therefore, k and n are constants. The value of the reaction order agrees reasonably well with values of ~ 0.7 obtained for other nuclear graphites (Overholzer, 1965). However, the reaction order at low concentrations of H₂O (≤ 10 ppmv) may be different from that obtained above; in addition, the reaction orders with respect to H₂ and CO are of great interest. These parameters will be examined during the next quarter.

The temperature dependence of the overall reaction rate for steam-PGX graphite was investigated using $\sim 0.86\%$ H₂O. Plots of $\ln k$ (obtained from Eq. (2.3)) versus the reciprocal of the reaction temperature, T_r , are displayed in Figures 2.15 and 2.16 for PGX-1A and PGX-5A, respectively; the former sample contains <40 ppm Fe as determined by Mössbauer spectrometry. The datum indicated by "x" in Figure 2.16 corresponds to the $\ln k$ value obtained from the intercept in Figure 2.14. The solid straight lines correspond to approximate best fits assuming that the relationship is linear throughout the temperature range employed. These give rise to activation energies, E_a , of 35-45 kcal/mole for PGX-1A and 45-55 kcal/mole for PGX-5A, in keeping with values generally obtained for Fe-catalyzed oxidation of graphites (Walker, 1959).

The scatter obtained in the low-temperature regime is quite high, however, and is strikingly similar for both samples. Each datum represents a steady-state value, corrected to 0.24% burnoff, which was reached no sooner than 1 1/2 hours after temperature equilibration; the values are reasonably reproducible as indicated by the 3 points on each plot near 800°C, which were at the beginning and at the end of these series of experiments. It is believed that the precision of the data is better than it appears to be from the fitted straight lines. Thus, there exists a possibility that $\ln k$ is not a linear function of $1/T_r$ throughout the temperature range considered and that truer fits may be obtained with the dashed broken lines connecting the data in Figures 2.15 and 2.16. This treatment would give rise to unusually low activation energies below $\sim 730^\circ\text{C}$ and activation energies close to that for the uncatalyzed reaction above that temperature. This result is not totally unprecedented. Marsh and Adair, 1975, obtained some baffling data on CO₂ oxidation of polyfurfuryl alcohol carbon doped with ~ 400 ppm Fe in

Figure 2.14 Plot of $\log (-dm_c/dt)$ vs. $\log P_{H_2O}$ for PGX-5A (>1000 ppm Fe) at 818°C.

Figure 2.15 Arrhenius plot of steam-graphite reaction for PGX-1A (<40 ppm Fe) with $P_{H_2O} \sim 0.0086$ atm.

Figure 2.16 Arrhenius plot of steam-graphite reaction for PCX-5A (>1000 ppm Fe) with $P_{\text{H}_2\text{O}} \sim 0.0086 \text{ atm.}$

which the Arrhenius plot had a definite sigmoid shape: the high- and low-temperature regions gave activation energies lower than usual, even for catalysis, while the intermediate temperatures gave an E_a at least as high as the non-catalytic rate.

If the transition(s) in E_a observed here are real, they may be accompanied by change(s) in the reaction mechanism. It should be noted that the flow rate employed in this work is low enough that secondary reactions will occur; it was for this reason that P_{CO_2} and P_{CH_4} , as well as P_{CO} , were measured. The reverse water-gas ($H_2 + CO = H_2O + C$) and Boudouard ($2CO = CO_2 + C$) equilibria tend toward higher carbon formation at lower temperatures (Walker, 1968); this will certainly affect the rate constants determined from product formation and will affect the values obtained from weight loss measurements if carbon deposition occurs on the sample. Likewise, the effect of the reaction $2H_2 + C = CH_4$ may have to be considered. Although the latter equilibrium lies to the right up to $\sim 800^\circ C$, the relative yield of CH_4 was very small throughout the temperature region employed in this study.

The yield of CH_4 is more sensitive to changes in P_{H_2O} than either CO_2 or CO , as would be expected if the overall reaction order for CH_4 formation is higher than that for the steam-PGX graphite reaction. On the other hand, the relative temperature dependence of the 3 products appears to follow the opposite trend: increasing the temperature by $100^\circ C$, for example, may lead to an observed 2- to 5-fold increase in CH_4 production, while CO_2 formation may increase by an order of magnitude, and CO formation may jump by a factor of 50. The complex nature of the steam-PGX graphite reaction makes it imperative that high flow rates, wherein negligible secondary products are formed, be used to repeat these studies.

The effect of burnoff on the reaction rate was also explored. Plots of the reaction rate versus percent burnoff at an intermediate temperature are displayed in Figures 2.17 and 2.18 for PGX-1A and PGX-5A, respectively. Approximately 0.86% H_2O was used in these experiments; for PGX-5A H_2 was added at $\sim 1\%$ burnoff to give $P_{H_2}/P_{H_2O} \sim 10$. Inlet and outlet P_{H_2O} values were averaged to minimize the effect of the decrease in P_{H_2O} during reaction.

The curve generated in Figure 2.17 is startling in that the expected continuous increase in reaction rate with percent burnoff is not obtained. The data, obtained from product analysis, were corroborated by weight loss rate data (not shown), which did in fact exhibit the same trends. This oscillatory behavior is difficult to understand, but suggests that the effect may be related to the catalytic behavior of Fe; one may speculate that worm-holing is taking place and that the mobility of the Fe catalyst is erratic, i.e., the Fe is able to travel to a location with new active sites and is impeded in its progress at that point. Catalytic oxidation ensues, with the consequent removal of the barrier, at which point the Fe moves on to a new location, etc. To determine whether worm-holing is indeed occurring microscopic analysis of the sample surfaces will be done.

In Figure 2.18 weight-loss rate data are plotted alongside the chromatographi data. The latter appear to give consistently larger reaction rates, but, again, the trends observed are the same. Large continuous increases in the rates observed at low burnoffs indicate a high, homogeneous rate of surface development, as has

Figure 2.17 Effect of burnoff on rate of steam-graphite reaction for PGX-1A (<40 ppm Fe) with $P_{H_2O} \sim 0.0086$ atm. at 810°C .

Figure 2.18 Effect of burnoff on rate of steam-graphite reaction for PGX-5A (>1000 ppm Fe) with $P_{H_2O} \sim 0.0086$ atm. at 818°C.

been observed for other coarse-grained graphites (Blakely, 1965). This effect becomes less pronounced at higher burnoffs; addition of H_2 appears to enhance this effect linearly with percent burnoff. The degree of enhancement observed appears to be much less than had been observed previously with other Fe-rich PGX samples reacted at $750^\circ C$ (Growcock, 1977). The majority of this discrepancy can be attributed to the large amount of H_2 generated during reaction (in the absence of added H_2) and the higher rate of reduction of the Fe impurity at $818^\circ C$ than at $750^\circ C$; these effects lead one to assert that even at low burn-offs the steam-PGX graphite rates measured at this temperature were catalytic rates.

2.4 Helium Impurities Loop (L. G. Epel)

The Helium Impurities Loop (HIL) was used during the reporting period to begin generating basic information on the kinetics of CO and CO_2 . The HIL is composed of a number of segments, constructed of various materials and having various flow cross sections. The helium which contains the CO- CO_2 mixture experiences different temperatures, for various time intervals as it progresses through the circuit. The flow path that the helium "sees" in the experiments reported here is shown in Figure 2.19 which also indicates the temperatures the helium is likely to encounter in its trip around the circuit.

The first set of experiments involved the injection of CO in various amounts so that the initial concentrations in the loop would be between about 1000 ppmv and 6000 ppmv; the CO_2 concentration initially was always nil. The results of 4 separate runs were consistently that the CO concentration declined monotonically while the CO_2 concentration increased over a period of a day or two. These results are illustrated in Figure 2.20, where the amounts of CO initially injected are noted for each set of curves. The declining curves in all cases represent the CO; the increasing ones represent the CO_2 concentrations.

The concentrations at the end points can be used to obtain a "pseudo-equilibrium" constant which, in turn, corresponds to a reaction temperature. When this is done for the data shown in Figure 2.20 the apparent reaction temperature for the 20 cm^3 injection run is around the temperature of the retorts. The apparent reaction temperatures for successively larger CO injections were successively higher (i.e., in the direction of higher final CO concentrations and lower CO_2 concentrations). It may be conjectured that for the higher CO injection runs the system did not reach steady state by the end of the run and that had the tests been prolonged, the CO/ CO_2 ratio would have continued to decline.

The second set of experiments involved the injection of CO_2 into purified loop helium. Again, there were 4 separate runs which resulted in a range of initial CO_2 concentrations about the same as the initial CO concentrations had been in the CO injection runs. During these runs the amount of CH_4 , H_2 , and H_2O were virtually zero (as they were during the previous 4 runs) but this time the changes in CO and CO_2 concentrations were insignificant. The temperatures corresponding to the pseudo-equilibrium constants for these runs are at and below retort temperature.

Figure 2.19 Schematic and Operating Parameters in Helium Impurities Loop.

Figure 2.20 Behavior of CO and CO₂ in the Helium Impurities Loop.

At present, there is no clear explanation for the difference in results between the CO injection runs and the CO₂ injection runs. This phenomenon will be investigated further by first repeating some of the CO injection experiments to see how reproducible the results are.

2.5 Safety Instrumentation and Control Systems (S. Nicolosi)

Brookhaven has planned to install a research mass spectrometer into Fort St. Vrain as part of a novel effort to survey the coolant gas of an operating power reactor. Interest is directed to a description of the coolant composition with regard to all gaseous impurities. In addition to technical data, this is an opportunity to gain practical working experience in an operating power reactor.

The mass spectrometer is still under construction by the Nuclide Corporation. Recent progress includes the installation and operability of components necessary for beam modulation (which is considered to be 90% complete). Additional components await installation and computer hardware has arrived although it awaits installation and programming.

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3. Structural Evaluation

3.1 Core Seismic (P. Bezler, M. Reich, H. Goradia)

The extended computer code, OSVERT-2, has been used to study the response of a three column, nine element array. Computer graphics pictures of the response at 4 cycles/sec have been processed and are being studied.

Investigations of the effects of simultaneous horizontal and vertical excitations have continued during this period. The test rig was redesigned so that greater vertical components could be introduced. Previously, teflon pads were used to guide the horizontal motion. For this arrangement, vertical accelerations were limited to less than 1 g. A new driving adapter was made and has been used to conduct tests with vertical accelerations greater than 1 g. Preliminary results indicate only a weak coupling effect between the vertical and horizontal inputs. This is for a single column loaded only with its own weight, the coupling effect should increase if an increased load is applied to the topmost block.

At the same time, in support of the test work, OSVERT-3 is being developed to introduce the capability of simultaneous vertical and horizontal excitation. With this code version, interactive effects will be studied analytically.

The investigations of the dynamics of a single degree of freedom system with a cubic nonlinearity is also continuing. A decaying exponential term is being introduced into the individual terms of the forcing function. This investigation was started because of the significant effect that the earthquake duration has on the response of the system. The equation being studied is:

$$m\ddot{x} + c\dot{x} + \alpha x + \beta x^3 = F_1 e^{-\alpha_1 t} \cos \omega t - F_2 e^{-\alpha_2 t} \cos 3 \omega t \quad 3.1$$

Preliminary results are in accordance with our former conclusions dealing with the subharmonic effect. More specific results will be available in the next quarter.

The extension of both the shake test work and the analytical work to a three-dimensional system continues. Design drawings of the three-dimensional test rig are in preparation. Modifications of the OSVERT code series designed to minimize running times have been undertaken. Any minimization of running times will be of direct benefit to the three-dimensional formulations and will be incorporated in them.

3.2 Steam Generator Tube Weld Evaluation (M. Reich, M. Subudhi, T. Tanaka*, P. Bezler)

This is the third reporting on the investigations of the structural integrity of the HTGR steam generator tubes. During this period the progress included:

* was on leave from Japan Atomic Energy Research Institute

- (1) completion of the elastic analyses of weldments as per information supplied by General Atomic;
- (2) completion of a validation study of the LEFM finite element code APES;
- (3) completion of a preliminary report on the LEFM studies of the stress conditions at the welds; and
- (4) the initiation of inelastic time-independent analysis of the welded structure.

In addition, the work on FEPLLOT initiated during the last quarterly period continues. The temperature contour plot routines are in operating condition but bugs remain in the stress contour plotting routines.

3.2.1 Elastic Analyses

The data supplied by General Atomic applies to current high temperature structural designs. All welds associated with high temperatures are located either in a stagnant gas zone, a shielded zone, or a zone of low gas side heat transfer. Thus the location of the Case I weld, I-800 to I-800 weld in the superheater bundle, is in a shielded area where little or no heat transfer to the tube is anticipated. Similarly, for the second case, a weld in the reheater bundle is in a zone completely shielded from the gas. Finally, the bi-metallic weld between I-800 and 2 1/4 Cr - 1 Mo is located at a zone where no heat transfer to the tube is expected. By such design, the temperature gradient across the wall thickness for each weldment has been reduced significantly. However, whether this design practice was followed in the operating Fort St. Vrain nuclear plant remains an open question.

A detail of the typical weld geometry is shown in Figure 3.1. The General Atomic supplied data on the tube dimensions together with full-load temperatures and pressures at the different weld locations are summarized in Table 3.1 and Table 3.2 respectively.

TABLE 3.1

Finite Element Model Data (GA)

Case	Outside Diameter (inch)	Thickness (inch)	Dimension 'B' (inch)
I	1.26	0.184	.105
II	0.906	0.088	.061
III	1.26	0.134	.082

TABLE 3.2

Full-load Temperatures and Pressure Loadings

Case	Fluid Temperatures (°F)		Tube Temperatures (°F)*		Pressure (PSI)	
	Water/Steam	Helium	Average Wall Temp.	Radial Temp. Gradient	Internal	External
I	956	1200	990	52	2490	710
II	1002	1315	848	60	605	725
III	760	1100	782	63	2510	710

* Based on the cold tube wall temperature conditions.

Comparing these with data from Gassar, as reported in the previous quarterly report, the tube size in the reheater bundle has been reduced by 50 percent in the current design and the thickness of the bimetallic weld has been reduced to 0.134 inches. As far as the loading conditions are concerned, the pressure effects remain almost unchanged. Since 1350°F is considered to be the reference temperature corresponding the postweld heat treatment condition, the bimetallic weld experiences a more severe temperature loading as compared to the previous analysis.

All assumptions regarding the finite element models and the material properties remain the same as reported in the previous quarterly. The average wall temperature is assumed to occur at the mid-wall thickness of the tube.

The radial, longitudinal, and circumferential stress distributions from the inside to the outside surface of the I-800/I-800 weldments are shown in Figure 3.2. No significant change in the stress patterns is observed with the new data except that the weldment in the reheater bundle is found to be less critical because of the change in tube size. The stress condition in the I-800 of the bimetallic weldment is found to be more severe as compared to the previous results. The results for this case are shown in Figure 3.3. Stress distributions along the inner and outer wall surfaces are given in Figure 3.4 for all three cases.

In the present analyses the weld groove angle was reduced to 30 degrees as against 75 degrees assumed in the previous studies. Hence, the better material compatibility should reduce the stress intensities at the fusion zone. However, the new loading conditions are found to offset this effect. As a result, there is no significant change in the stress conditions at the fusion zone due to the change in the weld groove angle.

It should be noted that in all the elastic analyses no accurate evaluation of the residual stresses is made. Some accounting is taken by assuming the postweld heat treatment temperature as the stress-free state. A more accurate accounting for these residual stresses should be made particularly in the fracture initiation and propagation studies. These residual stresses, superimposed on the other normal loading stresses, may easily bring the weld to the critical plastic strain accumulation at the fusion zone and hence to cause catastrophic failures in the tube structure.

FIGURE 3.1
TYPICAL WELD GEOMETRY

FIGURE 3.2

STRESS DISTRIBUTIONS WITHIN THE TUBE WALL OF I-800 WELDMENTS FOR NORMAL OPERATING CONDITIONS CORRESPONDING TO GA COLD TUBE DATA

S_1 =RADIAL

S_2 =LONGITUDINAL

S_3 =HOOP

S_e =EFFECTIVE

FIGURE 3.3

STRESS DISTRIBUTIONS WITHIN THE TUBE WALL OF A BIMETALLIC WELDMENT IN SUPERHEATER FOR NORMAL OPERATING CONDITIONS CORRESPONDING TO GA COLD TUBE DATA

S_1 =RADIAL

S_2 =LONGITUDINAL

S_3 =HOOP

S_e =EFFECTIVE

INSIDE WALL

OUTSIDE WALL

FIGURE 3.4

STRESS DISTRIBUTIONS ALONG INSIDE AND OUTSIDE WALL OF WELDMENTS
FOR NORMAL CONDITIONS CORRESPONDING TO GA COLD TUBE DATA

3.2.2 Validation of APES Fracture Mechanics Calculation

The APES computer code was modified to increase the number of nodes (400 → 1500), elements (50 → 200) and nodes across the front (40 → 80), and to include the capability of analyzing thermal loading conditions. The code was checked out with the supplied, as well as newly developed test problems. The validation of the APES fracture mechanics calculations is described below.

(a) Single-Edge Crack in a Compact Tension Specimen

The problem of a plate five units square and containing a central edge crack of length $a = 1.5$ units was considered. The problem is symmetric about the crack line and treated as a plane strain problem. The reference value for K for this specimen geometry is 4.016, i.e. BOWIE and NEAL (1965). The APES results for K (4.096 and 4.080) were 2.0 percent higher than the reference value.

(b) Forty-Five Degree Slant Crack in a Tension Specimen

This example is a combined mode plane strain problem. The reference values of K_I and K_{II} are 1.86 and 0.88. The results indicate that the value of K_I varied from 4.0 percent below to 2.4 percent above the reference value and that the value of K_{II} varied from 2.9 percent below to 1.4 percent above the reference value. For an isothermal loading case the values of K_I and K_{II} are zero as expected.

(c) Cracked Bar

This problem was a bar with a circumferential crack with a depth of half the bar radius. The results indicate that the value of K was 7.6 percent below the reference value.

(d) Cylinder with Internal Circumferential or Internal Axial Cracks

For the analyses cylinders with internal circumferential or internal axial cracks were evaluated. Loading conditions similar to those used for the Inco-loy-800 superheater tube were used. The results are compared in Table 3.3 with those developed by HELIOT and VAGNER (1977) using the weight function concept.

TABLE 3.3

Stress Intensities for Circumferential and Axial Cracks

		<u>Reference Value</u>	<u>APES Value</u>
Circumferential Crack	Plane Strain	100,000	109468.5
	Axisymmetric	32,266	32544.8
Axial Crack	Plane Strain	3,355	3589.7

3.2.3 LEFM Studies (Gassar Data)

Small flaws or cracks may grow when subjected to cyclic loads (fatigue), aggressive environments (corrosion fatigue and stress corrosion), or a combination of all these factors. A crack in a tube wall will propagate perpendicularly to the main stress axis. Thus, a crack will advance through the wall thickness at a rate faster than it elongates in the longitudinal or circumferential directions. Having extended through the wall, the crack produces either a leak or a rupture, depending on whether the crack has reached a critical length. A subcritical crack producing leakage may grow longitudinally causing a bulging failure.

To assess the integrity of the HTGR steam generator tube welds, linear elastic fracture mechanics methods were used to evaluate the characteristics of circumferential cracks in tubes with representative dimensions supporting operating loads. In these analyses, the materials were assumed to retain their virgin material mechanical properties. As a refinement of this procedure, the change in the mechanical properties of these materials due to the long-term exposure to elevated temperatures must be made.

The present analyses were conducted with the APES finite element computer program. This code uses a singularity function formulation to model elastic bodies with singular points. The latest version of APES contains subroutines that calculate the state of strain at the tip of a crack in either plane stress, plane strain, or axisymmetric geometries. Linear isotropic stress-strain material properties are used and small strain theory is assumed.

The weld geometry, material properties, and the model assumptions remain the same as reported in the previous quarterly report for the elastic analyses.

For the fracture mechanics analyses, only circumferential cracks were considered. These result from either stress corrosion cracking or sustained load cracking and are commonly observed in tubes. For such cracks the longitudinal load or stress field is the dominant load parameter affecting both crack severity and growth characteristics. For a given weldment the most detrimental circumferential crack will be located at the point where the longitudinal stress component attains a maximum. From the elastic analyses this point is the fusion line at the inner surface for all the cases. This was taken as the crack location for all the fracture analyses.

For the fracture runs, enriched element crack tip models were employed. The gross finite element grid was similar to that used in the elastic analyses with adjustments in the vicinity of the crack. Each weldment was analyzed for the 12.5 percent crack while the I-800/I-82/I-800 superheater weldment was analyzed for all the crack lengths.

The computed stress intensity factors range from 1 to 4 $\text{Ksi}\sqrt{\text{in.}}$ and are summarized in Table 3.4. The highest computed factor is still below K_{th} (6 $\text{Ksi}\sqrt{\text{in.}}$ @ 1000°F) for the material and consequently, there is no possibility of crack growth. For the deep cracks, the presence of the crack itself markedly reduces the through-wall thickness stress gradients and peak stresses which results in low values of the stress intensity factors. This implies that if a

TABLE 3.4

Computed Stress Intensity Factors ($\text{psi}\sqrt{\text{in.}}$ Units)

	<u>Crack Length Thickness</u>	<u>Superheater Tube</u>		<u>Reheater Tube</u>	
		<u>I-800/I-82/I-800</u>	<u>I-800/I-82/2 1/4Cr-Mo</u>	<u>I-800/I-82/I-800</u>	
Operating Temperature	0.125	3834.4	3046.0	4040.2	
	0.125	3172.1(temp. alone)		3931.8(temp. alone)	
	0.125	662.3(press. alone)			
Stress Free at 1350°F	0.25	3799.6			
	0.50	2589.2			
	0.75	2460.8			
	0.875	3918.2			
	0.125	2690.0	966.3	1781.5	
	0.25	1149.3			
Room Temperature Stress Free at 1350°F	0.50	-1027.9			
	0.75	- 594.6			
	0.875	1519.0			

small crack propagates in a tube wall having a steep stress gradient, crack arrest will occur after some propagation.

It is concluded that circumferential cracks will not propagate to the present pipe geometries and load conditions. For thermally induced stress gradients, crack arrest may be expected if initial crack propagation does occur. Since the hoop stress is found to be the most dominant, longitudinal cracks might be more critical than circumferential cracks.

3.2.4 Time-Independent Inelastic Analysis

Since the bimetallic weld was found to experience the most severe stress conditions at the fusion line an inelastic analysis for this weldment, when subjected to the normal operating conditions, is under consideration. Results of this will be reported in the next quarterly. In addition, if information regarding accident induced transient loadings become available, corresponding inelastic evaluations will be made.

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4. Analytical

4.1 Gas Dynamics in the Containment Vessel (H. Takahashi, J. Skalyo, Jr., I. Omata, J. Beerman)

In the previous quarterly report, the calculation of gas circulation using the CIRC code and 8 x 4 cells was reported. In order to study the effect of the mesh size for the same problem, calculations using 16 x 8 cells (4 times the number of cells used in the previous calculation) were performed. Figure 4.1 shows the case with the horizontal velocity input from the left side of the two upper cells; the results show the same velocity and flow pattern as a previously calculated 4 x 8 cell case. Another case was calculated in which the gas was introduced from the left side of only the topmost cell. From the conservation of mass, the input velocity is double that of the example depicted in Figure 4.1. Figure 4.2 shows flow and temperature patterns which are very similar to Figure 4.1. Comparing Figures 4.1 and 4.2 to the earlier 4 x 8 cell calculations, it may be reasonable to say that 4 x 8 cells are sufficient for our calculation. These figures also show that the momentum of the jet is not sufficient to force circulation of all of the gas in the CV and only the upper part of the gas circulates. Therefore, the layering model used in the HAZARD code (Omata, 1977) is more consistent with the results of this calculation than the complete mixing model. The temperature profiles shown in the figures indicate this layering; these temperature profiles are very similar to the ones calculated by the HAZARD code. The present CIRC code is limited to a uniform size mesh. In order to remove this limitation, the new difference equation for the variable mesh size grid has been formulated, and this formula has been implemented into the CIRC code.

The user's manuals for the CIRC code and the HAZARD code were written as BNL reports and these will be published in the next quarter.

Following the scaling law analysis for small-scale experiments described in the last quarterly report, the experimental preparation is in progress. The test system under consideration is the following: the model CV diameter will be 46 cm, giving a scale of about 1:100 in linear dimension. The top of the model PCRV will consist of an interchangeable plate to allow testing of different orifice sizes. A small heater and thermocouple in the PCRV will allow changes in the PCRV gas temperatures. A fast-acting valve will initiate depressurization. Eventual modification of the apparatus for testing off-center and side leaks from the PCRV will also be possible. For preliminary tests, a pyrex CV will be used to allow recording of the depressurization and layering using high-speed photography and a dye gas in the PCRV.

Various dye gases are under consideration. One of the most common is Al_2O_3 particles of 5-micron diameter. These particles are easily available and would be charged into the 3-liter, stainless-steel sampling cell that models the PCRV prior to final pressurization. The use of Al_2O_3 particles would also permit high initial temperatures in the PCRV. The abrasive nature of Al_2O_3 must however be considered; hence, it may be better to use alternative methods.

A practical alternative appears to be NH_4Cl particles. These will be produced by reacting some HCl and NH_3 gases directly in the stainless-steel PCRV prior to pressurization. The final pressurization of the PCRV would serve to evenly distribute the particles. The appropriateness of the particle size

FIGURE VELOCITY VECTOR FIELD
TIME = 10.00 SEC., $U_{inlet} = 3.93$ M/SEC

FIGURE VELOCITY VECTOR FIELD
TIME = 20.00 SEC., $U_{inlet} = 3.93$ M/SEC

FIGURE VELOCITY VECTOR FIELD
TIME = 30.00 SEC., $U_{inlet} = 3.93$ M/SEC

FIGURE VELOCITY VECTOR FIELD
TIME = 40.00 SEC., $U_{inlet} = 3.93$ M/SEC

FIG. TEMPERATURE CONTOUR LINE
AT 10.00 SEC., HI = 273.03, LOW = 66.15 C

FIG. TEMPERATURE CONTOUR LINE
AT 20.00 SEC., HI = 253.10, LOW = 92.22 C

FIG. TEMPERATURE CONTOUR LINE
AT 30.00 SEC., HI = 286.25, LOW = 109.90 C

FIG. TEMPERATURE CONTOUR LINE
AT 40.00 SEC., HI = 304.64, LOW = 122.41 C

Figure 4.1 Case 1C (8 x 16 cells; two inlet cells).

FIGURE VELOCITY VECTOR FIELD
TIME = 2.00 SEC. — = 10.02 M/SEC

FIGURE VELOCITY VECTOR FIELD
TIME = 4.00 SEC. — = 10.02 M/SEC

FIGURE VELOCITY VECTOR FIELD
TIME = 6.00 SEC. — = 10.02 M/SEC

FIGURE VELOCITY VECTOR FIELD
TIME = 8.00 SEC. — = 10.02 M/SEC

FIGURE VELOCITY VECTOR FIELD
TIME = 10.00 SEC. — = 10.02 M/SEC

FIG. TEMPERATURE CONTOUR LINE
BT 2.00 SEC. HI = 152.01, LOW = 35.51 C

FIG. TEMPERATURE CONTOUR LINE
BT 4.00 SEC. HI = 172.34, LOW = 44.15 C

FIG. TEMPERATURE CONTOUR LINE
BT 6.00 SEC. HI = 191.34, LOW = 50.35 C

FIG. TEMPERATURE CONTOUR LINE
BT 8.00 SEC. HI = 204.23, LOW = 56.25 C

FIG. TEMPERATURE CONTOUR LINE
BT 10.00 SEC. HI = 210.34, LOW = 61.14 C

Figure 4.2 Case 1D (8 x 16 cells; one inlet cell).

distribution obtained will have to be determined since too large a particle will tend to settle and not follow the gas flow. The NH_4Cl particles are limited in high-temperature studies by a sublimation temperature of 1100°R .

Quantitative studies will be done where the velocity flow patterns can be measured by laser anemometry. This technique also requires the use of smoke particles to give a measurable signal; hence, here also the perturbing effect of too large a particle size must be avoided. The use of the laser technique eliminates the problem of the hot-wire anemometer calibration (the latter would depend on the gas mixture concentration and would be changing with time).

Suitable fast response pressure and temperature transducers will be placed in the CV with the data multiplexed to a storage device. The gas concentration as a function of time and position will also be measured by a sniffer probe placed in the CV and connected to a mass spectrometer.

Sufficient data are needed to properly scope larger 0.1 scale experiments. These are necessary to prove the models set forth and increase the confidence wherein the results can be applied to full-scale predictions.

The large-scale model is envisioned as made of steel so that final pressures of 2-3 bar can be sustained. At this stage, some knowledge of the heat transfer of the impinging jet on the CV will be obtained. The heat transfer data will be necessary as input to computer codes that determine the final pressure in the full-scale CV following depressurization. Due to the economic penalty involved, it is expected that the designed pressure limit of the CV will not be overly conservative. Here, we have dealt with the case where the penetration is in the top of the PCRV and gas jets into the relative open space of the top of the CV. The various effects of hot jet impingement upon the CV wall may well be more important when the PCRV penetration is close to the CV; this is a problem for future study.

4.2 HTGR Code Library (J. Beerman, J. Colman)

The efficiency of the computer code CHAP (Composite HTGR Analysis Program) (Gilbert, 1977), has been investigated and much of the time-consuming section of the code appears to have no alternative to the present form without extensive research and development of a new code section. However, after further investigation of the existing code in this section a number of minor modifications have been made which have given approximately a 15% overall computer time reduction when running the sample case. Work is continuing on the understanding of the CHAP code and its individual modules.

Work has begun on adaptation of the QUIC/QUIL codes (Lunsford, 1977) for execution on the BNL CDC7600 computer.

Table 4.1 summarizes the status of the 60 codes now being developed or maintained in the HTGR Safety Code Library.

Table 4.1

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.
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.

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.

Table 4.1 Cont'd.

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
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.
TWIGL	OP	NP	Performs two-dimensional light water reactor kinetics calculations.
TAC-2D	OP	NP	Performs two-dimensional, transient conduction analyses.
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	C	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.
SORSO	OP	P	Computes the release of volatile fission products from an HTGR core during thermal transients.
GOPTWO	OP	NP	Analyzes the steady state graphite burnoff 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.

Table 4.1 Cont'd.

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
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.
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.
HILDA	OP	NP	Analyzes data acquired from the Helium Impurities Loop.
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.

Table 4.1 Cont'd.

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
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 Mössbauer spectrometer.
INREM	OP	NP	Calculates internal radiation doses.
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	NP	Calculates fluid dynamics for two-dimensional time-dependent recirculating flows.
CHAP	OP	NP	Simulates the overall HTGR plant with both steady state and transient solution capabilities.
EVAP	B	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	L	NP	Calculates fission product release from a reactor containment building.
SUVIUS	L	NP	Solves the behavior of fission gases in the primary coolant of a gas-cooled reactor.
FYSMOD	L	NP	Calculates the two-dimensional solution of HTGR core blocks subjected to external motion.
NONSAP-C	L	NP	Calculates static and dynamic response of three-dimensional reinforced concrete structures, in addition to creep behavior.

Table 4.1 Cont'd.

<u>Program</u>	<u>Status</u>	<u>Proprietary</u>	<u>Function</u>
LARC-1	L	NP	Calculates fission product release from BISO and TRISO fuel particles of an HTGR during the LOFC accident for single isotopes.
LARC-2	L	NP	Similar to LARC-1; in addition, handles release from isotope chains.
QUIL	C	NP	Solves complex equilibrium distributions in chemical environments.

4.3 Preliminary Investigation of Turbulent Reactive Mixing in PCRV/CV Gas Mixtures (J. L. Boccio, J. Colman)

The question of the possible flammability hazards within the CV due to combustible gas inleakage after a penetration failure (Macnab, 1974) or the question of flammability within the CV during a penetration failure (Omata, 1977) have been addressed under the assumptions of homogeneous or partial PCRV/CV gas "mixedness" and instantaneously fast chemical reaction kinetics. Notwithstanding the extreme remoteness of possible flammability hazards within the CV during a penetration failure, a consequence of gas layering and normal buoyant exchange of the unmixed CV air and PCRV gas after depressurization is the possible production of combustible mixtures which are extremely close to the best current estimate of conventional combustibility limits (Palmer, et al).

However, the presumption in knowing apriori the degree of PCRV/CV gas "mixedness" (either fully mixed as in CONTEMP-G or partially mixed as in HAZARD) and the assumption of chemical equilibrium amongst gas-species components requires further investigation with codes which realistically model the subsequent turbulent mixing and possible concomitant reaction kinetics. In particular, these two factors, viz:

- . turbulent diffusive mixing
- . finite-rate chemical kinetics

are extremely relevant in post-penetration failures, especially if gas layering is indeed possible. In this regard, it is conceivable that fluid-mechanic flow times in turbulent, buoyant plumes are comparable to chemical-reaction times in an H/C/O system (with N_2 and He considered as inert diluents) necessitating investigations into diffusion-controlled as well as chemically-controlled mixing processes.

Accordingly, during this quarter, work has been initiated in developing a computer code to investigate the subsequent development of turbulent, reactive shear layers. The salient features of the mixing process and the associated reaction kinetics are embodied by the classical problem of a turbulent, chemically-reacting jet exhausting into an infinite co-flowing, oxidizing stream. A so-called "two-equation" turbulence model, in the spirit of Launder and Spalding, 1976, wherein the turbulence exchange coefficients are related directly to the mean turbulent kinetic energy, k , and its dissipation rate, ϵ , is linked to a chemical kinetics code describing the oxidation of CO and H_2 with He and N_2 considered as inert diluents. The governing conservation equations of mass, momentum, energy, and species and the transport equations of turbulent kinetic energy and dissipation are, for numerical convenience, recast in a mapped streamline coordinate system according to Patankar, 1970, and appropriate to flows having free boundaries. Special attention in solution technique is required by the species conservation equations which are inherently "stiff" due to the presence of the chemical production terms. An uncoupling process, to be described, however, renders the subsequent finite-difference formulation into a hybrid implicit/explicit technique which reduces, to some extent, the numerical restrictions imposed in solving a system of parabolic differential equations with stiff coefficients. Progress, to date, in code implementation is also discussed.

4.3.1 Governing Equations for Turbulent Reactive Shear Flows

Referring to Figure 4.3, the problem presently under consideration is the free, turbulent mixing of two, possibly chemically reacting, co-flowing streams, involving N chemical species made up of L elements and undergoing R chemical reactions. This axisymmetric flow field is analyzed employing standard boundary-layer approximations; a binary, Fickian diffusion law is assumed; turbulent mass and heat exchanged coefficients are considered known and constant; and the turbulent eddy viscosity is considered to be related to the turbulent kinetic energy and dissipation rate, each of which are expressible by a transport equation according to Spalding's "two-equation" turbulence model. Thus, the governing equations are:

Momentum:

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = r^{-1} \{ \rho r (\mu + \mu_t) \frac{\partial u}{\partial r} \} - \frac{dp}{dx} + g (\rho_e - \rho)$$

Energy:

$$\begin{aligned} \rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial r} = r^{-1} \{ & \frac{\rho r \mu_t}{Pr} \left[\frac{\partial H}{\partial r} + \left(\frac{Pr}{Pr_t} - 1 \right) \frac{\partial k}{\partial r} + (Pr - 1) \frac{\partial u^2/2}{\partial r} \right. \\ & \left. + \frac{Pr}{Pr_t} (Le_t - 1) \sum_{i=1}^N h_i \frac{\partial \alpha_i}{\partial r} \right] \} \end{aligned}$$

Global Continuity:

$$\frac{\partial}{\partial x} (\rho u r) + \frac{\partial}{\partial r} (\rho v r) = 0$$

Species Continuity:

$$\rho u \frac{\partial \alpha_i}{\partial x} + \rho v \frac{\partial \alpha_i}{\partial r} = r^{-1} \frac{\partial}{\partial r} \left\{ \frac{\rho r \mu_t}{Sc} \frac{\partial \alpha_i}{\partial r} \right\} + \dot{w}_i$$

$$i = 1, 2, 3, \dots, N-L$$

Elements:

$$\rho u \frac{\partial \tilde{\alpha}_j}{\partial x} + \rho v \frac{\partial \tilde{\alpha}_j}{\partial r} = r^{-1} \frac{\partial}{\partial r} \left\{ \frac{\rho r \mu_t}{Sc} \frac{\partial \tilde{\alpha}_j}{\partial r} \right\}$$

$$j = 1, 2, \dots, L$$

In these equations, u and v represent the mean axial (x) and radial (r) components of velocity, respectively; ρ is the mean gas density; p , the pressure; H , the total enthalpy ($H \approx h + 1/2(u^2 + v^2)$); α_i and $\tilde{\alpha}_j$, the mass fraction of species i and element j , respectively; $\dot{w}_i$, the mass rate of production of species i due to chemical reaction; μ_t , the turbulent eddy viscosity coefficient; Pr_t , Sc_t and Le_t the turbulent Prandtl number, Schmidt number, and Lewis number.

Figure 4.3 Schematic of Mixing Flow Region

In addition to the above, the turbulence correlation terms are modeled by the transport equations of turbulent kinetic energy and dissipation rate, (Launder and Morse, 1976) viz:

Turbulent Kinetic Energy:

$$\rho u \frac{\partial k}{\partial x} + \rho v \frac{\partial k}{\partial r} = r^{-1} \frac{\partial}{\partial r} \left\{ r \mu_t \sigma_k^{-1} \frac{\partial k}{\partial r} \right\} + \mu_t \left(\frac{\partial u}{\partial r} \right)^2 - \rho \epsilon$$

Turbulence Dissipation:

$$\rho u \frac{\partial \epsilon}{\partial x} + \rho v \frac{\partial \epsilon}{\partial r} = r^{-1} \frac{\partial}{\partial r} \left\{ r \mu_t \sigma_\epsilon^{-1} \frac{\partial \epsilon}{\partial r} \right\} + C_{\epsilon 1} \frac{\epsilon}{k} \mu_t \left(\frac{\partial u}{\partial r} \right)^2 - C_{\epsilon 2} \frac{\rho \epsilon^2}{k}$$

where the exchange coefficients σ_k and σ_ϵ are considered constant along with the proportionality factors $C_{\epsilon 1}$ and $C_{\epsilon 2}$. The turbulent eddy viscosity, μ_t , is given by

$$\mu_t = C_\mu \rho k^2 / \epsilon$$

The instantaneous mass rate of production per unit volume is, through the law of mass action, expressed as:

$$\dot{w}_i = W_i \sum_{j=1}^R (v_{ij}'' - v_{ij}') k_{f,j} \rho_j^{n_j} \prod_{i=1}^N (\alpha_i / W_i)^{v_{ij}'} G_j$$

where

$$G_j \equiv 1 - \rho_j^{m_j} k_{c,j}^{-1} \prod_{i=1}^N (\alpha_i / W_i)^{v_{ij}'' - v_{ij}'}$$

$$n_j \equiv \sum_{i=1}^N v_{ij}'$$

$$m_j \equiv \sum_{i=1}^N (v_{ij}'' - v_{ij}')$$

where the forward rate constant, $k_{f,j}$, and the equilibrium constant $k_{c,j}$ are based upon the molar concentrations, for the j^{th} chemical reaction

$$\sum_{i=1}^N v_{ij}' M_i \xrightleftharpoons[k_{b,j}]{k_{f,j}} \sum_{i=1}^N v_{ij}'' M_i$$

$$j = 1, 2, \dots, k$$

and the stoichiometric coefficients v_{ij}' and v_{ij}'' . The fluid is assumed to be

comprised of a mixture of ideal gases; thus, the equation of state is:

$$p = \rho R_o T \sum_{i=1}^N (\alpha_i / W_i) = \rho R_o T / W_{\text{mix}}$$

In practice, the temperature, T , is determined by an iterative solution to:

$$h = \sum (\alpha_i / W_i) h_i^{(o)}(T) \approx H - 1/2 (u^2 + v^2)$$

where, by definition, $h_i^{(o)}(T)$ is the sum of the sensible enthalpy and chemical energy of species i at 0°K for the standard state and is presumed to be expressible by the polynomial:

$$h_i^{(o)}(T) = \sum_{k=1}^P a_{i,k} T^{(k-1)}$$

The above system of partial differential equations together with the attendant, constitutive, algebraic relations form a complete, closed system and can be solved subject to the following initial and boundary conditions:

$$x = x_o: u = u(r), H = H(r), k = k(r), \epsilon = \epsilon(r), \alpha_i = \alpha_i(r)$$

$$r = 0: \partial u / \partial r = \partial H / \partial r = \partial k / \partial r = \dots \partial \alpha_i / \partial r = 0$$

$$r \rightarrow \infty: u = u_E, H = H_E, k = \epsilon = 0, \alpha_i \rightarrow \alpha_{iE}$$

The associated chemical kinetic system along with the forward rate constants are presented in Table 4.2.

4.3.2 Governing Equations in Transformed Plane

Following Patankar, the conservation equations of mass, momentum, and energy and the second-order closure turbulent energy-dissipation model equations are recast from the physical (x, r) plane to a mapped streamline coordinate plane (x, ω) . The mapping variable, ω , is defined by

$$\omega = \frac{\psi - \psi_I(x)}{\psi_E(x) - \psi_I(x)}$$

where E and I , respectively, represent the external and inner boundaries of the mixing zone; the terms $(\psi_E - \psi_I)$ give a measure of the mass flow in the mixing layer, viz:

$$\psi_E - \psi_I = \int_{r_I}^{r_E} \rho u r dr$$

By this process global continuity is automatically satisfied and the lateral domain of the mixing region is defined by $0 \leq \omega \leq 1$ rather than $r_I(x) \leq r \leq r_E(x)$.

Table 4.2

Chemical System (He/H/C/O/N)

Reaction Number/Chemical Reaction	Forward Rates $k_f = AT^N \exp(-E/RT)$		
	A	N	E/R
1. $\text{CO} + \text{O} + \text{M} \rightleftharpoons \text{CO}_2 + \text{M}$	6.1E-33	0	1872
2. $\text{CO} + \text{O} \rightarrow \text{CO}_2$	1.4E-18	0	1308
3. $\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$	2.5E-17	1.3	-388
4. $\text{H}_2 + \text{OH} \rightleftharpoons \text{H} + \text{H}_2\text{O}$	3.6E-11	0	2607
5. $\text{H} + \text{O}_2 \rightleftharpoons \text{OH} + \text{O}$	3.7E-10	0	8505
6. $\text{OH} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}$	1.0E-11	0	554
7. $\text{O} + \text{H}_2 \rightleftharpoons \text{OH} + \text{H}$	3.0E-14	1	4509
8. $\text{H} + \text{H} + \text{M} \rightleftharpoons \text{H}_2 + \text{M}$	1.8E-30	-1	0
9. $\text{O} + \text{O} + \text{M} \rightleftharpoons \text{O}_2 + \text{M}$	3.8E-30	-1	171
10. $\text{O} + \text{H} + \text{M} \rightleftharpoons \text{OH} + \text{M}$	2.0E-32	0	0
11. $\text{OH} + \text{H} + \text{M} \rightleftharpoons \text{H}_2\text{O} + \text{M}$	6.1E-26	-2	0

(1) Species order: H_2 , CO , CO_2 , H_2O , H , N_2 , O_2 , O , OH , He

(2) $[\text{A}] = \text{cm}^{3n}/(\text{particles})^n/\text{sec}$
 $n = 1$ for second-order reactions
 $n = 2$ for third-order reactions

(3) M = third body or collision partner

Under these assumptions, and mapping law, the governing partial differential equations take the general form:

$$\frac{\partial}{\partial x} \vec{\phi} + (a + b\omega) \frac{\partial}{\partial \omega} \vec{\phi} = \frac{\partial}{\partial \omega} (C_{\phi} \frac{\partial \vec{\phi}}{\partial \omega}) + \vec{d}_{\phi}$$

where

$$\vec{\phi} \equiv (u, H, k, \varepsilon, \alpha_1, \alpha_2, \dots, \alpha_{N-L}, \bar{\alpha}_1, \bar{\alpha}_2, \dots, \bar{\alpha}_L)^T$$

$$a \equiv - (d \psi_I / dx) / (\psi_E - \psi_I)$$

$$b \equiv d/dx [\ln (\psi_E - \psi_I)]$$

$$C_{\phi} \equiv \rho u r^2 \mu_T / \sigma_{\phi} / (\psi_E - \psi_I)^2$$

and where the source-term vector, $\vec{d}_{\phi}$, and the coefficients σ_{ϕ} are given in Table 4.3.

4.3.3 The Numerical Integration Procedure

The numerical procedure also follows the approach of Patankar and supplements it with a particular calculation of the chemical and diffusive contributions to the source-term for the species conservation equations. The resulting scheme is a hybrid implicit/explicit one; hence, some stepsize controls are required as detailed later in this section.

With reference to the computational grid network and notation of Figure 4.4, Patankar reduces the integration process to the solution of a system of linear algebraic equations of the form:

$$\phi_{i,j} = A_j \phi_{i,j+1} + B_j \phi_{i,j-1} + C_j$$

$$j = N2-1, N2-2, \dots, N1+1$$

obtained by integrating the differential equations over small control volumes (shown shaded in the figure) and assuming the variation of the dependent variables therein. For an interior point (i,j), the coefficients A_j , B_j and C_j are defined by the following equations:

$$\begin{aligned} A_j' &= [(2)(r_{j+1} - r_j)^{-1} (r \mu_T / \sigma_{\phi})_{j+1/2}]_{i-1} - [(\psi_E - \psi_I) (a + b \omega_{j+1/2})]_{i-1} \\ &\quad - [(1/4) (\psi_E - \psi_I) (1/\Delta x - b) (\omega_{j+1} - \omega_j)]_{i-1} \end{aligned}$$

$$\begin{aligned} B_j' &= [(2) (r_j - r_{j-1})^{-1} (r \mu_T / \sigma_{\phi})_{j-1/2}]_{i-1} + [(\psi_E - \psi_I) (a + b \omega_{j-1/2})]_{i-1} \\ &\quad - [(1/4) (\psi_E - \psi_I) (1/\Delta x - b) (\omega_j - \omega_{j-1})]_{i-1} \end{aligned}$$

Table 4.3

Source Terms in Transform Equations

ϕ	σ_ϕ	d_ϕ
u	1	$(1/\rho u) \{gr_j/u_j^2 (\rho_e - \rho) - (\phi_j/\rho_j u_j^2) dp/dx\}$
H	Pr_t	$(u_j^2/H_j) \partial/\partial\omega \{[\rho u r^2 \mu_t/\Delta\psi^2] (1 - 1/Pr) \partial/\partial\omega (u^2/2)\}$
k	σ_k	$(1/\rho u) \{[\rho^2 u^2 r^2 \mu_t/\Delta\psi^2] (\partial u/\partial\omega)^2 - \rho\epsilon\}$
ϵ	σ_ϵ	$(1/\rho u) \{[\rho^2 u^2 r^2 C_{\epsilon_1} \mu_t/\Delta\psi^2] (\epsilon/k) (\partial u/\partial\omega)^2 - C_{\epsilon_2} \rho\epsilon^2/k\}$
α_i	Sc_t	$(1/\rho u) \{\dot{w}_i\} \quad i = 1, 2, \dots, N-L$
$\tilde{\alpha}_j$	Sc_t	0 (see note below)

Note: The L differential equations for $\tilde{\alpha}_j$ can be replaced by L algebraic equations by invoking the conservation of elements, i.e.,

$$\tilde{\alpha}_l = \sum \mu_{k,l} \alpha_k W_l/W_k \quad l = 1, 2, \dots, L$$

where $\mu_{k,l}$ defines the number of atoms of element, l , in species, k . The differential equations for $\tilde{\alpha}_l$ have relevance in chemical equilibrium flows where the $\dot{w}_i$ in the specie conservation equations are mathematically undefined.

- ϕ varies linearly between adjacent cross-stream steps, i.e.,

$$\omega = \omega_{i,j+\frac{1}{2}}: \quad \phi = \frac{1}{2} (\phi_{i,j} + \phi_{i,j+1})$$

- ϕ varies in a stepwise manner between adjacent streamwise steps, i.e.,

$$x_{i-1} < x \leq x_i: \quad \phi = \phi_{i,j}$$

Figure 4.4 Details of Control Volume for an Interior Point

$$C_j' = \{ (1/4) (\psi_E - \psi_I) (\Delta x)^{-1} [3\phi_j (\omega_{j+1} - \omega_{j-1}) + \phi_{j+1} (\omega_{j+1} - \omega_j) + \phi_{j-1} (\omega_j - \omega_{j-1})] \}_{i-1} + 2 S_{i,j}$$

$$D_j' = A_j' + B_j' + (\omega_{j+1} - \omega_{j-1}) [(\psi_E - \psi_I)/\Delta x]_{i-1}$$

$$S_{i,j} = (1/8) (\psi_E - \psi_I) (\omega_j - \omega_{j-1}) [d_{j+1} + d_{j-1} + 6 d_j]_{i-1}$$

and $A_j = A_j'/D_j'$, $B_j = B_j'/D_j'$, $C_j = C_j'/D_j'$. Values at the endpoints of the grid network (i.e., $j = N2$ and $j = N1$) are prescribed from boundary conditions in the external stream and internal jet stream or from symmetry conditions on the axis when the mixing layer has reached the symmetry axis.

Now, since the coefficients A_j , B_j and C_j are based upon flow properties at the $(i-1)$ station, the solution of the system of algebraic equations can proceed independently and sequentially for H , u , k , ϵ . However, special attention is required by the species conservation equations which are "stiff" due to the presence of the chemical source term. Following the uncoupling process of Ferri, 1965, for each marching step $\Delta x = x_i - x_{i-1}$, the species mass fractions, α_k , which are governed by the equation:

$$\frac{\partial \alpha_k}{\partial x} + (a + bw) \frac{\partial \alpha_k}{\partial \omega} = \frac{\partial}{\partial \omega} (C_{\alpha_k} \frac{\partial \alpha_k}{\partial \omega}) + \frac{\dot{w}_k}{\rho u}$$

$$k = 1, 2, \dots, N$$

are divided into two components $\alpha_k = \alpha_k^{(D)} + \alpha_k^{(C)}$, respectively, controlled by the equations:

$$\frac{\partial \alpha_k^{(D)}}{\partial x} + (a + bw) \frac{\partial \alpha_k^{(D)}}{\partial \omega} = \frac{\partial}{\partial \omega} (C_{\alpha_k} \frac{\partial \alpha_k^{(D)}}{\partial \omega})$$

and

$$\frac{\partial \alpha_k^{(C)}}{\partial x} = \frac{\dot{w}_k}{\rho u}$$

Thus, the numerical integration procedure just described can proceed independently and sequentially for the subset of dependent variables H , u , k , ϵ , $\alpha_1^{(D)}$, $\alpha_2^{(D)}$, $\dots$, $\alpha_N^{(D)}$. By contrast, the differential equation involving the chemical source term is recast into the form:

$$\frac{d\alpha_k^{(C)}}{dt} = -A_k(T, \alpha_i) \alpha_k + B_k(T, \alpha_j)$$

$$k = 1, 2, \dots, N$$

$$j \neq k$$

upon substitution of the law of mass action which yields for the elements A_k and B_k :

$$A_k = \sum_{m=1}^R (v_{mk}'' - v_{mk}') \left\{ k_{f,m} L_{k,m} \prod_{i=1}^N (\rho \alpha_i / W_i)^{v_{mi}'} - k_{b,m} (L_{k,m} - 1)^2 \prod_{i=1}^N (\rho \alpha_i / W_i)^{v_{mi}''} \right\} \alpha_k$$

$$B_k = \frac{W_k}{\rho} \sum_{m=1}^R (v_{mk}'' - v_{mk}') \left\{ k_{f,m} (L_{k,m} - 1)^2 \prod_{i=1}^N (\rho \alpha_i / W_i)^{v_{mi}'} - k_{b,m} L_{k,m} \prod_{i=1}^N (\rho \alpha_i / W_i)^{v_{mi}''} \right\}$$

where $L_{k,m} = 1$ if the molecularity of reaction m , for species k , i.e., if $(v_{mk}'' - v_{mk}')$ is negative or $L_{k,m} = 0$ if the molecularity is positive. The backward reaction rates $k_{b,m}$ can be obtained knowing the forward rate constants $k_{f,m}$ as given in Table 4.3 and the equilibrium constant k_c which can be obtained from expressions yielding the Gibbs Free Energy.

For non-reacting turbulent mixing, i.e., $\dot{w}_i = 0$, the numerical finite-difference formulation is implicit since there is no need for the uncoupling procedure just described. Accordingly, stability is insured even for large numerical steps; however, reasonably small step sizes are desired for good accuracy. One procedure is to make the step length proportional to the thickness of the mixing layer. A variant to this approach is to make the step length equal to the minimum physical spacing between grid points, i.e.,

$$\Delta x^{(D)} = \{\min [r_{j+1} - r_j]\}_{i-1}$$

For reacting, turbulent flow, the chemical production terms are non-zero and the uncoupling procedure and solution technique renders the system into a hybrid implicit/explicit scheme. The explicit nature for the calculation of $\alpha_k^{(C)}$ poses an additional step-size constraint on numerical stability and accuracy. Under these conditions, one can show that stability is dictated by the maximum eigenvalue, λ , for the Jacobian matrix $J = \{\gamma_{\ell k}\}$ where $\gamma_{\ell k} = \partial \dot{w}_\ell / \partial \alpha_k$. Difficulties in determining this eigenvalue are reduced if it is assumed that the chemical rates are such that the diagonal element of the Jacobian matrix, γ_{kk} , is dominant. Accordingly, the allowable step size can be shown to be:

$$\Delta x^{(C)} = u_{jet} \min \left\{ \alpha_k \left(\frac{d\alpha_k^{(C)}}{dt} \right)^{-1} \right\}_{i-1}$$

where $(d\alpha_k^{(C)}/dt)_{i-1}$ is readily evaluated. In practice the actual step size taken is determined by combining the above two expressions according to:

$$(\Delta x)_{act} = \left\{ \frac{1}{\Delta x^{(D)}} + \frac{1}{\Delta x^{(C)}} \right\}^{-1}$$

which implies that under diffusion-controlled situations, $\Delta x^{(D)}$ is the pre-dominant factor while under kinetically-controlled mixing $\Delta x^{(C)}$ determines the marching step.

4.3.4 Numerical Results

For non-reacting turbulent flows, Rodi, 1972, and Launder, et al, 1976, have presented the results of many comparisons of numerical predictions based upon the "two-equation" turbulence model, just described, with experimental data culled from the world's literature. These data are related to steady, two-dimensional "parabolic" flows such as plane jets, wakes and mixing layers; wall jets; boundary layers of various kinds; and flows in pipes and annuli. Agreement with experimental data is, as reported by these authors, to vary from good to very good. For reacting flows, Boccio, et al, 1976, have extended the above numerical technique in predicting, with reasonable success, the afterburning characteristics of fuel rich exhaust jets. It is for these reasons, that the numerical technique will be implemented in the investigation of possible combustion hazards within the containment vessel.

As a possible prelude to direct application to containment vessel response, several select numerical experiments were run to check the qualitative behavior of the numerical prediction. In this regard, two test cases were performed to date. Specifically, initial PCRV inventory was presumed composed of 100 moles of CO and H₂ and 5246 moles of He. A jet-to-free-stream temperature ratio of 3.3 was considered with jet-to-free-stream velocity ratio being either 100 (Test Case 1) or 10 (Test Case 2); the former approximating early stages of a non-mechanistically postulated penetration failure, the latter, approximating the final stages of such a failure. Computer-generated plots of the spatial variation of temperature, and mole fraction of He, CO, H₂, H₂O and CO₂ for these two cases are presented in Figures 4.5 and 4.6.

A cursory examination of the results as portrayed by these figures indicates the following:

- (1) For both test cases the initial conditions are such that a turbulent diffusion flame is generated.
- (2) Mixing is more rapid under Test Case 1 conditions ($u_j/u_E = 100$ @ $x = 0$) than under Test Case 2 conditions ($u_j/u_E = 10$ @ $x = 0$).
- (3) Oxidation of CO and H₂O production occur sooner under Test Case 2 conditions where rather sudden changes in axial temperature gradients occur within the mixing layer about two jet radii downstream as compared to larger temperature gradients occurring approximately 7 jet radii downstream for Test Case 1.
- (4) Both cases exemplify, somewhat, a two-stage combustion process wherein the hydrogen-oxidation stage occurs first thereby acting as a ignition source for the slower CO→CO₂ reaction kinetics.

Figure 4.5(a) Computer-Generated Plot. Test Case 1 - Temperature

Figure 4.5(b) Computer-Generated Plot. Test Case 1 - Helium Mass Fraction

Figure 4.5(d) Computer-Generated Plot. Test Case 1 - Carbon Monoxide Mass Fraction

Figure 4.5(e) Computer-Generated Plot. Test Case 1 - Water Mass Fraction

Figure 4.5(f) Computer-Generated Plot. Test Case 1 - Carbon Dioxide Mass Fraction

Figure 4.6(a) Computer-Generated Plot. Test Case 2 - Temperature

Figure 4.6(b) Computer-Generated Plot. Test Case 2 - Helium Mass Fraction

Figure 4.6(c) Computer-Generated Plot. Test Case 2 - Hydrogen Mass Factor

Figure 4.6(d) Computer-Generated Plot. Test Case 2 - Carbon Monoxide Mass Fraction

Figure 4.6(e) Computer-Generated Plot. Test Case 2 - Water Mass Fraction

Figure 4.6(f) Computer-Generated Plot. Test Case 2 - Carbon Dioxide Mass Fraction

(5) The spatial variation of temperature and other variables precludes to some extent the use of analytical similarity distributions as are used in existing CV-response codes.

Although these results are highly preliminary, it does tend to indicate that the phenomena of turbulent reactive mixing should be investigated and numerical procedures like the above should be judiciously utilized as to their potential use in analyzing HTGR plant response under certain accident situations.

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II. LMFBR SAFETY EVALUATION

SUMMARY

Engineering design for the hydrodynamic dispersion test has been completed. It has been found, however, that the large volume throughputs of vapor necessary to achieve liquid dispersal considerably beyond the Kutateladze criteria, require gas injection tubes having a large potential effect on the void dynamics and flow regimes. An evaluation of these effects will be accomplished using the dispersed boiling pool apparatus. Regarding dispersion and heat transfer in two phase boiling systems, analysis has continued to describe the behavior in open and closed systems. Estimations of flow regime transitions between bubbly and churn turbulent flows and between churn turbulent dispersed flows are presented, considering the effects of pool depth and pool power ratio.

In non-dispersed boiling pools, it has been determined that within the accuracy of existing data the local heat transfer coefficient may be expressed in dimensionless terms in a manner identical to that for laminar, single-phase, free convective heat transfer. This result indicates that it is only necessary to determine the thermodynamic state, depth, and local difference in density between the pool and the heat transfer surface in order to determine the local heat transfer rate. Preliminary analytical methods are demonstrated to provide these predictions. The new boiling pool apparatus is complete with the exception of the boron-nitride plate assembly which should be completed shortly. It is expected that these tests at various angles of inclination will be begun in the near future.

Testing and analysis regarding two-phase solidification dynamics of flowing core debris have continued during the last quarter. The analysis has emphasized the utilization of appropriate dimensionless parameters so as to enable direct application to the in-core situation to be made. It has been predicted and experimentally verified that the entrapment of voids in the solidified layer can be a significant factor in determining the time required for solidification, the amount of material relocated prior to solidification, and the extent to which melting will occur in structural regions where solidification is occurring. The question of void structure appears to be an important one and is being pursued. Excellent agreement has been obtained between the data for Wood's metal and the analysis, including void fractions between 0 and 40%. It is expected that the extent of void entrapment in the solidified layer will be strongly dependent on the Prandtl number of the liquid phase.

A major milestone on the SSC Code Development Program was achieved during this reporting period. A version of the SSC-L code was made operational on September 26, 1977 -- a few days ahead of its scheduled milestone of October 1. The test case that was successfully run simulated a scram transient in LMFBRs.

The SSC Code Validation effort consisted of finalizing the first phase of building up the data base of thermohydraulic tests and updating a work plan for SSC Validation using FFTF preoperation tests. The final results on the application of the sensitivity methods to DEMODA4 have been reported in a topical report to be issued in mid-November 1977. The results of the pre-analyses of proposed BIZET-B safety-related critical experiments were also summarized and issued in a topical report.

1. Fast Reactor Assessment - Accident Sequence Studies (O. C. Jones)

1.1 Hydrodynamic Characteristics of Two-Phase Dispersal Systems (T. Ginsberg)

A. Experimental Investigations

The prior Quarterly Progress Report (Ginsberg 1977a) describes the proposed design of the hydrodynamic dispersal test section. This apparatus will be used to obtain data which simulates the two-phase hydrodynamics of volume-heated boiling pools. In order to provide data which can be extended to molten boiling pools of UO_2 and steel, the system is being designed to provide both water/air and mercury/air simulations (Ginsberg 1977b). The experimental concept calls for volume-distributed injection of gas, through a horizontal bank of porous tubes into a long duct closed at the bottom. With this system, the axial variation of gas injection rate can be controlled and measured.

It may be expected that the presence of the gas injection tubes (normal to the axial flow direction) will introduce some disturbance to the two-phase flow field. A design objective is to identify the possible disturbance modes, and to minimize their effects if possible.

A gas injection simulation experiment was reported by Luk (1977) in a study of the heat transfer to the bounding walls of a simulated boiling pool. Air was injected into the water through a sparger consisting of approximately 30 stainless steel tubes, which contained holes drilled along their length. The injector tubes were inserted vertically into the system, and the tubes occupied about 0.2% of the pool volume. Calculations showed that the pressure gradient (10^{-4} cm-water/cm) due to flow past their tubes was small. From this it was concluded that the tubing was responsible for negligible resistance to circulation within the pool. An experimental determination of the effect of the tubes was not performed.

At the relatively low gas injection rates encountered by Luk (1977), the two-phase flow field was gravity-dominated. Acceleration and frictional effects were of second order. In contrast, the experiments designed here are planned to simulate volume boiling with large effective volumetric vapor generation rates. Large gas injection rates will be encountered, and superficial vapor velocities of up to 1000 cm/s will exist.

In order to estimate the influence of the injection tubes on the two-phase flow field, a momentum balance analysis was performed on the test section. Contributions to the pressure drop by friction, acceleration, gravity, and drag on the porous tubes were computed using a homogeneous, one-dimensional model of the two-phase flow.

The total pressure drop is given by

$$\left. \frac{dp}{dx} \right|_{\text{total}} = \left. \frac{dp}{dx} \right|_{\text{gravity}} + \left. \frac{dp}{dx} \right|_{\text{friction}} + \left. \frac{dp}{dx} \right|_{\text{accel}} + \left. \frac{dp}{dx} \right|_{\text{tubes}} \quad (1.1)$$

where p is pressure, and x is the axial coordinate. The first three of these are given, respectively, by

$$\left. \frac{dp}{dx} \right|_{\text{gravity}} = \rho_m g \quad (1.2)$$

$$\left. \frac{dp}{dx} \right|_{\text{friction}} = \frac{2c_f \rho_m U^2}{D_h} \quad (1.3)$$

$$\left. \frac{dp}{dx} \right|_{\text{accel}} = G \frac{dU}{dx} \quad (1.4)$$

where ρ_m is the mixture density, g is the gravitational acceleration, c_f is the flow friction factor, U is the mixture flow velocity, D_h is the hydraulic diameter of the duct, G is the mixture mass flux, S is the vapor generation rate per unit volume of liquid.

For large tube spacing (spacing to tube diameter ratio greater than approximately 4) the pressure gradient across the tube bank was taken as (Boucher 1948)

$$\left. \frac{dp}{dx} \right|_{\text{tubes}} = \frac{4f}{L} \frac{\rho_m U^2}{2} \quad (1.5)$$

where for large spacing (s/d_t)

$$f = \frac{C_D d_t}{4s} \quad (1.6)$$

where C_D is the single tube drag coefficient, L is the distance between tube rows, d_t is the tube diameter, and s is the transverse tube spacing.

The acceleration pressure drop was approximated by a vapor balance equation across an element of volume $A\Delta x$, where A is the duct cross-sectional area:

$$\begin{aligned} \text{change in volume flux across } \Delta x &= \text{net vapor generated in volume } A\Delta x \\ A\Delta j_g &= S(1 - \alpha)A\Delta x \end{aligned} \quad (1.7)$$

or

$$\frac{dj_g}{dx} = S(1 - \alpha). \quad (1.8)$$

In addition, the mixture density was approximated by

$$\rho_m = \rho_l (1 - \alpha). \quad (1.9)$$

where ρ_l is the liquid phase density, and α is the void fraction. Note that the superficial vapor velocity at the top of the pool is given by

$$j_g = SH_o \quad (1.10)$$

where H_o is the liquid height with no gas generation. Equation (1.10) is obtained by equating the volume flux at the top of the pool to the total quantity of vapor generated within the pool. The velocity U in Equations (1.1)-(1.4) was approximated by j_g , given by Eq. (1.10).

Calculations were performed using the following: $\rho_l = 1 \text{ gm/cm}^3$,
 $C_d = 1.0$, $d_t/s = 0.1$, $\alpha = 0.5$, $L = 2.5 \text{ cm}$.

Figure (1.1) shows the fractional contribution of the various components of pressure drop to the total. It is observed that for S less than 2, corresponding to $j_g \cong 75 \text{ cm/s}$, the flow is gravity dominated. For larger S , however, the pressure drop in the absence of the tubes would be governed by acceleration. The gas injection tubes introduce a disturbance which, in terms of momentum considerations, is of the same order as the acceleration component of pressure drop.

The impact on the dynamic behavior of the two-phase flow field of a disturbance, whose magnitude in terms of pressure drop is represented in Fig. (1.1), is uncertain. Would the void dynamics and phase interchanges be significantly affected? Would the flow regimes be influenced? How would the dispersion characteristics of the flow be influenced? These questions must be answered in the initial phase of the experimental study. The program is being directed towards this end.

1.2 Dispersion and Heat Transfer in Two-Phase Boiling Systems (T. Ginsberg)

A. Analytical Investigations

It has been shown (Ginsberg 1977c) that the rate of vapor generation in closed internally heated boiling pools is strongly dependent upon condensation heat transfer at the system boundaries. For adiabatic pools, it was shown that the rate of vapor generation is less than one percent of the vapor generated in open systems. Since the "dispersive" properties of boiling systems are strong functions of the vapor production rate, it is expected that dynamic behavior in adiabatic, closed pools will differ markedly from that in open pools.

The analysis presented earlier (Ginsberg 1977c) can be used to compute the vapor generation rate in a closed, uniformly-heated, uniformly vapor-generating boiling pool of UO_2 and steel. The superficial steel vapor velocity above a pool is, assuming all heat generated is transferred to the steel,

$$\frac{j_g}{j_g^*} = \frac{Q_c}{Q} + \frac{M_{sv}}{M_{sl}} \left(\frac{h_{fg}}{C_{ls} T_s} \right)^2 \frac{C_{ls}}{R} \left[1 - \frac{Q_c}{Q} - \frac{Q_N}{Q} \right] \quad (1.11)$$

where

- c_{ls} = heat capacity of liquid steel
- h_{fg} = steel heat of vaporization
- j_g = superficial velocity of steel vapor at top of a closed pool of liquid height H
- j_g^* = superficial velocity of steel vapor at top of an open pool of liquid height H

Fig. 1.1 Relative Contributions to Total Pressure Gradient vs. Vapor Source Strength

H = boiling pool liquid height
 M_{sv} = mass of steel vapor
 M_{sl} = mass of steel liquid
 R = steel gas constant
 T_s = steel saturation temperature
 Q = energy generation rate
 Q_c = condensation heat loss rate
 Q_N = non-condensation heat loss rate

For an adiabatic closed system, Eq. (1.11) yields

$$\frac{j_g}{j_g^*} = \frac{M_{sv}}{M_{sl}} \left(\frac{h_{fg}}{C_{ls} T_s} \right)^2 \frac{C_{ls}}{R} \quad (1.12)$$

where

$$j_g^* = \frac{QH}{\rho_g h_{fg} V} \quad (1.13)$$

and V is the fuel volume, and ρ_g is the steel vapor density. j_g^* is the superficial vapor velocity in an open pool.

It has been suggested that (Fauske 1975a) boiling pools of UO_2 and steel are "dispersive," and flow regime maps have been proposed (Fauske 1975b) which support this point of view. The superficial vapor velocity for transition from bubbly flow to churn-turbulent flow was given by

$$\frac{j_g \sqrt{\rho_l}}{\sqrt[4]{g \sigma (\rho_l - \rho_g)}} = 0.3 \quad (1.14)$$

where ρ_l is the liquid density, σ is the surface tension and g is the gravitational acceleration. The transition from churn-turbulent to dispersed flow was assumed to be defined by

$$\frac{j_g \sqrt{\rho_g}}{\sqrt[4]{g \sigma (\rho_l - \rho_g)}} = 0.14. \quad (1.15)$$

The superficial vapor velocity at the top of an internally heated boiling fuel/steel pool is a function of the static fuel height (H = fuel volume/pool area), and also of the energy generation rate. This is expressed in Eq. (1.13).

For a given energy generation rate, Q_1 , a pool height (H_1) can be calculated at which the superficial vapor velocity will equal one of the velocities given by Eqs. (1.14) and (1.15). The parameters Q_1 and H_1 , therefore, represent a flow regime limit. For Q_1 fixed, if $H > H_1$, one regime exists; if $H < H_1$, another regime exists. In this manner a flow regime map may be constructed (Fauske 1975b).

This technique was used to construct maps for adiabatic open pools and for adiabatic closed pools. It is expected that the results for the two cases will be significantly different, since the vapor generation rates can be two orders of magnitude different.

For open pools, Eqs. (1.13-1.14) were combined to yield the bubbly to churn flow transition:

$$\frac{QH}{Q_o H_o} = 0.3 \frac{\rho_g V h_{fg} \sqrt[4]{g\sigma(\rho_l - \rho_g)}}{Q_o H_o \rho_l^{1/2}} \quad (1.16)$$

For the churn to dispersed flow transition, the result is

$$\frac{QH}{Q_o H_o} = 0.14 \frac{\rho_g V h_{fg} \sqrt[4]{g\sigma(\rho_l - \rho_g)}}{Q_o H_o \rho_g^{1/2}} \quad (1.17)$$

where Q_o is the energy generation rate at full power, and H_o is the liquid pool height assuming all the fuel would melt down into a pool configuration.

For the closed pools, Eqs. (1.12)-(1.15) were combined to give for the dispersed flow boundary,

$$\frac{QH}{Q_o H_o} = 0.14 \frac{\rho_g^{1/2} h_{fg} V \sqrt[4]{g\sigma(\rho_l - \rho_g)}}{Q_o H_o} \left[\frac{M_{sv}}{M_{sl}} \left(\frac{h_{fg}}{C_{ls} T} \right)^2 \frac{C_{ls}}{R} \right]^{-1} \quad (1.18)$$

Equations (1.16) and (1.17) are plotted as dashed lines in Fig. (1.2); Eq. (1.18) appears as solid lines. In Fig. (1.2), $\bar{\alpha}$ represents the average vapor fraction within the pool, and V_{SL} represents the volume fraction occupied by steel liquid.

The dashed line in Fig. (1.2) represents the churn-to-dispersed flow transition in open pools. The solid lines represent the transitions in closed pools. This figure shows that in order to reach the dispersal limit in a liquid pool of height H , power densities are needed in a closed, adiabatic pool which are two orders of magnitude greater than for an open pool. For example, the dispersal limit will be attained at $H/H_0 = 1$ at one percent of full power density in an open pool. On the other hand, 100 percent of full power density is required in a closed, adiabatic pool.

The physical reason for the above behavior is that in a closed, adiabatic pool most of the energy generated is used to increase the sensible heat of the liquid. Only a small fraction of the available energy is used to generate vapor.

1.3 Boiling Pools with Internal Heat Generation (G. A. Greene, C. E. Schwarz)

(a) Heat Transfer Correlation Modeling:

The vertical wall boiling pool heat transfer data are correlated as an extended laminar natural convection phenomenon of the form

$$Nu(x) = K[Gr^*(x) \cdot Pr]^n \quad (1.19)$$

where $Gr^*(x)$ is a modified Grashof number based on the local void fraction, $\alpha(x)$ (Greene 1977). The typical Grashof number may be easily derived from the laminar free convection boundary layer equations as,

$$Gr(x) = \frac{g\beta(T_w - T_\infty)x^3}{\nu^2} \quad (1.20)$$

Recognizing that

$$\rho_w - \rho_\infty = \beta\rho(T_\infty - T_w) \quad (1.21)$$

and substituting into (1.20) we find

$$Gr^*(x) = \frac{g(\rho_w - \bar{\rho}_\infty)\rho x^3}{\mu^2} \quad (1.22)$$

Fig. 1.2. Flow Regime Map for Closed (Solid Line) and Open (Dashed Lines) Systems.

where subscripts w and ∞ refer to wall and infinity, respectively, and a thermophysical property without a subscript is evaluated at the film temperature given by

$$T_f = \frac{T_w + T_\infty}{2} \quad (1.23)$$

Define the density difference as

$$\rho_w - \bar{\rho}_\infty = \rho_w - (1 - \alpha)\rho_{l\infty} \quad (1.24)$$

where $\rho_{l\infty}$ is the density of the liquid fraction in the two-phase boiling core region at T_∞ . This may be substituted into Eq. (1.22) to yield

$$Gr^*(x) = \frac{g[(\rho_w - \rho_{l\infty}) + \alpha\rho_{l\infty}]\rho x^3}{\mu^2} \quad (1.25)$$

Generally for boiling pools it is a good approximation that $\alpha\Delta\rho_{l\infty} \gg (\rho_w - \rho_{l\infty})$. In this case we ignore the single-phase driving force and take

$$\rho_w \sim \rho_{l\infty} \sim \rho_{\text{film}} \quad (1.26)$$

so the modified Grashof number may be written in approximate form as

$$Gr^*(x) \sim \frac{g\alpha x^3}{\nu^2} \quad (1.27)$$

The form of Eq. (1.25) is preferred, however, where void effects are small.

For boiling pools with inclined walls, where the angle of inclination of the wall to the vertical plane is small, it may be shown in rigorous form that the modified Grashof number becomes (Fujii 1972)

$$Gr^*(x, \theta) = \frac{g\alpha x^3 \cos \theta}{\nu^2} \quad (1.28)$$

where θ is the angle from the vertical.

The vertical wall boiling pool data (Gustavson 1976) has been correlated on the basis of $\text{ZnSO}_4/\text{H}_2\text{O}$ solution properties and local void fraction as mentioned. Comparison of the correlation to the single phase natural convection correlation of Fujii (1972) is seen in Fig. (1.3) where the correlation of Fujii (1972) is

$$\text{Nu}(x) = 0.56[\text{Gr}(x) \cdot \text{Pr}]^{.25} \quad (1.29)$$

and the presently discussed boiling pool data are better correlated by

$$\text{Nu}(x) = 0.76[\text{Gr}(x) \cdot \text{Pr}]^{.25} \quad (1.30)$$

It is thus seen that prediction of local heat transfer coefficient in boiling pools has been basically resolved into a need for accurately predicting local void fraction.

(b) Analysis of Vertical Wall Void Distribution

Analysis of the local void fraction distribution based on a two-phase drift flux model, has begun to use with Eq. (1.30) in determination of the wall heat flux. The effects of volumetric power density, $\dot{Q}'''$, heat of vaporization, h_{fg} , initial pool depth, h_o , bubble terminal rise velocity, U_∞ , and vapor density ρ_v , are included.

Consider a volumetric boiling pool such that the volumetric vapor source term and liquid source term may be written as

$$\Gamma_v = \frac{\dot{Q}'''}{h_{fg}} (1 - \alpha) \quad (1.31a)$$

and

$$\Gamma_l = -\frac{\dot{Q}'''}{h_{fg}} (1 - \alpha) \quad (1.31b)$$

where the term $(1 - \alpha)$ identifies that the volumetric heating is proportional to the local liquid volume fraction, and Γ_k is the volumetric source of phase k .

For most low power boiling systems, $\frac{\Gamma_v}{\rho_v} \gg \left| \frac{\Gamma_l}{\rho_l} \right|$ so the vapor continuity equation may be written as

$$\frac{dj_g}{dz} = \frac{\Gamma_v}{\rho_v} = \frac{\dot{Q}'''}{h_{fg}\rho_v} (1 - \alpha) \quad (1.32)$$

Fig. 1.3. Laminar Natural Convection Heat Transfer Correlation for Volumetric Boiling Heat Transfer to Vertical Wall.

where $j_g = U_v \cdot \alpha$ and for churn-turbulent flow, the drift flux may be written, from Zuber and Findlay (1965),

$$j_{gj} = \frac{U_{\infty} \alpha (1 - \alpha)}{1 - C_o \alpha} \quad (1.33)$$

Since (for $j_l \ll j_g$) $j_g = j_{gj} / (1 - \alpha)$, Eq. (1.32) becomes

$$\frac{d}{dz} \left[\frac{j_{gj}}{1 - \alpha} \right] = \frac{\dot{Q}''' h_o}{h_{fg} \rho_v} (1 - \alpha) \quad (1.34)$$

which may be rewritten as

$$\frac{d}{d\xi} [F(\alpha)] = K(1 - \alpha) \quad (1.35)$$

where

$$F(\alpha) = \frac{\alpha}{1 - C_o \alpha} \quad (1.36)$$

C_o = Zuber-Findlay distribution parameter

$$K = \frac{\dot{Q}''' h_o}{h_{fg} U_{\infty} \rho_v} \quad (1.37)$$

subject to the initial condition

$$F(\alpha) \big|_{\xi=0} = 0.0 \quad (1.38)$$

The solution to this equation for various values of the vapor source parameter, K , has been calculated and compared to the vertical wall boiling pool void data for characteristic experimental values of K . This comparison may be seen in Figs. (1.4) and (1.5).

Fig. 1.4 Comparison of Void Fraction Data to Analytical Solution
($K = 0.57$)

Fig. 1.5 Comparison of Void Fraction Data to Analytical Solution
($K = 1.70$)

(c) Design and Instrumentation

The design and instrumentation is nearing completion with the exception of the remaining tasks:

1. Install flow meters and thermocouples to measure wall heat losses.
2. Plate and install thermocouples in boron nitride test wall.
3. Complete wiring of 150°F reference junction.

It is believed that the difficulties previously reported (Greene 1977) with the Boron nitride plate have now been solved and that testing will begin shortly.

1.4 Two-Phase Solidification Dynamics of Flowing Core Debris (G. A. Greene)

a. Experiment

The experimental transient freezing program of a two-phase non-condensable gas/liquid mixture has continued, using Wood's metal and N₂ gas. Additional runs have been performed at an inlet temperature of 80°C (5°C above the Wood's metal fusion temperature) and at each of seven void fractions to investigate the reproducibility of the test apparatus and data acquisition technique. The data acquisition has been smoothed by recognizing that the Cross Bar Scanner was exceeding the sampling rate of the IDVM and causing data scatter. Slowing down the scan rate eliminated the difficulty.

The smooth mass displaced data is now being differentiated to determine the mass flow rate of Wood's metal and thus the measure is the quality (and void fraction).

Marked effects of average inlet void fraction, $\langle \alpha \rangle$, have been observed on the mass displaced and plugging time as is outlined in Table (1.1). Since the ratio of inlet sensible heat in the liquid to the heat of fusion is very small, i.e.,

$$\frac{C_p (T_i - T_f)}{h_{fs}} \ll 1.$$

The effect cannot be explained solely on this basis, but primarily on the basis of freezing entrapment of the non-condensable void fraction. (See Fig. 1.6a-c). The analytical model presently being developed for transient crust growth assumes 100 percent void entrapment. The 76°C runs will eliminate any effect of sensible heat and allow verification of this hypothesis. The 80°C Wood's metal/N₂ gas freezing data is summarized in Table (1.1).

We are beginning to take data with Wood's metal and N₂ gas at 76°C to see if there is much influence of sensible heat at 80°C on the freezing process ($T_f = 74.8^\circ\text{C}$). For these runs, both mass displaced and flow rate

Average Void Fraction (α)	Plugging Time (exp) (sec) t_p	Mass Displaced (exp) (kg) m_d	Plugging Time* (analysis) (sec) τ_p
0.00	17.3	15.3	12.09
0.05	13.3	11.6	11.5
0.09	11.4	8.5	
0.10			10.9
0.20	10.8	7.7	9.7
0.23	9.4	5.5	
0.26	11.1	6.2	
0.30			8.45
0.33	7.5	3.3	
0.40	6.2	3.1	7.3

Non-condensable gas, N_2 .

Inlet Temperature 80.0°C

* $N_{PH} = 0.07$, based on $h_{fs}^* = h_{fs} + C_p(T_i - T_f)$ since $T_c > T_f$.

Table 1.1. 80°C Wood's Metal-- N_2 Gas Two-Phase, Non-Condensable Freezing Data.

data are measured. This data will be compared to the analytical model through plugging time and mass flow rate comparison (See Fig. 1.7) at the same phase change number, (inverse of the Stephan Number),

$$N_{PH} = \frac{C_p (T_f - T_w)}{h_{fs}}$$

and over a range of average inlet void fraction, $\langle \alpha \rangle$ from 0.00 to 0.40.

(b) Analysis of Two-Phase Non-Condensable Transient Freezing

An approximate analytical model is being developed for the transient crust thickness of a solidifying two-phase non-condensable mixture entering a circular channel at the liquid freezing temperature. The model assumes homogeneous two-phase flow and total void freezing, i.e., low Prandtl number. The wall temperature is assumed constant and lower than the freezing temperature. The results are presented for variable phase change number,

$N_{PH} \equiv C_p (T_f - T_w) / h_{fs}$, and variable void fraction, $\langle \alpha \rangle$, in Figs.

(1.8-1.9). Preliminary comparison to the data is performed in Table (1.1).

The data is for $T_i = 80.0^\circ\text{C}$, and the model is for $T_i = T_f = 75.0^\circ\text{C}$. A more meaningful comparison will be available when more 76°C Wood's metal data are available. This comparison is based on $N_{PH} = .05$ where h_{fs}^* is computed as an effective heat of fusion,

$$h_{fs}^* = h_{fs} + C_p (T_i - T_f)$$

combining the inlet sensible heat plus the time heat of fusion. If this correction did not have to be performed, N_{PH} would be larger and T_{plug} would be correspondingly lower as indicated in the figures. This is expected to yield better agreement with the 76°C data to be taken. It should be noted that significant uncertainty exists in the values of $\langle \alpha \rangle$ listed since the determination of $\langle \alpha \rangle$ is somewhat inaccurate.

(a) $\alpha_o = 0.0$ (b) $\alpha_o = 0.2$ (c) $\alpha_o = 0.33$

Fig. 1.6 Comparison of Two-Phase Transient Freezing Data
($T_i = 80^\circ\text{C}$)

TWO PHASE TRANSIENT FREEZING

Fig. 1.7 Typical Transient Solidification Data, Mass Displaced, Mass Flow Rate
 $(T_i = 76.0^\circ\text{C})$

TRANSIENT FREEZING, $T(1) = T(F)$

Fig. 1.8. ANALYTICAL RESULTS: DIMENSIONLESS
CRUST THICKNESS VS DIMENSIONLESS TIME

TRANSIENT FREEZING, $T(I) = T(F)$ Fig. 1.9. DIMENSIONLESS CRUST THICKNESS, SINGLE PHASE, VARIABLE N_{PH}

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2. Technical Coordination of Structural Integrity (M. Reich)

A third report in the series of reports dealing with fracture mechanics applications to reactor structural components is in preparation. In this report a critical in-depth review of some of the data sources that were delineated in the first report (BNL-NUREG-50650) was undertaken.

Specifically, the following areas were singled out for study:

- (1) application to doubly curved (shell) structures;
- (2) part-through crack problems;
- (3) leak-before-break analysis;
- (4) triaxial constraint effects;
- (5) fatigue-crack propagation;
- (6) fracture and limit load, enlarged strain general yield conditions; and
- (7) time-dependent nonlinear creep behavior.

3. SSC Code Development (A. K. Agrawal)

The Super System Code (SSC) development program deals with the development of an advanced benchmark thermohydraulic code to simulate transients in LMFBs. So far, the work was concentrated on developing a version of this code, SSC-L, for the analysis of transients in loop-type LMFBs. The scheduled date for completion of an operational code was October 1, 1977. During this quarter, the SSC-L code was made operational on September 26, 1977 -- a few days ahead of the date scheduled more than two years ago. In the following, progress made during this quarter is reported. Reference is made to the previous quarterly progress report (Agrawal, 1977) for a summary of accomplishments prior to the start of the current period.

3.1 Transient Fuel Heat Transfer and Coolant Flow Computation (J. W. Yang)

The coupling of transient fuel heat transfer and coolant flow has been completed. The computation procedures are shown in Figs. 3.1 and 3.2. Because of the multi-time step method used in the SSC code, fuel heat transfer and coolant flow are computed separately with different time steps. They are interconnected through the extrapolation/interpolation of the boundary conditions. All temperature-dependent properties are evaluated at temperatures linearly extrapolated from two previous temperatures.

Figure 3.1 shows the procedure of transient coolant computation. There are four major regions in the vessel: lower plenum, core, bypass channel and upper plenum. Since the core is the most important region of the vessel, its lower and upper boundary conditions are not extrapolated from previous times. The boundary conditions are provided by the lower and upper plena, which are computed in advance, as illustrated in Fig. 3.1. The transient fuel computation is shown in Fig. 3.2. Three different sections of rod -- fuel, blanket and fission gas plenum -- are treated according to the material index specified by the user. Checks of melting of pellet or clad are done during the computation. If the computed pellet temperature is above the specified melting temperature, a simple molten fuel model will be used to replace the solid-phase heat transfer model. The molten model is not available at present, but will be added in the code to compute the fraction of fuel melted. Melting of clad, as stated previously, is the index of terminating the transient computation. Calculation of hoop stress and comparison with the fission gas pressure are performed for every channel. Release of fission gas is indicated, as the fission gas pressure is higher than the hoop stress. Boundary conditions of gas bubble formation are transmitted to the coolant model for the initialization of bubble computation. It is assumed that rupture of clad has no effect on clad heat transfer calculations.

3.2 Heat Transport System (I. K. Madni and E. G. Cazzoli)

3.2.1 System Hydraulics

An equation to determine the vessel inlet pressure, which utilizes information from the primary loop hydraulic equations, as well as from vessel coolant dynamics, has been formulated. For illustrative purposes, two-loop simulation of an $(n+1)$ loop plant, with break after pump in loop 1, and the n unaffected loops being lumped together, will be used. The code has the more

FIGURE 3.1: TRANSIENT COOLANT COMPUTATIONS

FIGURE 3.2: TRANSIENT FUEL COMPUTATIONS

general formulation. The equations thus obtained are: Mass conservation at vessel inlet yields

$$W_c = nW_{2,2} + W_{3,1} \quad (3.1)$$

or, differentiating both sides,

$$\frac{dW_c}{dt} = n \frac{dW_{2,2}}{dt} + \frac{dW_{3,1}}{dt} \quad (3.2)$$

From loop hydraulics (see Agrawal, 1977),

$$\frac{dW_{2,2}}{dt} = \frac{P_{out,2} - P_{inV} - (\Delta P_{f,g})_{2,2}}{\sum_{2,2} \frac{L}{A}} \quad (3.3)$$

and, assuming break after pump:

$$\frac{dW_{3,1}}{dt} = \frac{P_{out,b} - P_{inV} - (\Delta P_{f,g})_{3,1}}{\sum_{3,1} \frac{L}{A}} \quad (3.4)$$

Core flow can be expressed as

$$W_c = \sum_j W_j \quad \text{where } j = 1, (N6CHAN + 1) \quad (3.5)$$

Differentiating both sides of Eq. (3.5) and substituting along with Eqs. (3.3) and (3.4) in Eq. (3.2), gives

$$\sum_j \frac{dW_j}{dt} = \frac{n[P_{out,2} - P_{inV} - (\Delta P_{f,g})_{2,2}]}{\sum_{2,2} \frac{L}{A}} \quad (3.6)$$

$$+ \frac{[P_{out,b} - P_{inV} - (\Delta P_{f,g})_{3,1}]}{\sum_{3,1} \frac{L}{A}} \quad (3.6)$$

Simplifying and rearranging yields the vessel inlet pressure as:

$$P_{inV} = \left(\frac{\frac{n[P_{out,2} - (\Delta P_{f,g})_{2,2}]}{\sum_{2,2} \frac{L}{A}} + \frac{[P_{out,b} - (\Delta P_{f,g})_{3,1}]}{\sum_{3,1} \frac{L}{A}} - \sum_j \frac{dW_j}{dt}}{\left[\frac{n}{\sum_{2,2} \frac{L}{A}} + \frac{1}{\sum_{3,1} \frac{L}{A}} \right]} \right) \quad (3.7)$$

3.2.2 Centrifugal Pump

Pony Motor: While the arrangement of the primary and intermediate loops is expected to be such that natural circulation will provide sufficient heat transport for safe decay heat removal in the event of loss of all pumping power, the pumps may be equipped with pony motors (as is the case with CRBR) and supplied with normal and emergency power to provide forced circulation decay heat removal. Therefore, an option for pony motor operation was added to the pump model. The pony motor is assumed to come into play when the main motor coasts down to a user-specified fraction of its rated speed. Once the pony motor takes over, the angular momentum balance equation (see Agrawal, 1976) is bypassed since pump speed stays constant, i.e., $dw/dt = 0$. All other calculations remain the same.

Pump Characteristics: Pump characteristics have been extended into one more region of operation, i.e., reverse pump. This corresponds to positive flow and negative impeller rotational speed, and can occur during the later stages ($t > 60$ sec) of the transient following pipe break, without pony motor. As tabulated values are not available for this region, these were generated from the Karman-Knapp Circle diagram (Donsky, 1961), and then polynomial relations were curve-fitted to these values.

3.2.3 Guard Vessel

As a safety feature to minimize the effects of a pipe-break accident, guard vessels are provided around the reactor vessel, IHX, primary pump and all piping which is below the elevation of the tops of the guard vessels, while their volume is such that reactor vessel coolant level does not fall below the outlet nozzle, so that the core is always submerged in coolant. If a leak occurs such that coolant spills into the guard vessel, eventually the vessel will fill up to the leak height. Any level rise above that will create back pressure against further leakage.

An example configuration of a guard vessel for a break in the reactor vessel is shown in Fig. 3.3. At any time t during the transient following a pipe break, the volume of sodium collected in the guard vessel can be determined by

$$V_{GV} = \int_0^t \frac{W_b}{\rho} dt \quad (3.8)$$

where W_b , the break flow rate (for the case illustrated), is

$$W_b = W_{2,1} - W_{3,1}$$

and ρ is the density of coolant at break.

To determine the height of sodium in the guard vessel (Z_{GV}) requires detailed knowledge of configuration and dimensions of the annular and bottom space between the component and its guard vessel. However, a simpler and more general approach is to have a functional relationship between Z_{GV} and V_{GV} in the form of a polynomial equation as follows:

FIGURE 3.3: GUARD VESSEL CONFIGURATION
FOR BREAK IN RV INLET REGION

$$\text{If } V_{GV} \leq V_{MIN}, \quad Z_{GV} = 0$$

$$\text{If } V_{GV} > V_{MIN}$$

$$Z_{GV} = c_1 + c_2(V_{GV} - V_{MIN}) + c_3(V_{GV} - V_{MIN})^2 \quad (3.9)$$

where c_1 , c_2 , c_3 are user-input coefficients depending on the geometry of the guard vessel space.

V_{MIN} is the volume required to fill up to nozzle centerline of the lower pipe. This is also a user-input quantity, and will be different for different guard vessels.

V_{GV} is limited by V_{MAX} , the maximum capacity of the guard vessel. It seems reasonable to assume V_{MAX} to be the same for all guard vessels based on the volume contained in the upper plenum between the operating level and the minimum safe level. Z_{GV} is limited by Z_{MAX} , the height of the guard vessel. This can be different for different guard vessels.

The pressure external to the break during the transient is determined by

$$\begin{aligned} P_{ext} &= P_{atm} && \text{if } Z_{GV} \leq Z_b \\ &= P_{atm} + \rho g \cdot (Z_{GV} - Z_b) && \text{if } Z_{GV} > Z_b \end{aligned} \quad (3.10)$$

A sample test case corresponding to break at vessel inlet has been successfully run. A comparison of system hydraulic response in terms of flow rates for this accident, with and without guard vessel, will be shown in the next quarterly report.

3.2.4 HTS Module Development

The modules for transient thermal calculations in the primary and intermediate heat transport systems were coded, debugged, and then tested individually and together for pump coastdown with scram boundary conditions. The IHX routine was rearranged and modified to allow separate evaluation of primary and secondary sodium temperatures.

The hydraulic modules were updated to accommodate the new models described in the preceding subsections.

Work was initiated on a file containing the entire HTS transient code interfaced with the main driver for the plant-wide calculations, as well as with SSC (steady state). The code was first examined and corrected for inconsistencies, then cleaned of parts that, in running thermal and hydraulic modules together, were no longer needed. The entire thermal-hydraulic code was run for 80 seconds transient without any forcing function, to check for consistency with steady state. However, additional bugs were uncovered on

running pump coastdown transient. These were also removed, and subsequently, the code has been successfully tested for both steady state (no forcing function) and pump coastdown with scram.

3.3 Steam Generating System (W. L. Weaver III and J. G. Guppy)

The work during this quarter was directed toward debugging the coding of the transient model of the steam generating system. The original integration method was found to be both stiff and unstable for time steps of interest (> 25 msec). Methods were found to remove the instability but not the stiffness. Because the stiffness could not be removed from the original integration method, a new linearized, fully implicit integration method was derived.

A simplified steam generator model was developed to account for the heat removal by the tertiary loop while the new integration method is being coded and debugged.

3.3.1 Simplified Steam Generator Model

In the simplified model, as applied to the CRBR generating system, each heat transfer module (evaporator and superheater) and the steam drum are represented by a single node. These three nodes are interconnected by five flow paths (feedwater to drum, drum to evaporator, evaporator to drum, drum to superheater and superheater to turbine). The mass and energy conservation equations are applied to each node and the conservation of momentum equation is applied to each flow path.

The conservation equations for nodes containing two-phase fluid mixtures yield three differential equations for the pressure in the node, the mass of saturated liquid in the node and the mass of saturated vapor in the node. Only two differential equations are needed for nodes containing single-phase fluid; i.e., equations for the pressure and enthalpy in the node. The momentum equation yields a single differential equation for the rate of change of flow rate in each flow path. Thus, this simplified model of the steam generator tertiary side consists of thirteen differential equations, three equations for the steam drum, three equations for the evaporator, two equations for the superheater and five flow path equations. These differential equations are integrated in time by an explicit integration package (see Lucas, 1976).

This model of the tertiary side of the steam generating system has been coded, debugged and tested. It is included in the present version of the SSC-L code.

3.3.2 Improved Integration Technique

The model equations for the steam generating system are grouped into two sets of equations. The first set of equations describes the enthalpy and flow rate distributions in flow segments consisting of linear networks of pipes, pumps and heat exchangers. The second set of equations describes the pressure and enthalpy in accumulators. The two sets of equations are coupled by the interconnections between the flow paths and accumulators. A momentum integral flow model has been chosen for describing the flow segments because it is appropriate for the types of transients to be analyzed by the initial version

of the SSC-L code (see Meyer, 1961). The fluid compressibility was removed from the momentum integral model by assuming that the fluid pressure is spatially constant and using this reference pressure in the evaluation of the fluid properties. In the version of the momentum integral utilized for the SSC code, the reference pressure was allowed to be time dependent. The time-dependent reference pressure reintroduced the effects of fluid compressibility into the model equations for the flow loops. The stiffness observed in the original integration scheme in which explicit coupling was used between the two sets of equations was a result of this fluid compressibility.

To relax the time step limitations imposed by the explicit nature of the coupling between the two calculations, a fully implicit integration method was developed. The equations comprising the momentum integral model were linearized so that the conditions at any location in the flow segment at the advanced time could be written as a linear combination of the advanced time pressures and enthalpies in the accumulators. The linear relations were then used to eliminate the flow segment terms in the implicit form of the conservation equations for the accumulators. This results in a coupled set of linear algebraic equations for the conditions in the accumulators at the advanced time. Once this set of equations has been solved, the conditions in the flow segments at the advanced time can be reconstructed from the linearized flow segment equations. A memorandum describing this integration method in more detail will be prepared during the next quarter.

3.4 System Integration Method (J. G. Guppy)

The logic and time step hierarchy of the multi-step scheme (see Agrawal, 1977) used in SSC had to be modified slightly. It was decided that the in-vessel coolant fluid dynamics calculations would, in general, need to be calculated more often than the fuel heat conduction calculations. This is particularly true when flow redistribution calculations are performed. Thus, the coolant fluid dynamics time control logic had to be nested within the fuel heat conduction logic instead of vice versa as had been done previously.

Numerical stability studies were conducted using the Runge-Kutta-Merson (RKM) integration package (Lucas, 1976) which was proposed for use in advancing the loop hydraulics equations. The system of equations used during these studies was in good approximation of that actually included in the SSC-L package. These numerical stability studies showed that the range of stability of the RKM package for this system of equations lies within 0.5 to 1.0 seconds. In addition, the RKM package requires five calls to the derivative update modules per time step. Although the RKM package requires less storage than more sophisticated packages, its numerical stability restrictions and the multiple number of derivative calculations required indicate that a more efficient integration package may be desirable in SSC.

3.5 Code Development (J. G. Guppy, R. J. Kennett, T. E. Nepsee and E. S. Srinivasan)

The first working version of the SSC-L transient package was successfully run on September 26, 1977. The case simulated was reactor scram with simultaneous pump coastdown.

The major computational modules of the SSC-L transient portion are shown in Fig. 3.4. Briefly, these modules do the following:

- MAIN9T - Drives all other modules and handles overall time step control.
- FUEL5T - Computes reactor power and fuel heat conduction.
- COOL6T - Computes in-vessel coolant dynamics and coolant heat convection.
- LOOP1T } - Compute all energy calculations in all primary
LOOP2T } and intermediate loops, respectively.
- FLOW1T } - Compute all hydraulic calculations in all primary
FLOW2T } and intermediate loops, respectively.
- STGN3T - Handles the thermal and hydraulic calculations in the steam generator.

During this quarter, stand-alone versions of all seven major computational modules were obtained, interfaced with the steady-state package, interfaced with the main driver (MAIN9T) and interfaced with each other where applicable.

A restart option is now operable such that the transient portion of SSC-L may be run alone (i.e., without having to reinitialize) by simply reading the previously computed steady-state data from tape.

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FIGURE 3.4: MAJOR SSC-L COMPUTATIONAL MODULES

4. SSC Code Validation (A. K. Agrawal and R. J. Cerbone)

The Code Validation work this quarter covers the following areas:

- 4.1 Analysis of Integral Thermohydraulic Experiments
- 4.2 SSC-L Needs
- 4.3 Sensitivity Analysis Methods
- 4.4 Critical Experiments

The Analysis of Integral Thermohydraulic Experiments covers the evaluation of proposed experiments, such as the preacceptance tests in FFTF, and analysis of natural convection tests that were performed in the EBR-II reactor. A list of key assumptions that were made in the SSC-L code is noted in Section 4.2 under SSC-L Needs for its verification. The Sensitivity Analysis work covers the use of statistical methods for SSC validation, and the Critical Experiments work covers the design of the RSR experiments in the BIZET series on the UKAEA-Winfrith critical facility ZEBRA.

4.1 Analysis of Integral Thermohydraulic Experiments (A. K. Agrawal, R. J. Cerbone and D. Majumdar)

During this quarter, work was continued on building up a data base for SSC Code Validation. Reports were collected and reviewed for relevant SEFOR, FERMI and EBR-II experiments. This work is being compiled into a topical report to be issued by October 31, 1977. Although these experiments are expected to provide checks on some of the models and data used in SSC, a major thrust of the code validation effort will be utilization of FFTF preoperation tests. In particular, the natural convection tests are expected to provide data which can be used to check the adequacy of SSC to model natural convection.

An updated work plan for SSC Validation using FFTF has been prepared and discussed with ARSR staff. Accordingly, this program will focus on examining the adequacy of preoperation tests in FFTF to quantify models used in the SSC-L code. Work on EBR-II will also be carried out, albeit at a low level, due to the priority being given to interfacing SSC with FFTF.

4.2 SSC-L Needs (A. K. Agrawal)

As a part of the program, a list of key assumptions made in various modules of the SSC-L code along with the pertinent issues and comments was prepared. This list is a partial one and is detailed in Table 4.1.

4.3 Sensitivity Analysis Methods (C. Durston and T. Krieger)

During the quarter, work was directed toward implementing and testing the methods developed and reported in the previous quarter (Agrawal, 1977). The methods were applied to the DEMODA4 (Albright, 1977) thermohydraulic code to determine whether important or key variables could be identified in a complex code without their prior knowledge. To this end, a numerical experiment was performed with DEMODA4 in order to evaluate the efficacy of the methods to identify and rank key variables in a specified accident scenario. Since the results are being incorporated into a topical report, only a brief summary will be given here.

TABLE 4.1

A Partial List of Assumptions and Validation Needs
for the SSC-L Code

<u>Area</u>	<u>Current Method/Assumptions</u>	<u>Issue</u>	<u>Comments</u>
Thermohydraulic modeling for in-core (without coolant boiling)	N-parallel 1-D channels	Intra-assembly incoherency	A channel represents one or many assemblies. Radial temperature profile may not be as critical for single-phase coolant. In the event of sodium boiling, this issue becomes a major one.
	Channels coupled neutronically and hydraulically through lower and upper plena.		
	No cross-flow terms between different channels considered.	Channel selection method	Computed results may depend upon how various channels are selected.
	Axial heat conduction in a channel neglected.	Flow reversal in only some of the channels -- potential coolant stagnation.	There appears a possibility of setting up internal convection within the core.
	Interchannel heat conduction ignored.	Coupling method for heat transfer between different channels.	The interchannel heat transfer may be an important factor for long-term transients.
		Interchannel flow redistribution	The observed flattening of temperature profile for natural convection transients may be explained by flow redistribution alone. Or, the radial heat conduction may have to be included.

TABLE 4.1 (cont.)

A Partial List of Assumptions and Validation Needs
for the SSC-L Code

<u>Area</u>	<u>Current Method/Assumptions</u>	<u>Issue</u>	<u>Comments</u>
Thermohydraulic modeling for in-core (without coolant boiling) (cont.)		Effect of cross- flow on transients with scram	Temperature variation across a fuel assembly should accentuate for low flows. In fact, for a zero-flow rate case, the temper- ature distribution will be para- bolic.
		Lumping of spacer wire and structural materials	In an axisymmetric channel rep- resentation, spacer wire and other structural material has to be lumped together.
		Method of selecting channels	Computed response may depend upon the method of selecting channels.

TABLE 4.1 (cont.)

A Partial List of Assumptions and Validation Needs
for the SSC-L Code

<u>Area</u>	<u>Current Method/Assumptions</u>	<u>Issue</u>	<u>Comments</u>
Sodium boiling model	Single-bubble, slug model	Sodium boiling at low flow and low heat flux may differ sig- nificantly from that under LOF conditions.	Time delay between reaching saturation temperature and superheated condition is small for LOF (high heat flux). This should be evaluated for transients with scram.
		The effect of superheat	There appears to be growing interest in dispersed model for sodium boiling, as opposed to inhomogeneous slug model.
		The effect of quality on boiling	Low quality boiling may be encountered as well as reasonably high quality.

TABLE 4.1 (cont.)

A Partial List of Assumptions and Validation Needs
for the SSC-L Code

<u>Area</u>	<u>Current Method/Assumptions</u>	<u>Issue</u>	<u>Comments</u>
Coolant mixing in lower plenum	Perfect mixing	Extent of pressure variation in the radial direction	Discharge rate through a break in the inlet leg depends on it.
	One-dimension in axial direction	Coolant stratification in the event of reverse flow in some or all of the reactor channels.	Thermal conditions needed to continue channel-dependent thermohydraulic analysis.
		The effect of passage of gas or vapor bubble from one channel into the vessel plenum	While vapor bubble may be quenched readily, the gas bubble is noncondensable.
Coolant mixing in upper plenum	Two-zone model	Layering or stratification	An accurate assessment of stratification is needed to get sodium conditions at the vessel outlet.
	All structural material and bypass flow considered.	Effect of channel selection	Since zones are selected on the basis of average jet penetration height, different schemes for getting averages should be examined.
	Zoning based on average jet penetration height.	Effect of structural material and bypass flow	Analysis has shown a significant effect on layering and temperature calculations.

TABLE 4.1 (cont.)

A Partial List of Assumptions and Validation Needs
for the SSC-L Code

<u>Area</u>	<u>Current Method/Assumptions</u>	<u>Issue</u>	<u>Comments</u>
Power generation in the core	Point kinetics for fission heating; tabular or functional input for decay heating	Relative fraction of fission and decay heating during transient	SSC code is written in general terms to account for the variation in the two fractions. The sensitivity of calculations to different modes of normalization should be examined.
Radial blanket assembly	Treated as one or more equivalent channels	The effect of power tilt on hot channel factors during transient	The intra-assembly incoherency effects appear to be the largest in blanket assemblies. Methods for calibrating channel parameters must be examined.
Pipe Break	Double-pipe arrangement is modeled as either free-flow or confined flow.	Time delay in scram due to the presence of guard pipe	In the presence of guard pipe, coolant drainage from the inner pipe can be substantially less than that without guard pipe. Resulting slower depressurization leads to delayed scram possibilities.

The total number of input parameters in the DEMODA4 code is 1394. Of these, 661 were actually varied from a base or "reference" value. The reactor transient analyzed is the consequence of a one-square-foot rupture at the reactor inlet. The reactor was scrambled by the first applicable function. The effect of varying the 661 variables on the maximum hot channel clad temperature (MHCCT) was investigated.

A total of 64 runs were performed. The first or reference run was made with all variables set equal to their respective nominal or base values. A discrete change of +1% or -1% was assigned to each variable, and 63 subsequent runs were made, each with increments of random sign on each of the 661 variables. Thus, 64 values of MHCCT were obtained corresponding to 64 known sets of input parameters, 63 of which were random.

The data were analyzed by means of two methods previously developed for detecting sensitivity coefficients (Agrawal, 1977). Each method yields an approximate ranking of the absolute magnitude of the sensitivity coefficients. The "true" sensitivity coefficient for a variable was found by perturbing only this variable and keeping all others to their respective base values. With the help of these "one-at-a-time" runs to obtain true sensitivities (assuming the code is linear over the small incremental range), it was found that of the top six coefficients (as determined by the more accurate of the two methods mentioned above), five were in fact effective. Of the top thirteen, seven were found to be effective.

It is important to recognize that the sensitivities referred to here do not take into account uncertainties in the specification of the input variables. The variation in any output quantity of a code due to variation in a given input parameter depends on both the associated sensitivity (which is essentially a derivative) and the increment or uncertainty in that input parameter. In the present work, we consider only the sensitivities which are determined by the code and not by any imprecision of input data.

It is concluded from the results of the verification test that the efficiency of the methods proposed for the detection of effective input parameters without resorting to human judgment is reasonable. The efficiency will naturally increase as the number of runs increases. The results with DEMODA4 were obtained with a ratio of runs to variables of less than 1/10. To obtain 100% efficiency (assuming a linear system) would require this ratio to be unity, i.e., 661 runs.

4.4 Critical Experiments (H. Ludewig)

During the last reporting period, the pre-analysis of the proposed BIZET-B safety-related critical experiments was completed and a report outlining the work was written (Ludewig, 1977). The major conclusion reached in this report was the desirability of these experiments, since they extend the data base in the direction of commercial-sized breeder reactors. Such experiments are necessary to validate reactor physics techniques for large reactors. These techniques will then be used in answering the various safety and licensing questions concerning commercial LMFBRs.

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III. LIGHT WATER REACTOR SAFETY

SUMMARY

Modeling has continued in the development of constitutive relationships for non-equilibrium phase change and flashing flows. The model previously developed to express the volumetric vapor generation rate in flashing incorporated a parameter which was dependent upon the interfacial area density. Calculations of the interfacial area density and thus the area density parameter have been made based on the existing data of Reocreux.

Mechanical construction of the test facility is virtually complete except for some vendor supplied components yet to be installed in places provided. Work has begun on the electrical system. The venturi and venturi supports for the test section have been completed and the detailed drawings for the balance of the test section are nearly complete. The material for sources and detectors for the gamma densitometer have been received and the source capsules have been fabricated. Ordering is in progress for the balance of the electronic system.

Methods have been demonstrated to provide corrections for simultaneously recorded data where temporal incoherencies exist between recording channels, and these methods have been verified. In addition, analytical methods have been provided which allow the reconstruction of actual signal behavior from the recorded behavior, taking into account the attenuation and phase lag characteristics of the recording device. These methods have also been demonstrated and results are included in this report.

Repeatability of the results previously reported regarding the velocity sensitivity in the optical probe output has been demonstrated. This was accomplished by fabricating a completely separate probe and rerunning the tests. The results indicate that a single device such as the one we have constructed should be capable of providing both local void fraction and local interface velocity measurements. It is believed that the physical principles underlying this behavior have been determined and can be explained in terms of thin film withdrawal theory. Numerical results calculated from this theory appear to agree reasonably well with our experimental results, and provide information as to the way design change can have a potential effect on the behavior. Further analysis is being accomplished and these ideas will be tested shortly.

As an alternative to the optical probe for purposes of obtaining a local void fraction and velocity measurements, a probe based on radio frequency (r-f) transmission/detection principles has been constructed and tested. It has been determined that the technique has considerable promise for the intended purpose. Void fraction information can be obtained from residence time data in a manner similar to that accomplished with the optical probe. In addition, velocity information can be obtained from transit time considerations taking into account the dimensions of the probe and a detailed knowledge of the behavior of the probe response. It appears as though neither maxima nor minima are affected by local flow conditions in a fixed geometric configuration. However, there does appear to be an effect due to surrounding geometry which may alter the calibration. On the other hand, since velocity and void fraction information are obtained from purely temporal considerations coupled

with the fixed and well-known geometry of the probe, it may be that changes in signal amplitude due to variable geometric input with the r-f field will not be important.

Finally the development of the signal analysis system has continued with implementation of the intermediate speed, multiplexed, analogue/digital conversion sub-system. Data can now be continuously recorded at throughput rates of 50 kHz for periods of approximately 25 seconds. Systems software has been developed to allow both overall and "zoom" capability in data examination, and to provide numerical output on specific and interesting details of the signals. In addition, fast Fourier direct and inverse transform capability has been implemented and the development of a flexible, user-oriented, macro-instruction environment for block manipulation has been instituted. This system has been utilized in performing the signal incoherency and reconstruction demonstrations referred to previously.

Work on the THOR code development continued in the following areas:

The single-loop PWR program was developed using an explicit numerical scheme, which was found to be unstable. It was, therefore, decided to switch to a semi-implicit scheme, known to be numerically stable.

A two-region core model using the kinematic shock approach for tracing the flow regime interface was completed, and initial results are shown.

Modeling and programming of the steam generator and the pressurizer has been progressing.

1. Light Water Reactor Thermal/Hydraulic Development Program (O. C. Jones)

1.1 Development of Constitutive Relations

1.1.1 Analytical Modeling

(a) Effect of Pressure Change (P. Saha)

In the previous Quarterly Progress Report (Saha 1977), the following expression for the volumetric vapor generation rate for flashing flow was developed:

$$\Gamma_v = C_\Gamma \frac{k_\ell (T_\ell - T_{\text{sat}})}{\sqrt{a_\ell t}} \frac{[\alpha(1 - \alpha)]^{2/3}}{\Delta i_{fg}} \quad (1.1)$$

where C_Γ is a free parameter to be determined from the experimental data, k_ℓ is the thermal conductivity of the liquid, a_ℓ is the thermal diffusivity of the liquid, t is the transport time from the net vapor generation point, $(T_\ell - T_{\text{sat}})$ is the instantaneous liquid superheating, α is the area-averaged void fraction, and Δi_{fg} is the latent heat of vaporization.

During the reporting quarter, work started in evaluating the above model with the data of M. Reocreux (1974). In this experiment, the pressure and the diametral-averaged void fraction were measured along the length of the test section. However, the cross-sectional averaged void fraction was not measured. Therefore, for model evaluation purposes, the measured diametral void fraction has been taken as the area-averaged void fraction, α .

Given a distribution of area-averaged void fraction and pressure, one can write the following expressions for actual vapor quality, x , and the rate of vapor generation, Γ_v :

$$x = \frac{\alpha \left[C_o \frac{\rho_g}{\rho_\ell} + \frac{\rho_g V_{gj}}{G} \right]}{\left[1 - \alpha C_o \frac{\Delta \rho}{\rho_\ell} \right]} \quad (1.2)$$

and

$$\Gamma_v = \frac{Gx}{\alpha \left[1 - \alpha C_o \frac{\Delta \rho}{\rho_\ell} \right]} \frac{d\alpha}{dz} + \frac{[\alpha C_o G(1-x)/\rho_\ell + \alpha V_{gj}]}{\left[1 - \alpha C_o \frac{\Delta \rho}{\rho_\ell} \right]} \frac{d\rho_g}{dp} \frac{dp}{dz} \quad (1.3)$$

where G is the mass-flux, C_o is the void distribution parameter, V_{gj} is the vapor drift velocity, z is the axial co-ordinate, and ρ_k is the density of phase k .

Eq. (1.3) is valid for a constant area duct, an incompressible liquid, a constant vapor drift velocity, V_{gj} , and a constant void distribution parameter, C_o . Two sets of M. Reocreux's data (Run nos. 403 and 400) have been used to calculate the actual rate of vapor generation from Eq. (1.3), using a value of unity for C_o , and the value for bubbly churn-turbulent upflow for V_{gj} .

Because of the large scatter in the data, the derivatives $d\alpha/dz$ and dp/dz have been calculated in two ways: (a) by center-differencing the adjacent data points, and (b) differentiating the best-fit, second-order polynomials through the data points. The study has also been confined to the constant area portion of the test section.

The local liquid superheating, $(T_\ell - T_{sat})$, was calculated from the mixture thermal energy equation, and the value of C_Γ was determined by equating Eq.

(1.1) to Eq. (1.3). The interfacial area density, A_s , was also calculated by assuming the net interfacial heat flux q_s to be equal to $k_\ell(T_\ell - T_{sat})/\sqrt{a_\ell t}$. Results are shown in Figs. (1.1) and (1.2).

However, no conclusion can be drawn at this time because of the small amount of data analyzed and because of the scatter of the data. More data will be analyzed in the near future.

Fig. 1.1 Calculated Values of Vapor Generation Rate, Liquid Superheat, and Interfacial Area Density from Reocreux's Data.

Fig. 1.2 Calculated Values of C_T from Reocreux's Data.

1.2 Design, Construction, and Checkout of Experimental Equipment

(a) Flow Circuit (W. J. Leonhardt and J. H. Klein)

All major loop piping and loop components have been installed and welded with jumpers in place of some commercial elements not yet received. Construction efforts have been limited by the availability of craft welders. However, rapid progress has been made in the last part of the quarter by the addition of two temporary technicians to the staff. The components installed during this quarter include the flash tank, booster pump, make-up pump, high temperature seals for the main pump, among others. Major components which now remain to be installed to make the system complete are the test section, heaters, pressurizer, and cooling tower. The cooling tower has been delivered, put in place, and will be connected shortly.

A vendor was chosen to fabricate the heating system after competitive bids were evaluated. Outside fabrication was chosen over in-house fabrication, which yielded a cost savings of 21 percent. Fabrication of the pressurizer has been delayed because preliminary drawings of the heating system have not been received. Since the pressurizer must mate with the heating system, its final design dimensions cannot be determined until these drawings arrive.

The electrical interlock system has been reviewed and approved. Currently, electrical schematic drawings are being prepared, and it is expected that wiring of all controls and sensors will be completed next quarter. Conversion of the old generator room to a control room for the flow circuit is virtually complete.

(b) Test Section (W. J. Leonhardt, J. H. Klein, J. Seeberger)

Detail drawings for the test section are now nearly complete, and fabrication is in progress in both vendor and BNL shops. Bids are still being received for fabrication of the probe rake, and vendor selection is expected to be made shortly.

Fabrication of the venturi has been completed. This was accomplished by the use of a spinning technique. The finished venturi was held to extremely close tolerances, and the wall thickness varies only from 0.569 mm to 0.597 mm. Once completed, the venturi was used as a template to fabricate the venturi support. This support is the single most costly item to fabricate in the entire test section. The completed support was delivered at the close of the quarter, and it is expected to be joined to the venturi early next quarter using a brazing technique. Figure (1.3) shows the venturi and the venturi support before joining.

The problems with the probe seal that were discussed in the last quarterly seem to have been solved. Ethylene propylene ter-polymer (EPT) has been chosen as the sealing material. Autoclave testing has shown no apparent

Fig. 1.3. Venturi Tube and Mating Support

detrimental effects on this material at our expected operating conditions. In addition, a simpler design has been developed using a standard, readily available cross-sectional shape. Delivery has been taken on a sufficient amount of sealing material to allow several changes in the test section if needed.

A precision traversing motor system has been specified, and an order is currently being placed. The system will provide independent positioning of both axes of the probe and the gamma densitometer. This system should provide repeatable positioning on any axis with an accuracy greater than 0.025 mm.

(c) Global Densitometer (W. J. Leonhardt, N. Abuaf)

The two channel layout for the gamma densitometer has been expanded to two banks of five channels each. It is felt that five is the optimum number per bank possible considering the geometrical constraints of the current test section design. Sufficient material for sources and detectors have been received, including spares. Aluminum capsules to hold the thulium sources have been designed and fabricated. Removable modules holding five sources or five detectors remain to be designed and fabricated.

A vendor has been chosen who can supply all the necessary electronics associated with the gamma densitometer, and an order is currently being placed to allow construction of a ten channel system.

(d) Facilities (W. J. Leonhardt, J. H. Klein)

Development of both the optical and r-f probes requires a small high speed air-water loop to simulate actual test section velocities. A loop has been designed and is presently being constructed. It includes a pump with a flow rate of 1500 l/min at a total dynamic head of 600 kPa. Air injection is provided in the loop to simulate water/steam two-phase flow. In addition to the test sections housing the optical and r-f probes, the flutter test apparatus and a spare venturi will also be included. The inclusion of a spare venturi will allow bench testing of the gamma densitometer system. Both a turbine flow meter and an orifice plate will be used to measure the flow rate. It is planned that additional studies can be made with this flow loop to evaluate the effects of two-phase flow through a turbine flow meter during the next fiscal year.

1.3 Development of Instrumentation Techniques

1.3.1 Analytical Modeling (N. Abuaf, A. Swoboda, G. A. Zimmer)

Concerning the methods for correlation incoherencies in data acquisition hardware, an analytical method was presented in the April-June 1977 Quarterly Report (Abuaf 1977). It was shown that the cross correlation function could be used between the two recordings to derive an expression for

the time incoherency τ_l between two recording channels. Continuing this activity, a computer program was written where two stationary time functions can be used as an input. These two discrete functions can be generated analytically or recorded through the data acquisition system. The program calculates and plots the cross correlation (covariance) between the two functions. As a typical example, Figs. (1.4a and 1.4b) present two sine waves which were shifted by five time units with respect to each other, so that the function, X, lags the function Y by five time units. Fig. (1.5) plots the cross covariance of X and Y as a function of the time lag, τ , and shows a maximum at a time lag τ_l equal to five time units, which is consistent with the input and the previous predictions.

For the signal enhancement, the following analysis was conducted and a computer program debugged and rendered operational. If $y(t)$ is an input function to an instrument whose transfer function, $h(t)$, is known then the output function can be expressed as

$$Z(\omega) = H(\omega) \cdot Y(\omega) \quad (1.4)$$

where $Y(\omega)$ and $H(\omega)$ are the Fourier transforms of $y(t)$ and $h(t)$ respectively and ω is the frequency. The output in the time domain will be given by the inverse Fourier transform of $Z(\omega)$;

$$z(t) = F^{-1}[Z(\omega)] \quad (1.5)$$

For the practical case, we wish to reconstruct the actual signal producing a recorded signal $z(t)$ through a device where the transfer function of the instrument can be determined. The input function can be reconstructed from

$$Y(\omega) = \frac{Z(\omega)}{H(\omega)} = \frac{Z(\omega) \cdot H^*(\omega)}{H(\omega) \cdot H^*(\omega)} \quad (1.6)$$

where $H^*(\omega)$ is the complex conjugate of the Fourier transform of the transfer function. Performing the inverse Fourier transform operation on $Y(\omega)$ provides the input function to the instrument

$$y(t) = F^{-1}[Y(\omega)] \quad (1.7)$$

A typical example was solved and will be presented in the section dealing with signal analysis.

1.3.2 Design, Construction, and Checkout of Experimental Equipment

(a) Local Instruments (N. Abuaf, A. Swoboda, T. Feierabend, G. A. Zimmer)

Optical Probe. An optical probe built in the laboratory was tested in the

Fig. 1.4 Time Functions $X(T)$ and $Y(T)$, where $X(T)$ is lagging $Y(T)$ by five time units.

Fig. 1.5 Cross correlation (covariance) between $x(t)$ and $y(t)$ as a function of time lag, τ .

calibration set up described in the April-June 1977 Quarterly Report (Abuaf 1977). The amplitude of the probe output (in mv) was observed to decrease with the bubble velocity. In order to check that this observation is not due to some electronic response limitations of the amplifying circuit, some additional experiments were conducted. First a light emitting diode driven by a signal generator was placed in front of the probe tip, and the probe output was monitored as a function of input pulse width and repetition frequency. No reduction in output intensity was observable for pulses as small as 50 μ sec in width and at a repetition rate of 40 msec. The rise time of the circuit was 20 μ sec, and the amplifier was able to reproduce signal pulses, 100 μ sec in width. This time corresponds to a 0.1 mm long bubble moving at 100 cm/s, while in reality we had 1 cm bubble moving at 100 cm/sec, giving pulses 10 msec long. Thus it was concluded that this reduction in signal intensity is not due to electronic limitations.

In order to check the repeatability of the results, a second optical probe was built and checked in the same test apparatus. The probe output at various bubble velocities divided by the steady probe signal in air (Zero being the water level) provided a normalized graph which is presented in Fig. (1.6). A thin film of silicon grease applied to the probe tip to make it non wetting, still produced a similar decrease in the optical probe signal output with bubble velocity. This behavior of the probe response seemed to indicate a water film thickness left at the probe tip which increases with bubble velocity. A literature search on wire withdrawal showed that the film thickness left along a small wire increases with withdrawal velocity (White 1967). This theoretical prediction was also checked experimentally for various liquids. The dimensionless film thickness was related (Tallmadge 1968) to a Capillary Number,

$$N_{ca} = \frac{\mu u_w}{\sigma} \quad (1.8)$$

and a Goucher Number,

$$N_{Go} = \frac{R}{a} \quad (1.9)$$

where μ and σ are the viscosity and surface tension of the liquid, u_w is the withdrawal velocity, R is the wire radius, and a is the capillary length defined as $(2\sigma/\rho g)^{1/2}$. Their predictions are presented in Fig. (1.7).

For our experiments, $N_{Go} = 0.066$ and N_{ca} which is related to the bubble velocity. For $u_w = 100$ cm/s, $N_{ca} = 0.0137$. Calculation of the film thickness left on the wire, under the above mentioned conditons, gives $h \sim 0.016$ mm. These values are quite close to the critical film thickness of $h \sim 0.020$ mm, calculated in the January-March 1977 Quarterly Report (Jones 1977).

Fig. 1.6 Probe signal amplitude at a given bubble velocity I , divided by the steady signal in air, I_0 vs. bubble velocity (Results obtained by two separate probes).

Fig. 1.7 Plot of Film Thickness Capillary Number from Wire Withdrawal Predictions (Tallmadge and White, 1968).

This critical thickness was the water film that can rest on the probe tip and will cause the probe to see an all water situation. In addition to this, White and Tallmadge (1966) observed that experiments conducted with distilled water provided film thicknesses almost twice those predicted by their theory. This fact is still unexplained.

The possible explanation of the decrease of the probe signal with velocity seemed to cast some doubt on the successful operation at high velocities. This presumption will not hold true if at very high velocities the water film is stripped completely by the high shear rates. A high velocity loop is being built to check the probe response at high flow velocities. The probe developed operates successfully in the bubble velocity range considered and is able to provide local void fraction and interphase velocities after proper calibration.

The r-f Probe. In parallel with the optical probe development, a second local probe operating on a radio wave frequency (r-f probe) was also developed, built and is being tested. The probe as presented in Fig. (1.8) consists of two shielded insulated wires inside a stainless steel tube. The probe tip is formed by the two insulated wires, projecting from the end of the stainless steel tube. One of the wires is used as an emitter and fed a sine wave. The second wire is used as a receiving antenna, and its output is fed to an oscilloscope after proper amplification.

The probe output depends on whether or not the two wires at the tip are immersed in water or in air. The probe was tested in the test facility described in the April-June 1977 Quarterly Report (Abuaf 1977). A static calibration of the probe output showed that the signal amplitude varies with the input frequency both in air and in water. Fig. (1.9) depicts the variation of the output divided by the input (22.7 v) as a function of input frequency in air and in water. The probe seems to act as a band pass filter. The r-f probe output also varies with the surrounding media and the immersion depth, showing a maximum in the output before leveling off at the all water level. One more fact observed is that the output vs input frequency curve varies with the pipe size in which the probe is immersed.

The r-f probe with a 500 kHz, 22.7 v peak-to-peak sine wave input was also checked dynamically in the set up mentioned above for various bubbles moving at different velocities. The bubble velocity and size were also recorded independently by two light sources and detectors, using the following procedure. The output of the two light source-detectors were recorded on a FM channel, and the r-f probe output was recorded on a direct record channel, using a Honeywell 9600 tape recorder at a tape speed of 120 in/s. The tape was played back at 7.5 in/s and the data recorded on a disc through the Neff multiplexed ADC subsystem at a rate of 50 kHz for 25 seconds. The disc data was then analyzed and plotted on the Varian printer-plotter.

The signal analysis allowed observation of total output, while a "zoom" capability provided the possibility of concentrating on specific and interesting parts of the data by examining details of expanded time frames. Typical detailed results are presented in the next section for the particular response discussed in the next paragraph.

Fig. 1.8 Schematic representation of the r-f probe.

Fig. 1.9 Ratio of the r-f probe output to input as a function of input wave frequency for the probe tip immersed in air or in water (1/4" ID tube).

Fig. (1.10) is a zoom graph of the r-f probe response during the passage of the bubble. The response of the probe appears to be consistent under static or dynamic operation conditions. Fig. (1.11) shows a comparison between the bubble velocities as determined by the r-f probe and the output of two light sources and detectors. The agreement is satisfactory and can be determined from the passage of either interface (air-water or water-air) along the insulated wires. The r-f probe output levels for water or air do not change with the bubble velocity (Fig. 1.12) in the range considered (30-160 cm/sec). Considering the void fraction measurements, Fig. (1.13) depicts agreement (± 10 percent) between the bubble sizes as determined by the two independent methods (r-f probe and two light sources detectors). The bubble lengths recorded by the r-f probe are 10 percent higher at the low velocity range (30 cm/sec), probably due to surface tension effects.

The r-f probe seems to have a relatively simple construction and once tuned properly to the geometry, seems to provide the required information. New probes will be tested to check repeatability, and results will be extended to higher flow velocities.

(b) Signal Analysis (G. A. Zimmer, A. L. Swoboda, T. Feierabend, N. Abuaf)

The Mensor Quartz Pressure Standard (QPS) was received. A calibration procedure and program was developed for differential pressure transducers. The advantage of this system is the ability to keep track of specific devices for calibrational consistence and incipient failure, and to provide quick and accurate, tabular and graphical information on calibrational adequacy, (open hysteresis curves), deviation from linearity, dead band, and repeatability.

The Neff multiplexed ADC subsystem was received. A continuous 50 kHz data through-put to the disc was demonstrated.

In the study of the r-f probe response, outputs were recorded on FM, and direct record channels of the Honeywell 9600 tape recorder. The tape was then played back at a slower speed, and the data of the two channels was acquired and stored onto the disc through the Neff multiplexed ADC subsystem at a rate of 50 kHz for 25 seconds.

The stored data was then analyzed and plotted on the Varian printer-plotter. The signal analysis software was developed to allow observation of the total output or of the output at selected time intervals. A "zoom" capability was included to allow one to concentrate on specific parts of recorded time sequence and examine details of expanded time frames of selected data. Typical examples are presented in Figs. (1.14-1.17). Figs. (1.14-1.16) present the output of the two light detectors as observed upstream of the probe. Here the voltage output of the detectors connected in series is presented as a function of time. (In order to convert this abscissa to real time, one has to multiply it by 7.5/120 which is the ratio of the tape speeds.) The two large dips display the passage of the bubble through the two light detectors. Figs. (1.17) and (1.10) presents similar results for the r-f probe output, where Fig. (1.17) is the total output and Fig. (1.10) "zooms" on the probe response during the passage of the bubble similar to Figs. (1.15) and (1.16) for the detectors. The signal analysis software was also written to allow determination and print out the various voltage levels associated with phenomenologically interesting times such as the start of a change in average slope, local maximum or local minimum.

Fig. 1.10 Typical r-f probe output

Fig. 1.11 Comparison of bubble velocity as determined by two independent methods, r-f probe and two light source detectors.

Fig. 1.12 r-f probe output for water and air as a function of bubble velocity.

Fig. 1.13 Ratio of bubble length as determined by the r-f probe and two light sources-detectors as a function of bubble velocity.

Fig. 1.14 Output of the two light detectors (1.2) as a function of time (true time = time x 7.5/120) showing the passage of one bubble. Exp. 1.4. Bubble 1 th = 1.58 cm.

Fig. 1.15 Output of detector 1 as a function of time (expanded time scale). Zoom onto the first signal.

Fig. 1.16 Output of detector 2 as a function of time (expanded time scale). Zoom onto the second signal.

Fig. 1.17 Output of the r-f probe as a function of time showing the passage of the bubble.

A program to compute the discrete Fast Fourier transform of a time series was debugged and rendered operational. The same program also allows calculation of the inverse Fourier transform. Using the latter program and complex algebra incorporated in the signal analysis system, a program was used to solve a typical example for the signal enhancement procedure described in Section 1.3.1.

A function of time $y(t)$ consisting of two pulses was chosen as the input function in Fig. (1.18). The transfer function of the instrument was chosen to be equal to $h(t) = e^{-t}$, which corresponds to a first-order instrument with unity gain and a time constant $\tau = 1$ sec. The Fourier transform of both functions was calculated, and their multiplication provided us with the real and imaginary parts of the output function $z(t)$ in the frequency domain Fig. (1.19). The inverse Fourier transform of $Z(\omega)$ is shown in Fig. (1.20) and corresponds to the output function, $z(t)$. To obtain the input function from the output and the transfer function of the instrument, first the Fourier transforms of $z(t)$ and $h(t)$ were calculated respectively. The expression $Y(\omega) = Z(\omega)/H(\omega)$ provided us with a means of calculating the real and imaginary parts of $Y(\omega)$ in the frequency domain. An inverse Fourier transform of $Y(\omega)$ provided us with the input function $y(t)$ which is the original reconstruction of the input function of two pulses (Fig. 1.21). This program will allow us to reconstruct input function to instruments once the output and its transfer functions are known.

Fig. 1.18 Input Function $Y(T)$, $T = \text{time}$.

a. real part

b. imaginary part

Fig. 1.19 Fourier transform of the output function

Fig. 1.20 .Output Function, $Z(T)$.

Fig. 1.21. Reconstructed input function, $Y(T)$.

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2. THOR CODE DEVELOPMENT

(P. G. Kroeger, G. S. Srikantiah and W. Wulff)

2.1 General Program Objectives and Approach

The THOR Code Development Program is designed to produce an advanced computer code for the prediction of accident-induced thermo-hydraulic transients in water-cooled nuclear reactors.

The primary objectives are:

1. The model should include the effects of thermal non-equilibrium, as well as non-equal velocities between the vapor and liquid phases.
2. The reactor components should be modeled to include the specific characteristics of each component.
3. The axial variation of the transient fission power must be modeled.
4. The program should include the capability for an initial steady-state computation.
5. The code structure should be modular, permitting its application to different system configurations, as well as providing for ready improvement of individual component and process subroutines.
6. The code should be executing rapidly, for instance, for frequent application in parametric studies.

To achieve the above objectives a lumped parameter approach has been formulated for the various component models and a semi-implicit solution scheme is being followed.

2.2 Status and Current Goals

A considerable portion of the work directed towards the above objectives was done and has been reported in previous quarterly reports. This includes in particular the formulation of lumped parameter models of components with nonhomogeneous non-equilibrium flow; a system steady-state formulation and demonstration, as well as process models for drift flux relationships and choking conditions. A model of the 1-dimensional neutron kinetics including the axial variation of fission power was completed during the current quarter.

To demonstrate the feasibility of using the previously selected explicit solution scheme for the specific set of ordinary differential equations and algebraic equations resulting from the lumping method selected for THOR, a single-loop blowdown case was formulated and programmed. This explicit solution scheme was found to be unstable. Therefore, the decision was made to change to a semi-implicit numerical solution scheme.

2.3 Current Achievements

2.3.1 Single Loop PWR Blowdown Program (D. I. Garber, G. S. Srikantiah, R. Krasny and A. Dubow)

Final stages of debugging and modifications of the Single Loop PWR program were completed. The program in its final form has the following features:

A container array where all addresses of all the variables are available; a FORTRAN written preprocessor which controls the addressing for block decomposition of the system of equations and interfacing with the nonlinear equation solver (ZSYSTEM) for solution; separate sections of the code to handle the initialization, steady state computation and initiation of the transient, a routine called DUMP EQUATIONS which produces an output of all equations as programmed as well as the computed numbers printed below each term, a transient routine which interfaces with the ODE solver (both first order and higher order ODE solvers have been used) and finally an output routine which produces line printer plots of all nodal variables as well as standard printouts of all nodal variables.

The solution procedure is as follows:

Starting from the vector of volume averaged variables, $\langle Y \rangle$, obtain a solution of the (70 x 70) non-linear algebraic system consisting of 15 momentum balances, 13 mass balances, 36 nodal enthalpy and vapor mass equations (flow direction dependent) and 6 coupling or constraint equations which will produce current values of all the nodal variables and of $\langle G \rangle$ in all the components except in the core, next the values of the remaining $\langle Y \rangle$'s are obtained from the ODE's in which these $\langle Y \rangle$'s are single cited thus producing the complete $\langle Y \rangle$ vector. This process involves calls to the various component subroutines. The ODE solver then produces a new set of $\langle Y \rangle$ corresponding to the next time step.

This program was set up to simulate a series 800 semiscale test. This test is a single loop blowdown experiment. The loop comprises a hot channel connected to plena at either end. The upper plenum is connected to a heat exchanger by pipes. The loop is completed by cold leg piping connecting the heat exchanger to the lower plenum via a pump. This system is ideally suited for simulation by the hardwired system program described above.

Several test runs were conducted. First a steady-state solution was obtained. Second, the transient was turned on without any system perturbation. The object of this calculation was to see if the system steady-state could be maintained. Next, the system transient was computed for a break initiated at the lower plenum. The results of all these computations are briefly shown in Figures 2.1 and 2.2.

Numerical instabilities were observed in these computations. Firstly, it was not possible to maintain a steady-state in the system when no external transient was imposed. Secondly, when a break was initiated as indicated above, instabilities in the shape of "rocking" around average values developed and grew in time. It was noticed that this type of instability arose as a consequence

Geometry

BLOWDOWN

Spatial and temporal distribution of flow, $\text{Kg/m}^2 \text{ sec}$.

Figure 2.1 Single loop blowdown

BLOWDOWN

BLOWDOWN

Figure 2.2 Single loop blowdown. Spatial and temporal distribution of pressure and enthalpy.

of the "explicit" computational scheme applied to the system of algebraic and ordinary differential equations. According to this scheme, the end point variables must be computed after specifying the volume averaged value in any component. Since an end point variable is common to two adjacent components, even slight differences in the average values gave rise to this "rocking" behavior in order to satisfy linear profile relationships.

Furthermore, a preliminary computation of the eigenvalues of this system were completed by the same procedure, i.e., by first stipulating the average values of the variables and computing the $\langle Y \rangle$'s by perturbing one average value at a time. The real parts of many of the eigenvalues turned out to be positive. This shows that the system is unconditionally unstable.

2.4 Component Modeling for Two-Loop PWR

2.4.1 Reactor Core Modeling (C.J. Ruger, P.G. Kroeger, J.M. Kaufman)

The two region non-homogeneous thermal-equilibrium model with a moving flow regime interface represented by a kinematic shock has been solved and results were obtained. The important assumptions in the model were the use of average pressure to evaluate flow properties, uniform heating, pressure derivatives small compared to heating terms and linear enthalpy profiles.

The lumped parameter formulation for each zone consists of first combining the mixture mass and mixture thermal energy balance and integrating the result to obtain an algebraic expression (GAE) for the exit mass flux in terms of the entrance value. A further spatial integration yields a relation (IGAE) between the average zone mass flux and the entrance value. In addition the mixture thermal energy balance is volume averaged over each zone (ME) and the mixture momentum balance is volume averaged over the entire channel (MOM).

The interface between the two regions is defined by specification of the void fraction on the inflow side, which directly yields the enthalpy h_{2-} , see Figure 2.3. Since all properties are evaluated at an average pressure no internal pressures are needed and only two jump conditions are required. The first is the mixture mass jump (SH1). The second should naturally be the mixture energy jump, however, since it is simpler the vapor mass shock jump was used instead (SH2). For the case of thermal equilibrium these should be equivalent and have been numerically shown to yield identical results.

Figure 2.3 shows the solution procedure schematically. Equation GGG represents the summation of the individual average mass fluxes ($\langle G \rangle_T = f(\langle G \rangle_1, \langle G \rangle_2)$). The p profile is assumed constant at the average pressure and the enthalpy profiles are assumed linear. Upward flow is considered and the corresponding boundary conditions are the entrance pressure and enthalpy and the exit pressure.

Three transient calculations were made; one in which the exit pressure alone decreases, another with both pressures dropping at the same rate and one with the pressure at the exit dropping faster than at the entrance.

Figures 2.4 through 2.6 show the history of the pressure, overall average mass flux and interface location for case 1 for the transient starting at 10 seconds. The pressure decrease at the top causes the flow to accelerate. Since

given

 p_3

$$h_3 = \text{H PROF2}; G_3 = \text{GAE2}$$

$$\langle h \rangle_2 = \text{ME2}$$

$$\langle G \rangle_2 = \text{IGAE2}$$

$$h_{2+} = \text{SH2} ; G_{2+} = \text{SH1}$$

$$h_{2-} = \text{ALPHA}; G_{2-} = \text{GAE1}$$

$$U = \text{ME1}$$

$$\bar{p} = \text{P PROF}$$

$$\langle G \rangle_T = \text{MOM}$$

$$\langle h \rangle_1 = \text{H PROF1}$$

$$\langle G \rangle_1 = \text{GGG}$$

$$G_1 = \text{IGAE1}$$

given:

 h_1, p_1

FLOW DIRECTION

Figure 2.3 Schematic of solution

Figure 2.4 Case 1 - Pressure history

Figure 2.5 Case 1 - Overall average mass flux

Figure 2.6 Case 1 - Interface location

Figure 2.7 Case 1 - Interface void fractions

the entrance enthalpy and the heat input are fixed the increase in mass flow results in a greater length being required in region 1 to reach the enthalpy corresponding to the flow regime transition. Therefore, the interface, which is defined by $\alpha = 0.2$, moves up. Figure 2.7 shows the discontinuity in void fraction existing across the interface.

In the second case where both pressures drop at the same rate, Figure 2.8, the mass flux remains essentially constant. However, due to the overall pressure decrease the interface enthalpy (at fixed α) will decrease as shown in Figure 2.9. For fixed entrance enthalpy and fixed heating the interface must move toward the entrance as shown in Figure 2.10.

The third case in which the exit pressure is dropped slightly faster than the entrance, Figure 2.11, represents a superimposition of the first two cases. The mass flux increases due to the more rapid pressure drop at the top, Figure 2.12. However, the interface enthalpy drops due to overall pressure decrease. This effect will eventually take over resulting in the interface motion as shown in Figure 2.13. Figure 2.14 shows that while the entrance drift velocity remains essentially constant due to its weak pressure dependence the entrance mixture velocity increases since the mass flux increases and the density is a weak function of pressure.

2.4.2 Pressurizer (P. Saha and A. Dubow)

A new simplified model for the pressurizer has been formulated during the reporting quarter. Illness of a key person responsible for the earlier model initiated the present effort.

The present model is comprised of the following simplifications:

1. Based on the semi-scale tests, the convective term of the rate of pressure change, i.e., $u \frac{\partial p}{\partial z}$, is neglected compared to the local rate of pressure change, i.e., $\frac{\partial p}{\partial t}$. Therefore, the rate of vapor generation in the low-void two-phase region is taken as (assuming thermodynamic equilibrium)

$$\Gamma_g = \frac{1}{h_{fg}} \left[1 - \rho_m \left(\frac{dh_f}{dp} + c \frac{dh_{fg}}{dp} \right) \right] \langle p \rangle$$

where the symbols have their usual meanings.

2. In the low-void two-phase region, linear axial profiles for the vapor mass concentration, c , and the mixture mass-flux, G , are used as first approximations.

Besides the above simplifications, the present model is essentially the same as the earlier model in relation to the high-void, two-phase region and the single-phase liquid region.

A stand-alone computer program has been written using a semi-implicit numerical scheme, and the program is being debugged at this time.

Figure 2.8 Case 2 - Pressure history

Figure 2.9 Case 2 - Mixture enthalpy above interface

Figure 2.10 Case 2 - Interface location

Figure 2.11 Case 3 - Pressure history

Figure 2.12 Case 3 - Overall average mass flux

Figure 2.13 Case 3 - Interface location

Figure 2.14 Case 3 - Entrance drift flux and mixture velocities

2.4.3 Steam Generator (J. H. Jo, S. Stein)

A model of the thermohydraulics of one side of a steam generator for non-homogeneous, thermal equilibrium flow, permitting any number of flow regimes has been formulated to serve as a first step towards the final two-side, thermal non-equilibrium model. A stand-alone code in semi-implicit form is being programmed. The model accounts for pressure change with respect to time ($\partial p / \partial t$). Originally an effort was made to account also for the spatial pressure variation in the energy equation ($\partial p / \partial z$); however, to avoid inconsistencies this requires an exact integration of a term involving the sonic velocity, which was not possible. A simple numerical check showed that the terms involving $\partial p / \partial z$ are negligibly small when compared to the heat flux terms. Therefore, the $\partial p / \partial z$ terms in the energy equation were dropped.

The model will be able to track the interfaces between flow-regimes using the kinematic shock equations also used in the core model.

A separate program to track appearances and disappearances of flow regimes has been written and debugged.

Work is presently in progress to express this single side model as a primary side and a secondary side model and to couple them together. Further work to include non-equilibrium effects and flow reversal is planned for the next quarter.

A simplified back-up program using a single-zone, homogeneous, thermal-equilibrium model for each side of the steam generator has also been prepared. This simpler model uses a single zone on each side, without interface tracking, but allows multi-phases (liquid, two-phase, vapor) in the same component and uses different density profiles in each phase. Debugging of this model has just been completed.

2.4.4 Pipe Branches ("Wyes" and "Tees") (J. M. Kaufman)

After a search of the available literature it was decided that the hydraulic head loss due to branching in the pipes will be evaluated using Ginzburg's (1973) formulations. There are two formulations, one for converging flow, where two pipes discharge into one, and one for diverging flow, where one pipe discharges into two.

The head losses primarily depend on the angle of deflection of the streams and, therefore, the above two formulations for converging or diverging wyes and tees cover all flow configurations.

A subroutine to calculate the loss coefficients has been written including a routine to calculate the branch angles from the pipe coordinates which can be used, if the angles are not supplied. The two routines have been debugged. The routines will be tested for all foreseeable flow situations. If unreasonable results arise from using these coefficients available empirical parameters can be introduced.

2.5 System Modeling

2.5.1 Semi-Implicit Solution Scheme Applied to a Simple Pipe-Pump Loop (G. S. Srikantiah, S. V. Lekach)

Since instabilities arose due to the numerical scheme adopted for the single loop PWR, alternative methods of integration were pursued using a single loop made up of pipes and pumps as a test case (Figure 2.15).

The problem considered is two-phase flow of water in this single loop during start-up of the pump, attainment of steady-state and coast down after motor power is cut off. A semi-implicit scheme of integration was developed for the system of algebraic equations and ordinary differential equations arising out of volume integration of the drift flux model partial differential equations with linear profiles in the pipes. The results of the computation are shown in Figure 2.15 and Table 2.1. The "explicit" method of integration was also used for the identical set of equations, assumptions and profiles for comparison. While the semi-implicit scheme produced stable and accurate (when compared with discrete calculations) solutions the "explicit" scheme produced a steady-state only after a relatively long run time and with some residual "rocking".

2.5.2 Development of a General Code Structure Using the Semi-Implicit Scheme (S. V. Lekach)

A generalized code structure has been developed which can handle systems of pipes, pumps, tees and area changes in the form of single or multiple loops. Once the system topology is specified, the code is capable of treating the system made up of lumped or distributed parameter components or a combination of both. This code has been applied to a loop made up of pipes and pump described above. The pipes were described by the lumped parameter model (Rohatgi, et.al., 1977). Two different models for the pump were used, viz., a simplified model which impressed a head between the inlet and the outlet of the pump and the current best estimate THOR model which utilizes the homologous curves. Computations were carried out as described in Section 2.5.1 by applying the semi-implicit integration scheme. The results are as shown in Figure 2.15. The running time for the lumped model was 3-5 times faster compared to a discrete calculation.

Currently this code is being extended to incorporate realistic lumped parameter models of the components as well as nonlinear boundary conditions.

Fig. 2.15 Simple pipe pump loop: pump start-up and coast down

TABLE 2.1 COMPARISON OF NUMERICAL METHODS

	<u>STABILITY</u>	<u>COMPUTING SPEED</u>
DISCRETE (6 NODE)	REF.	1.0
LUMP - (SEMI-IMPLICIT)	EXCELLENT	4 - 5
LUMP - EXPLICIT	POOR	---

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3. APPRAISAL OF ANALYSIS DEVELOPMENT IN FOREIGN COUNTRIES

(Liliane Schor)

3.1 NICKY - A multi-region equilibrium blowdown program (G. Forti, Euratom, Italy)

The code (Forti, 1974) calculates the mass and enthalpies inventories, pressures and mass flows in the primary circuit during blowdown. Input for the code are: the break flow and enthalpy, the heat input and output (heat exchangers) in each region of the system and the flows and enthalpies added through feedwater and/or emergency refill systems.

The leakage flow is calculated using Moody's correlation for two-phase choked flow as a known function of the stagnation pressure behind the break, the sink pressure, the stagnation enthalpy and the L/D ratio. The pressure is chosen as the independent variable in the calculation, and the time increments are derived as dependent variable.

The primary circuit of a reactor or experimental apparatus is represented by up to 30 nodes connected by a maximum of 50 junctions (up to 10 independent loops with up to 4 pumps acting on them). For every volume the code solves, the energy and mass continuity equations plus the state equation for the coolant at thermodynamic equilibrium. The momentum equations are ignored for an open-tree circuit and only one recirculation equation for every closed loop is considered, imposing the total recirculation rate according to the specification of the pumps acting on each loop.

Each node can be a homogeneous fluid volume or a phase separation volume. The phase separation has two options: complete separation of phases or fluid quality in the mixture region to be specified in input. For every junction leading to a phase separation volume the input specifies the function of volume above the connection.

The code can calculate only BWR problems due to the fact that in a PWR plant, the high resistance to flow in the pressurizer's surge line will cause a high pressure difference with respect to the rest of the system. Since the code considers no pressure differences in the primary circuit, to treat PWR problems a separate pressurizer model is needed.

No comparisons with experiments are yet available for this code.

3.2 NORCOOL - A model for analysis of a BWR under LOCA conditions (J.G.M. Andersen et al., RISO Research Establishment, Denmark)

NORCOOL is a LOCA code, intended to formulate the behavior of a BWR after the termination of the blowdown and to evaluate the core heat up transients for a fuel element and the performance of the emergency core cooling system.

NORCOOL consists of two basic models, a fuel rod model and a model for the two-phase flow (Andersen, J.G.M., 1976). The fuel rod model is a one dimensional heat conduction model except at the quenching front, where a quench

front velocity correlation is used to represent the multi-dimensional effects which are present. The model can simulate groups of fuel rods or single rods and all or part of the channel box.

The two-phase flow model is a one dimensional simulation for steam, liquid droplets and surface films. The two-phase flow model is used to simulate the liquid film on fuel rods and the coolant flow in the fuel element, bypass channel and the corresponding part of the primary system, which is scaled down to one fuel assembly. The coolant regions are divided into steam regions and two-phase regions. Five two-phase regions are modeled: single phase liquid, bubbly flow, inverse annular flow, film flow and dispersed flow.

Since the velocities are small in the two-phase regions, the flow is assumed to be quasi-steady state and a drift flux model is applied to account for the bubble rise. In the steam region, three sets of balance equations are written (mass, momentum, energy) for liquid, vapor and droplets. For the steam flow a quasi-steady approach is used for the momentum equation. If a water lock does not exist in the lower plenum, the momentum integral method is used.

The coupling between the fuel rod model and two-phase flow model is done through a number of physical models and correlations of heat transfer, which includes conduction, convection and radiation. The differential equations above and below the two-phase level are solved using a partially implicit donor cell technique. The heat-transfer is solved explicitly.

The NORCOOL code is finished, it is implemented in the BNL computer but it is not yet able to handle real plant transients.

No comparison with experiments are available.

3.3 BRUCH-S - A code to investigate blowdown of BWR (H. Karwat, Laboratories für Reaktorregelung and Anlagensicherung, Munchen, Germany)

BRUCH-S is a multi-node point model which describes the behaviour of a BWR during a rupture of a primary steam line or a rupture of a primary recirculation line.

In the formulation of the code a separation of the primary system into nine different pressure models was assumed as shown in Figure 3.1.

For every node the mathematical model consists of the mass, volume, energy and momentum balance. The water state equation is introduced in a special differential form which is needed to avoid numerical difficulties. For every volume, four fluid properties are calculated: mass, energy, pressure and mass flux, which are considered to be uniform within a control volume.

The ordinary differential equations are solved by the DIFFSYS sub-program (Burlich, 1966). Special considerations are taken for the core fuel region (for the boiling length) and for the steam dome and separator. Some additional basic assumptions are made within BRUCH-S code which are necessary to describe the system:

Figure 3.1 Pressure node distribution of a boiling water reactor

- the heat addition rates to each pressure node are assumed to be known input functions.
- Moody's model is used to calculate the flow rate through the break.
- For some calculations, such as a break of a steam line, the efficiency of the steam separators must be given as an input.

Examples of calculations of a steam line break and a recirculation line break are presented (Karwat, 1969). The results published in the BRUCH-S report show a main sustained (Figure 5) flow oscillatory behavior with a frequency of two cycles per second, and smaller oscillations with a period of the order of one tenth of a second. It is evident that the integration time step for BRUCH-S must be smaller than the shorter oscillation period if the computed solution is to have any meaning. No comparisons with experiments are available.

3.4 BRUCH-D - A digital computer program to analyze loss of coolant accidents in PWR (K. Wolfert, Laboratorium fur Reaktorregelung und Anlagensicherung, Technische Universitat, Munchen, West Germany)

The computer program BRUCH-D simulates the thermodynamic and fluid dynamic response of the PWR primary coolant system for a LOCA (Karwat, 1970). The primary coolant system is represented by a fixed number of nodes (23). The physical model is based on the solution of the conservation equations for mass, energy, a special form of the state equation for water and steam, and the momentum equation.

Within the nodes, which are of constant volume, thermodynamic equilibrium is assumed. Four parameters are calculated within every volume: pressure, mass, enthalpy and mass flow rate (Karwat, 1975). The difference between BRUCH-S and BRUCH-D is the inclusion in the latter, of some additional features:

- point neutron kinetics for the core
- a core heat transfer calculation using a multi-node pin conduction model
- a pump model
- simulation of steam generators.

For critical flow, the code BRUCH-D includes three correlations: Bernoulli equation for subcooled conditions, homogeneous equilibrium model and Moody correlations.

The first order, mostly nonlinear differential equations are integrated using the subroutine IMEX. IMEX combines the implicit trapezoidal rule with the explicit midpoint rule with starting and stabilizing steps. It uses an extrapolation algorithm (Burlich-Stoer), a test for convergence and an automatic step size control (Hofer, W., 1973).

The results of the code were compared with a quarter scale LOFT blowdown experiment. The code was also tested against RELAP-3 for a 3540 MW-PWR. (A cold leg and a hot leg double ended rupture were simulated).

3.5 RISQUE - A one dimensional two-fluid code, by M. D. Andersen, et. al., - RISO Research Establishment, Denmark.

The RISQUE code is a two-fluid, one dimensional model intended to be used in the NORCOOL code (Andersen, M.D., 1976).

The two-fluid model consists of conservation equations (mass, momentum, energy) for each phase. The equations were obtained by averaging the three dimensional formulation of Ishii over the flow area. The pressures of the two phases are considered to be equal, and constitutive equations were derived for the interfacial transfers of mass, momentum and energy. The code can calculate closed loops and pipes (with critical flow).

To avoid the presence of complex characteristics the authors modified the momentum equation by the introduction of a momentum transfer (Andersen, P.S., 1976) based on virtual mass considerations. With an arbitrary choice of coefficients in this transfer term, the characteristics are real for void fraction below an upper limit.

Turner (Turner, 1977) considers that the choice of coefficients much larger than 1 (up to 10^4 are analyzed) has no physical basis. Also, the inclusion twice of the virtual mass effect (in the time rate of change of total momentum and again in the momentum exchange term) is not satisfactory. The partial differential equations are solved by approximating them by finite difference equations using an extended form of the differencing scheme suggested by Turner (Turner, 1972).

No comparison with experimental data are available.

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