

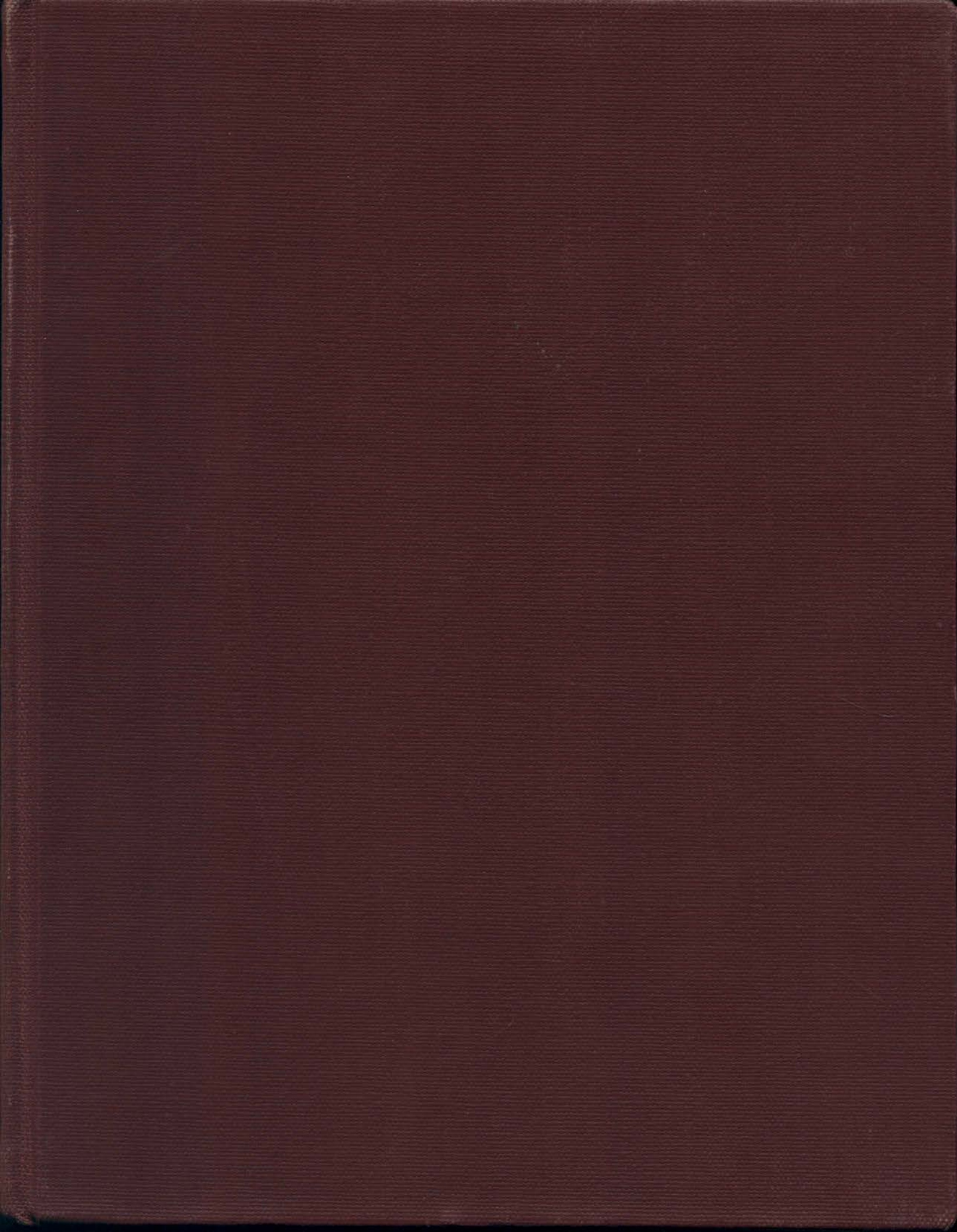
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The Effect of Volatile Fission Products on Fuel Motion in Nuclear Fuel Elements

Paul Sasa

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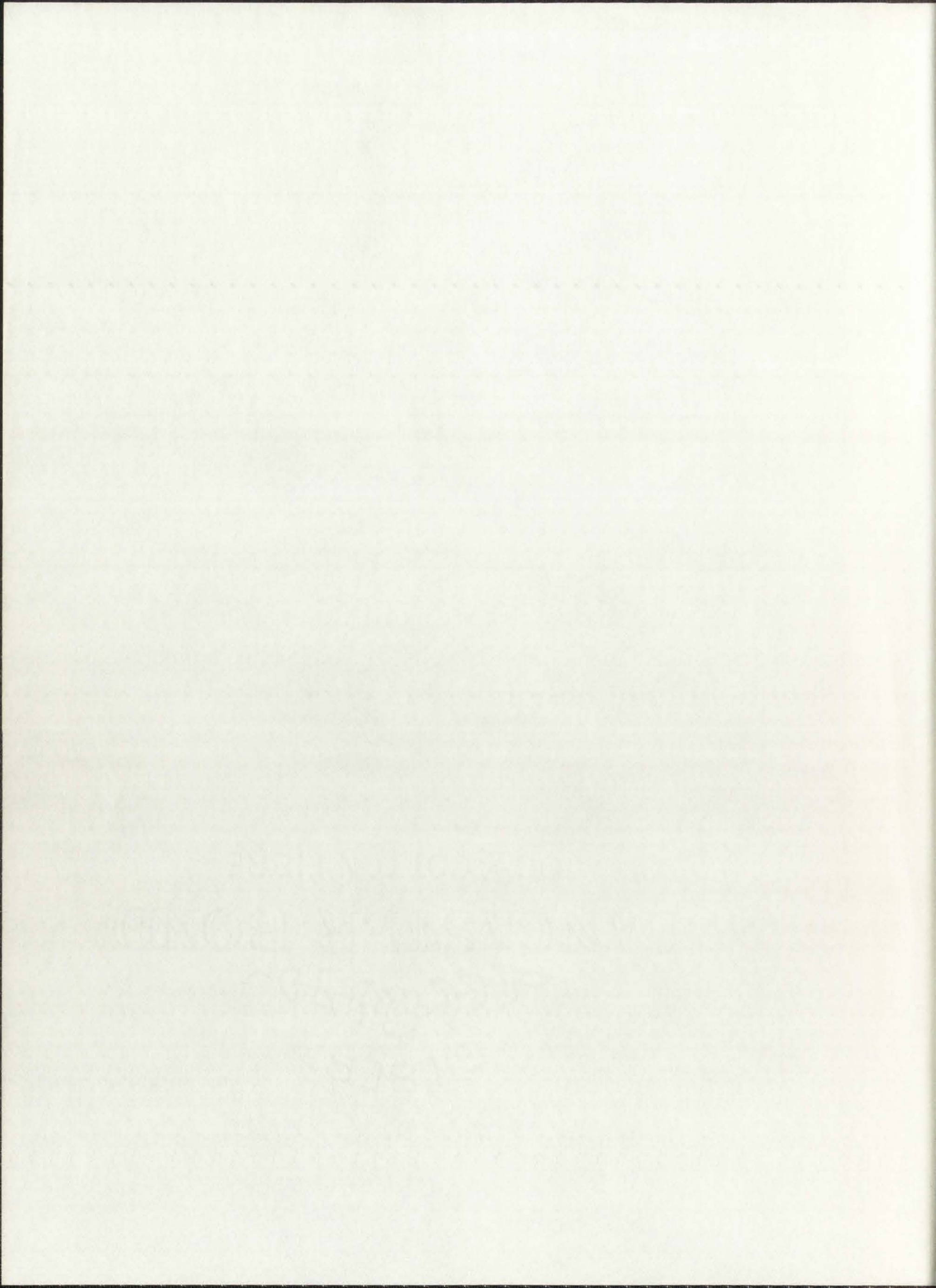
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Paul Sasa

Candidate

Chemical and Nuclear Engineering

Department

This dissertation is approved, and it is acceptable in quality and form for publication on microfilm:

Approved by the Dissertation Committee:

August Crenney

, Chairperson

Jay E. Baudron

R. S. Nuttall

Michael M. Lerner

Ronald Krief

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Dean, Graduate School

December 6, 1978

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THE EFFECT OF VOLATILE FISSION PRODUCTS ON
FUEL MOTION IN NUCLEAR FUEL ELEMENTS

by

Paul Sasa

B.S., University of Colorado, 1968

M.S., University of New Mexico, 1974

DISSERTATION

Submitted in Partial Fulfillment of the
Requirements for the Degree of
Doctor of Philosophy in Nuclear Engineering
in the Graduate School of
The University of New Mexico
Albuquerque, New Mexico
December 1978

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Finally, a special thanks goes to his wife, Janet, for just believing in him.



THE EFFECT OF VOLATILE FISSION PRODUCTS ON
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ABSTRACT OF DISSERTATION

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THE EFFECT OF VOLATILE FISSION PRODUCTS ON FUEL
MOTION IN NUCLEAR FUEL ELEMENTS

Paul Sasa, Ph.D.

Department of Chemical and Nuclear Engineering

The University of New Mexico, 1978

Stringent licensing procedures for commercial nuclear reactor operation require an in-depth analysis of the phenomena associated with postulated reactor core overheating accidents. One aspect of nuclear reactor safety assessment is a prediction of fuel behavior associated with such postulated overheating events, which includes an assessment of the role of fission product inventory contained within irradiated fuel elements on fuel relocation potential. In general the gaseous fission product, such as Xenon and Krypton, have been considered the most likely candidates for fuel relocation due to gas dissolution from the fuel matrix and bubble expansion during fuel overheating; thus, such gaseous fission products have received considerable attention in fuel modeling efforts associated with accident code development work. However, the fissioning of UO_2 fuel in both a fast and slow neutron spectrum also results in the generation of a significant quantity of metallic fission products such as Barium, Iron, Molybdenum, and other metallic species. Metallurgical analysis of irradiated fuel indicates

Department of Internal Medicine, University of Chicago
The Journal of the American Medical Association
Chicago, Ill., June 1, 1953

Dear Sir:

I have your letter of May 27, 1953, regarding the
report of the Committee on the Medical Profession
and the American Medical Association, and in reply
to inform you that the American Medical Association
has no objection to the publication of the report
in the Journal of the American Medical Association
and that the American Medical Association has no
objection to the publication of the report in the
Journal of the American Medical Association.

Sincerely,
W. H. C. [Signature]

that such metals aggregate into inclusions found throughout the fuel matrix. During normal reactor operation such metallic inclusions are in a solid state, but at the elevated temperatures expected for overheating accident transients, such inclusions may tend to volatilize, contributing to fuel motion. This work involves an assessment of the potential effect of such metallic fission product inclusions to fuel motion for accident analysis and is the first known attempt at such an assessment.

The first portion of this work involves a characterization of the metallic inclusions with respect to species composition, and inclusion size and distribution within fuel pellets under various irradiation conditions. Such characterization was accomplished through an extensive literature review of metallurgical assay of irradiated fuel rods. A typical inclusion composition for $(U_{.8} Pu_{.2}) O_2$ fuel irradiated in a fast neutron spectrum consists of Molybdenum (14.5 wt%), Ruthenium (43.3 wt%), Technetium (20 wt%), Rhodium (17.6 wt%), Palladium (2.1 wt%) and Iron (2.45 wt%); while for UO_2 irradiated in a thermal neutron spectrum inclusions consist of Molybdenum (41 wt%), Ruthenium (18 wt%), Technetium (18 wt%), Rhodium (5 wt%) and in addition Tellurium (2.1 wt%), Strontium (.9 wt%) and Barium (6.75 wt%).

An equation-of-state, based upon inclusion composition, was then developed from standard thermodynamic principles, considering the inclusions to be either homogeneous solutions of the different metals or complete immiscibility of the various metal constituents. A fuel motion model was then developed and the contributions due to metallic

The following experiments have been performed to study the effect of the temperature on the rate of the reaction between hydrogen peroxide and iodide ions. The reaction studied is:

$$2\text{H}_2\text{O}_2 + 2\text{I}^- + 2\text{H}^+ \rightarrow 2\text{H}_2\text{O} + \text{I}_2$$

The rate of the reaction was measured by the appearance of the color of iodine. The rate of the reaction was found to be proportional to the concentration of hydrogen peroxide and to the concentration of iodide ions. The rate was found to be independent of the concentration of hydrogen ions. The activation energy of the reaction was found to be 52 kJ mol⁻¹. The following table gives the experimental data for the reaction at different temperatures.

Temperature (°C)	Rate constant (s ⁻¹)
20	1.5 × 10 ⁻³
25	3.0 × 10 ⁻³
30	6.0 × 10 ⁻³
35	1.2 × 10 ⁻²
40	2.4 × 10 ⁻²

The following table gives the experimental data for the reaction at different concentrations of the reactants.

[H ₂ O ₂]	[I ⁻]	[H ⁺]	Rate (mol l ⁻¹ s ⁻¹)
0.1	0.1	1.0	1.5 × 10 ⁻³
0.2	0.1	1.0	3.0 × 10 ⁻³
0.1	0.2	1.0	3.0 × 10 ⁻³
0.1	0.1	2.0	1.5 × 10 ⁻³

The following table gives the experimental data for the reaction at different concentrations of the products.

[I ₂]	[H ₂ O]	Rate (mol l ⁻¹ s ⁻¹)
0.0	0.0	1.5 × 10 ⁻³
0.1	0.1	1.5 × 10 ⁻³
0.2	0.2	1.5 × 10 ⁻³

The following table gives the experimental data for the reaction at different concentrations of the catalyst.

[Catalyst]	Rate (mol l ⁻¹ s ⁻¹)
0.0	1.5 × 10 ⁻³
0.1	3.0 × 10 ⁻³
0.2	6.0 × 10 ⁻³

The following table gives the experimental data for the reaction at different concentrations of the inhibitor.

[Inhibitor]	Rate (mol l ⁻¹ s ⁻¹)
0.0	1.5 × 10 ⁻³
0.1	1.2 × 10 ⁻³
0.2	0.9 × 10 ⁻³

inclusion volatilization and fission gas bubble expansion were assessed. Predicted results were compared with previously obtained fuel motion data of irradiated fuel rods tested, in-pile, to elevated temperatures. Metallic inclusion volatilization potential was then assessed for both light water and fast reactor fuels, considering both UO_2 and $(Pu, U)O_2$.

The contribution to fuel expansion due to volatilization of the metallic fission product inclusions were calculated for $15/s$ transient overpower (TOP) accident, assuming 3 atom percent burnup. It was initially assumed that each individual species within the inclusion volatilized when its vapor pressure exceeded the internal fuel rod pressure, which for typical liquid metal fast breeder reactor (LMFBR) would be about 20 atm while for light water reactor (LWR) would be either 70 atm for boiling water reactor (BWR) or 160 atm for pressurized water reactor (PWR). For LMFBR conditions and $(Pu, U)O_2$ fuel, a maximum nodal (local) volume expansion (i.e. the percent volume increase from the original volume of 20-30% and a total fuel rod volume expansion of 1% was calculated prior to incipient fuel vaporization.

Thermodynamic consideration indicate that the metallic inclusion constituents may be mutually soluble; thus the effect of single-phase volatilization was also assessed. Making use of Raoult's law of partial pressure, the inclusion vapor pressure for a typical LMFBR type inclusions is found to be less than that required to overcome fuel rod internal constraints, such that fuel vaporization is predicted to occur before significant inclusion volatilization.

For the typical inclusion composition found for LWR fuel, the miscible inclusion vapor pressure was assessed to be much greater than that for LMFBR fuel due to the presence of small quantities of Tellurium, Strontium, and Barium not found in fast reactor fuel metallic inclusions. These three elements are more volatile than Palladium, Iron, and Antimony found in fast reactor fuel inclusions and contribute a minimum of 75% of the nodal volume expansion. The high volatility of the constituents for in LWR-type inclusions also causes expansion to occur much earlier in the transient. It thus appears that thermal reactor fuel may swell due to volatilization of metallic inclusions during an overpower transient, if either segregated or homogeneous inclusions are assumed.

Fission gas analysis and experimental results indicate that the expected fission gas driven fuel volume expansion is on the order of 0-40%, depending on steady state and transient irradiation conditions. In addition, fuel volume expansion due to the solid-liquid change of phase is estimated to be 10%.

In summation, it was found that LWR metallic inclusion volatilization can provide a substantial fuel motion driving potential during transient overheating. However, such is not the case for LMFBR fuels, where the metallic inclusions are not expected to play a role in fuel expansion during accident transients.

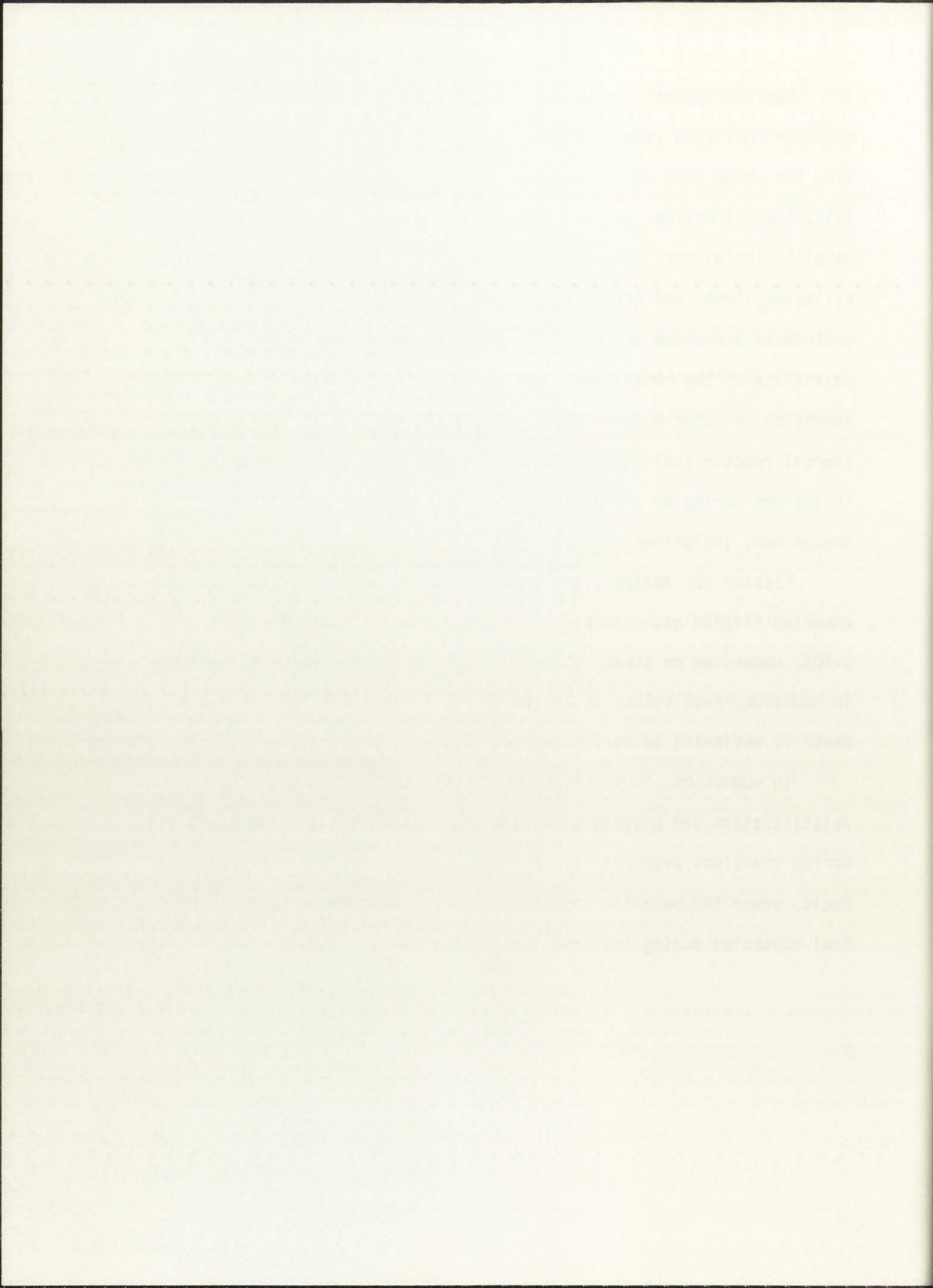


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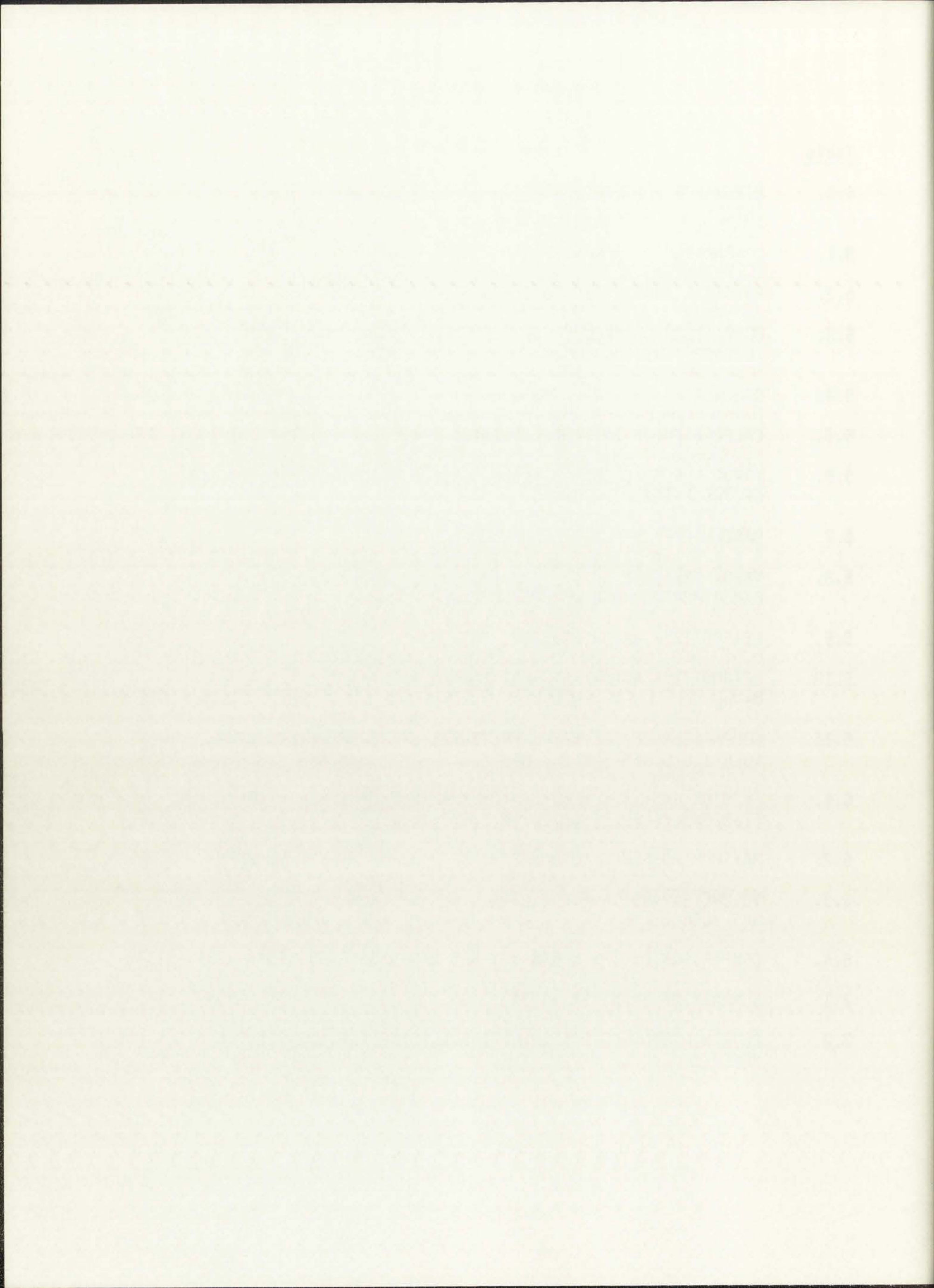
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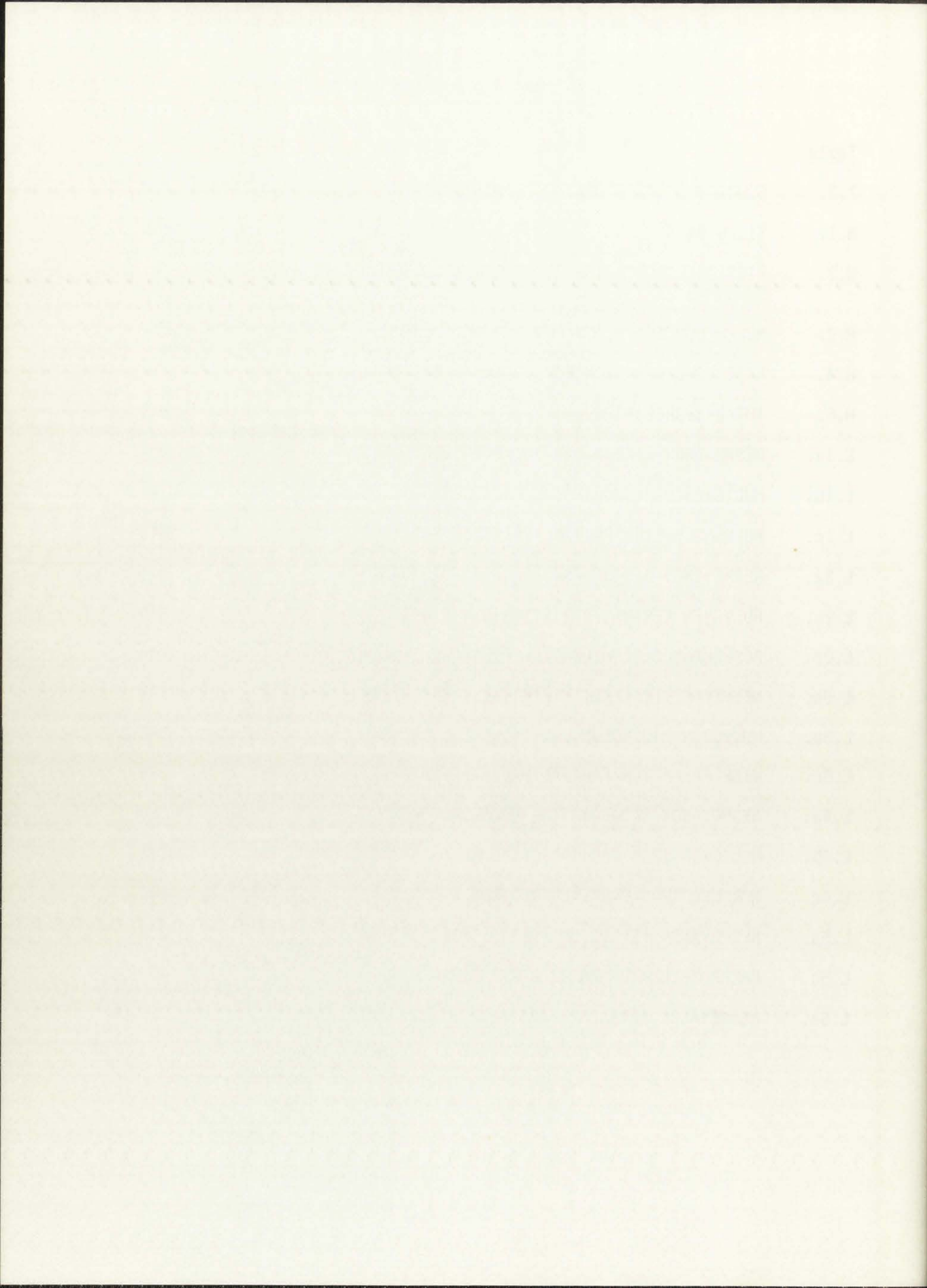
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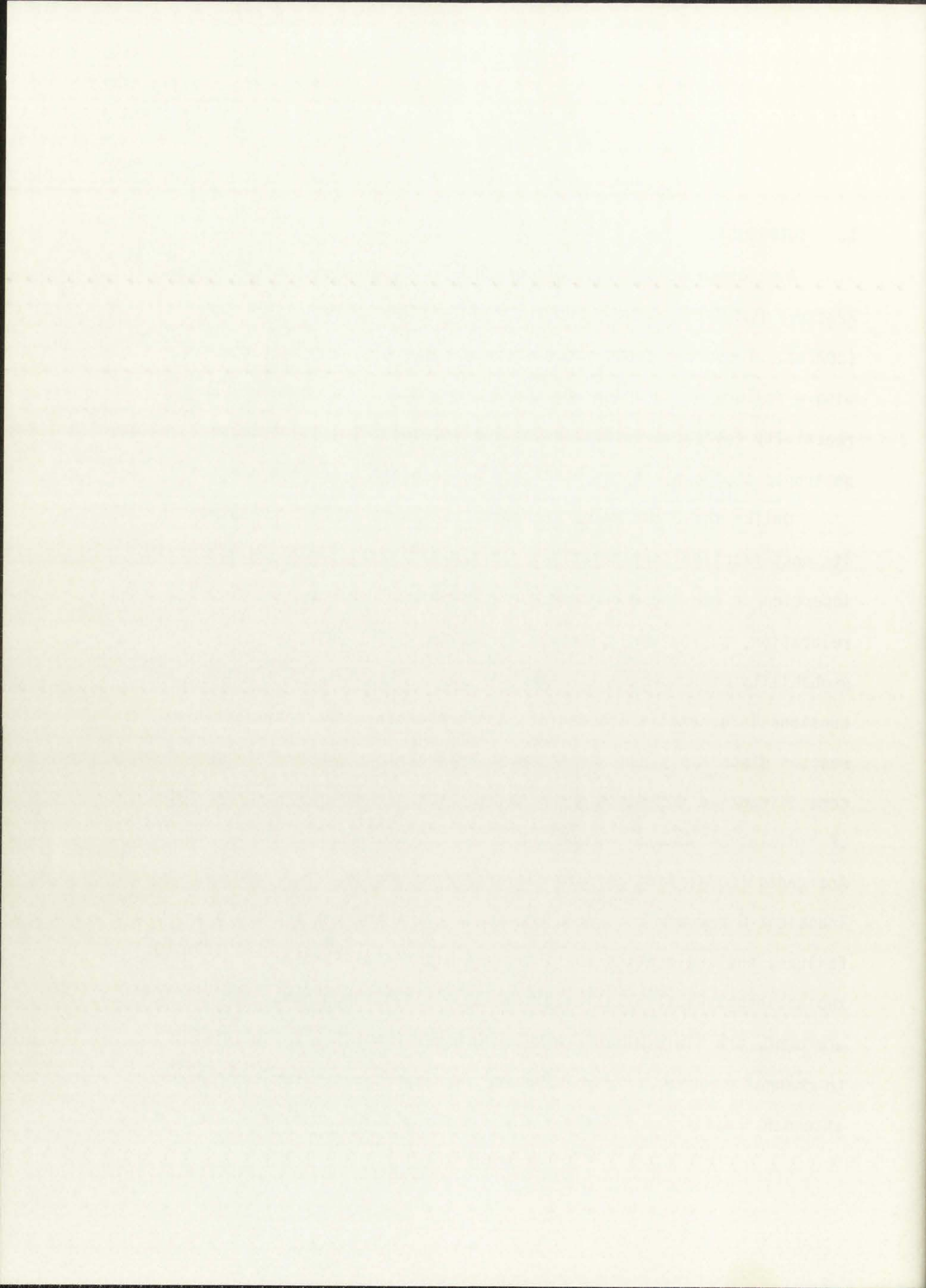
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1. INTRODUCTION

A major concern in the licensing of Liquid Metal Fast Breeder Reactors (LMFBR) is that of postulated Core Disruptive Accidents (CDA's). These accidents occur when an initiating event is coupled with a failure of the plant protection system. If such negative reactivity feedbacks as fuel expansion are insufficient to cause a neutronic shutdown, it can then only be achieved by core dispersal.

Unlike the Light Water Reactors (LWR), the LMFBR core is not in its most reactive configuration. Thus negative and positive reactivity insertion is very dependent on core dimensional changes and material relocation, making core disassembly accidents of concern even if their probability of occurrence is extremely low. The analysis of power excursions is generally broken into three phases: accident initiation, reactor disassembly, and containment evaluation. Two general groups of core disruptive accidents are usually described depending on the type of "initiation" phase. These two are: (1) Loss-Of-Flow Initiated Accidents (LOCA) such as pump failure, pipe breaks, etc., and (2) Transient-Overpower Initiated Accidents (TOP) such as control rod failure, fuel relocation to an area of higher reactivity, etc. These two accidents usually follow differing accident sequences. In the LOCA accident, the "initiation" phase progresses from the loss of coolant, to channel voiding, clad melting and resultant fuel slumping with an attendant rapid rise in temperature at the outside surface of the fuel

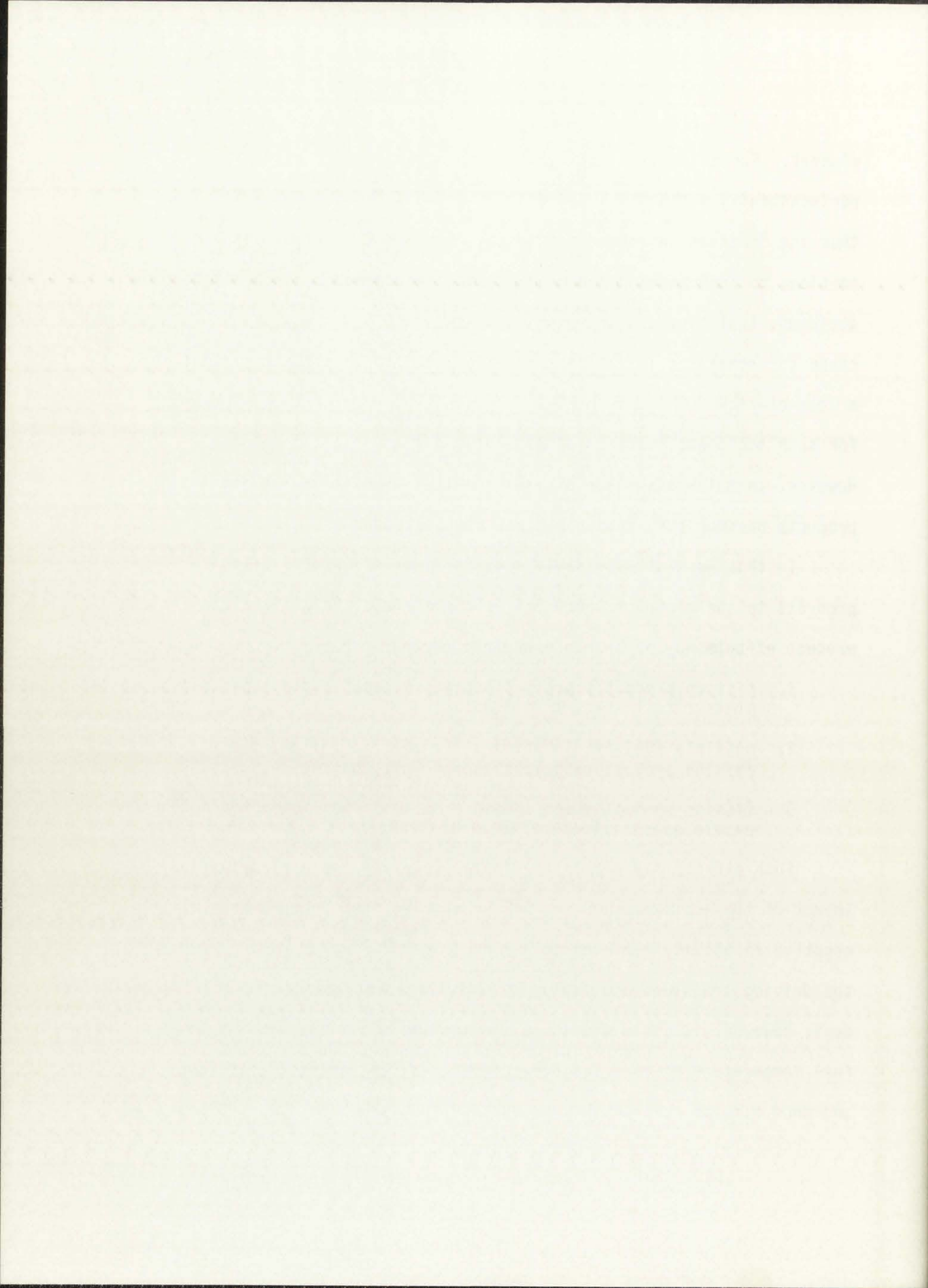


element. For a TOP type accident, the pin temperature rises preferentially at the fuel center due to the increased power level, thus the "initiation" phase progresses from positive reactivity insertion, to fuel heating and melting, to clad failure. In a LOF type accident, fuel slumping or movement to areas of high reactivity can cause the remaining intact pins to experience a TOP situation, that is, a loss-of-flow (LOF) driven TOP. To assess fuel relocation problems for such accidents, various codes and models have been developed. However, to date the effect of the potentially volatile fission products on such fuel motion has not been assessed.

In this work, the possible contributions of volatile fission products to the accident sequences is considered. Volatile fission product effects may be broken down into several groups:

1. fission product vaporization and release leading to pin pressurization and clad loading;
2. possible fuel axial motion prior to clad failure due to fission product vaporization and fuel foaming;
3. fission product vapor pressure as a driving force for fuel expulsion and dispersal at clad failure.

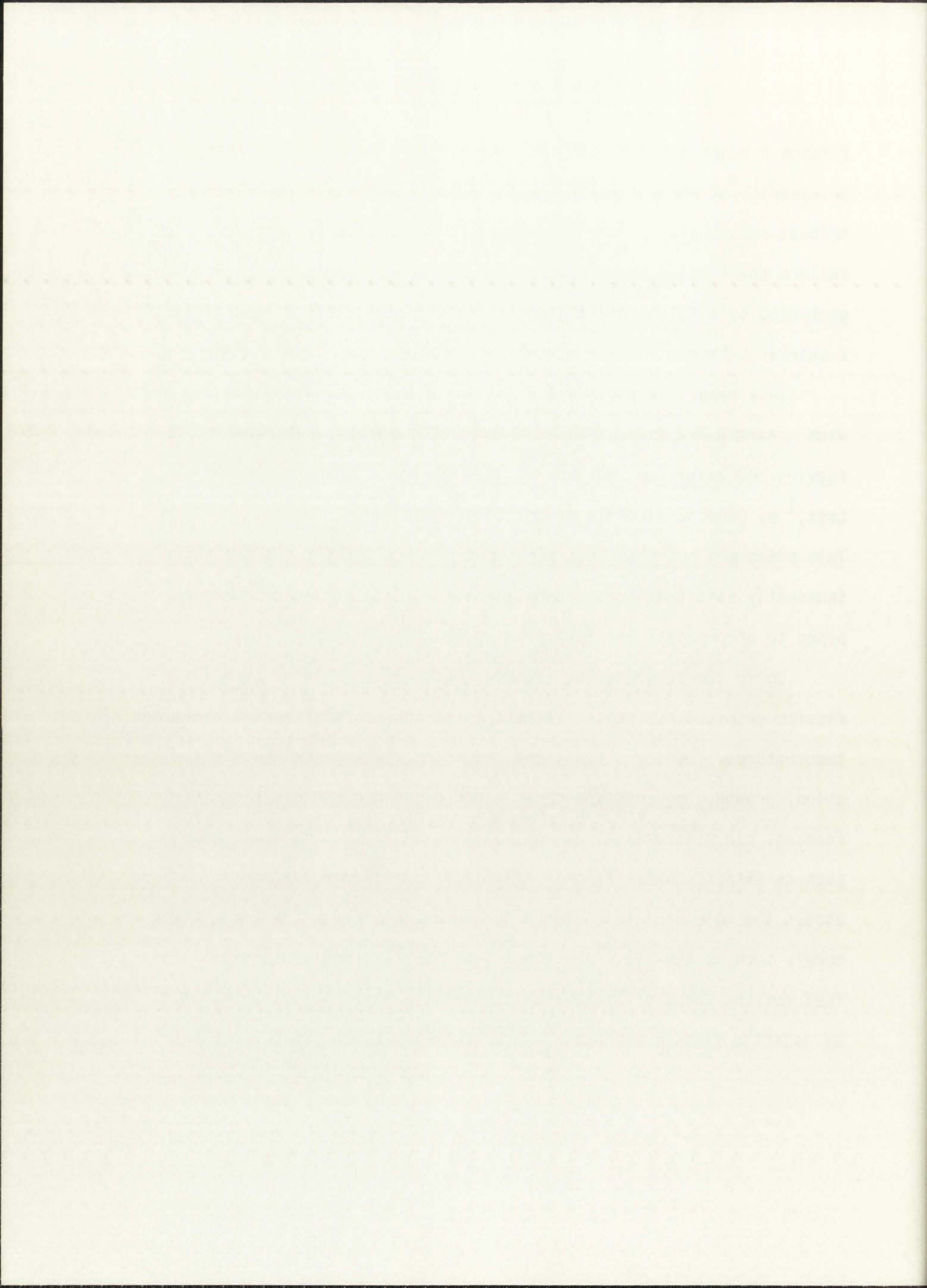
Such effects may either terminate or lessen the destructive impact of the accident sequence. For example, item 2 would provide a negative reactivity feedback to the core in a TOP which would decrease the driving transient and may or may not stop the core disruptive accident; however, it could provide a longer time sequence allowing lower fuel temperature at clad failure, probably a less energetic accident, and more time to control the reactor before disruption occurs. Some



fission product effects, such as item 1, might increase the energetics or severity of an accident. Fission product vaporization may contribute substantially to a decrease in time-to-clad-failure. At clad failure the fission product vapor could increase an impulse force generated by a FCI by driving more fuel into the coolant channel and in a shorter Δ time.

This report is concerned primarily with item 2 which could provide a safety reactivity feedback loop. Experimental evidence of fuel foaming and axial fuel motion has been reported by ANL in the F2 test,¹ by General Electric in the C3B,² C4A,³ and C5⁴ pins. This phenomena has also been mentioned in ANL-7963⁵ in the design of inherently safe fuel pins. Annular blankets and reflectors were proposed to accommodate the fuel foaming and the axial movement.

Up to the present, fuel foaming has been attributed totally to fission gases, i.e., those elements in gaseous form at normal operating temperatures. During a transient condition, fission gas bubble nucleation, growth, and coalescence will occur, also contributing to fuel foaming, pin pressurization, and possible axial fuel motion. Models such as GRASS,⁶ HOPE,⁷ FRAS⁸ - PFRAS,⁹ VENUSII¹⁰ are used to assess the role of fission gases during an accident situation. Other models such as BEHAVE3,¹¹ HOTPIM,¹² and TOFFII¹³ calculate axial fuel motion. None of these models, however, account for contributions by volatile fission products. This report assesses the potential of

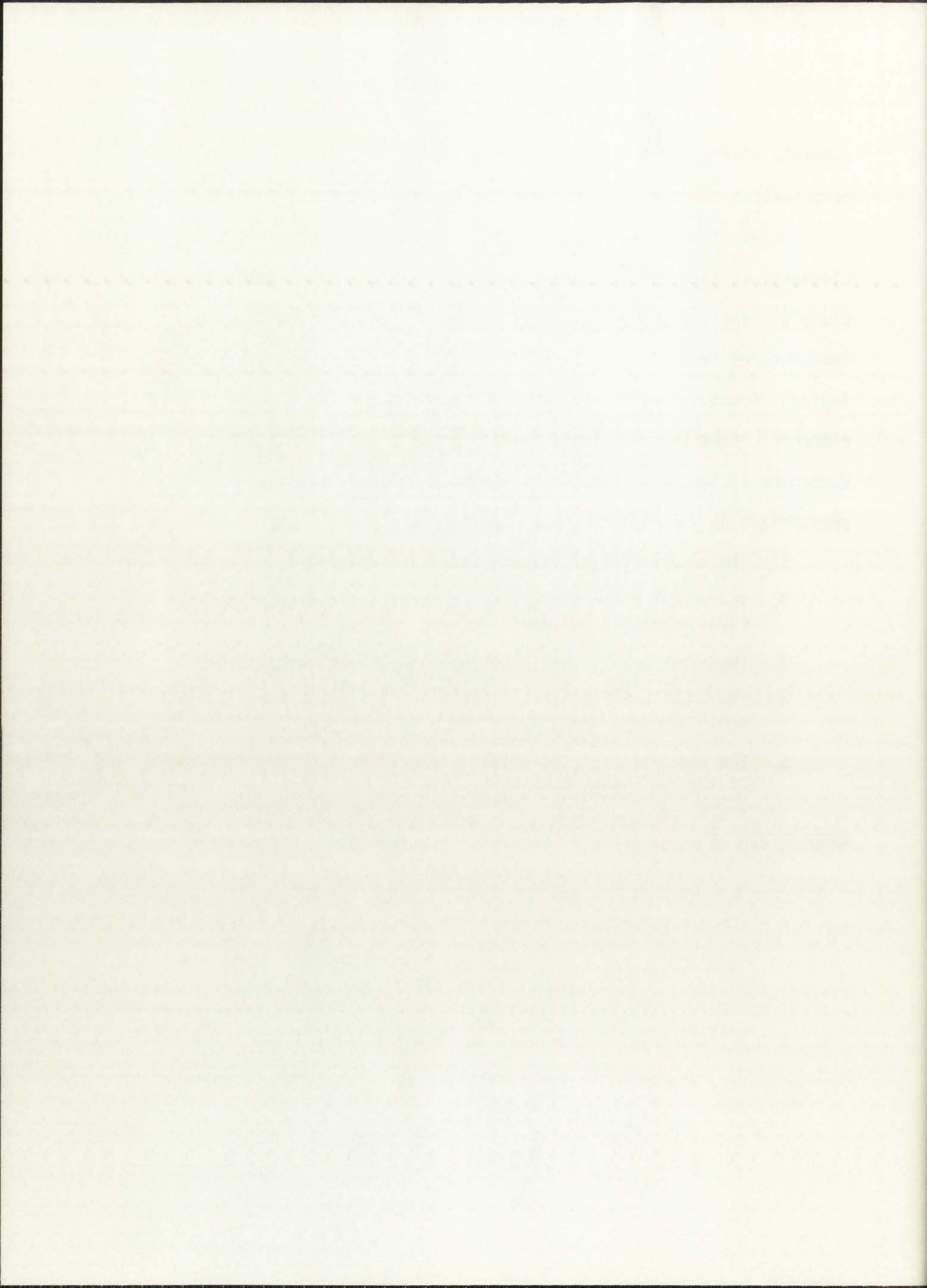


volatile fission products to fuel motion and, the magnitude of this contribution in comparison to that due to fission gases.

Irradiated oxide and mixed oxide fuels contain metallic inclusions, as seen in Fig. 1.1* made up of fission products that include elements which can volatilize in pure form at or below fuel temperatures reached in an accident situation. These aggregates are logical structures to investigate due to the concentration of volatile elements. Some key questions, however, must be answered in order to determine if the inclusions can contribute to fuel foaming and pin pressurization. Such questions include:

1. The composition of typical metallic inclusions;
2. The radial distribution and characteristic size of the inclusions within the fuel;
3. The vapor pressures of the inclusion constituents;
4. The phase diagram of the inclusion, i.e., whether the elements are in solid solution or if two or more phases exist;
5. The comparison of the total vapor pressure of the inclusion to the fuel vapor pressure.

*Photograph courtesy of W. F. Murphy, Argonne National Laboratory.



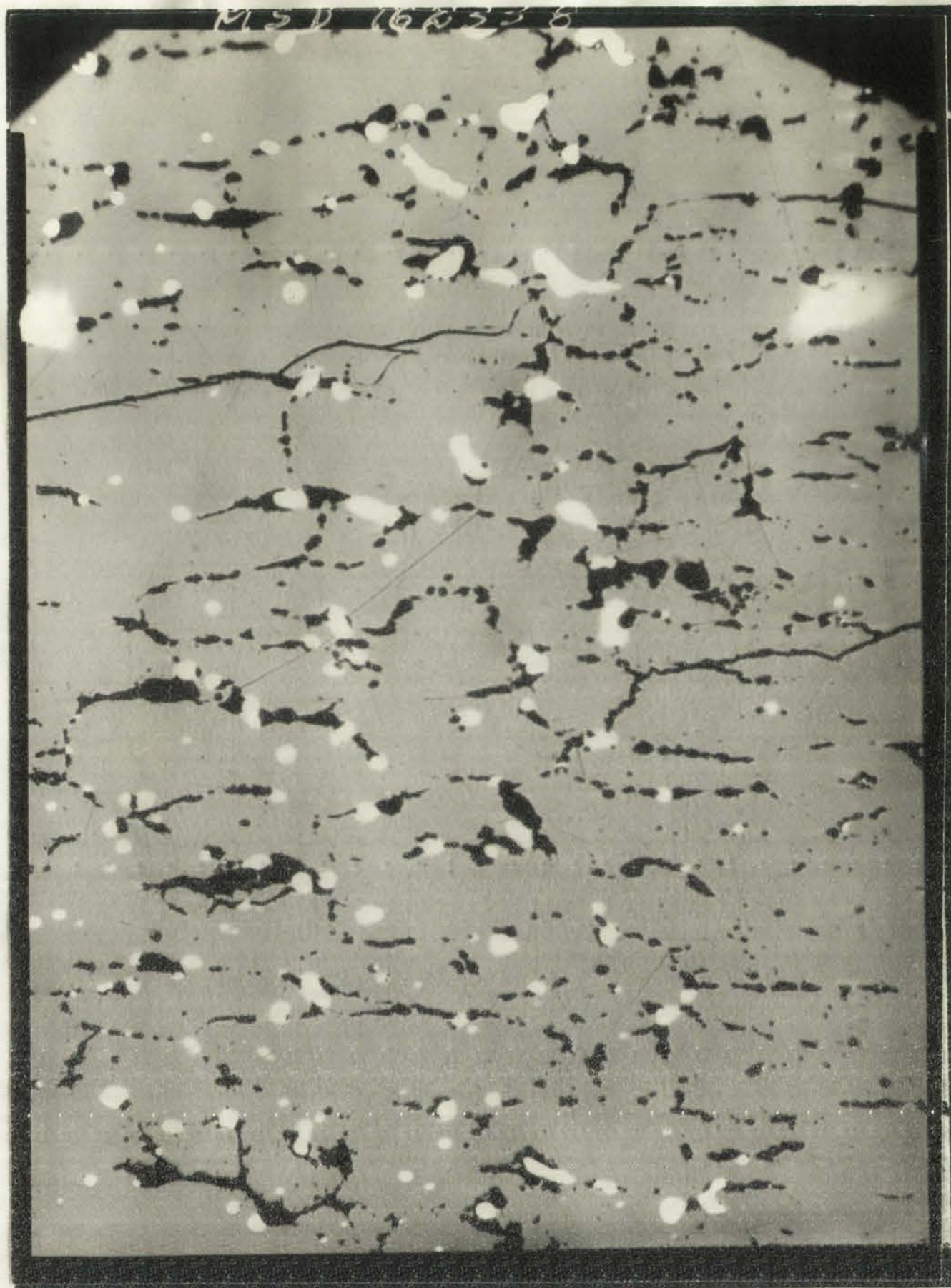
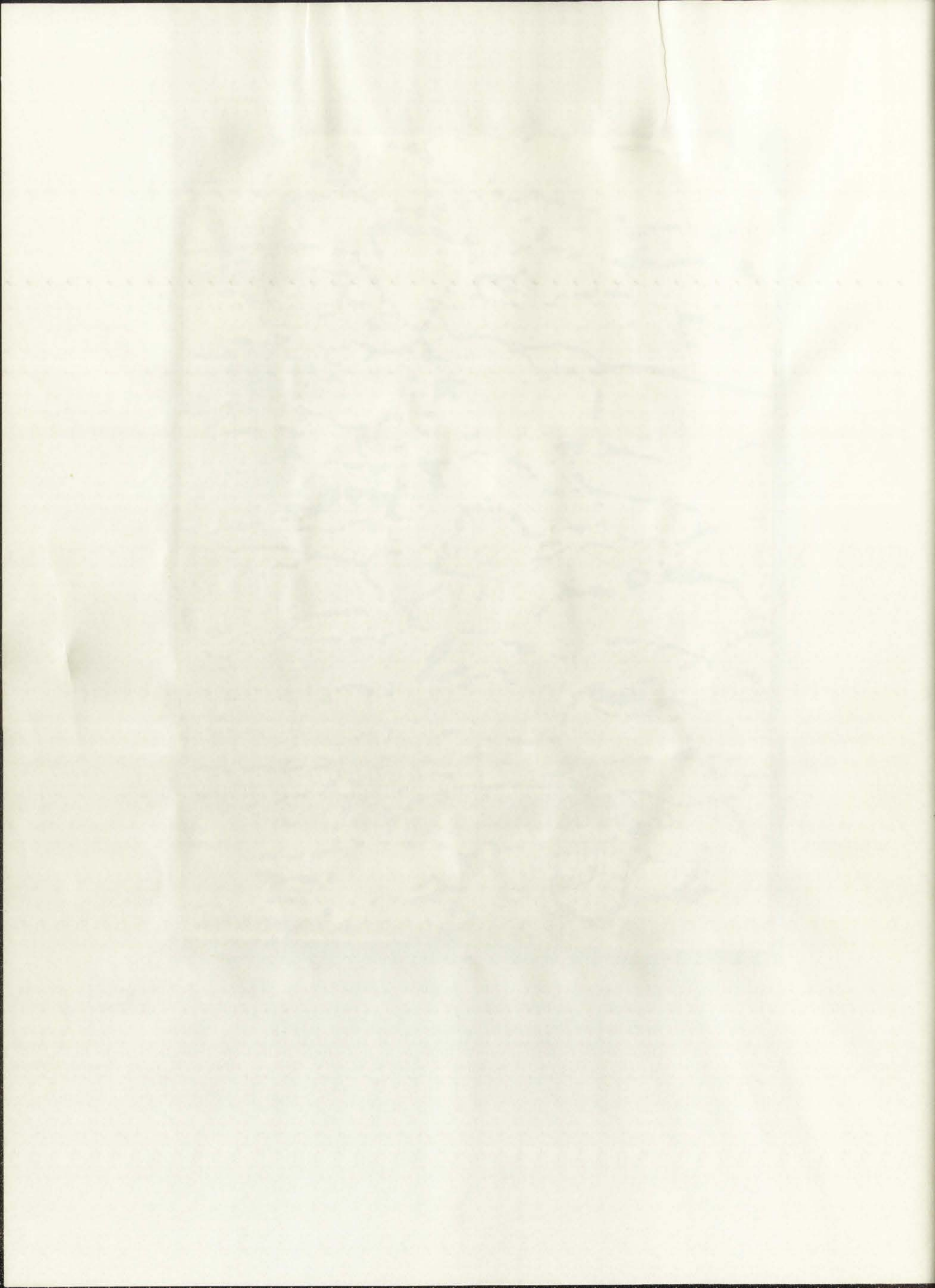
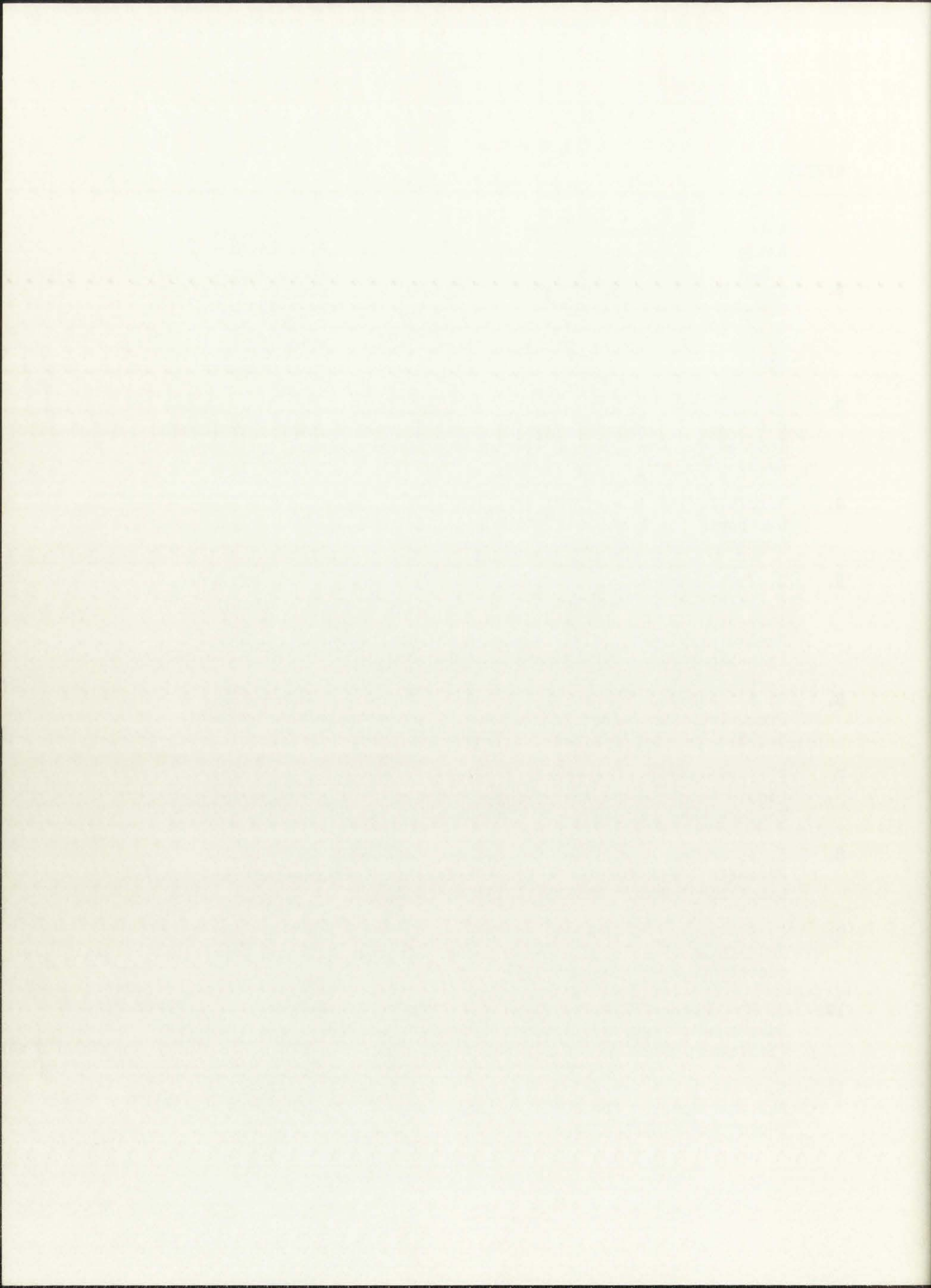


Figure 1.1
Micrograph showing the presence of metallic
inclusions. 250x.

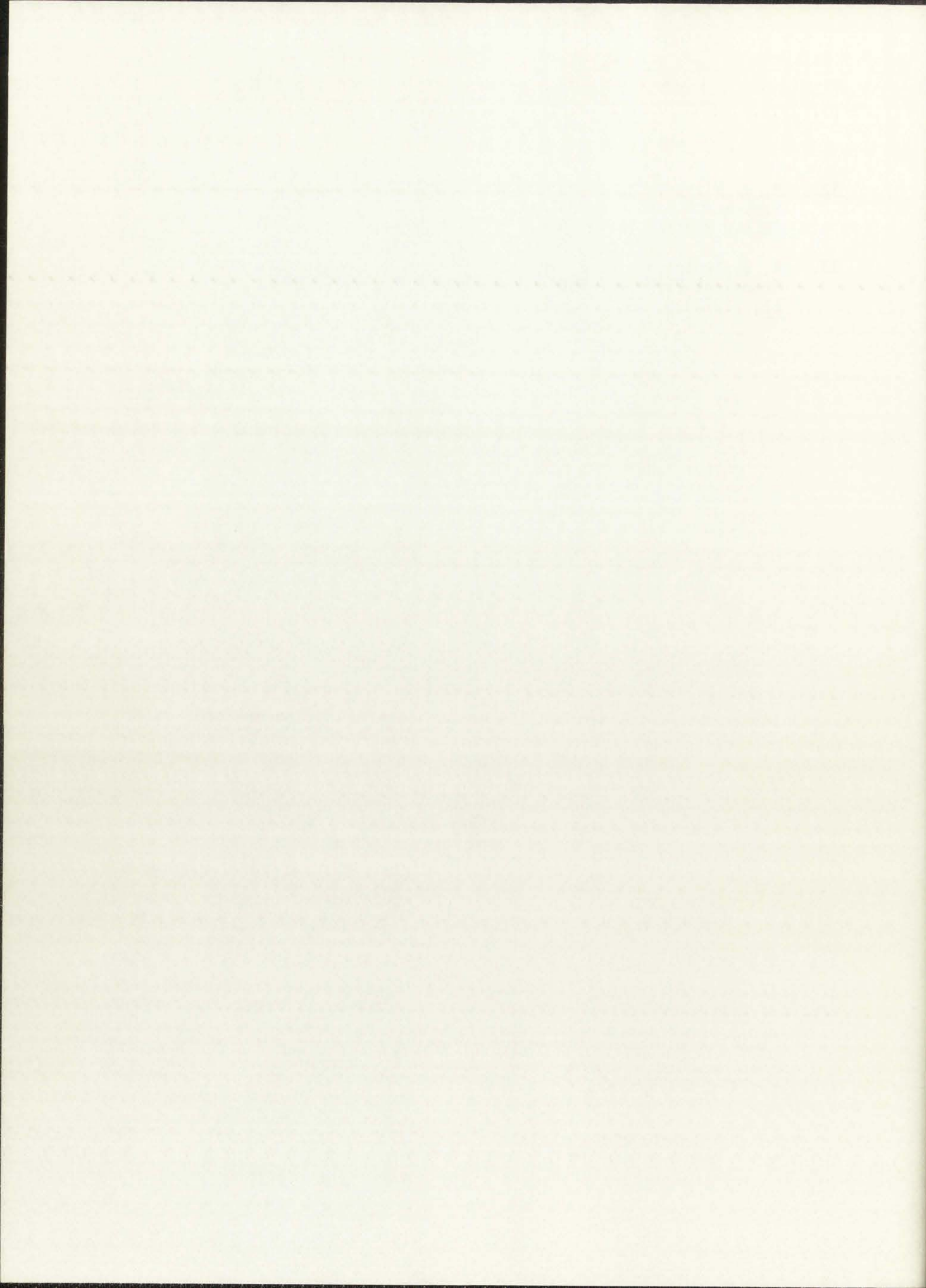


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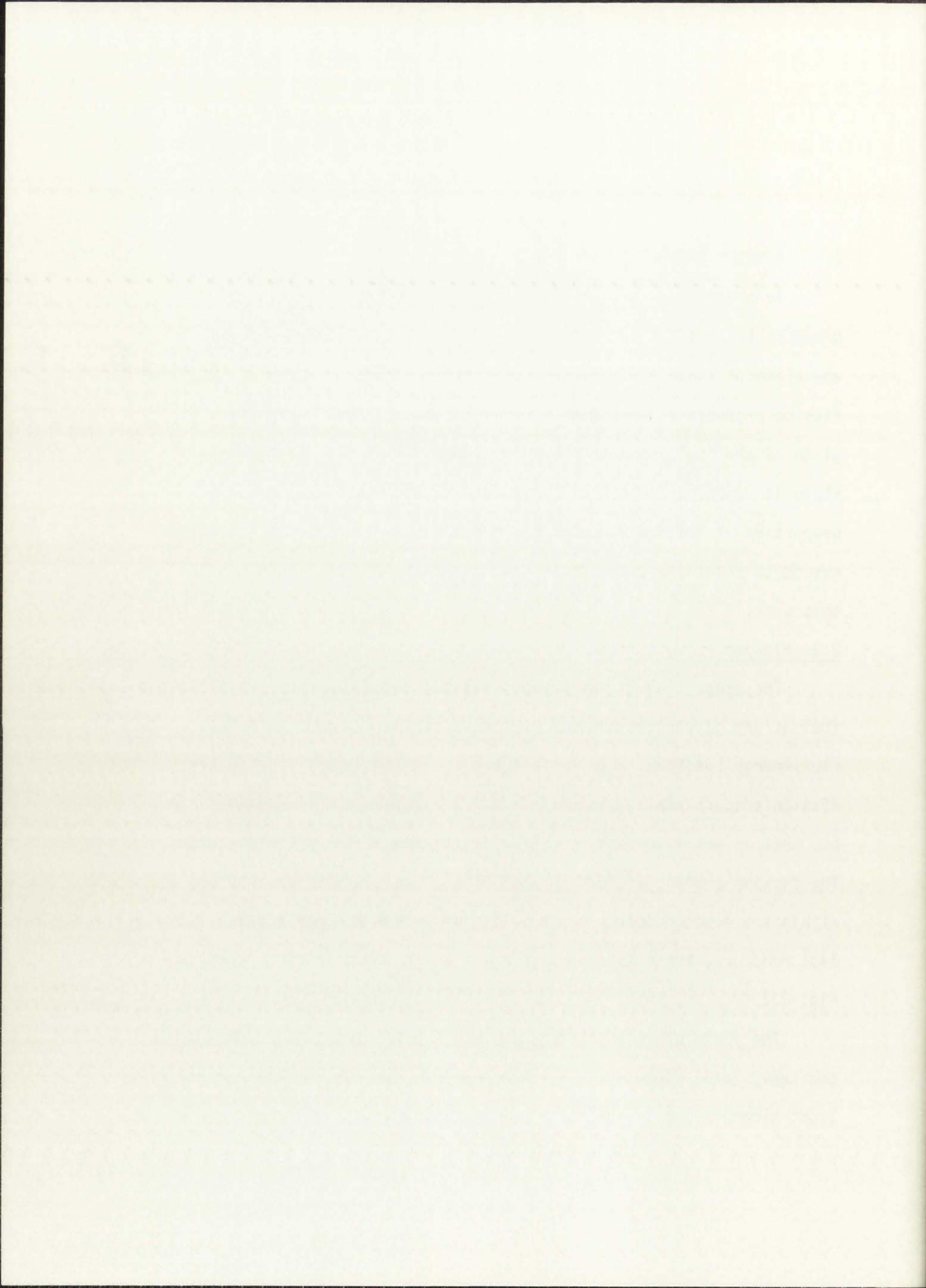
2. FISSION PRODUCT CHARACTERIZATION

In order to determine the possible contribution of fission products to accident scenerios, the location, quantity, and physical and chemical state of these products must be known. The quantity of fission products is dependent on fuel burnup and the fission product yield of the fuel species. The location and physical and chemical state is dependent on the oxygen potential and other thermodynamic properties of the individual fission products. These areas are discussed to determine the fission products that will be of concern in this work.

2.1 Fission Product Yield

The proportion of the various fission and decay products in the fuel at any given time depends on the particular fissile materials and flux/energy spectrum. For a short period of time after startup the fission product yield also depends on flux levels and irradiation time, but this is not important for fuels irradiated longer than 100 days. The fission product yield distribution does not change appreciably within the neutron energy range, a few Kev - few Mev, of concern with fast reactors, but does depend on the fissile composition as seen in Fig. 2.1.¹

The yield of mixed oxides, (U, Pu) O₂, is weighted somewhat to the heavy metal elements, i.e. atomic masses 100-110, at the expense of light elements due to the upward shift of the lower yield curve of



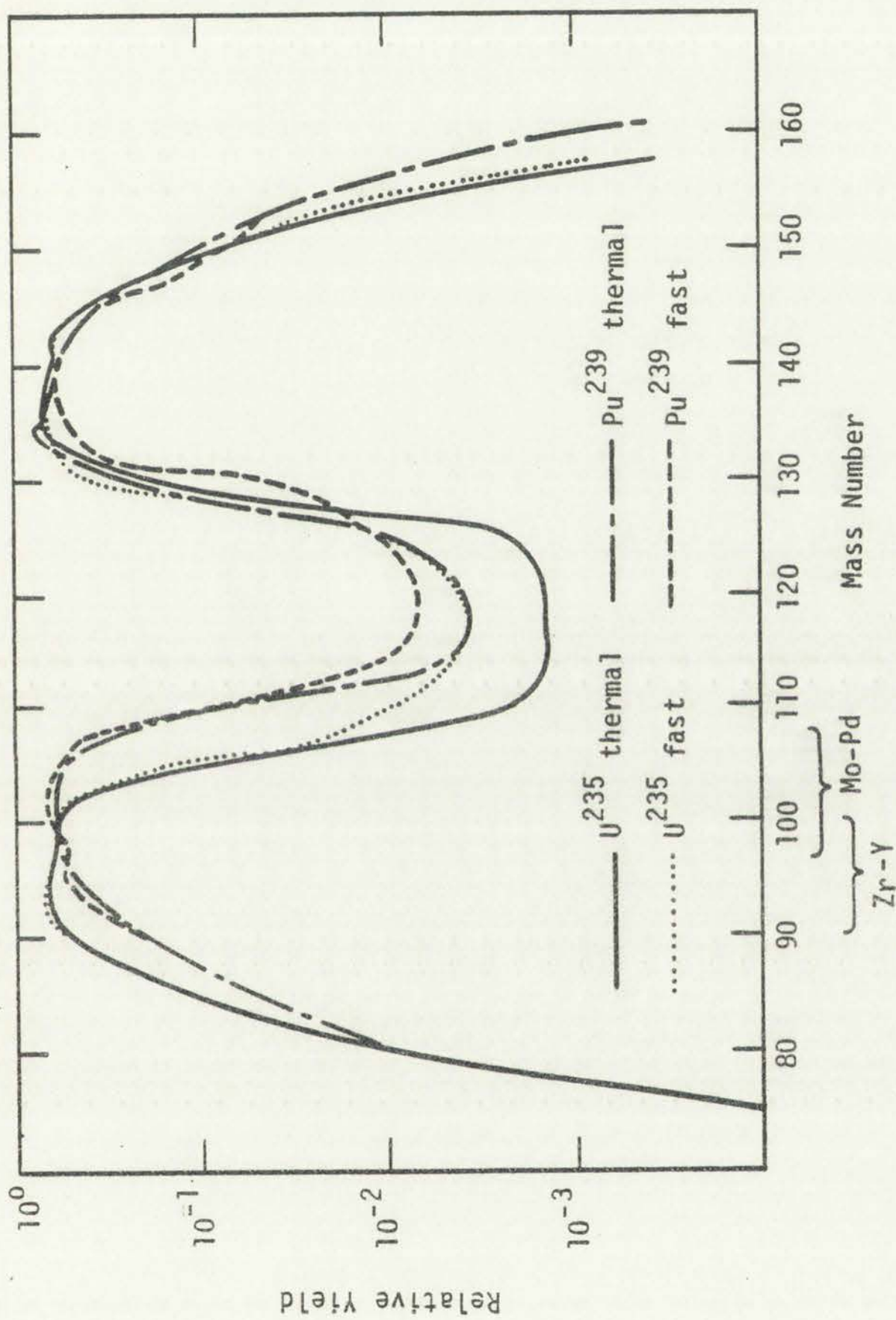


Figure 2.1. ²³⁵U and ²³⁹Pu fission yield spectra.

Figure 1: A plot of $\log_{10}(\text{relative error})$ versus $\log_{10}(\text{number of points})$.



Figure 1: A plot of $\log_{10}(\text{relative error})$ versus $\log_{10}(\text{number of points})$.

Pu^{239} vs U^{235} . For example, in the fissioning of Pu^{239} compared to U^{233} or U^{235} , there is a drop in the yield of zirconium isotopes from about 30% to 20% as well as a drop in the light elements cerium, strontium, with a corresponding increase in the noble metal products, rhodium, ruthenium, and palladium, as shown in Table 2.1.a¹ and Table 2.1.b²

Fission product yields have been calculated for oxide and mixed oxide fuels and various irradiation spectrums.²⁻⁷ Computations have shown that the effect of power rating and cooling time on composition are negligible for irradiations longer than 100 days. Obviously short lived products build up to very low equilibrium values, and it is the long half-life and stable products that become important. However, as will be mentioned later, the precursors of the stable or long lived products can have an effect on where their daughter nuclei will be spatially located in the fuel pin for the case where the diffusion time is shorter than the decay time. A few of these yield curves will be used in later analysis.

2.2 Oxygen Potential

The oxygen potential controls the chemical state of the fission products, and their interaction with and distribution throughout the fuel.

The valency, thus the oxygen requirements for the fuel and fission products, is controlled by the partial molar free energy or oxygen potential for the reaction:

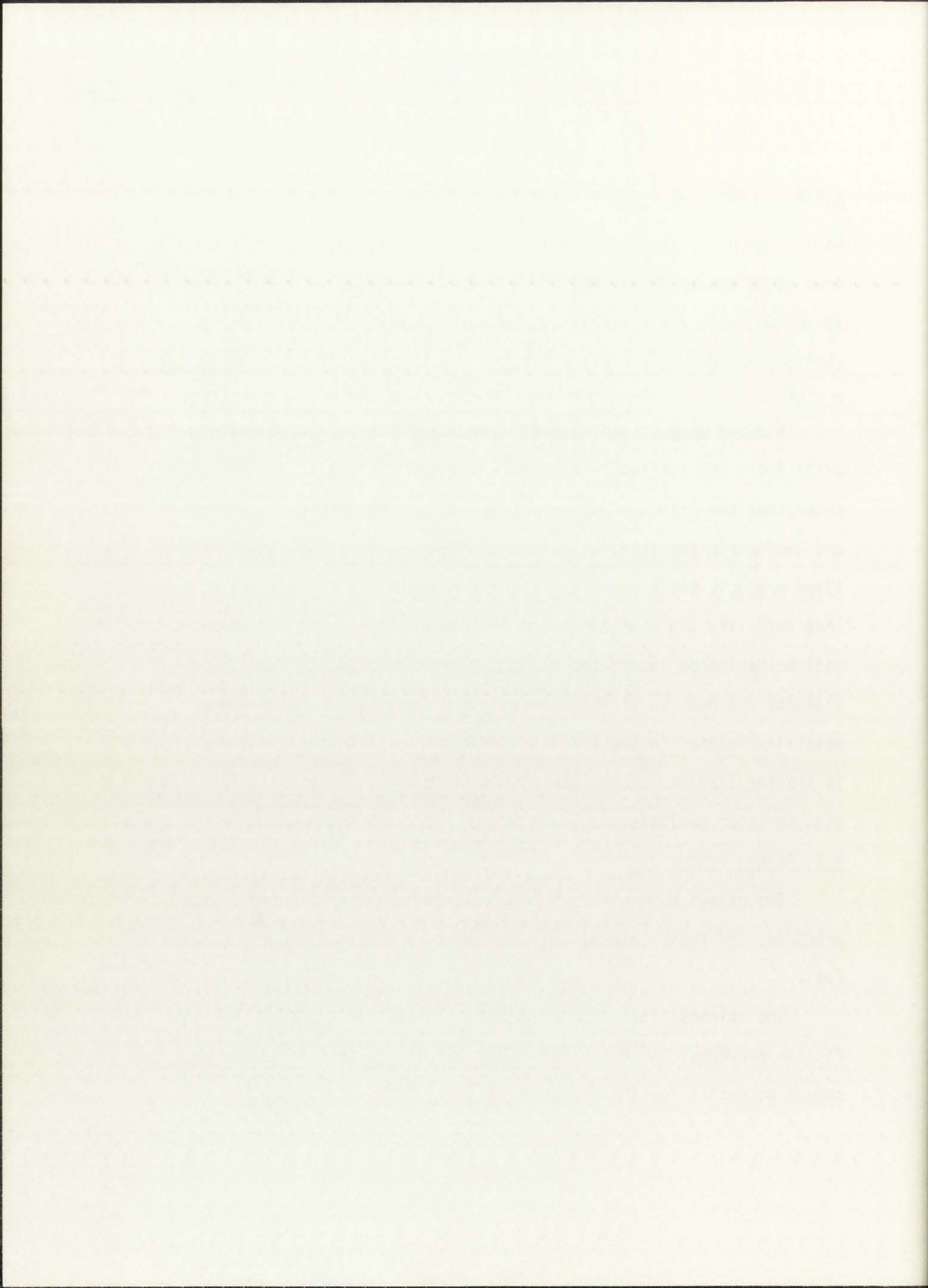


Table 2.1a
Atom Percent of Final Fuel Composition at 10% Burn-up.

Element	Thermal Fission (^{238}U .70, ^{235}U .30) O_2	Thermal Fission (U .70, Pu .30) O_2	Fast Fission (U .85, Pu .15) O_2
Y	.195	.084	.078
La	.216	.199	.177
Ce	.840	.691	.446
Pr	.139	.123	.164
Nd	.373	.328	.514
Pm	.063	.059	.063
Sm	.063	.106	.119
Eu	.006	.021	.021
Ba	.232	.215	.212
Zr	1.085	.740	.685
Sr	.416	.125	.140
Nd	.047	.038	.021
Mo	.676	.678	.665
Tc	.202	.197	.190
Ru	.444	.851	.695
Rh	.050	.099	.167
Pd	.042	.425	.419
Xe	.703	.755	.696
Cs	.625	.647	.605
Rb	.123	.049	.072

Table 2.1b
Atoms Per 100 Atoms Fast Fissioned,
135 Days Irradiated, 0 Days Cooling

Element	U^{235}	Pu^{239}
Zr	29.510	20.650
Ce	15.852	13.403
Sr	9.875	4.418
Ba	6.910	6.304
Mo	21.394	20.098
Tc	6.010	5.835
Ru	16.091	24.736
Rh	2.450	5.458
Pd	1.600	15.500

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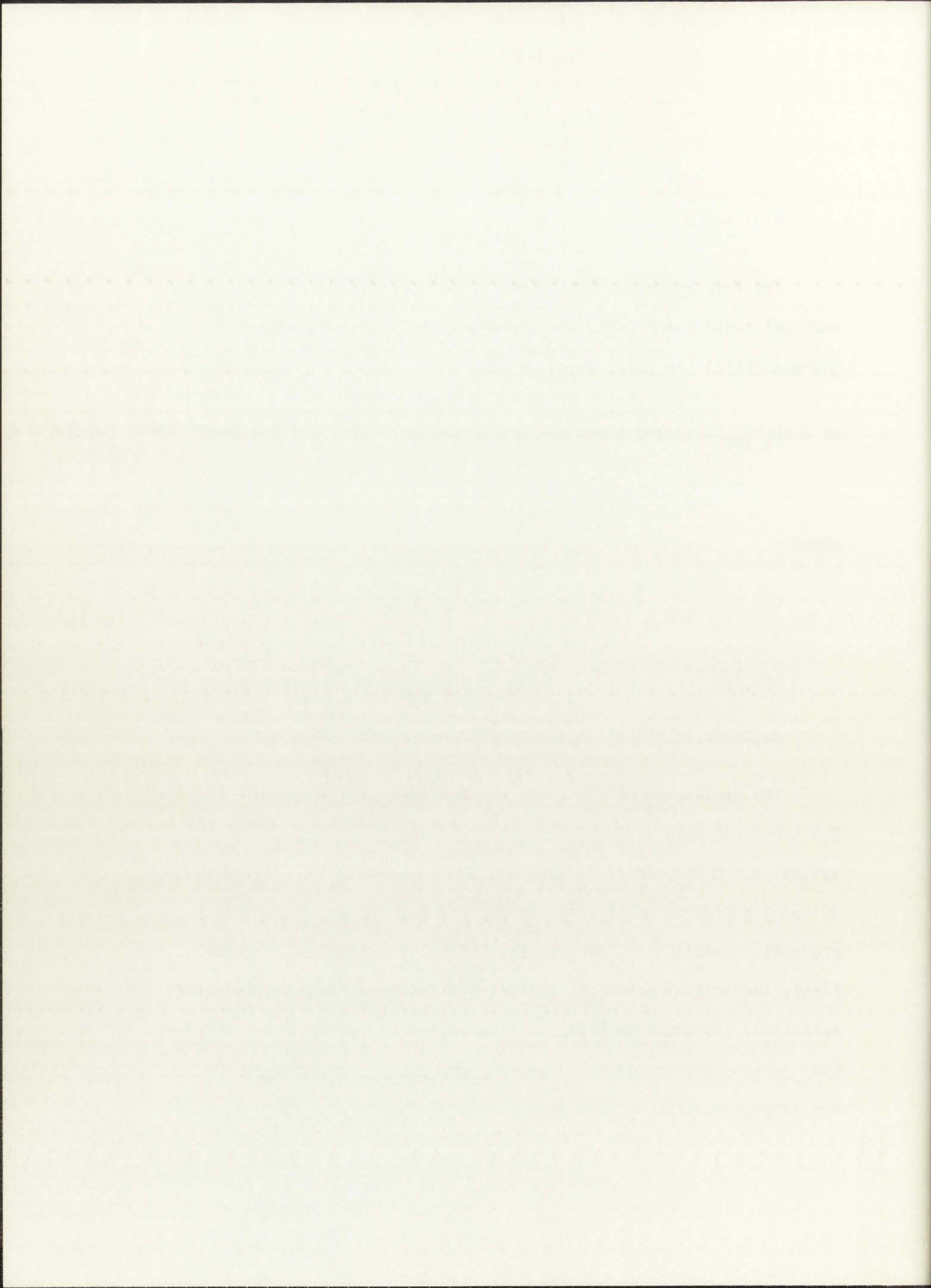
The free energy of formation for various fission product oxides and fuel systems are calculated from Eq. (2.2), based on the thermochemical constants given in Ref. 8;

$$\Delta F = \Delta H_{f,298} - (2.303 \Delta a) T \log T - \frac{1}{2} (\Delta b \times 10^{-3}) T^2 - \frac{1}{6} (\Delta c \times 10^{-6}) T^3 \\ - \frac{\frac{1}{2} (\Delta d \times 10^5)}{T} - T \Delta(B - a) + \Delta A \quad , \quad (2.2)$$

where

- ΔF = free energy of formation at T,
 T = temperature,
 $\Delta H_{f,298}$ = heat of formation of the oxide under consideration from the elements at 298 K,
 $\Delta a, \Delta b, \Delta c, \Delta d, \Delta(B-a), \Delta A$ = empirical constants.

The derivation of Eq. (2.2) can be found in Appendix A. Figure 2.2 shows the results for representative fission products. For a system in thermodynamic equilibrium, the free energy is a minimum, thus allowing a prediction of the chemical state of the various fission products. Complicating factors exist in this prediction, however. First, the initial state of the fuel has a large effect on its oxygen potential. As shown in Fig. 2.3⁹ the oxygen potential of UO_2 and PuO_2 is strongly dependent on whether the fuel is hypo- or hyperstoichiometric. The oxygen potential undergoes a rapid change



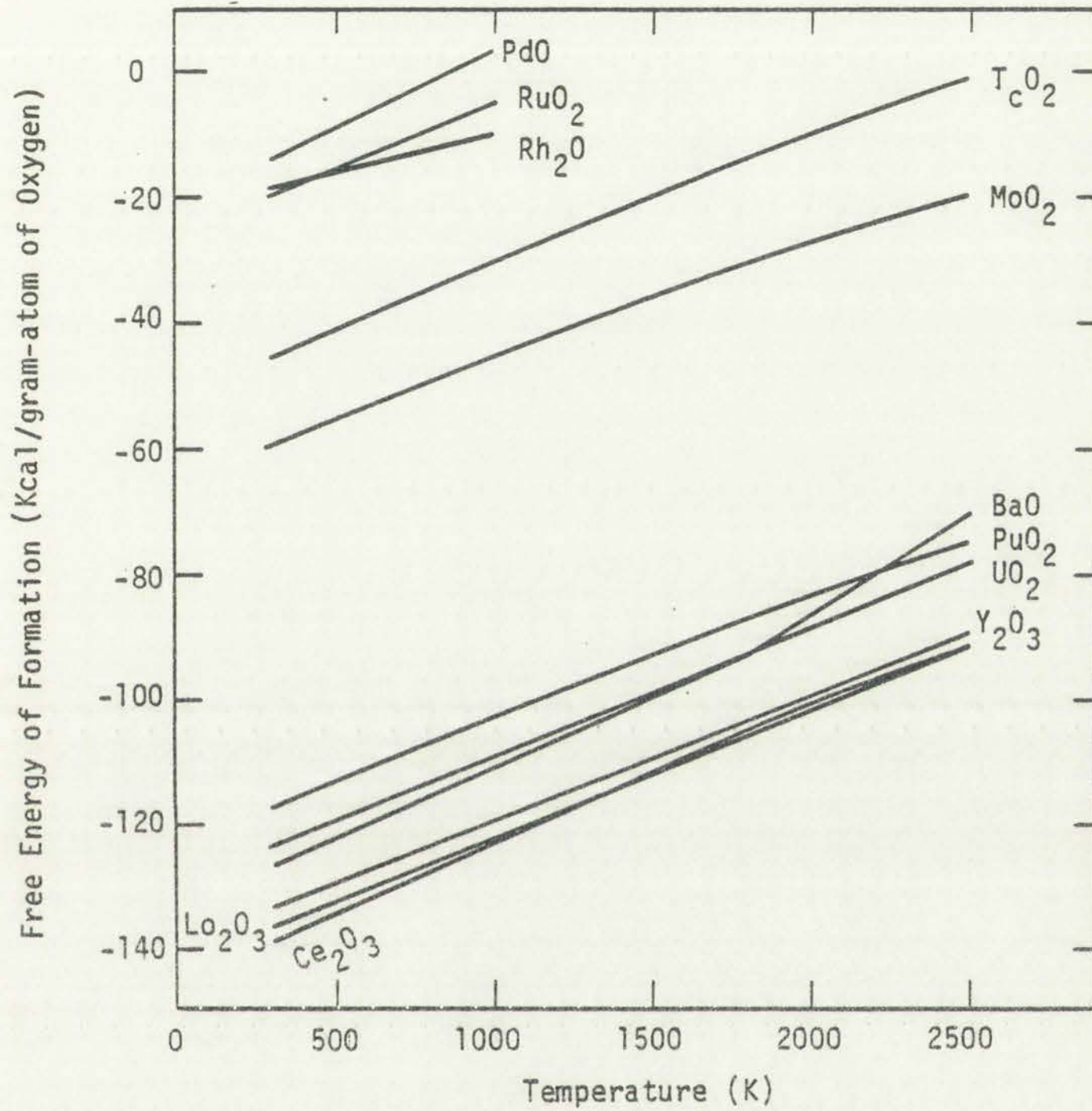


Figure 2.2.
Free energy of formation for various
fuels and fission products.



Figure 1: A line graph showing the relationship between variables X and Y. The x-axis represents X (1 to 10) and the y-axis represents Y (1 to 10). The graph displays multiple data series, each represented by a thin line, showing varying trends across the range of X.

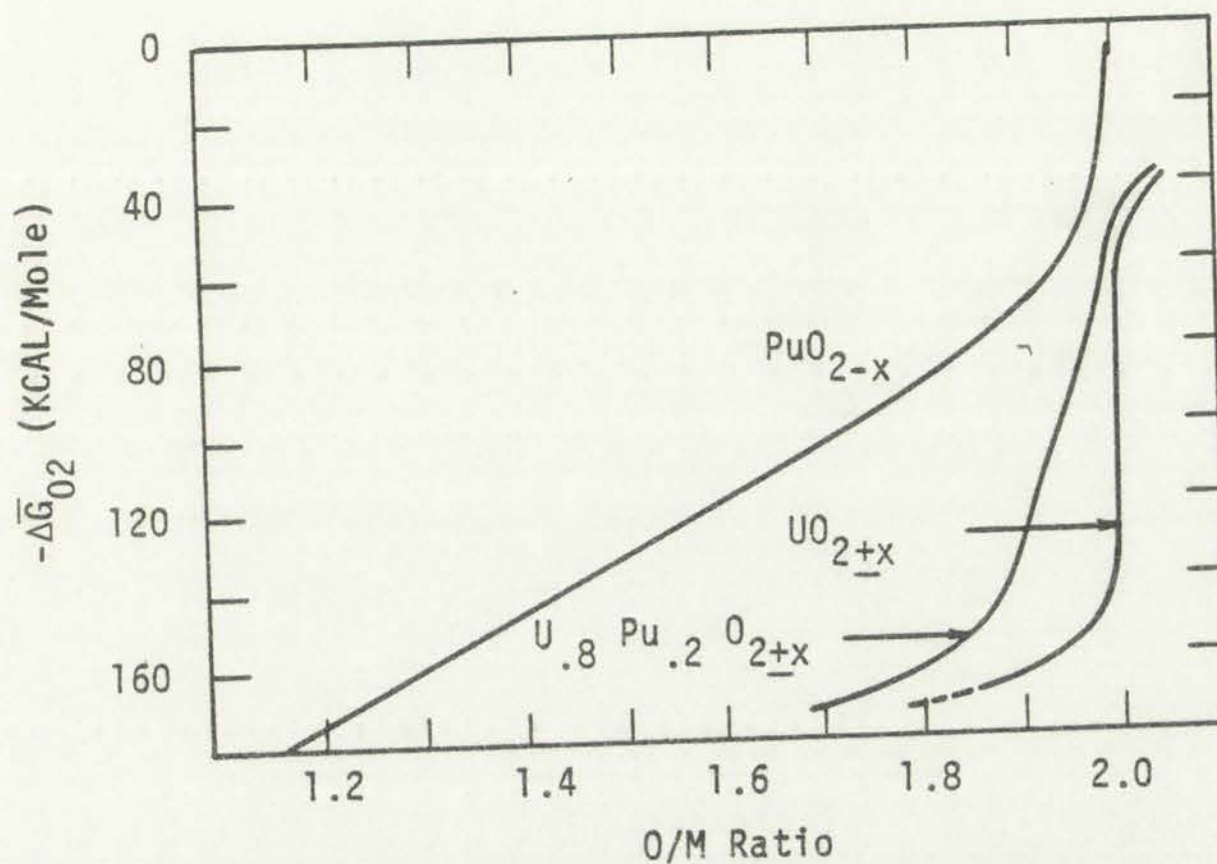


Figure 2.3.
Calculated oxygen potentials at 2513 K for
 UO_{2+x} , PuO_{2-x} , and $(\text{U}_{.8}\text{Pu}_{.2})\text{O}_{2+x}$.

between $\text{MO}_{1.99}$ and $\text{MO}_{2.01}$. In addition to the oxygen-to-metal (O/M) ratio, the total number of moles of uranium and plutonium, and the quantity of fission product elements available to go into solid solution in the fluorite phase change with burnup. The rate at which the O/M ratio increases with burnup is dependent on the fuel composition. Plutonium, with its increased yield of noble metals at the expense of lighter elements, has a lower average valency per fission product than U, i.e. 1.3^+ vs 1.7^+ ,¹⁰ leading to a larger increase in stoichiometry per atom % burnup.

As seen in Fig. 2.2, the oxygen potentials for the various fission products vary approximately linearly with temperature but have



Figure 1. Rate of reaction vs. time for the decomposition of KClO_3 at different temperatures. The rate of reaction increases with increasing temperature. The curves show that the rate of reaction is highest at 140°C and lowest at 100°C .

The rate of reaction is affected by temperature. As the temperature increases, the rate of reaction also increases. This is because the molecules have more kinetic energy and are able to overcome the activation energy barrier more easily.

The graph shows that the rate of reaction is highest at 140°C and lowest at 100°C . The curves for 120°C and 140°C are very close to each other, indicating that the rate of reaction is similar at these two temperatures.

The rate of reaction is also affected by the concentration of the reactants. In this experiment, the concentration of KClO_3 was kept constant, so the only variable was temperature.

The rate of reaction is also affected by the surface area of the reactants. In this experiment, the surface area of KClO_3 was kept constant, so the only variable was temperature.

The rate of reaction is also affected by the presence of a catalyst. In this experiment, no catalyst was used, so the rate of reaction was determined by the natural decomposition of KClO_3 .

differing slopes. Thus, a fuel pin having a temperature gradient leads to a gradient in the oxygen potential. Figure 2.4⁹ illustrates calculated and measured oxygen potentials vs temperature for $(U_{.8}Pu_{.2})O_{2+x}$ for various investigators. Such a gradient provides a driving force for the oxygen, U, Pu, and fission product concentrations to redistribute, involving a combination of solid-state diffusion and gaseous transport processes.* Figure 2.5 illustrates the effect on the oxygen distribution as calculated by Rand and Markin¹¹ for the various stoichiometries of fuel.

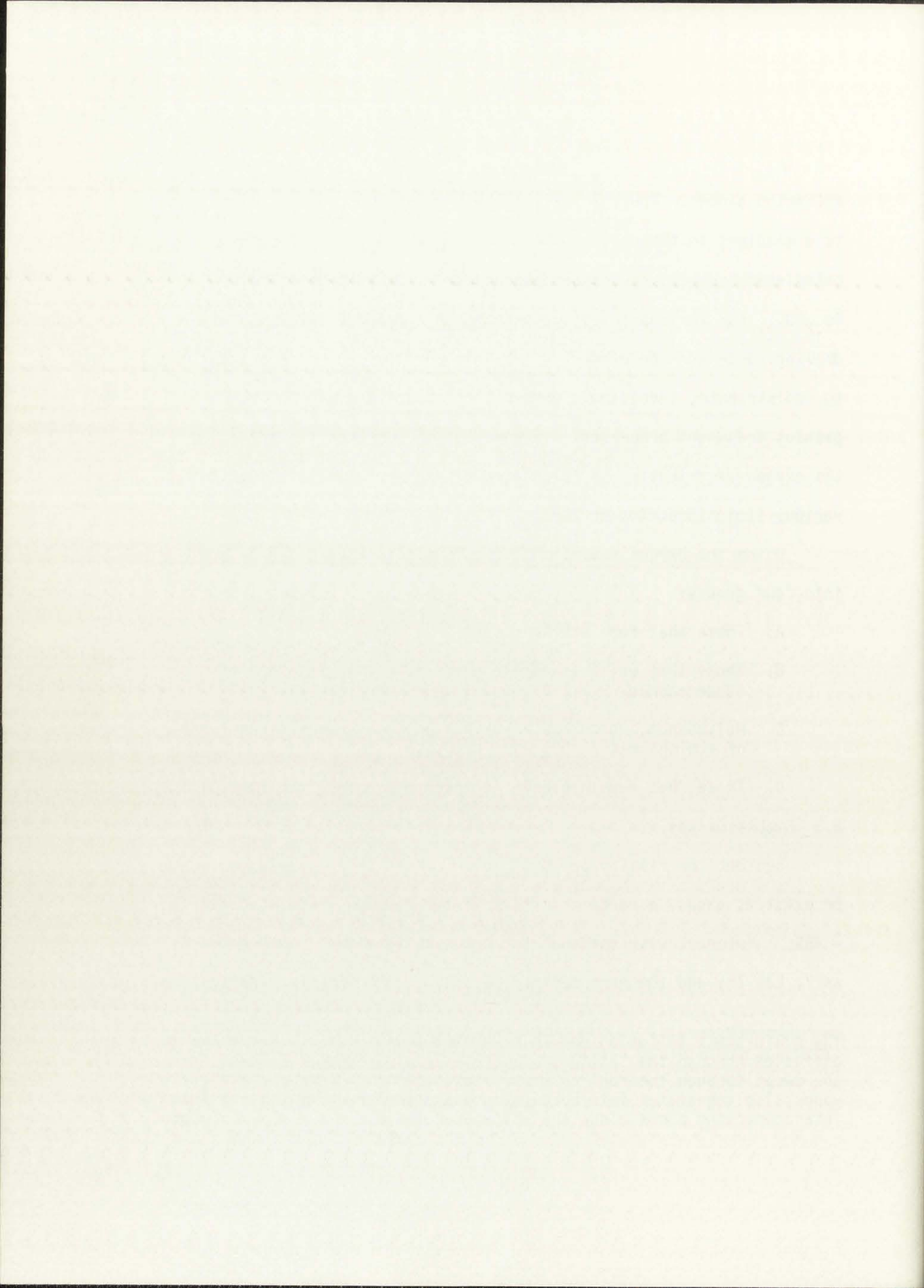
Using the oxygen potentials, the fission products can be broken into four groups:

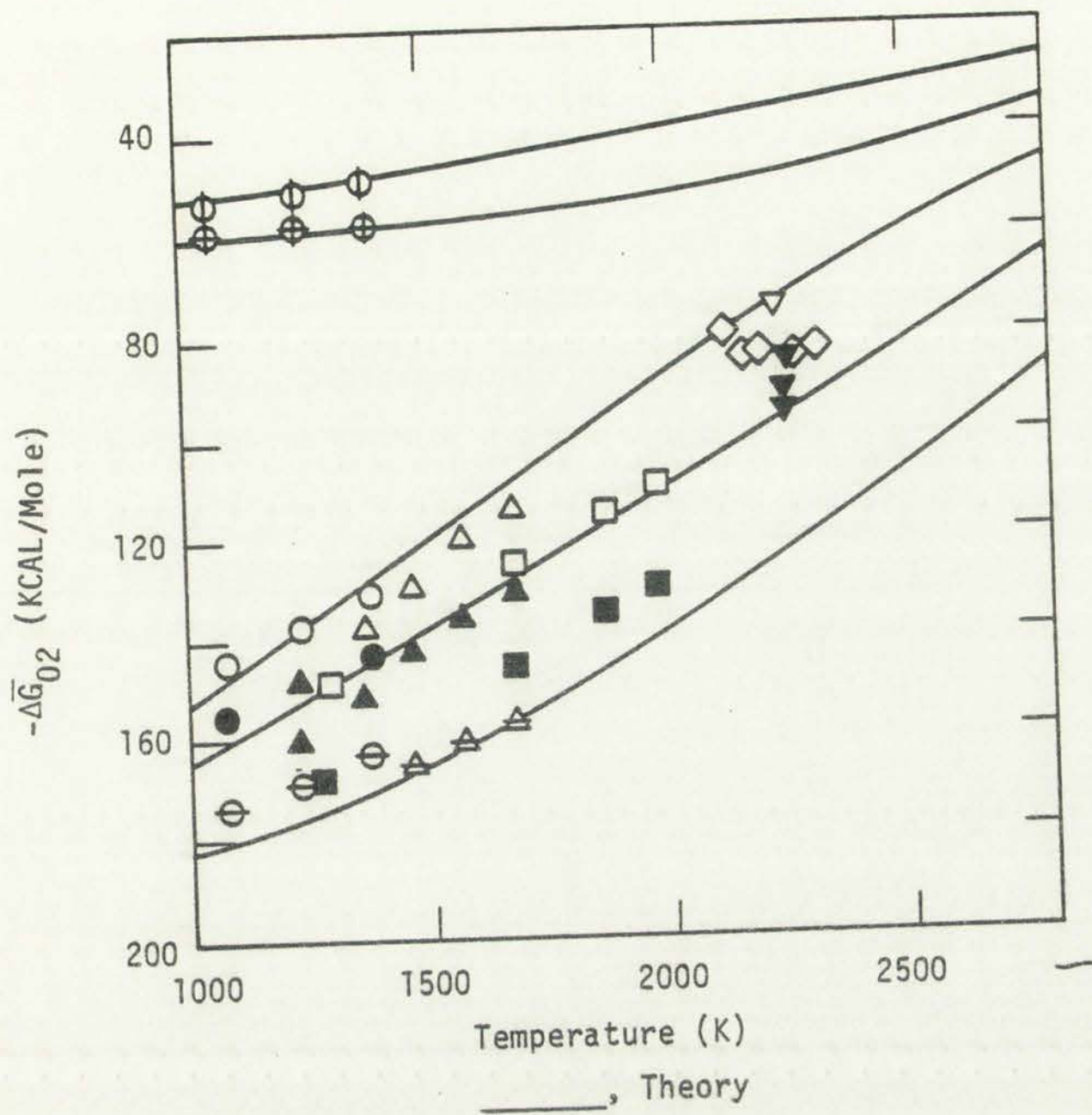
- A. Those that form stable oxides.
- B. Those that exist as stable gases at normal fuel operating temperatures.
- C. Molybdenum, which has an oxygen potential very close to that of stoichiometric UO_2 and $(Pu, U)O_2$.
- D. Those that remain stable in their elemental form (metallics).

2.3 Stable Oxides.

Besides the fission products which remain in their elemental form or exist as gases, a certain portion of the fission yield products, $\approx 45\%$,¹² interact with the fuel to form stable oxides. Such elements as Y, La, Zr, and the rare earths (Ce, Pr, Nd, Pm, Sm, Eu, and Gd) form

*By solid-state diffusion one is referring to individual atom or molecule diffusion through the lattice. In the gaseous transport process, atoms are swept through the fuel columnar region by lenticular pores. Gas or vapor also aggregates into bubbles in other fuel regions and can form interconnecting pores along the grain boundaries.





- | | | | | | |
|------|------|------|------|------|---|
| 2.05 | 2.01 | 1.91 | 1.95 | 1.98 | |
| ⊕ | ⊕ | ⊕ | ● | ○ | Markin and McIver |
| | | ⊕ | ▲ | △ | Woodley, normal to 20% Pu |
| | | ⊕ | ■ | □ | Javed and Roberts |
| | | ⊕ | ▼ | ▽ | Battles et al. |
| | | | ◇ | | Ohse and Olson, $U_{0.85}Pu_{0.15}O_{1.969}$
normal to $U_{0.80}Pu_{0.20}O_{1.98}$ |

Figure 2.4.
Calculated and measured oxygen potential vs temperature
curves for $(U_{.8}Pu_{.2})O_{2+x}$.



Figure 1
 Relationship between Temperature and % Diffusivity for various materials.

Legend:
 ○ - Material A
 △ - Material B
 □ - Material C
 ◇ - Material D
 × - Material E

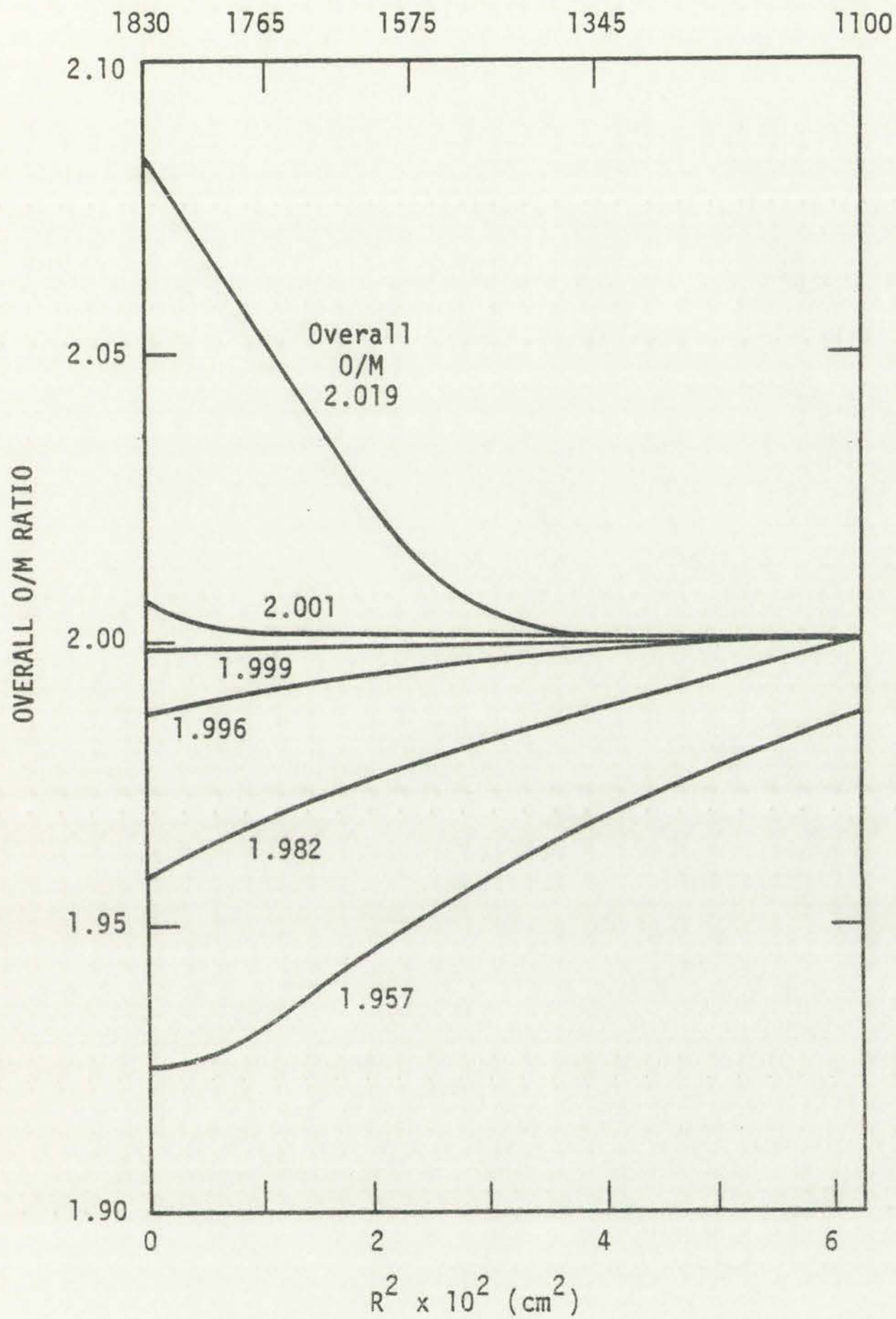


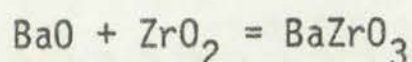
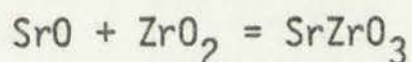
Figure 2.5
 Oxygen distribution in $(\text{U}_{.85} \text{Pu}_{.15}) \text{O}_{2+x}$ as computed
 by Rand and Markin.



Figure 1. Productivity vs. Time for a 10.5
 10.2
 10.0
 9.8
 9.5

oxides of greater stability than the initial UO_2 or $(U, Pu)O_2$. Even if there is not enough oxygen freed during the fission process, these elements will reduce the fuel matrix. Such elements are soluble fission products and their oxides enter the fuel crystalline structure.

Ba, Sr, and Nb also form stable oxides BaO , SrO , NbO_2 but are not in solid solution with the fuel,¹ but can be expected to form a separate oxide phase. As the fission product elements accumulate in the oxide matrix, however, physical-chemical phases most stable under the local conditions will form. As the concentration of Sr, Ba, and Zr increases, the tendency to form a separate phase of $SrZrO_3$ and $BaZrO_3$ will increase via the following reactions:

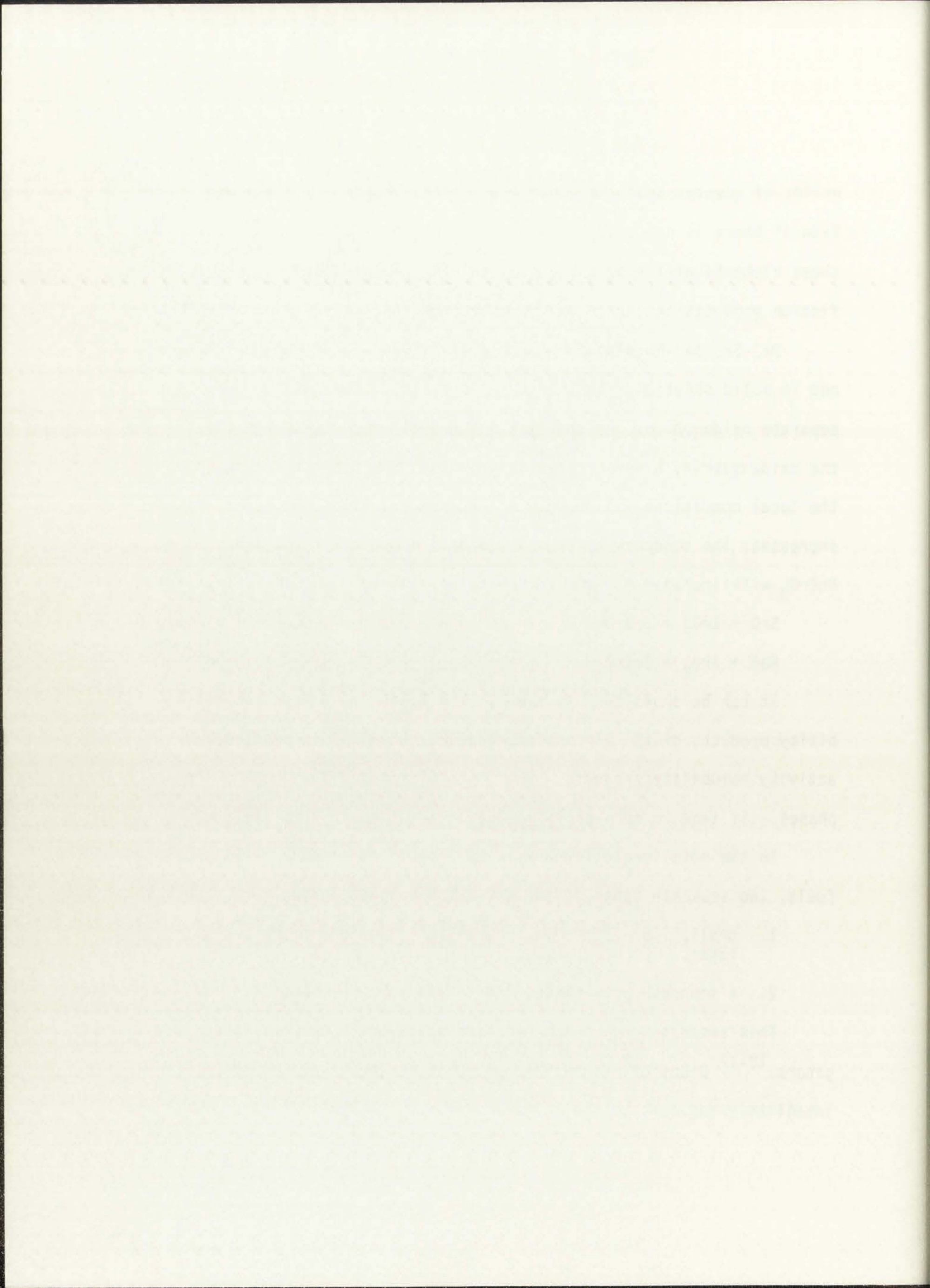


It can be shown that at even 1 atom %, the mole fraction solubility products of the zirconates, ($BaZrO_3$, $SrZrO_3$), exceed their activity solubility products. Thus, it is expected that both solid phases will tend to form early in the irradiation life of the fuel.

In the metallurgical analysis of irradiated oxide and mixed oxide fuels, two separate types of solid fission product states were observed:

1. small, $\approx 5 - \approx 10$ m dia., metallic inclusions to be discussed later,
2. a separate gray phase.

This separate gray phase had been observed by various investigators.¹²⁻¹⁷ O'Boyle¹² found this phase in the equiaxed region immediately adjacent to the columnar grains. Analysis of this gray



phase yielded a high concentration of Ba and Ce. Concentrations of U and Zr were low, but some Sr was present. The analysis does not support the formation of zirconates, where equal concentrations of Ba plus Sr, and Zr are expected. O'Boyle¹² believes the Ba and Sr existed in their oxide state. The Ce in or near Ba concentration is not unusual since La and Ce are daughter products of Ba-140 and Ba-142. During normal operation La and Ce from the decaying Ba redissolve into the fuel matrix. After shutdown, however, the migration and resolution processes virtually cease. Thus, in the analysis of this separate phase after shutdown, Ce is associated with the Ba.

The yields of Sr and Ba are fairly close; therefore, one would expect a measured concentration of Sr very close to that of Ba in the gray phase. This was not the case in any of the observed analyses,^{10,12,16,17,18} and may be due to the very short half life of the volatile precursors of Sr-90, i.e. 33 s for Kr, 2.74 m for Rb, and 28 y for Sr, which makes up approximately 60% of the total Sr yield. The volatile precursors of Ba-138, 5.9 s for I, 17 m for Xe, 32 m for Cs-Ba(stable), are much longer lived. Not only the volatility but also the decay time of precursors is important in determining the form and location of daughter products.

Kleykamp's¹⁵ analysis of the gray phase indicated that is predominantly metallic (Mo, Tc, Ru, Rh) in nature; thus the assumption that the gray phase is made up of fission product oxides or zirconates

1

The first step in the analysis of the data is to examine the distribution of the response variable. This is done by plotting the data and looking for any obvious patterns or trends. In this case, the data is normally distributed, which allows us to use standard statistical tests.

The second step is to calculate the mean and standard deviation of the data. The mean is the average value of the data, and the standard deviation is a measure of the spread of the data. In this case, the mean is 1.5 and the standard deviation is 0.5.

The third step is to calculate the probability of observing a value greater than or equal to the observed value. This is done by using the standard normal distribution table. In this case, the probability is 0.05.

The fourth step is to calculate the p-value, which is the probability of observing a value as extreme as the observed value, assuming that the null hypothesis is true. In this case, the p-value is 0.05.

The fifth step is to compare the p-value to the significance level. If the p-value is less than the significance level, then we reject the null hypothesis. In this case, the p-value is 0.05, which is equal to the significance level of 0.05.

The final step is to conclude the analysis. Since the p-value is equal to the significance level, we are at the threshold of rejecting the null hypothesis.

cannot be made. The analysis of fuel microstructure by Hanson¹⁴ found the gray phase located in the cooler portion of the fuel near the clad; thus, it could contain not only fission products, but also could be due to cladding attack. This phase, however, was not analyzed.

There have been analyses that support the formation of zirconates. Bazin¹⁷ did find a gray phase in UO_2 that had concentrations of Ba, Zr, and O very close to that needed for $BaZrO_3$. HEDL-TME 76-16¹⁶ also reported a ring of Ba-Zr deposits in the columnar grain region of the fuel. Bradbury¹⁹ analyzed inclusions that contained Ba and Zr in a 1:1 ratio. Jeffery¹⁸ in his inclusion analysis found a type of inclusion which contained Ba and Zr in a 4:5 ratio which is close to 1:1.

From the above analysis, it is known that a large portion of the stable oxides are in solution within the fuel structure, with Ba and Sr, however, tending to form a separate oxide or zirconate phase. From the experimental evidence, it appears that a high concentration of Ba is present in the gray phase, but one cannot make a conclusion about its state (oxide or zirconate).

2.4 Stable Gases

Elements that exist as vapor in the fuel include the inert gases Xe, Kr; the halogens Br, I; and the highly volatile elements (Ce, Te, Rb, Cd, Sn, Se, and Sb). It should be noted that Cd, Sn, Te, and Sb are listed both under stable metallics and also under stable gases. This is due to the fact that their vaporization temperatures are in the

The first part of the paper is devoted to a general discussion of the problem. It is shown that the problem is well-posed in the sense of Hadamard. The second part is devoted to the construction of the numerical algorithm. It is shown that the algorithm is stable and convergent. The third part is devoted to the numerical results. It is shown that the algorithm is efficient and accurate.

There have been many papers on this subject. However, the present paper is the first to consider the problem in the sense of Hadamard. It is shown that the problem is well-posed in the sense of Hadamard. The second part is devoted to the construction of the numerical algorithm. It is shown that the algorithm is stable and convergent. The third part is devoted to the numerical results. It is shown that the algorithm is efficient and accurate.

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range between the expected maximum and minimum fuel temperature at steady state operation. Since these elements exist as vapors in the columnar region they migrate by the same mechanism as the inert gases. Some of the fission products such as Cs are swept out with the Xe and Kr and condense in the cooler regions of the fuel, i.e., at the clad-fuel interface.

A radial concentration profile of Cs in a fuel pin shows high concentration of cesium in the unstructured region of the fuel and in the region of the fuel-clad interface. Cs was not detected within the columnar grains but was found in the cracks and voids in this region, supporting the idea that redistribution of cesium occurs by vaporization rather than by diffusion through the matrix.

2.5 Molybdenum

The chemical state of Mo and the oxygen balance in the fuel are interdependent. The extent of MoO_2 formation depends on such factors as temperature, fuel composition, oxygen potential, and initial O/M ratio.

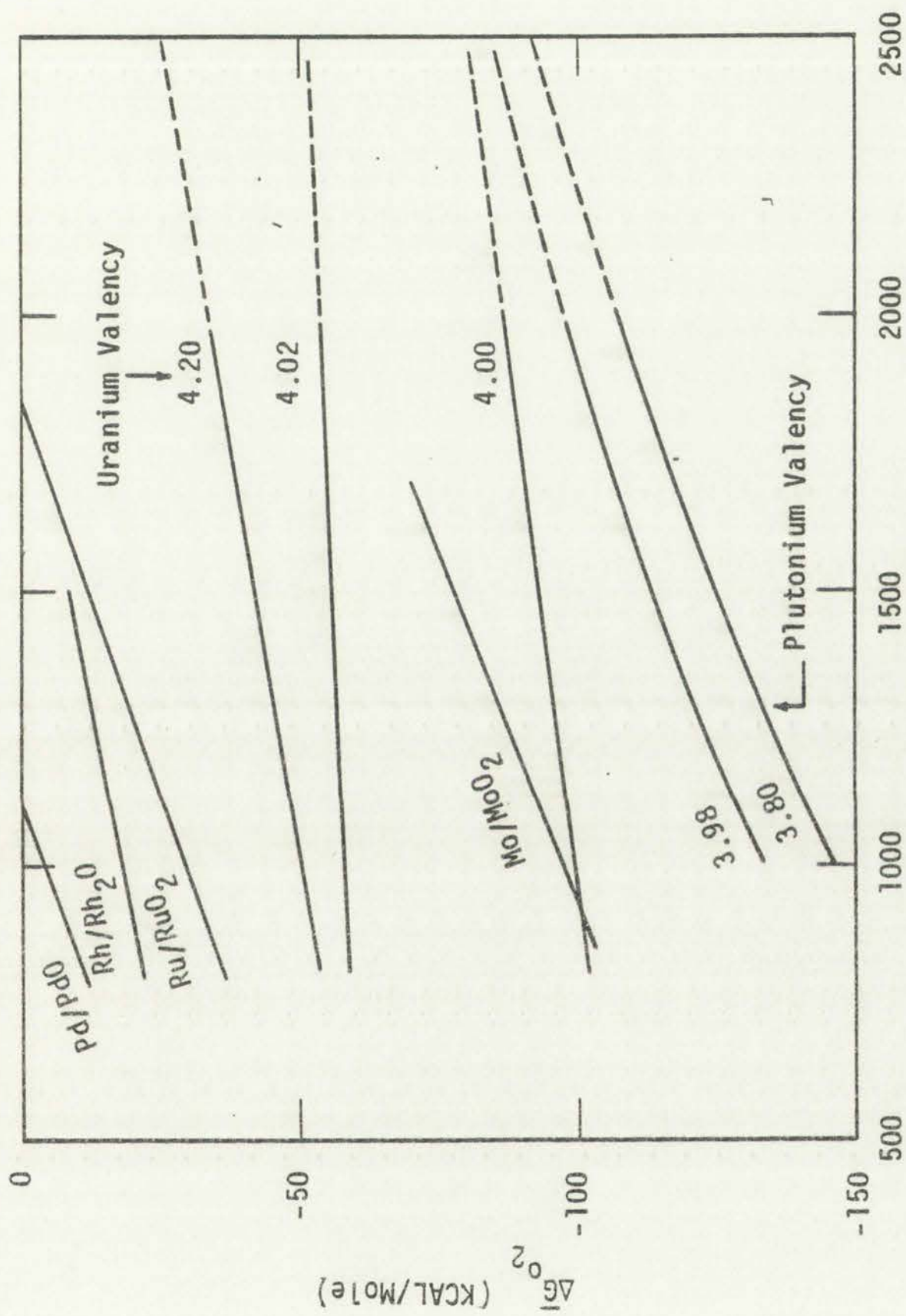
As seen in the Ellingham diagram, Fig. 2.6,^{1,11,20} the oxygen potential of MoO_2 is very close to that of stoichiometric fuel. The free energy of formation of Mo oxide is of the same order of magnitude as the fuel at low temperatures but increases rapidly with increasing temperature. It can also be seen that the oxygen potential of the fuel decreases as the fuel becomes more hypostoichiometric. Thus for hypostoichiometric fuel at temperatures of relevance to reactor

range between the constant average and minimum fuel temperatures at
steady state operation. These three elements exist in various degrees
of their region they exhibit by the same behavior in the first place
loss of the fuel's properties such as it was noted with the loss of
it and conductive in the fuel, which of the fuel, the, at the end-

fuel transfer.
A typical concentration profile for a fuel pin shows high
concentration of boron in the peripheral region of the fuel pin in
the region of the peripheral fuel pin. It was not detected within the
central region but was found in the center and outer in this region.
According to the fuel pin characteristics of design shown in Figure 1
this region may be diffusion through the walls.

3.1. Discussion

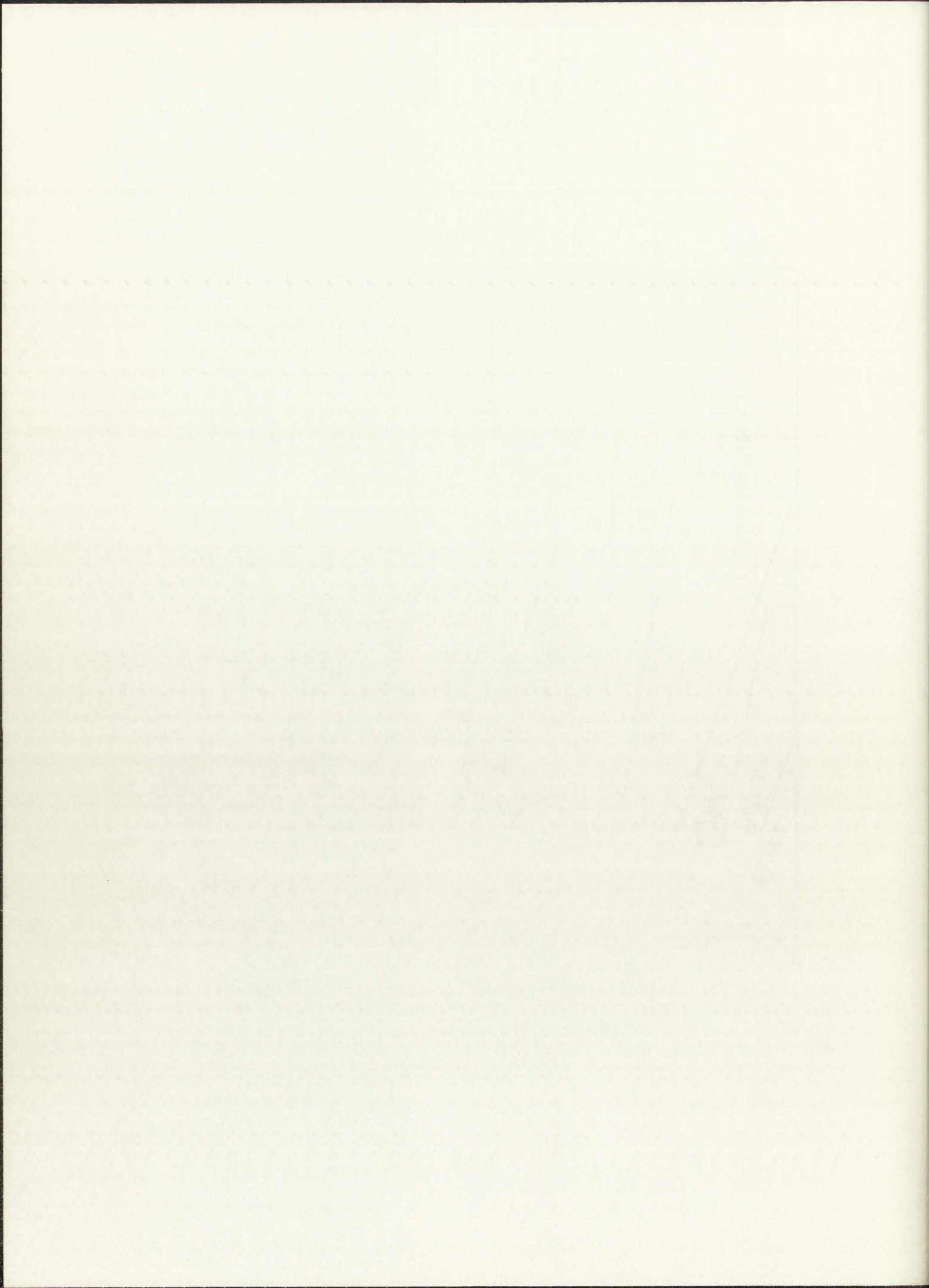
The chemical state of the fuel pin is dependent on the fuel pin
temperature. The extent of boron transfer depends on two factors
as temperature, fuel composition, oxygen potential, and initial boron
content. As seen in the literature diagram, Fig. 1, the oxygen
potential of the fuel is very close to that of atmospheric level. The
free energy of formation of boron is at the same order of magnitude
level as the fuel at low temperatures but increases rapidly with in-
creasing temperature. It can also be seen that the oxygen potential of
the fuel increases as the fuel temperature increases. The
for boron transfer fuel at temperatures of interest is shown



Temperature (K)

Figure 2.6

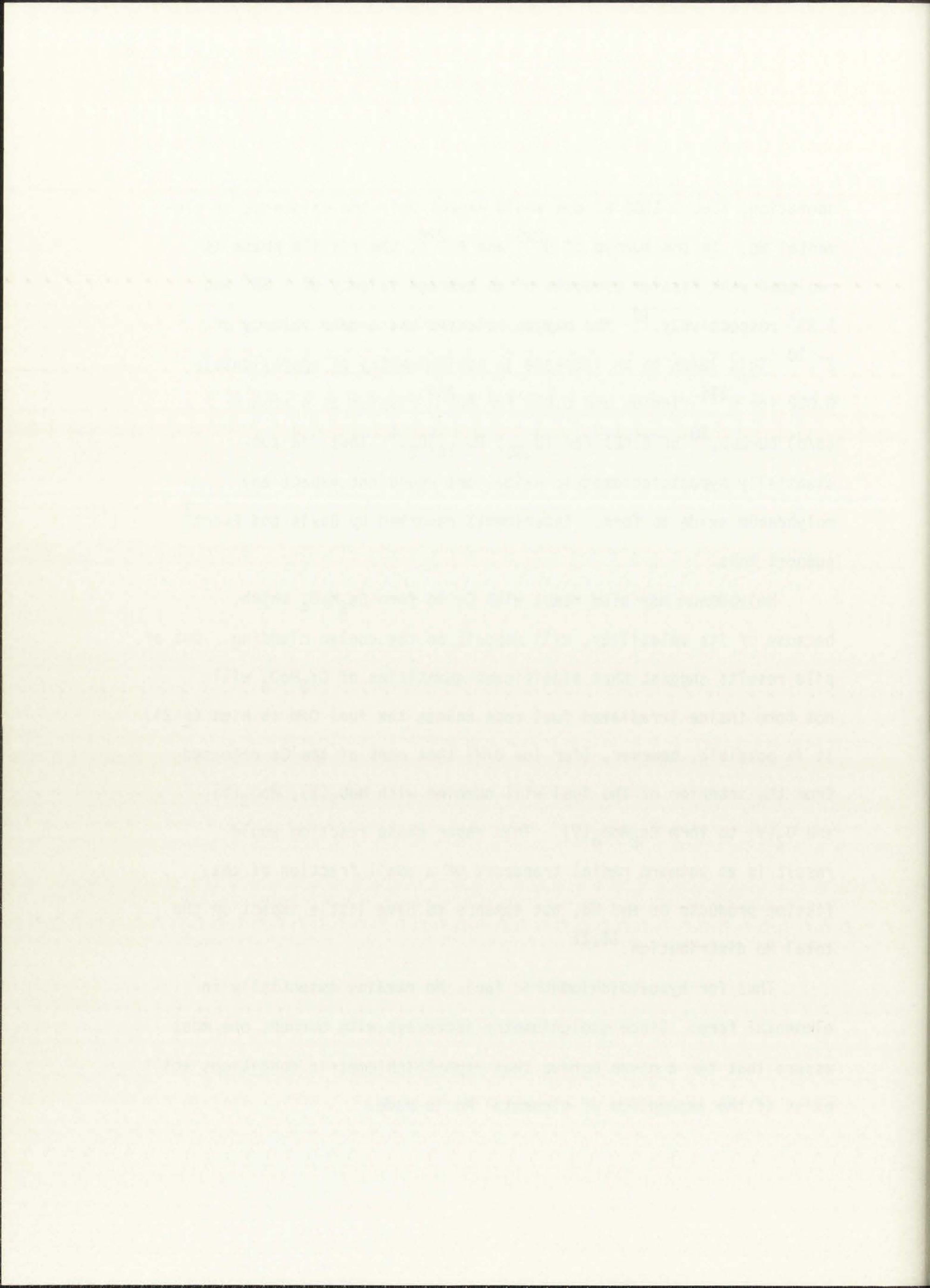
Ellingham diagram comparison of oxygen potentials of uranium, plutonium oxides as a function of U valency (> 4.00) and Pu valency (< 4.00) and some fission product metal/metal oxide couples.



operation, i.e. > 1000 K, one would expect only the existence of elemental Mo. In the burnup of U^{235} and Pu^{239} , the fissile phase is replaced with fission products of an average valency of 1.68^+ and 1.29^+ respectively.¹⁰ The oxygen released has a mean valency of 2^- .¹⁰ This leads to an increase in stoichiometry of approximately 0.012 for U^{235} fission and 0.028 for Pu^{239} fission at 4 atom % (a/o) burnup,¹⁰ or 0.021 for $(U_{.85}, Pu_{.15})O_2$.¹ Thus, in substantially hypostoichiometric oxide, one would not expect any molybdenum oxide to form. Experiments reported by Davis and Ewart¹ support this.

Molybdenum may also react with Cs to form Cs_2MoO_4 which, because of its volatility, will deposit on the cooler cladding. Out of pile results suggest that significant quantities of Cs_2MoO_4 will not form inside irradiated fuel rods unless the fuel O/M is high (≥ 2). It is possible, however, (for low O/M) that part of the Cs released from the interior of the fuel will combine with $MoO_2(V)$, $MoO_3(V)$, and $O_2(V)$ to form $Cs_2MoO_4(V)$. This vapor phase reaction would result in an outward radial transport of a small fraction of the fission products Cs and Mo, but appears to have little impact on the total Mo distribution.^{16,21}

Thus for hypostoichiometric fuel, Mo remains essentially in elemental form. Since stoichiometry increases with burnup, one must assure that for a given burnup that hypostoichiometric conditions still exist if the assumption of elemental Mo is made.



2.6 Stable Metallic State

The fission products As, Ge, Nb, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, and Mo exist in the metallic state or have oxides that are easily reduced at fuel operating temperatures. This is due to the fact that these elements have free energies of formation higher, and are thus less stable, than UO_2 and PuO_2 . Since the free energy of formation of some of the fission product oxides (Pd, Rh, Ru, Tc, etc.) is positive in the temperature range of interest (2000 to 2500 K), energy must be provided to form these oxides.

Microanalysis of irradiated fuel^{1,9,10,12-18,21-29} shows the presence of small inclusions, approximately 5 to 10 μm in diameter, believed to be the aggregation of these insoluble solid fission products (see Fig. 1.1). This form of fission products is a logical target for possible contribution to fuel swelling during an overpower transient. The inclusions are distributed throughout the columnar and equiaxed portion of the fuel pin and if vaporization or even partial vaporization of these inclusions occur, fuel foaming as a driving force for axial and/or radial fuel motion is a distinct possibility.

The composition of these metallic inclusions have been investigated by a number of people. Bradbury²⁵ analyzed inclusions found in UO_2 , irradiated in the thermal flux, PLUTO reactor to 4.6 atom % burnup with an estimated center temperature of 1720 K. He found two types of inclusions: one containing molybdenum and ruthenium and the other barium and traces of cerium; the two never combined. In a later

1.2. Particle Size Distribution

The particle size distribution of the reaction products was determined by means of a laser light scattering apparatus. The results are shown in Figure 1. It is seen that the distribution is very narrow and centered around 0.1 μ m. This is due to the fact that the reaction products are very small and uniform in size. The laser light scattering apparatus used was a Malvern 4700.

Micrographs of the reaction products were also taken. The results are shown in Figure 2. It is seen that the particles are very small and uniform in size. This is in agreement with the results of the laser light scattering apparatus. The particles are also very uniform in shape. This is due to the fact that the reaction products are very small and uniform in size. The micrographs were taken with a Zeiss 10A electron microscope.

The composition of these metallic inclusions has been investigated by means of energy dispersive X-ray analysis. The results are shown in Table 1. It is seen that the composition of the inclusions is very uniform. This is in agreement with the results of the laser light scattering apparatus. The inclusions are also very uniform in size. This is due to the fact that the reaction products are very small and uniform in size. The energy dispersive X-ray analysis was carried out with a JEOL JXA-733.

report,¹⁹ however, he stated that all inclusions contained molybdenum, ruthenium, technetium, and rhodium and that only 80 out of the 3723 inclusions contained in addition, barium, cerium, strontium, and zirconium. The relative concentrations of Mo, Ru, and Tc were estimated from count rate measurements using an electron microprobe and found to be

$$\text{Mo:Ru:Tc} = 3.7:1.6:1$$

which agrees well with the values calculated from fission product yield⁴ of 4.1:1.8:1. This leads one to conclude that the segregation of these fission products is almost total and that very little of these elements remains in solution in the fuel matrix.

Jeffery,¹⁸ using an electron microprobe, analyzed the same batch of 4.6% burnup material. He found the inclusions to be small (on the average less than 5 μ m in diameter). His microprobe analysis of 26 different inclusions revealed 3 basic types:

1. 70% contained Mo without Ba. Rhodium, ruthenium, technetium, and neodymium were always detected in the presence of Mo.
2. 15% of the inclusions contained both Mo and Ba. Rhodium, ruthenium, and technetium were also detected along with trace amounts of other elements.
3. 15% contained Ba without Mo. Cerium, neodymium, zirconium, and strontium were also detected.

Table 2.2 contains the average weight percents of the three type of inclusions. This low irradiation temperature fuel is nonprototypic, and Jeffery does not indicate in which section of the fuel pin either axially or radially these 26 inclusions were found. This may or may

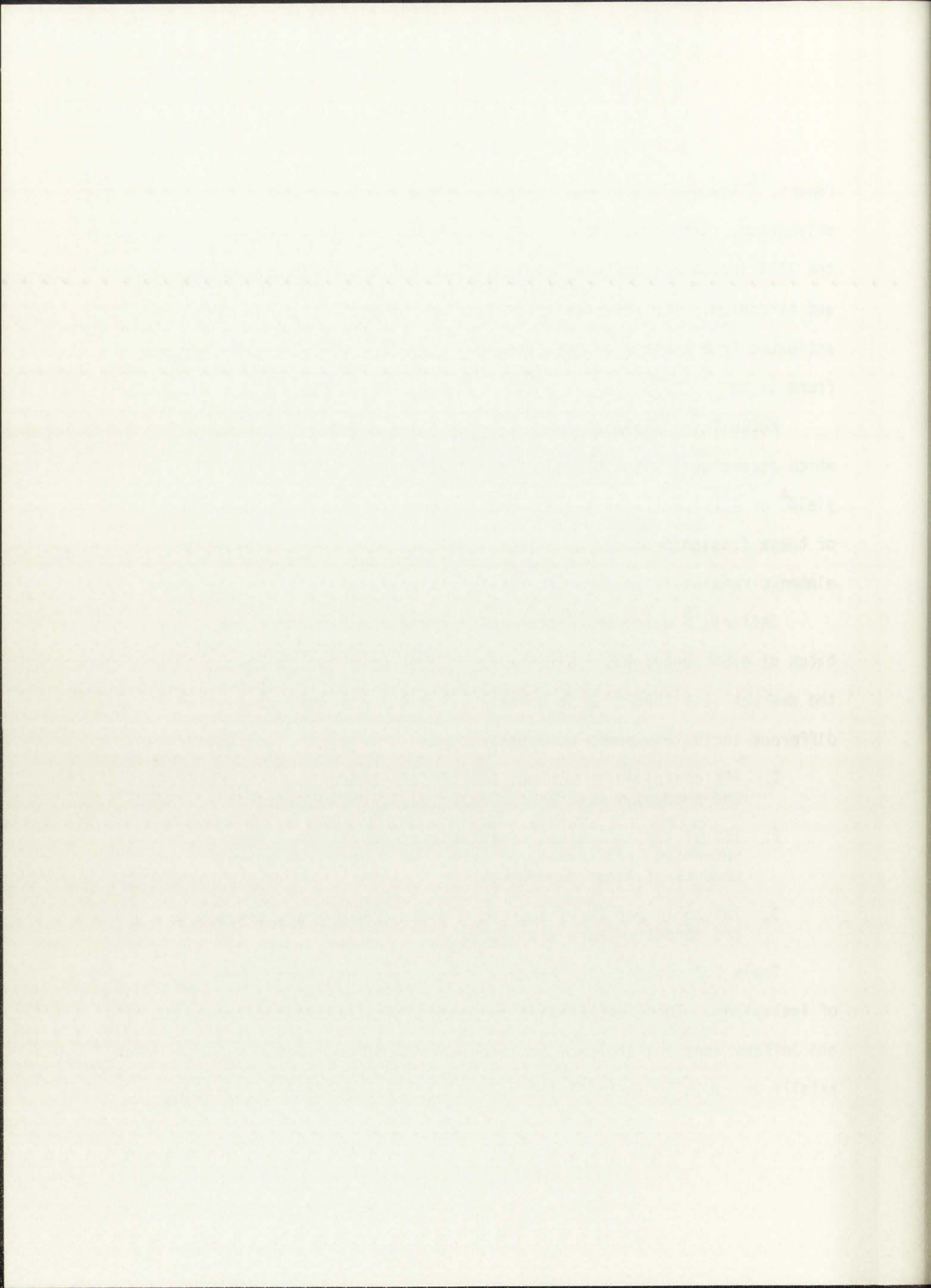


TABLE 2.2
COMPARISON OF INCLUSION COMPOSITIONS

Investigator	Fuel Description	Type of Inclusion	Constituent Weight %								Other Constituents
			Mo	Ru	Tc	Rh	Ba	Pd	Zr	Ce	
Bradbury 19	Highly enriched UO ₂ , thermal spectrum, low temp. (peak < 1800°k) 4.6 atom % B.U.	2%, Barium containing 98% Barium free	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Mo, Ru, Sr, Ce, Nd
Jeffery 18	Highly enriched UO ₂ , thermal spectrum, low temp. (peak < 1800°k) 4.6 atom % B.U.	70% Type 1	41	18	13	5	-	-	-	-	Te, Pd, Nd < 5 w/o
		15% Type 2	21	9	6		20	10	6	6	Sr, Nd, Rh < 5 w/o
		15% Type 3					25	10	5	5	Sr, Nd, Mo < 5 w/o
Bramman 29	(U.85, Pu.15) O ₂ , fast spectrum 8 - 8.5 atom % B.U. 2000°C < T < T melt	1 mm inclusion at center void 5-10 volume % of above incl.	41	32	15	7					
				2.5	11.9			38.4			
O'Boyle 12	(U.8, Pu.2) O ₂ , fast spectrum 2.7 atom % B.U.	6µm Inclusions	35	35	20	10					
				48	17						
Johnson 26	(U.8, Pu.2) O ₂ , fast spectrum 9.5 atom % B.U.	Averaged Type 1 inclusion from Pin, C-11, C-15	14.5	43.3	20	17.6			2.1		Fe = 2.45
		Type 2 Type 3	> 90						*72		Fe 13-30, Sb 1-2, Te .3-1.7

Year	1900	1901	1902	1903	1904	1905	1906	1907	1908	1909	1910	1911	1912	1913	1914	1915	1916	1917	1918	1919	1920	1921	1922	1923	1924	1925	1926	1927	1928	1929	1930	1931	1932	1933	1934	1935	1936	1937	1938	1939	1940	1941	1942	1943	1944	1945	1946	1947	1948	1949	1950	1951	1952	1953	1954	1955	1956	1957	1958	1959	1960	1961	1962	1963	1964	1965	1966	1967	1968	1969	1970	1971	1972	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025																																																							
Population	100	105	110	115	120	125	130	135	140	145	150	155	160	165	170	175	180	185	190	195	200	205	210	215	220	225	230	235	240	245	250	255	260	265	270	275	280	285	290	295	300	305	310	315	320	325	330	335	340	345	350	355	360	365	370	375	380	385	390	395	400	405	410	415	420	425	430	435	440	445	450	455	460	465	470	475	480	485	490	495	500	505	510	515	520	525	530	535	540	545	550	555	560	565	570	575	580	585	590	595	600	605	610	615	620	625	630	635	640	645	650	655	660	665	670	675	680	685	690	695	700	705	710	715	720	725	730	735	740	745	750	755	760	765	770	775	780	785	790	795	800	805	810	815	820	825	830	835	840	845	850	855	860	865	870	875	880	885	890	895	900	905	910	915	920	925	930	935	940	945	950	955	960	965	970	975	980	985	990	995	1000

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not have influenced the much higher percentage of barium rich inclusions found by Jeffery in the same fuel analyzed by Bradbury.

Jeffery compared the experimentally determined ratios of the concentrations of rhodium: ruthenium: technetium: molybdenum: barium (1:3.6:2.5:8.3:1.7) to the theoretical yield determined by Katcoff⁴ (1:3.6:2.0:8.1:1.9). Such agreement suggests that all five elements segregate almost completely into inclusions or at least do so in the same ratio as their fission yield. This applies only to regions where inclusions are formed, i.e. columnar and equiaxed.

In the work by Bramman et al.²⁹ $(U_{.85} Pu_{.15})O_2$ was irradiated to a maximum burnup of 8-8.5 atom % in the Dounreay Fast Reactor. The center temperature of the fuel was greater than 2273 K but less than the melting temperature of the fuel, hence representing more realistic operating conditions than the fuel analyzed by Jeffery. Microanalysis was performed on small metallic particles on the order of 1 mm diameter attached to the wall of the center void. X-ray analysis of one of the particles indicated the presence of Mo, Ru, Tc, and Rh with the following approximate concentrations:

Mo 41.0 wt. %, Ru 31.9 wt. %, Tc 14.9 wt. %, Rh 7.6 wt. %

Palladium was thought to be present in about 2 wt. %, but U and Pu, if present, were in a concentration less than .5 wt. % in the section exposed.

A separate phase existed adjacent to the fuel and constituted approximately one-tenth of the whole inclusion. Quantitative analysis

The first part of the paper describes the experimental setup and the results obtained. The second part discusses the theoretical aspects of the problem and compares the experimental results with the theoretical predictions. The third part presents the conclusions and the authors' suggestions for further research.

The authors are grateful to the National Science Foundation for the support of this work. The work was carried out at the University of California, San Diego.

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9. R. D. Burman, *Phys. Fluids*, **1**, 153 (1958).

10. R. D. Burman, *Phys. Fluids*, **1**, 153 (1958).

of this phase gave the composition as 25.4 wt. % U, 13.5 wt. % Pu, 38.4 wt. % Pd, 11.9 wt. % Rh, and 2.5 wt. % Ru. Tc and Mo were not present. Both phases contained no significant amount of oxygen and no other elements were present in excess of .5-1. wt. %.

Another interesting aspect of Bramman's work was the analysis of inclusions approximately 5 μm in diameter found within the fuel. A sample of $(\text{U}_{.85}\text{Pu}_{.15})\text{O}_2$ fuel irradiated in the Dounreay Reactor to 4.9% burnup was dissolved in nitric acid yielding an insoluble residue of the inclusions. These particles were analyzed with an electron microprobe and yielded the following composition:

35 wt. % Mo, 35 wt. % Ru, 20 wt. % Tc, 10 wt. % Rh.

As stated by Bramman, a probable error of $\pm 5\%$ exists on each figure because of the nature of the analysis. Palladium was also detected but only on the order of a few percent.

The initial O/M ratio of the mixed oxide was 2.004, slightly hyperstoichiometric. The relative proportion of molybdenum detected in the inclusions was approximately half of that predicted from a yield curve; therefore, as discussed in the previous section, the oxygen potential of the fuel is high enough for the formation of MoO_2 .

O'Boyle et al.¹² in their electron microprobe analysis of UO_2 -20 wt. % $\text{PuO}_{2.00}$, irradiated in a fast flux to a 2.7 atom % burnup, identified two separate types of solid-fission-product inclusions.

1. White metallic inclusion located in the equiaxed and columnar grain regions

2. A gray phase which was previously mentioned and located in the equiaxed grain region, thought to be insoluble oxides and zirconates.

The white metallic inclusions ranged in size up to $6\mu\text{m}$ in diameter. Ruthenium, molybdenum, and technetium account for approximately 90 wt. % of the inclusions with Rh and Pd making up the remaining 10%. The approximate concentrations can be seen in Table 2.2.

In ANL-7877²⁶ (Johnson) metallic inclusions from two mixed oxide pins irradiated in EBR-II were analyzed. The fuel description and irradiation history are given in Table 2.3.²⁶ Three distinctly different types of inclusions were found:

1. Noble-metal inclusions similar to those discussed previously found throughout the columnar-grain region and approximately midway through the equiaxed-grain region.
2. Inclusions with palladium as the principle constituent (60%-80%) alloyed with 10-30% of either iron, as an impurity in the fuel, or molybdenum or cladding constituents. These are generally found in the cooler equiaxed and unrestructured regions of the fuel.
3. Inclusions of essentially pure molybdenum alloyed with a few percent of other fission products. Only a few of these inclusions were found and were always located in the unrestructured region.

The summary electron microprobe analysis can be found in Table 2.2

It should be noted from Table 2.2 that none of the inclusions from $(\text{U}, \text{Pu})\text{O}_2$ examined thus far contain barium. Thus, it is unknown if the barium-bearing inclusions found in irradiated UO_2 occur in irradiated mixed oxide fuel. It may be possible that the increased yield of Pd at the expense of Zr in the fission of Pu may favor the formation of the palladium-rich, fissile-material phase, found by

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DOCUMENT SUMMARY

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Operator: Yvonne
Author: Sasa

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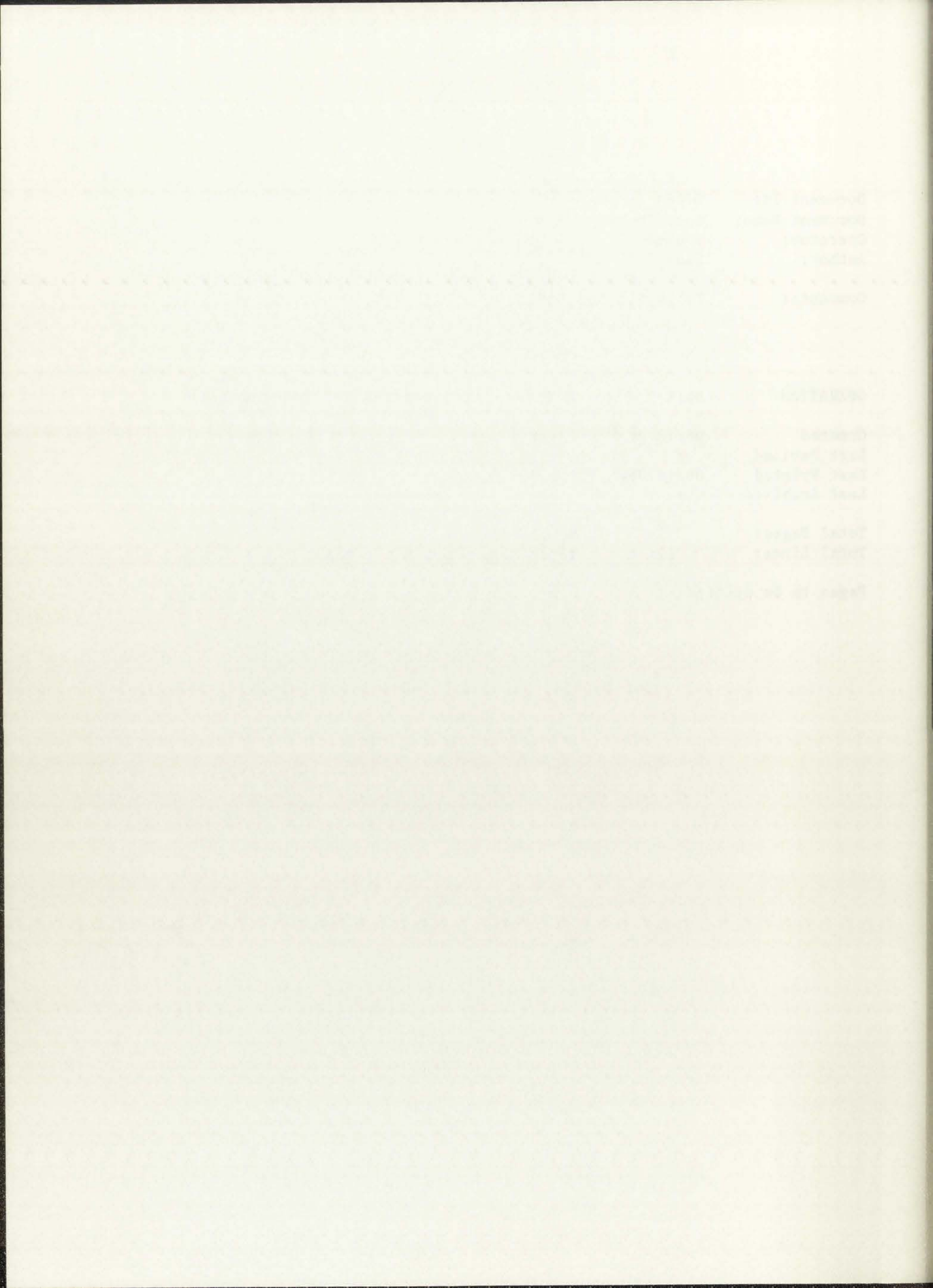
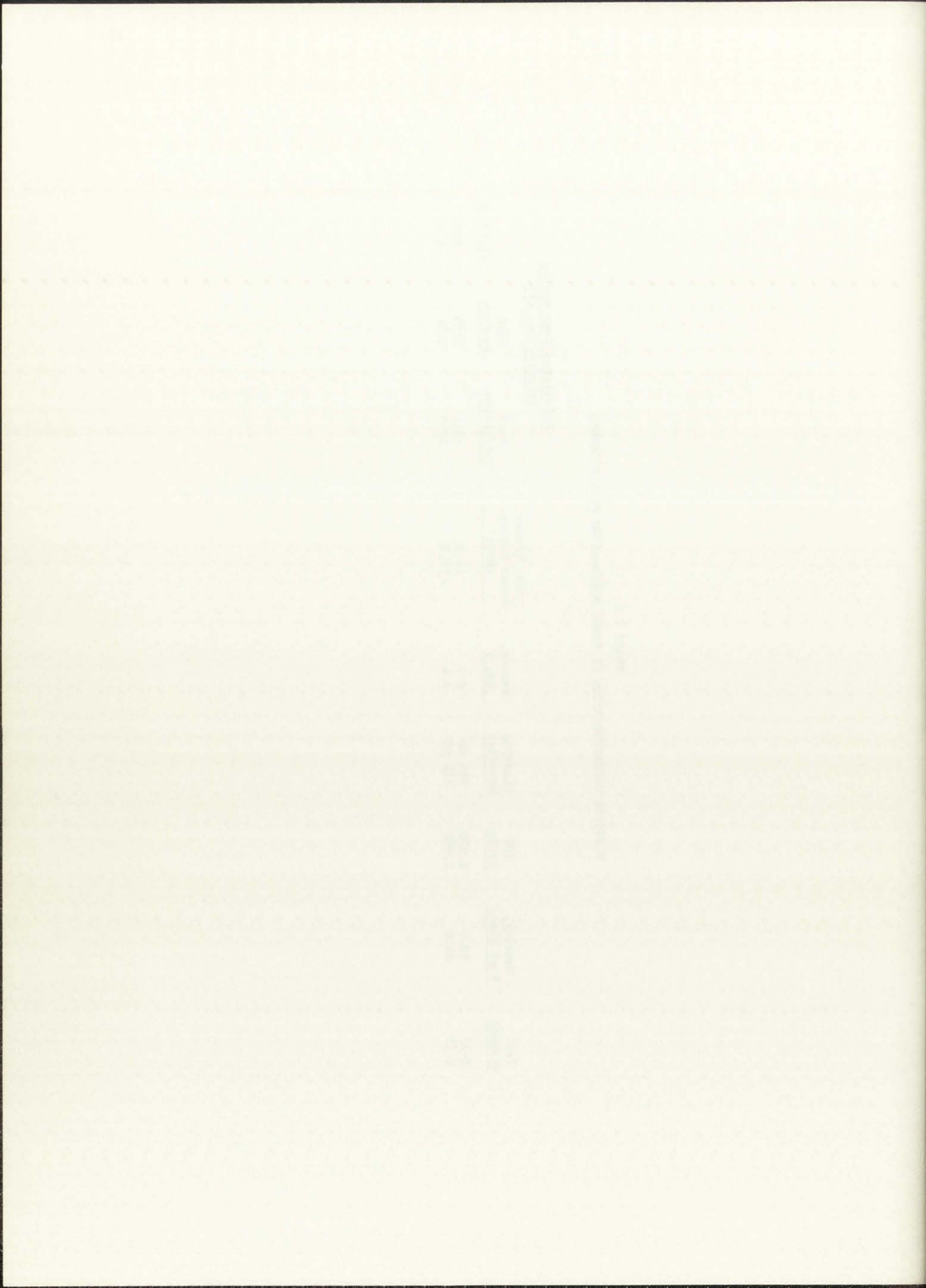


TABLE 2.3
 PHYSICAL CHARACTERISTICS OF NUMEC MIXED-OXIDE FUEL ELEMENTS

Fuel Element	Density, % of Theo.	O/M Ratio	Cladding Material	Burnup, at, %	Max. Linear Power Rating, kW/ft	Calculated Temp during Irradiation, (K)		
						Fuel Centerline	Fuel Surface	Cladding
C-11	90.6	2.000	316 SS	9.7	14.0	1511	1155	805
C-15	85.0	1.998	316 SS	9.4	12.9	2368	1166	814



Bramman, at the surface of metallic inclusions in preference to zirconate phases. The inclusion analysis also reflects the fact that plutonium fission favors the formation of Pd and Ru at the expense of Zr, Ce, and Sr.

In summary it can be seen that total agreement on inclusion composition has not yet been achieved. Many factors such as flux energy spectrum, original fuel stoichiometry, operating temperature, etc., affect the final composition. One does not expect total agreement, however, some inclusions differ quite markedly from the noble-metal inclusions which were found by all investigators. A graphic illustration (see Table 2.2) of this problem of fission product characterization is the nonagreement of the results of Bradbury and Jeffery analyzing the same fuel.

The mechanism by which metallic inclusions are formed is not completely understood. None of the molybdenum nuclides have volatile precursors with a half-life longer than 1 s. On the other hand, ruthenium and technetium nuclides all have molybdenum precursors. Some of the Ru and Tc nuclides are precursors of rhodium and palladium. It thus appears that molybdenum may be the diffusing species. Bramman, using an alloy of the same composition as the inclusion he found at the central void, found its melting point was between 2073-2173 K. It is possible that the inclusions close to the center may have been formed by the coalescence of molten fission products along cracks, but since inclusions have been observed in all parts of the mixed oxide fuel

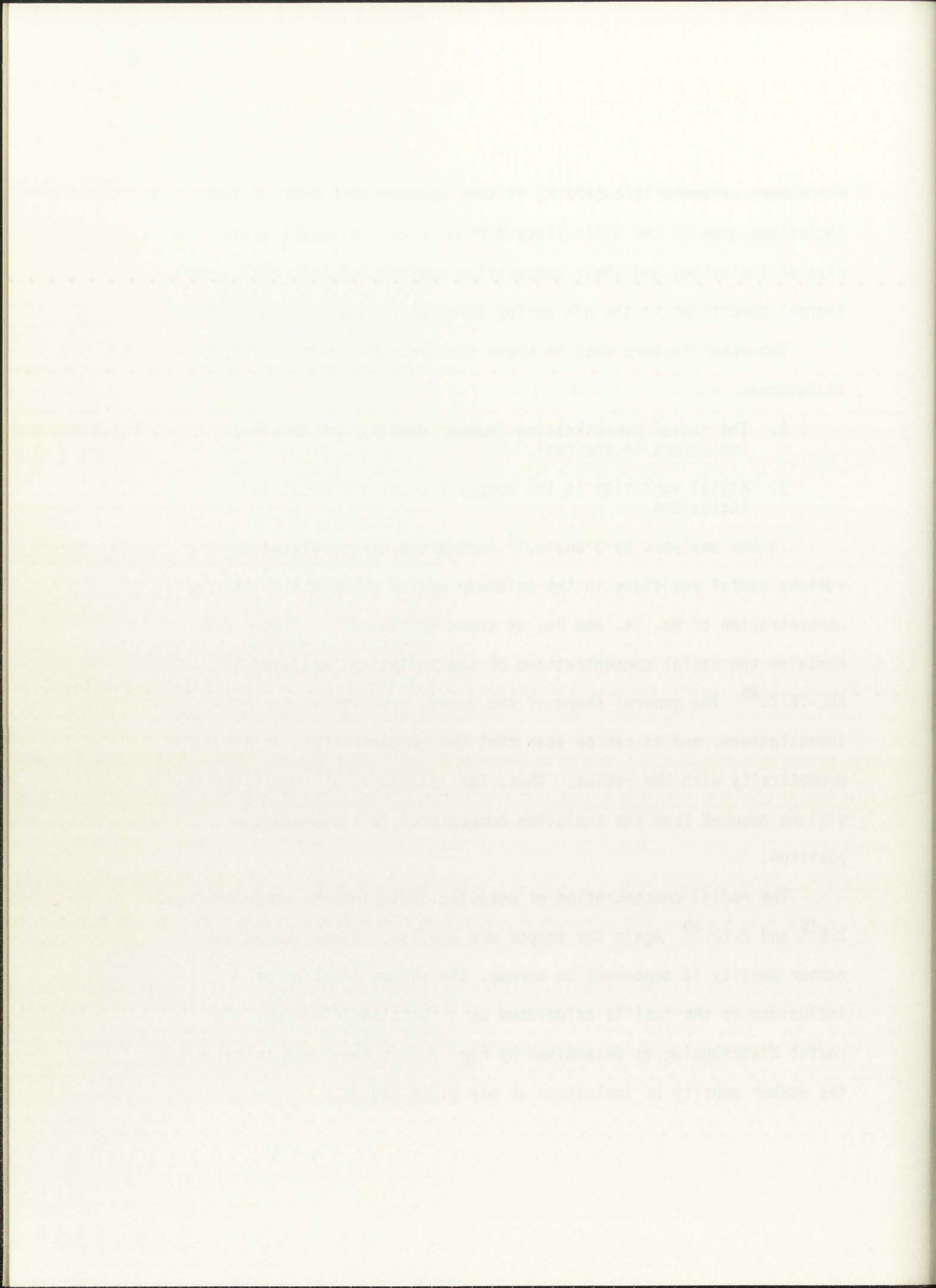
which have exceeded 1273-1473 K, it thus appears that most of the inclusions grow by the solid state diffusion of individual atoms. The size of inclusions and their composition must depend critically upon thermal conditions in the pin during irradiation and irradiation time.

Two other factors must be known to characterize the metallic inclusions:

1. The radial concentration (number density) of metallic inclusions in the fuel.
2. Radial variation in the composition of the metallic inclusions.

In the analysis by O'Boyle,¹² inclusions were analyzed at various radial positions in the columnar region to establish the radial concentration of Mo, Tc, and Ru, as shown in Fig. 2.7. Figure 2.8 contains the radial concentrations of the inclusions analyzed in ANL-7877.²⁶ The general shape of the curves are similar for both investigators, and it can be seen that the concentrations do not vary dramatically with the radius. Thus, for calculational simplicity it will be assumed that the inclusion composition is independent of position.

The radial concentration of metallic inclusions is shown in Figs. 2.9¹⁶ and 2.10.¹⁹ Again the shapes are similar. Since the actual number density is dependent on burnup, the volume fraction of inclusions in the fuel is calculated as a function of burnup. The radial distribution as determined by Fig. 2.9 is then used to calculate the number density of inclusions at any given radius.



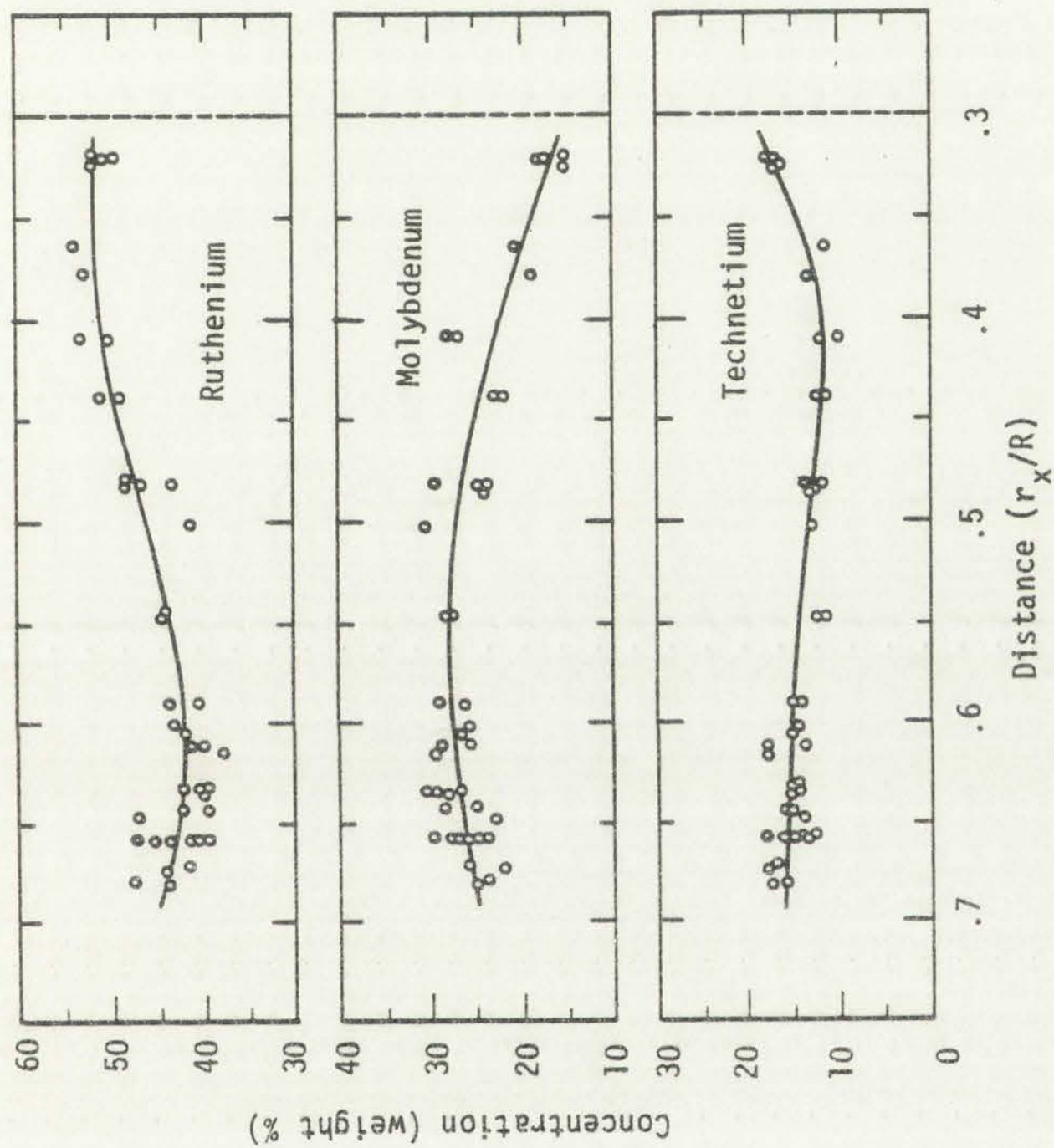


Figure 2.7.
O'Boyle's measured radial variation in Ru, Mo, and Tc concentrations in the metallic inclusions.

The concentration of the drug in the plasma is measured at various times after the start of the infusion. The concentration of the drug in the plasma is measured at various times after the start of the infusion.



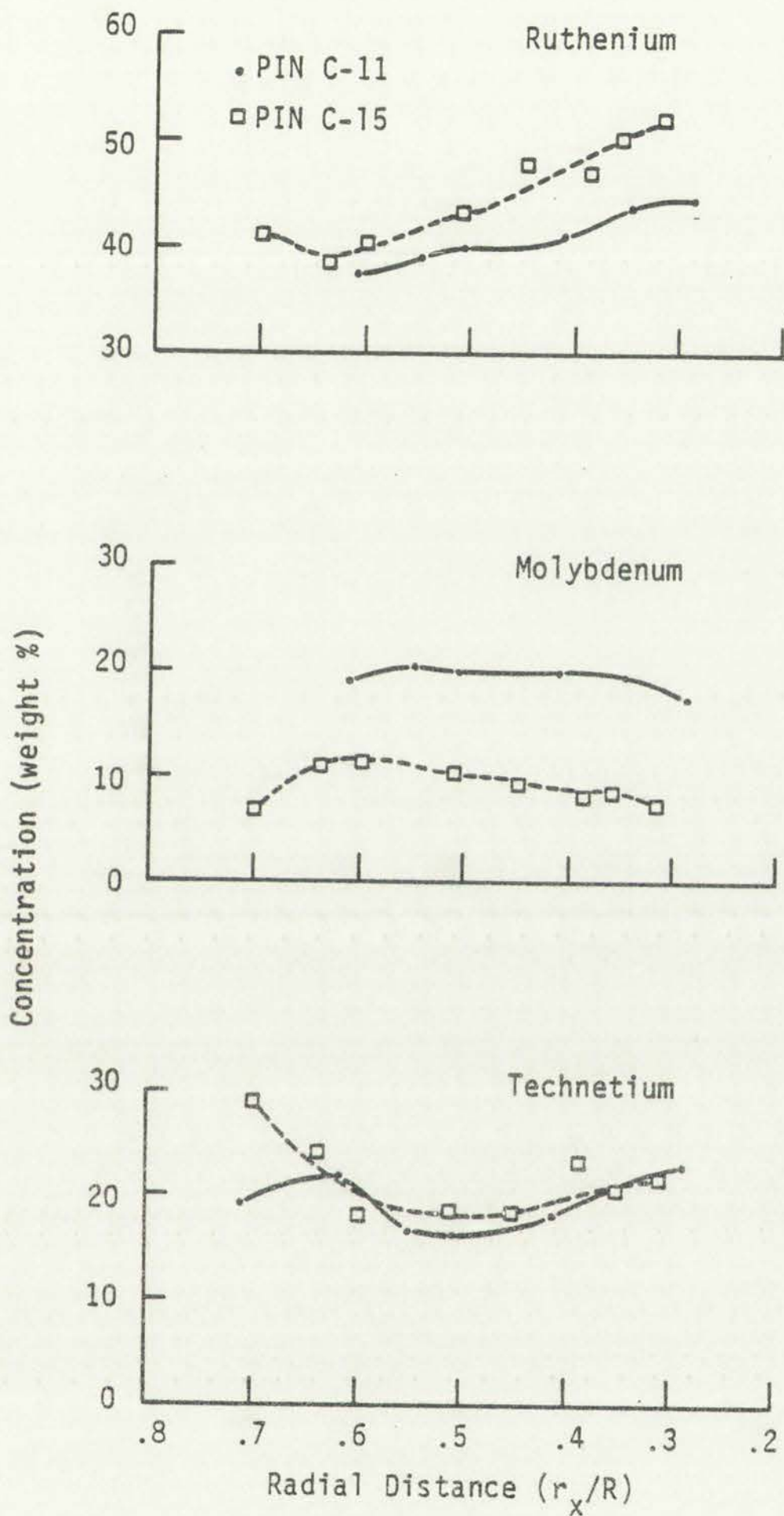
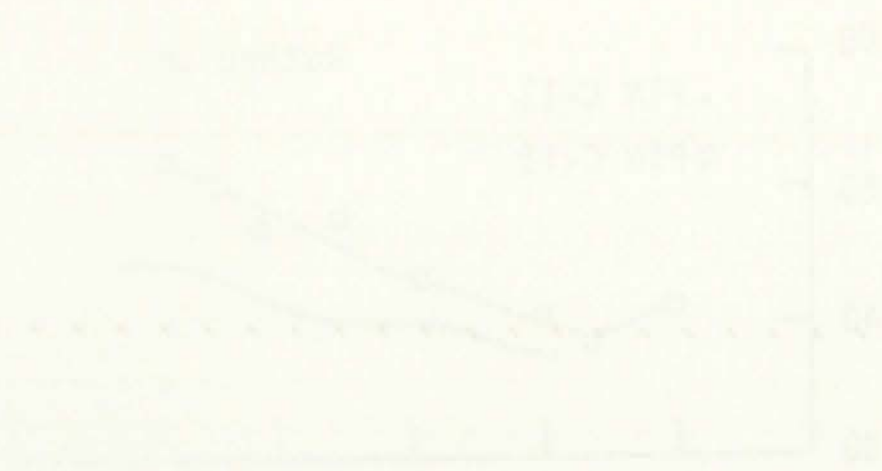


Figure 2.8.
Radial variation in composition
for Johnson inclusion.



(a) (b) (c)

Figure 1
 Effect of ...
 on ...

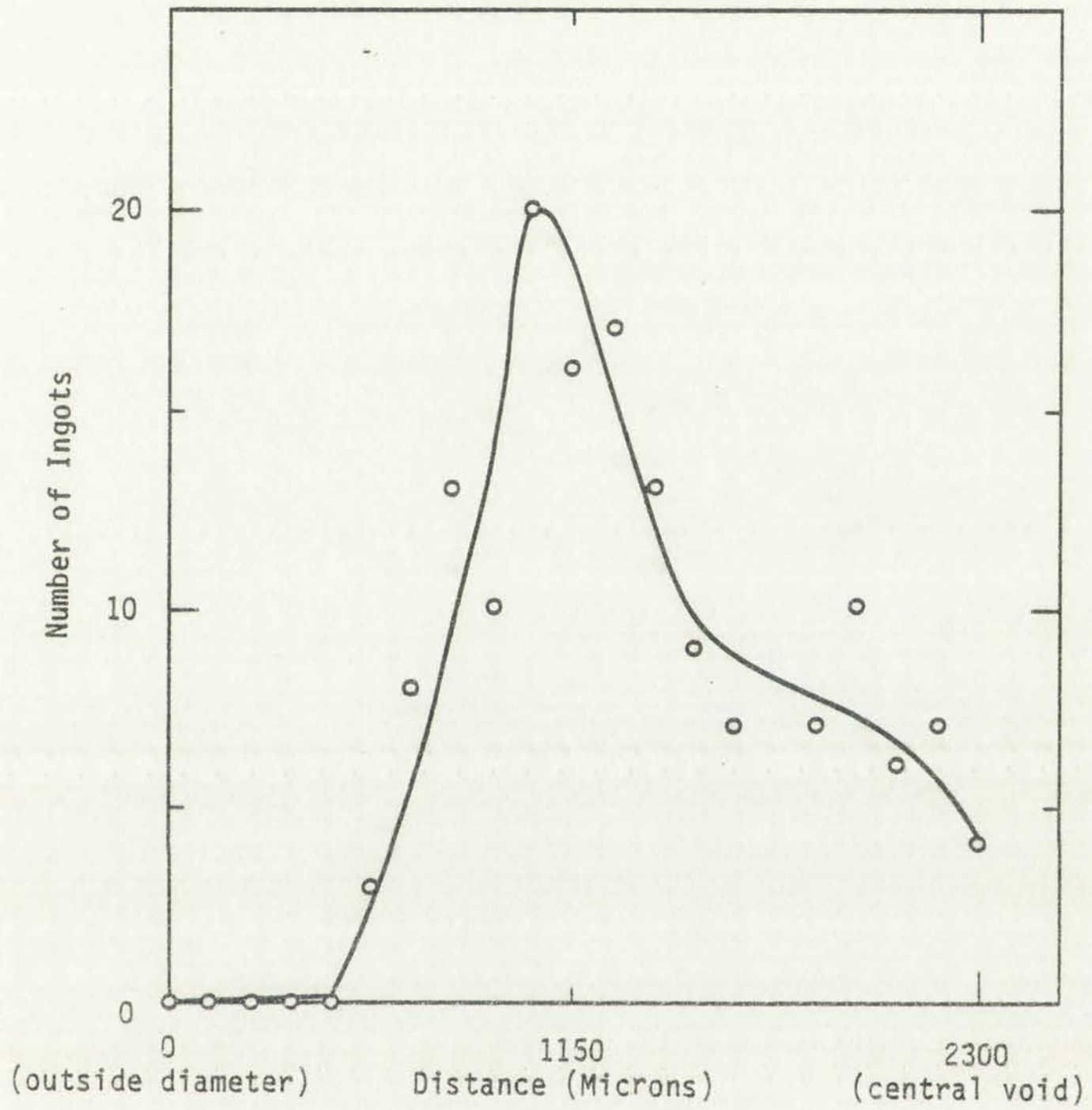


Figure 2.9.
Radial distribution of fission product ingots
in unit area found by Baird.¹⁶



Figure 1. Distribution of plants in a field. The x-axis represents distance in meters, and the y-axis represents the number of plants. The curve shows a peak at approximately 350 meters.

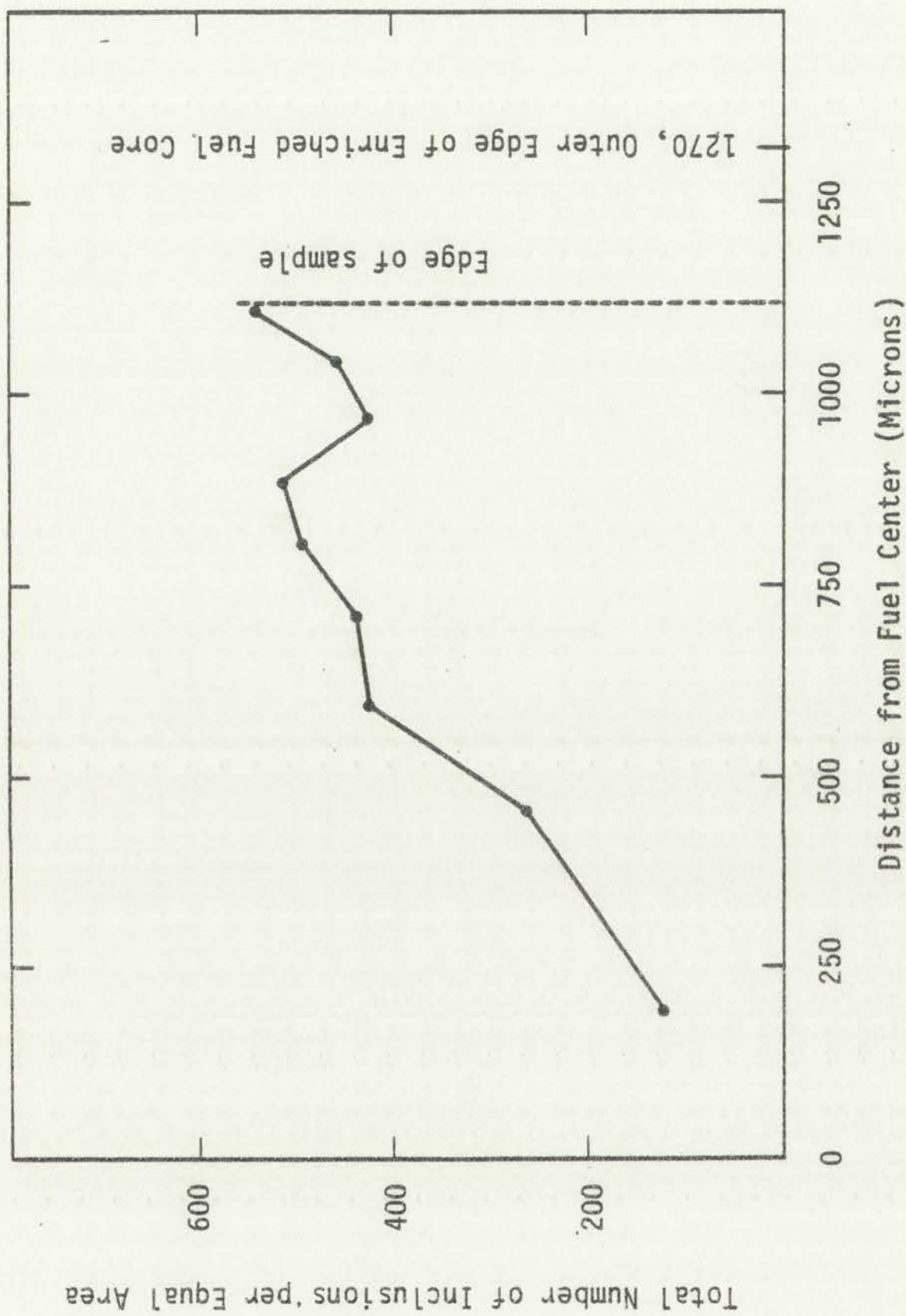


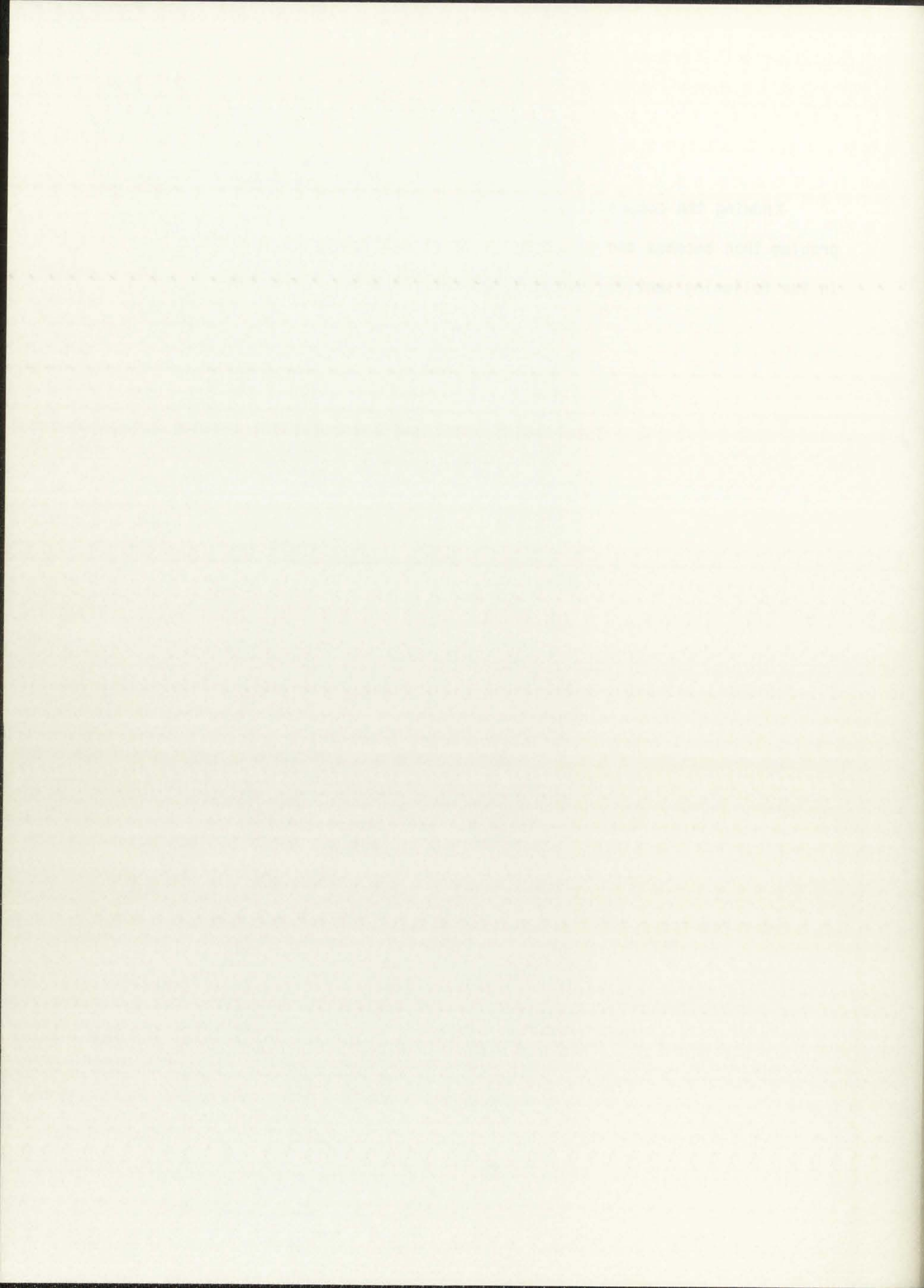
Figure 2.10.
Radial distribution of inclusions.

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2016-2017
2018-2019
2020-2021
2022-2023
2024-2025



Knowing the composition and distribution of inclusions, the problem then becomes one of assessing an effective equation-of-state. In the following section such an assessment is made.



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1. The first part of the report deals with the general situation of the country and the position of the various groups. It is a very interesting and well-written account of the country and its people. The author has done a great deal of research and has written a very interesting and well-written account of the country and its people. The author has done a great deal of research and has written a very interesting and well-written account of the country and its people.

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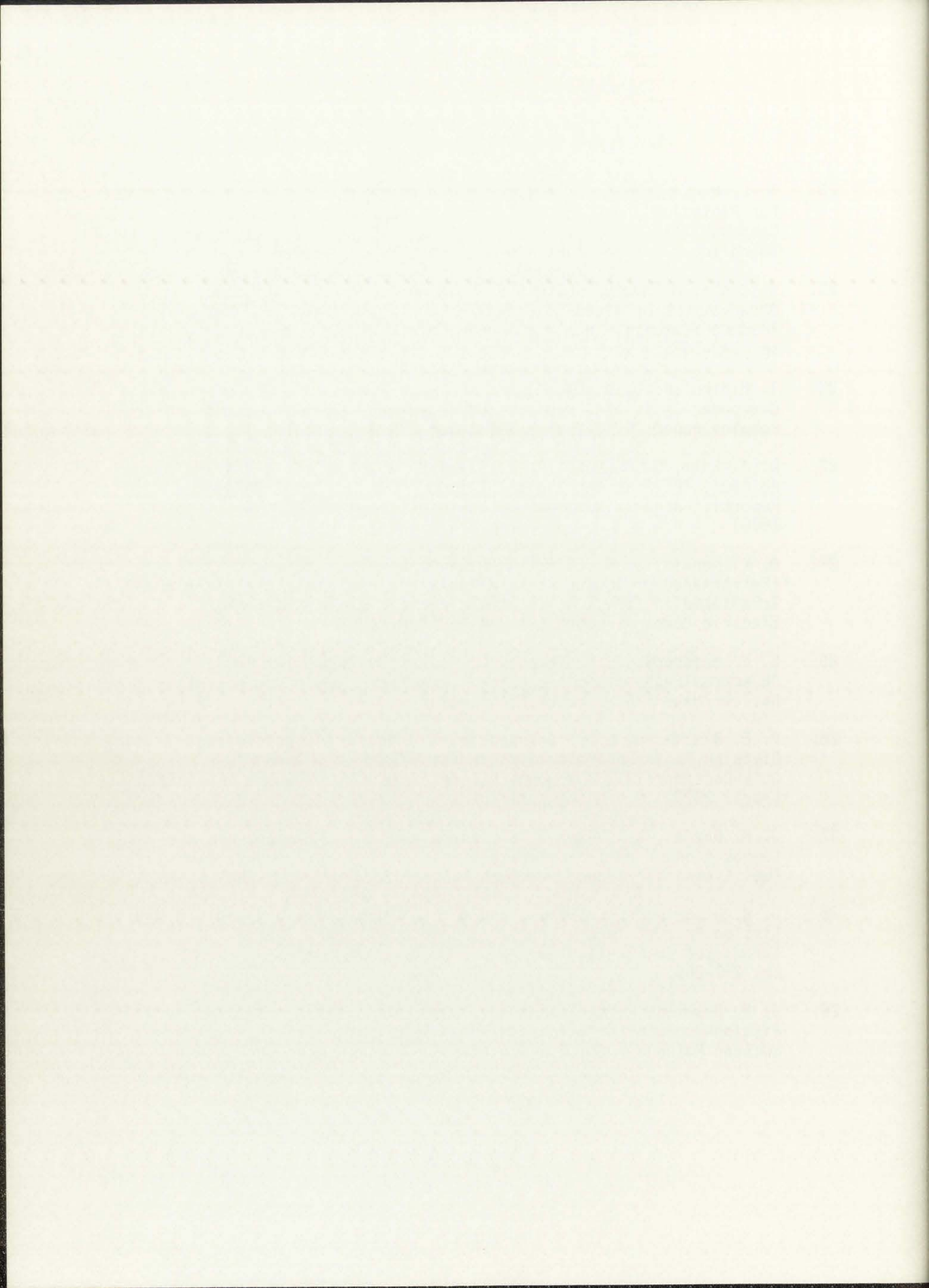
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3. EQUATION-OF-STATE

One problem that must be considered in determining the contribution of volatile fission products to the fuel motion is an appropriate equation-of-state (EOS) to model the PVT behavior for the various fission products.

Very little experimental PVT data currently exists in the literature for metal vapors with the exception of mercury, sodium, and cesium. Since cesium is a volatile fission product, various EOS's are used to calculate the molar volume of cesium to compare such calculated values with existing experimental data.¹⁻³ This is done over a range of pressures and temperatures in order to gain insight into the expected error in the molar volumes for the rest of the volatile species where little or no experimental data exists. The equations-of-state used to calculate the molar volumes are the Ideal Gas, the van der Waals, a modified hard-sphere, and the Redlich-Kwong EOS. In addition, calculations are performed using the generalized compressibility chart. Equations-of-state such as the Beattie and Bridgeman are not considered since they contain empirical constants which do not exist in the literature for the volatiles of interest, i.e. Pd, Fe, Sb, Te, Ba, etc.

3.1 Critical Points

The critical points for the volatiles are required in order to determine constants for the Van der Waals and Redlich-Kwong EOS. Using

The work of this study is presented in Chapter 2. The results of the study are discussed in Chapter 3. The conclusions of the study are presented in Chapter 4.

The first part of the study is a review of the literature on the topic. This is followed by a description of the methodology used in the study. The results of the study are then presented and discussed.

The second part of the study is a description of the methodology used in the study. This is followed by a description of the results of the study. The results are then discussed and compared to the literature.

The third part of the study is a discussion of the results of the study. This is followed by a discussion of the implications of the study. The study concludes with a summary of the findings and a list of references.

The fourth part of the study is a list of references. This is followed by a list of appendices. The study concludes with a list of references and a list of appendices.

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the technique of Young and Alder,⁴ the critical points are calculated assuming a mean-field approximation of the cohesive energy⁵ used in the classical van der Waals model; also required is the hard sphere atomic diameter,⁶ and the molar volume.⁵ The equations used and results are presented in Appendix B. Young and Alder⁴ compared calculated critical points with experimentally determined values. Their results indicate that the calculated critical volumes and temperatures are fairly close, usually within 30% of the experimentally determined values. The critical pressures, however, are off by as much as 100 to 200%. The calculated critical values listed by Gates⁷ differ substantially from those of Young.⁴ Thus analytical agreement has yet to be established. The values calculated in Appendix B will be used since more substantiated data is not available.

3.2 Equations

As stated previously, the equations-of-state compared are the Ideal Gas, the van der Waals, the modified hard-sphere, and the Redlich-Kwong. It should be noted, however, that in analyses of the fuel pin behavior during a transient, the local pressure and temperature are usually assessed or known and used to determine the molar volume of any volatiles present. Thus, the equations-of-state are solved in terms of the molar volume, with the pressure and temperature being independent variables.

The Ideal Gas Law expression is well known. It assumes no interaction between individual molecules and assumes the molecular volume as

insignificant. Its applicability is thus for very low density gas and this equation-of-state will not be expanded upon further. By using the critical isotherm,⁸ the van der Waals constants can be found in terms of the critical point as shown in Appendix C and, in particular, in terms of the more accurate V_c and T_c . The constants are put back into the general equation and solved in terms of the molar volume, yielding a cubic equation in term of the molar volume:

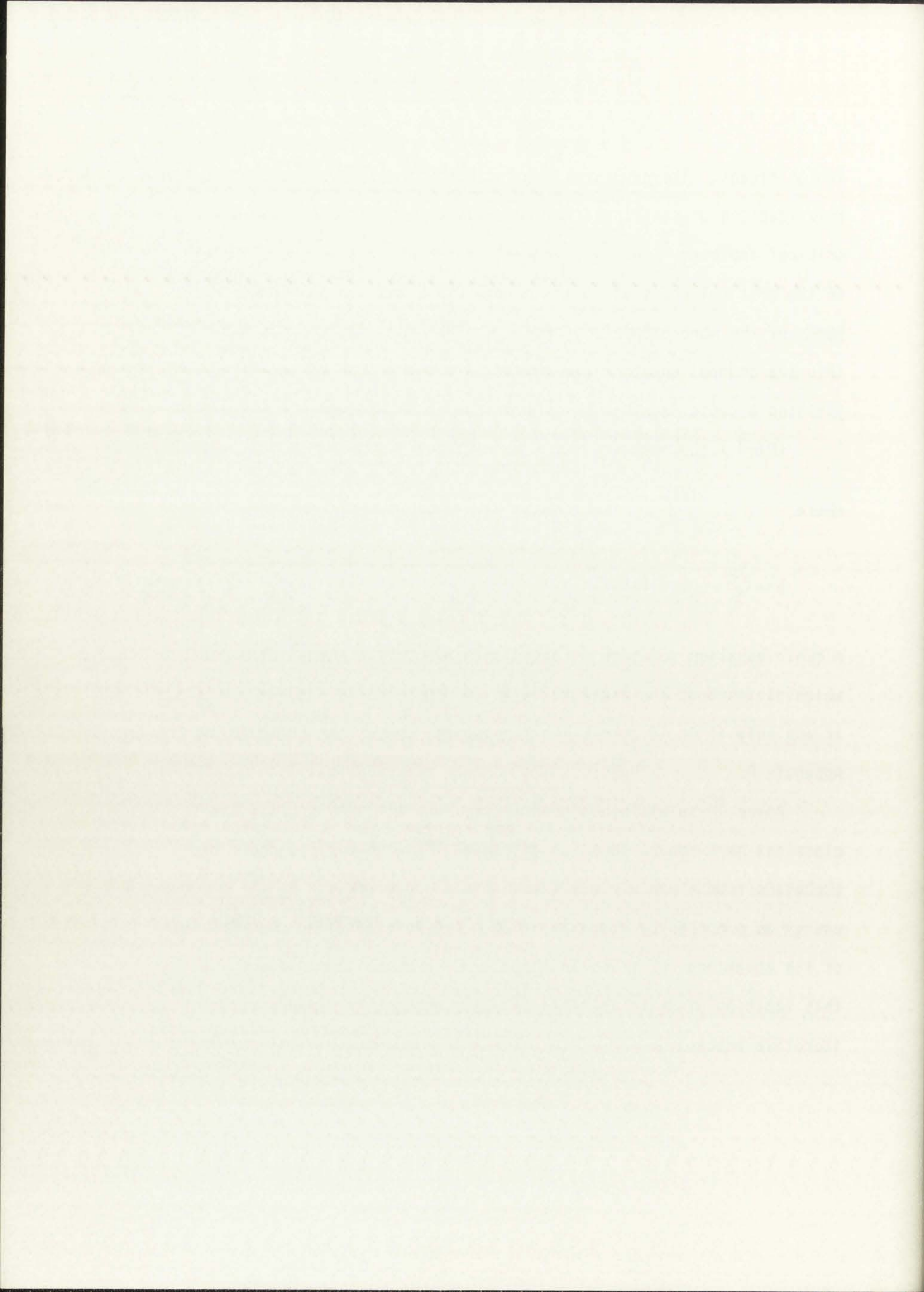
$$(P)v^3 - (bP + RT)v^2 + av - ab = 0 \quad (3-1)$$

where

$$b = \frac{V_c}{3} \quad , \quad a = \frac{27RbT_c}{8} \quad . \quad (3-2)$$

A cubic equation solution is based on d'Alembert's Lemma⁹ of algebra which states that the absolute value of a polynomial assumes a minimum if and only if it is zero. The subroutine, CUBIC, can be found in Appendix F.

Royce,¹⁰ in his equation-of-state work for metals, used the classical hard-sphere equation of state^{11,12} with a first order perturbation from a van der Waals mean-field approximation to the cohesive energy as proposed by Young and Alder.⁴ A more detailed description of the equations is given in Appendix D. Due to the complexity of this equation-of-state in terms of molar volume, it is solved by an iterative process.



The Redlich-Kwong equation of state^{13,14} is also included for comparison. As seen by this equation in Appendix E, its expansion is also cubic in terms of the molar volume. The numerical coefficients are determined empirically to fit moderate densities.

The generalized compressibility diagram¹⁴ is used to hand calculate the molar volume at a few of the experimental points. The results are listed in Table 3.1. Due to the lower limits on the compressibility diagram, only the experimental data points at high pressure and temperature could be analyzed. The critical values used are those calculated via Appendix B. It should be noted that since the compressibility, Z , must be read off the diagram, this technique to generate PVT information is not easily programmable, and would thus be unusable for future modeling. It does, however, provide a few points for comparison.

3.3 Results

A program to calculate the critical values and the molar volume as a function of P and T for the various equations-of-state can be found in Appendix F. This program is run at the experimental data points of cesium, and results are compared in Table 3.2. It can be seen that the Redlich-Kwong equation-of-state comes closer to predicting the experimental molar volumes than the remaining equations-of-state. It can also be seen that, as the molar volume becomes larger, the equations-of-state and the experimental value all approach ideal gas as required. At very low molar volumes, i.e. high

The first step in the analysis is to determine the critical values of the test statistic. This is done by comparing the observed test statistic to the critical values of the test statistic. The critical values are determined by the level of significance and the degrees of freedom of the test statistic.

The second step is to calculate the test statistic. This is done by using the formula for the test statistic. The test statistic is then compared to the critical values to determine whether the null hypothesis should be rejected. If the test statistic is greater than the critical value, the null hypothesis is rejected. If the test statistic is less than the critical value, the null hypothesis is not rejected.

The third step is to interpret the results of the test. This is done by comparing the test statistic to the critical values. If the test statistic is greater than the critical value, the null hypothesis is rejected. If the test statistic is less than the critical value, the null hypothesis is not rejected. The results of the test are then used to make a decision about the null hypothesis.

TABLE 3.1
CESIUM MOLAR VOLUMES FROM GENERALIZED COMPRESSIBILITY DIAGRAM

P_{ATM}	T °K	P_r	T_r	Z	$V = \frac{ZRT}{P}$ ℓ/g-mole	EXP. Value ℓ/g-mole	% Dev.
26.1	1533	.1155	.794	.905	4.3614	3.77	15.7
26.66	1667	.118	.864	.922	4.7303	4.406	7.36
124.13	2136.1	.549	1.107	.855	1.207	.585	106.36
64.96	1818.83	.287	.942	.860	1.976	1.442	37.01
75.07	1964.56	.332	1.018	.88	1.890	1.448	30.50
88.32	2168.61	.391	1.124	.90	1.8132	1.454	24.70

$$P_c = 226 \text{ atm}, P_r = \frac{P}{P_c}$$

$$T_c = 1930 \text{ °K}, T_r = \frac{T}{T_c}$$

$$R = .08205 \frac{\text{ℓ-atm}}{\text{°K mole}}$$

TABLE 1
 SUMMARY OF RESULTS FROM THE 1960-1961 CENSUS

Year	Age	Sex	Marital Status	Occupation	Income	Education	Health	Other
1960	15-24	M	Married	Professional	\$10,000	High School	Good	None
1960	25-34	F	Single	Service	\$5,000	High School	Fair	None
1960	35-44	M	Married	Managerial	\$8,000	High School	Good	None
1960	45-54	F	Married	Service	\$6,000	High School	Fair	None
1960	55-64	M	Married	Professional	\$12,000	College	Good	None
1960	65-74	F	Married	Service	\$4,000	High School	Fair	None
1960	75-84	M	Married	Professional	\$15,000	College	Good	None
1960	85-94	F	Married	Service	\$3,000	High School	Fair	None
1960	95-104	M	Married	Professional	\$18,000	College	Good	None
1960	105-114	F	Married	Service	\$2,000	High School	Fair	None

$\chi^2 = 10.5$
 $p < 0.05$
 $\chi^2 = 15.2$
 $p < 0.01$
 $\chi^2 = 20.1$
 $p < 0.001$

TABLE 3.2
COMPARISON OF CALCULATED AND EXPERIMENTAL RESULTS FOR CESIUM

P ATM	T °K	Specific Vol. μ/g_{mole}										
		Experimental Value	Ideal Gas	% Variation	Van der Maals	% Variation	Modified Hard Sphere	% Variation	Redlich Kwong	% Variation	Generalized Compressibility	% Variation
10.01	1677.	12.862	13.75	6.90	13.50	4.96	13.47	4.73	13.43	4.416		
6.73	1222.3	12.70	14.91	17.40	14.54	14.49	14.48	14.02	14.36	13.071		
5.02	1201.8	17.335	19.65	13.35	19.27	11.16	19.21	10.82	19.09	10.124		
4.79	1157.9	17.316	19.84	14.58	19.44	12.27	19.38	11.92	19.24	11.111		
1.12	980.5	66.46	71.83	8.08	71.32	7.31	71.27	7.24	71.06	6.921		
12.33	1586.8	9.595	10.56	10.06	10.30	7.35	10.26	6.93	10.21	6.410		
15.24	1404.44	6.245	7.561	21.07	7.246	16.03	7.201	15.31	7.121	14.027		
19.21	1668.4	6.29	7.126	13.29	6.876	9.32	6.847	8.86	6.805	8.188		
19.26	1527.9	5.468	6.509	19.04	6.226	13.86	6.189	13.19	6.129	12.089		
26.1	1533.	3.77	4.819	27.82	4.533	20.24	4.495	19.23	4.434	17.613	4.3614	15.7
33.21	1655.4	3.222	4.090	25.94	3.830	18.87	3.799	17.91	3.754	16.511		
3.23	1101.	24.99	27.97	11.92	27.55	10.24	27.48	9.96	27.32	9.324		
26.66	1667.	4.406	5.130	16.43	4.877	10.69	4.847	10.01	4.804	9.033	4.73	7.36
25.99	1513.3	3.693	4.778	29.38	4.485	21.45	4.446	20.39	4.383	18.684		
2.01	1684.2	67.7	68.75	1.55	68.51	1.20	68.49	1.17	68.45	1.108		
5.19	1659.7	25.367	26.24	3.44	25.99	2.46	25.96	2.34	25.92	2.180		
124.13	2136.1	.585	1.412	141.37	1.216	107.86	1.211	107.01	1.194	104.10	1.207	106.36
64.96	1818.83	1.442	2.298	59.36	2.060	42.86	2.037	41.26	2.006	39.11	1.976	37.01
75.07	1964.56	1.448	2.148	48.34	1.935	33.63	1.920	32.60	1.898	31.08	1.890	30.50
88.32	2168.61	1.454	2.015	38.58	1.832	26.00	1.826	25.58	1.812	24.62	1.8132	24.70

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pressure and low temperature, the equations-of-state inaccurately predict observed phenomena.

Based on this analysis, the Redlich-Kwong equation will be used. It appears from this analysis that an error in the molar volume for cesium of less than 30 to 40% can be expected in the projected temperature range, 2900 K to 6000 K, and pressure range, 25 to 100 atm., of interest. The error for the other volatiles, however, may be much higher. This depends on whether the vapor is monatomic or tends to form molecules, and on the accuracy of the calculated critical point and thus the Redlich-Kwong constants. For dense vapors, interatomic forces become important; thus the range of the quasistatic pressure used in later analysis will determine how seriously one must search for a more appropriate equation-of-state. It appears that for pressures less than 100 atms., the Redlich-Kwong equation-of-state is acceptable. One must also keep in mind that the Redlich-Kwong equation of state tends to overpredict the molar volume, and thus will tend to overpredict the quasistatic fuel motion also. A model for such fuel motion is presented in the following section.

The first part of the paper is devoted to a discussion of the general principles of the theory of the structure of the nucleus. It is shown that the structure of the nucleus is determined by the interaction of the nucleons, which are assumed to be point particles. The interaction is assumed to be of the Yukawa type, and the resulting equations are solved for the ground state of the nucleus. It is shown that the ground state is a bound state, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

In the second part of the paper, the structure of the nucleus is studied for excited states. It is shown that the excited states are also bound states, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

The third part of the paper is devoted to a discussion of the structure of the nucleus for large values of the mass number. It is shown that the structure of the nucleus is determined by the interaction of the nucleons, which are assumed to be point particles. The interaction is assumed to be of the Yukawa type, and the resulting equations are solved for the ground state of the nucleus. It is shown that the ground state is a bound state, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

In the fourth part of the paper, the structure of the nucleus is studied for large values of the mass number. It is shown that the structure of the nucleus is determined by the interaction of the nucleons, which are assumed to be point particles. The interaction is assumed to be of the Yukawa type, and the resulting equations are solved for the ground state of the nucleus. It is shown that the ground state is a bound state, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

where ϵ is the dielectric constant of the medium, \mathbf{E} is the electric field, \mathbf{H} is the magnetic field, \mathbf{J} is the current density, and ρ is the charge density.

The first part of the paper is devoted to a discussion of the general principles of the theory of the structure of the nucleus. It is shown that the structure of the nucleus is determined by the interaction of the nucleons, which are assumed to be point particles. The interaction is assumed to be of the Yukawa type, and the resulting equations are solved for the ground state of the nucleus. It is shown that the ground state is a bound state, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

In the second part of the paper, the structure of the nucleus is studied for excited states. It is shown that the excited states are also bound states, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

The third part of the paper is devoted to a discussion of the structure of the nucleus for large values of the mass number. It is shown that the structure of the nucleus is determined by the interaction of the nucleons, which are assumed to be point particles. The interaction is assumed to be of the Yukawa type, and the resulting equations are solved for the ground state of the nucleus. It is shown that the ground state is a bound state, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

In the fourth part of the paper, the structure of the nucleus is studied for large values of the mass number. It is shown that the structure of the nucleus is determined by the interaction of the nucleons, which are assumed to be point particles. The interaction is assumed to be of the Yukawa type, and the resulting equations are solved for the ground state of the nucleus. It is shown that the ground state is a bound state, and the binding energy is calculated. The results are compared with the experimental data, and it is shown that the theory is in good agreement with experiment.

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1. The first part of the paper deals with the general theory of the subject.

2. The second part of the paper deals with the application of the theory to the case of the subject.

3. The third part of the paper deals with the application of the theory to the case of the subject.

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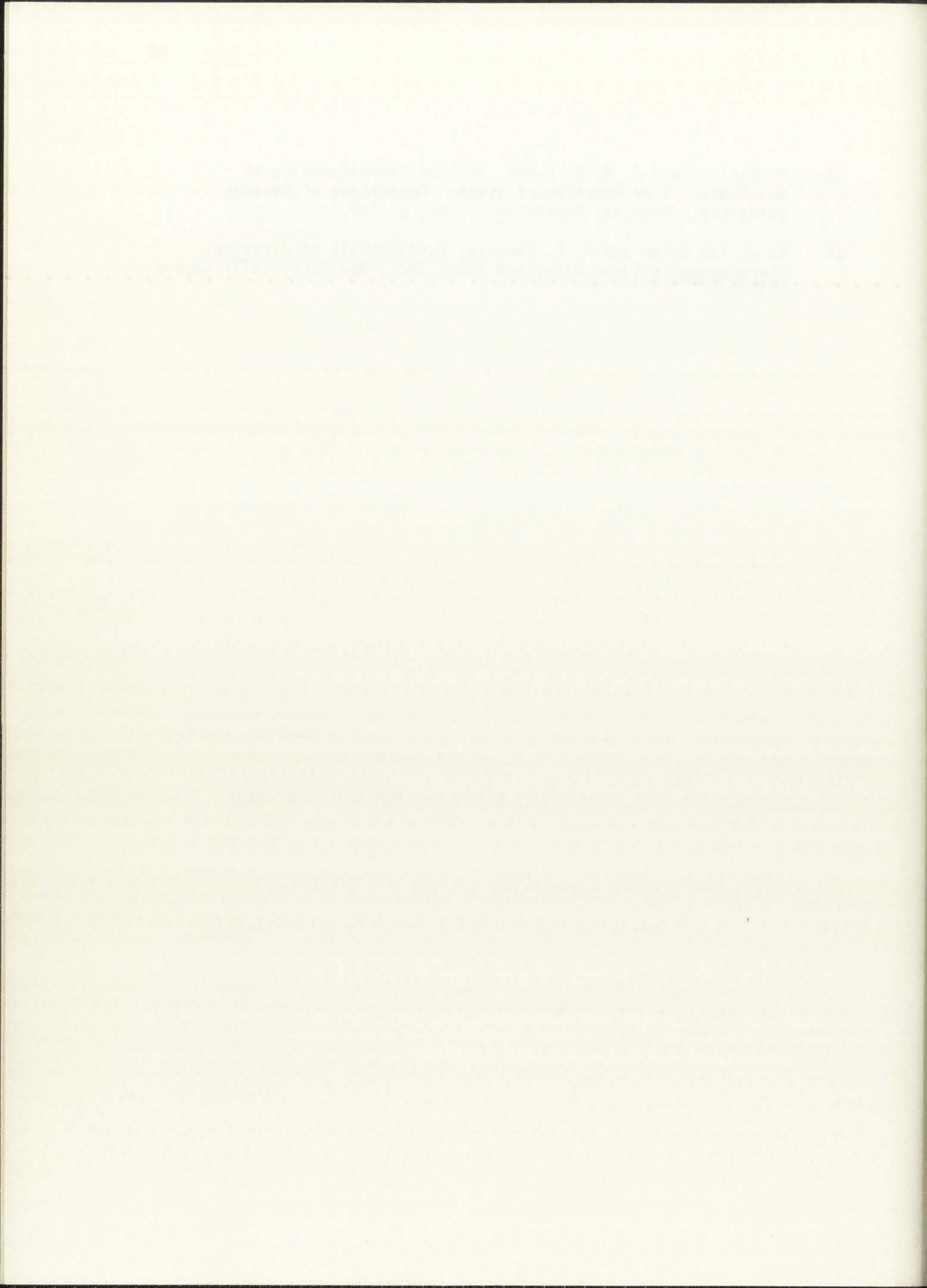
7. The seventh part of the paper deals with the application of the theory to the case of the subject.

8. The eighth part of the paper deals with the application of the theory to the case of the subject.

9. The ninth part of the paper deals with the application of the theory to the case of the subject.

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4. FUEL MOTION MODEL

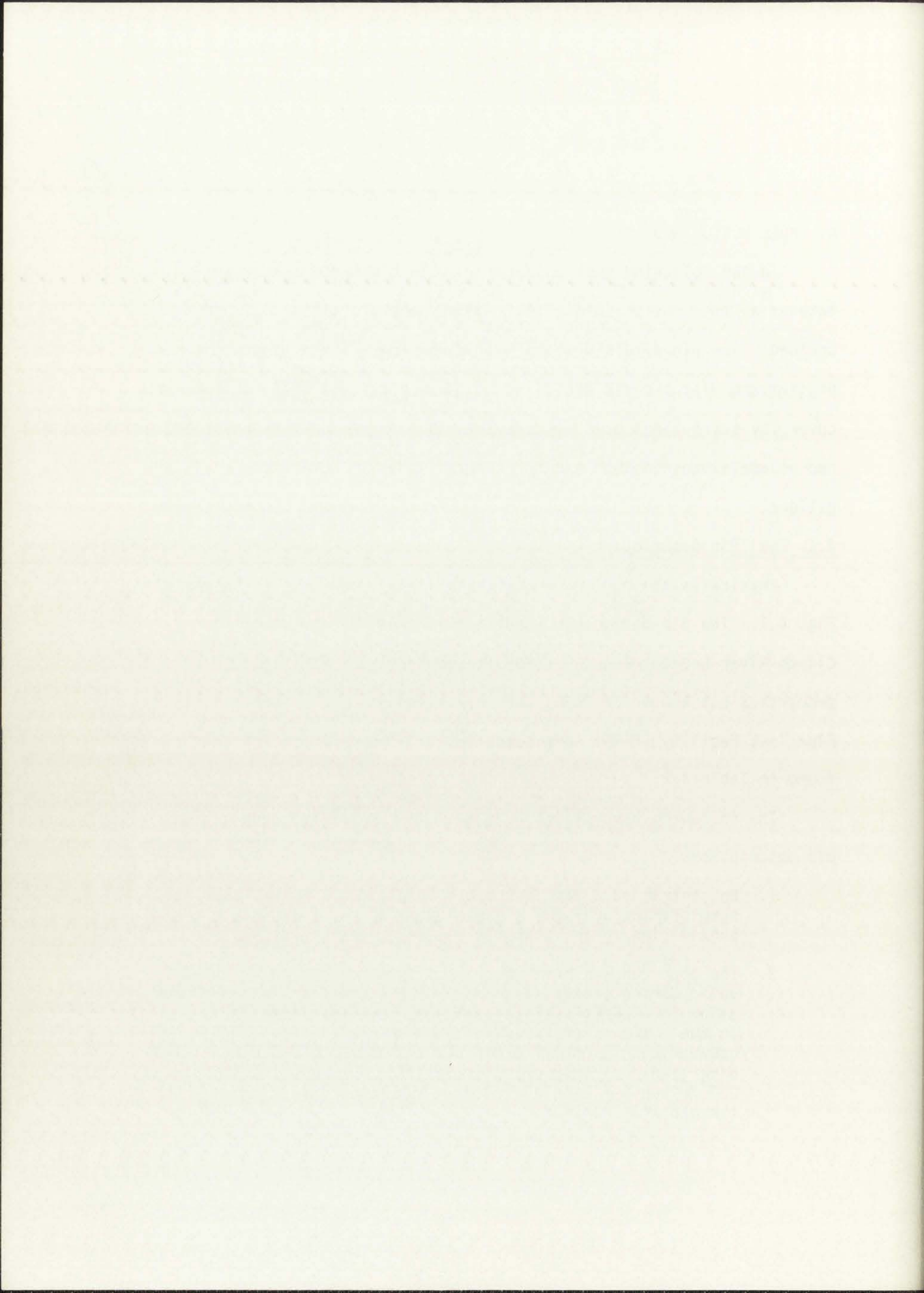
In the following sections, the input and program used to calculate axial fuel motion in a transient overpower condition will be described. The pin dimensions and inclusion compositions, input to the program, are discussed in the first two sections. The last two sections cover the subroutines used to calculate the pin temperature profiles and volume expansion that can be expected under the existing local conditions.

4.1 Fuel Pin Description

Physically the fuel pin model used in this analysis is shown in Fig. 4.1. The pin parameters used in this study are those of the Clinch River Breeder Reactor (CRBR) taken from HEDL-TME-75-12.¹ For properties not known for CRBR, the corresponding values from the Fast Flux Test Facility (FFTF) were substituted. These parameters can be found in Table 4.1.

The following assumptions were made concerning the general fuel pin description:

1. No central void was included. This assumption was made to simplify the analysis since only an order of magnitude approximation to the possible volume expansion was desired.
2. The bond gap was still present. This assumption is probably valid during steady state operation since for low power operation (≈ 7 kW/ft ave) the bond gap does not close until late in fuel life. For transient overpower accidents (TOP), however, differential temperatures between the fuel and cladding leads to rapid gap closure. For loss-of-flow (LOF) or a LOF driven TOP, the clad temperature may rise enough to keep the gap from closing.



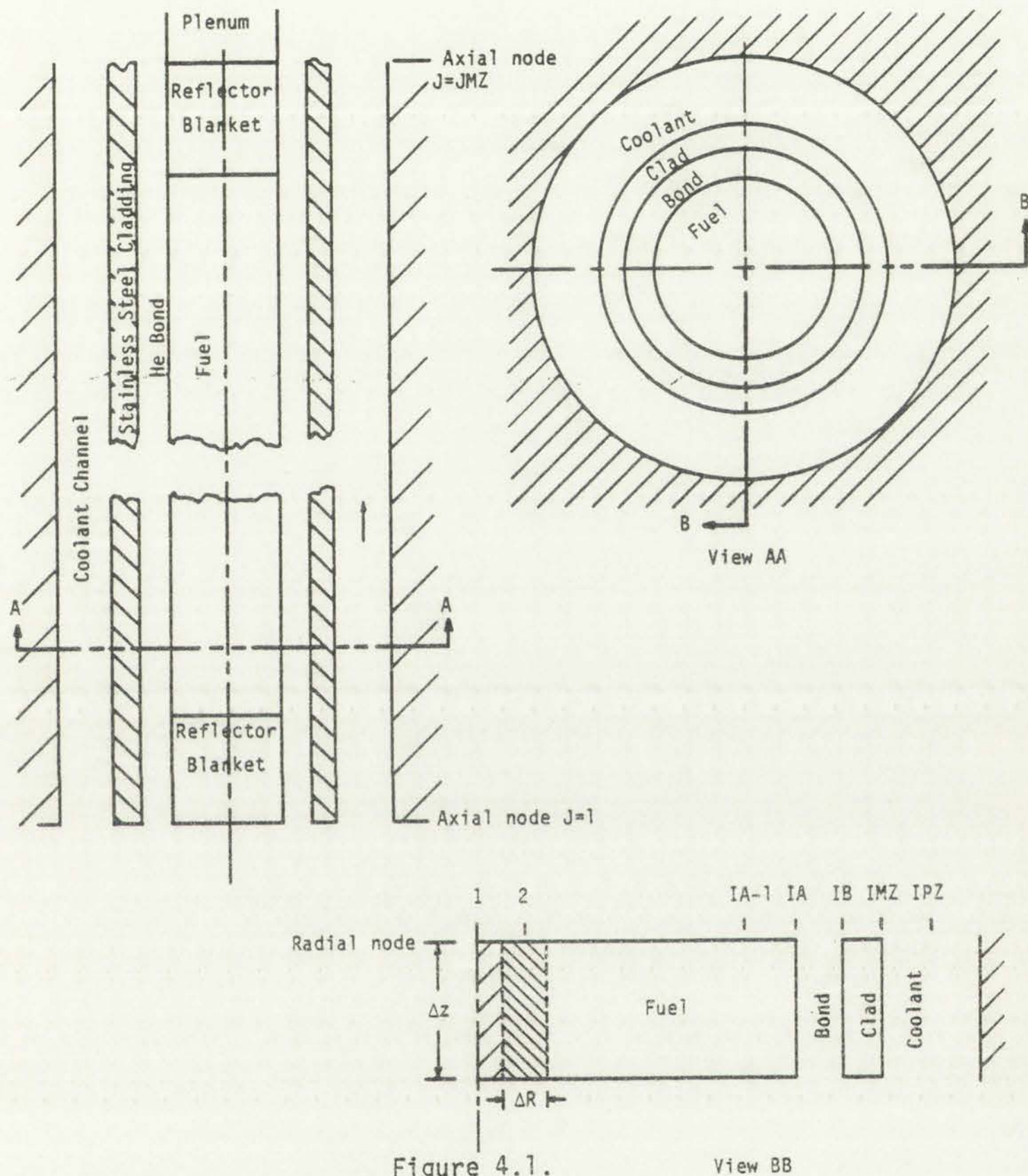


Figure 4.1. Schematic of fuel pin.



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TABLE 4.1
FUEL PIN DESCRIPTION

Description	CRBR	FFTF
A) Fuel		
Composition	UO ₂ - PuO ₂ (Driver Zone) UO ₂ (Axial Blanket)	(U, Pu)O ₂ (Driver Zone) UO ₂ Insulator Pellets Inconel Reflector
Stoichiometry	Sub Stoichiometric Assume 1.96	1.96
Enrichment Pu/(U + Pu)	Depleted (Blankets) 22% (Inner Zone) 32% (Outer Zone) (U Natural)	22.43 Weight % (w/o) Inner 27.37 w/o Outer
Radius	2.3876 mm (.094 in.)	2.48 mm
Length	914.4 mm (36 in.)	910 mm (\approx 36 in.)
Axial Blanket Length	355.6 mm (14 in.) (Upper) 355.6 mm (14 in.) (Lower)	
Density	Assume 90% T.D.	85.5% T.D. Smear 90.4% T.D.
B) Cladding		
Composition	316 Stainless Steel	Stainless Steel
Outer Diameter	5.842 mm (.23 in.)	5.84 mm
Wall Thickness	.381 mm (.015 in.)	.38 mm

Year	Month	Day	Time	Location	Activity	Remarks
1950	Jan	1	10:00
1950	Jan	2	10:00
1950	Jan	3	10:00
1950	Jan	4	10:00
1950	Jan	5	10:00
1950	Jan	6	10:00
1950	Jan	7	10:00
1950	Jan	8	10:00
1950	Jan	9	10:00
1950	Jan	10	10:00
1950	Jan	11	10:00
1950	Jan	12	10:00
1950	Jan	13	10:00
1950	Jan	14	10:00
1950	Jan	15	10:00
1950	Jan	16	10:00
1950	Jan	17	10:00
1950	Jan	18	10:00
1950	Jan	19	10:00
1950	Jan	20	10:00
1950	Jan	21	10:00
1950	Jan	22	10:00
1950	Jan	23	10:00
1950	Jan	24	10:00
1950	Jan	25	10:00
1950	Jan	26	10:00
1950	Jan	27	10:00
1950	Jan	28	10:00
1950	Jan	29	10:00
1950	Jan	30	10:00
1950	Jan	31	10:00

TABLE 4.1 (cont)

C) Bond	Inert Gas	Inert Gas
Composition	Inert Gas (He)	Inert Gas
Fuel-clad gap (at beginning of life)	.1524 mm (.006 in.)	.07 mm
D) General Parameters		
Gas Plenum Length	1219.2 mm (48 in.)	940 mm
Pin Pitch	P/D = 1.26	P/D = 1.24
Core Inlet Temp.	661°K	589°K
Core Outlet Temp.	808°K	755°K
Max. Can Temp.	930.4°K	943°K (Hot Spot)
Output Power	350 MWe/975 Mwt	400 Mwt
	Linear 14.5 kW/ft. Max. 7 kW/ft. Ave.	.39 MW/ft (Density)
Coolant	Sodium	Sodium
Burnup Goal	80,000 MWD/T (\approx 8.5 atom %) Peak	80,000 MWD/T (\approx 8.5 atom %) Peak

1940-1941	1940-1941	1940-1941	1940-1941
1942-1943	1942-1943	1942-1943	1942-1943
1944-1945	1944-1945	1944-1945	1944-1945
1946-1947	1946-1947	1946-1947	1946-1947
1948-1949	1948-1949	1948-1949	1948-1949
1950-1951	1950-1951	1950-1951	1950-1951
1952-1953	1952-1953	1952-1953	1952-1953
1954-1955	1954-1955	1954-1955	1954-1955
1956-1957	1956-1957	1956-1957	1956-1957
1958-1959	1958-1959	1958-1959	1958-1959
1960-1961	1960-1961	1960-1961	1960-1961
1962-1963	1962-1963	1962-1963	1962-1963
1964-1965	1964-1965	1964-1965	1964-1965
1966-1967	1966-1967	1966-1967	1966-1967
1968-1969	1968-1969	1968-1969	1968-1969
1970-1971	1970-1971	1970-1971	1970-1971
1972-1973	1972-1973	1972-1973	1972-1973
1974-1975	1974-1975	1974-1975	1974-1975
1976-1977	1976-1977	1976-1977	1976-1977
1978-1979	1978-1979	1978-1979	1978-1979
1980-1981	1980-1981	1980-1981	1980-1981
1982-1983	1982-1983	1982-1983	1982-1983
1984-1985	1984-1985	1984-1985	1984-1985
1986-1987	1986-1987	1986-1987	1986-1987
1988-1989	1988-1989	1988-1989	1988-1989
1990-1991	1990-1991	1990-1991	1990-1991
1992-1993	1992-1993	1992-1993	1992-1993
1994-1995	1994-1995	1994-1995	1994-1995
1996-1997	1996-1997	1996-1997	1996-1997
1998-1999	1998-1999	1998-1999	1998-1999
2000-2001	2000-2001	2000-2001	2000-2001
2002-2003	2002-2003	2002-2003	2002-2003
2004-2005	2004-2005	2004-2005	2004-2005
2006-2007	2006-2007	2006-2007	2006-2007
2008-2009	2008-2009	2008-2009	2008-2009
2010-2011	2010-2011	2010-2011	2010-2011
2012-2013	2012-2013	2012-2013	2012-2013
2014-2015	2014-2015	2014-2015	2014-2015
2016-2017	2016-2017	2016-2017	2016-2017
2018-2019	2018-2019	2018-2019	2018-2019
2020-2021	2020-2021	2020-2021	2020-2021
2022-2023	2022-2023	2022-2023	2022-2023
2024-2025	2024-2025	2024-2025	2024-2025

3. Constant fuel, clad, bond, and coolant properties were assumed, i.e. temperature, pressure, or time dependence of density, heat capacity, thermal conductivity, etc., were ignored.
4. An annular flow area was used for the coolant, the equivalent cross sectional area was determined from the pin pitch. As seen in Fig. 4.1, no interchannel heat transfer was allowed.

The theoretical and 90% theoretical density for CRBR fuel is calculated in Appendix G. This was done to account for the spread in densities quoted in the literature.

4.2 Inclusion Description

In the following analyses, inclusion compositions based on the investigations of O'Boyle,² Johnson,³ and Jeffery⁴ were utilized. O'Boyle² and Johnson's³ compositions were chosen since the pins they analyzed were of mixed oxides irradiated in a fast spectrum, thus approximating conditions in an LMFBR. Jeffery's⁴ inclusion composition was included to try to obtain a comparison of both inclusion composition and expected inclusion reaction to hypothetical accident situations between an LMFBR and a light water reactor (LWR).

For use as input data, an average Jeffery⁴ inclusion composition was calculated and can be found in Table 4.2. A value of 3 weight % was assigned to the constituents detected in the inclusions with a concentration of 5 weight %. It was then assumed that the fission product yield would segregate into inclusions in the weight % of Jeffery's average inclusion. The yield at 3 atom % burn-up for U, irradiated in a fast spectrum, was used. Appendix H contains the required yield data for U, Pu, and mixed oxides at 3 atom % burn-up. As

The theoretical and experimental results for the polymerization of styrene in the presence of a radical scavenger are presented. The experimental results show that the rate of polymerization is decreased in the presence of the scavenger. The theoretical results show that the rate of polymerization is decreased in the presence of the scavenger.

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TABLE 4.2
AVERAGE JEFFERY INCLUSION COMPOSITION*

Element	Mo	Ru	Tc	Rh	Ba	Pd	Zr	Ce	Sr	U	Te	Nd
Weight %	32.2	13.95	10.0	3.95	6.75	2.1	3.0	1.65	.90	20.3	2.10	3.0

*based on 70% type 1; 41 w/o Mo, 18 w/o Ru, 13 w/o Tc, 5 w/o Rh, 3 w/o Te, 3 w/o Pd, 3 w/o Nd, 14 w/o U

15% type 2; 21 w/o Mo, 9 w/o Ru, 6 w/o Tc, 20 w/o Ba, 10 w/o Zr, 6 w/o Ce, 3 w/o Sr, 3 w/o Nd, 3 w/o Rh, 19 w/o U

15% type 3; 25 w/o Ba, 10 w/o Zr, 5 w/o Ce, 3 w/o Sr, 3 w/o Nd, 3 w/o Mo, 51 w/o U.

mentioned previously the yield of U in a thermal spectrum is close to its yield in a fast spectrum. The results are shown in Table 4.3. The maximum inclusion number density for both 5 and 10 μm diameter inclusions, assuming a flat distribution, was calculated along with the concentration of the constituent fission products in the fuel. It should be noted that the density of the inclusions, based on an average Jeffery inclusion was on the order of 8.5 g/cm^3 versus the measured⁵ density of 11.3 g/cm^3 for UO_2 inclusions. The calculated density of Jeffery's Type 1 inclusion, disregarding the U content, is on the order of 10.5 g/cm^3 . The Type 1 inclusion is very similar to the noble metal inclusions found by all investigators. It appears that the Type 2 and 3 inclusions are predominantly barium zirconates. The fuel analyzed is highly enriched UO_2 irradiated in a thermal spectrum with low center temperature, and is thus dissimilar to

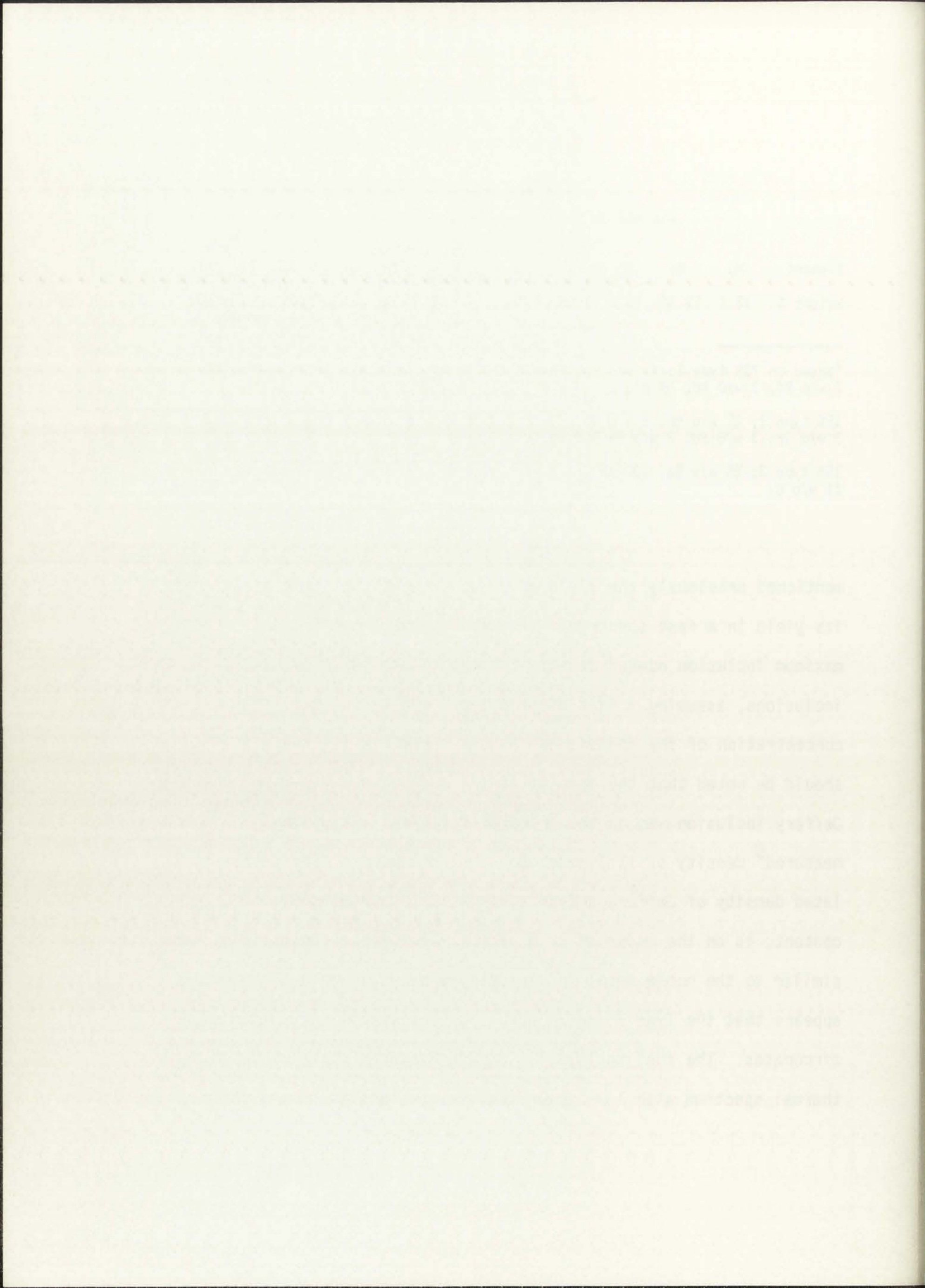


TABLE 4.3
ANALYSIS OF JEFFERY'S INCLUSIONS AT 3 ATOM % BURNUP

Constituent	Weight Yield* (gms/cm ³ Fuel) for Fast Irradi- ated U to 3 A/D B.U.	Average Inclusion Weight %	Weight Yield Inclusion w/o	Limiting Element	Maximum Weight Concentration (gms/cm ³ Fuel)	% of Yield in Inclusions	Maximum Concentration (Moles/cm ³ Fuel)	Maximum Volume of Inclusion (cm ³ of Elem./cm ³ of Fuel)	
Mo	2.29 x 10 ⁻²	32.3	7.09 x 10 ⁻²	Tc	2.11 x 10 ⁻²	92.2	2.17 x 10 ⁻⁴	2.04 x 10 ⁻³	
Tc	6.54 x 10 ⁻³	10.0	6.54 x 10 ⁻²		6.54 x 10 ⁻³	100.0	6.61 x 10 ⁻⁵	5.66 x 10 ⁻⁴	
Ru	1.81 x 10 ⁻²	13.95	1.30 x 10 ⁻¹		9.12 x 10 ⁻³	50.4	8.93 x 10 ⁻⁵	7.30 x 10 ⁻⁴	
Rh	2.77 x 10 ⁻³	3.95	7.01 x 10 ⁻²		2.58 x 10 ⁻³	93.3	2.50 x 10 ⁻⁵	2.07 x 10 ⁻⁴	
Pd	1.86 x 10 ⁻³	2.1	8.86 x 10 ⁻²		1.37 x 10 ⁻³	73.8	1.29 x 10 ⁻⁵	1.15 x 10 ⁻⁴	
Ba	1.05 x 10 ⁻²	6.75	1.56 x 10 ⁻¹		4.41 x 10 ⁻³	42.0	3.19 x 10 ⁻⁵	1.25 x 10 ⁻³	
Zr	3.04 x 10 ⁻²	3.0	1.01		1.96 x 10 ⁻³	6.5	2.09 x 10 ⁻⁵	3.06 x 10 ⁻⁴	
Ce	2.46 x 10 ⁻²	1.65	1.49		1.08 x 10 ⁻³	4.4	7.63 x 10 ⁻⁶	1.58 x 10 ⁻⁴	
Sr	9.68 x 10 ⁻³	.90	1.08		7.06 x 10 ⁻⁴	7.3	7.92 x 10 ⁻⁶	2.78 x 10 ⁻⁴	
Nd	2.67 x 10 ⁻²	3.0	8.9 x 10 ⁻¹		1.96 x 10 ⁻³	7.3	1.35 x 10 ⁻⁵	2.82 x 10 ⁻⁴	
Tc	3.37 x 10 ⁻³	2.10	1.60 x 10 ⁻¹		1.37 x 10 ⁻³	40.8	1.06 x 10 ⁻⁵	2.17 x 10 ⁻⁴	
Sb	3.10 x 10 ⁻⁴	< 1				3.10 x 10 ⁻⁴	100.0	2.51 x 10 ⁻⁶	4.57 x 10 ⁻⁵
Sn	4.56 x 10 ⁻⁴	< 1				4.56 x 10 ⁻⁴	100.0	3.79 x 10 ⁻⁶	6.14 x 10 ⁻⁵
In	3.54 x 10 ⁻⁵	< 1				3.54 x 10 ⁻⁵	100.0	3.08 x 10 ⁻⁷	4.85 x 10 ⁻⁶
Nb	1.54 x 10 ⁻³	< 1			5.22 x 10 ⁻⁴	34.9	5.25 x 10 ⁻⁷	6.11 x 10 ⁻⁵	
Ag	1.70 x 10 ⁻⁴	< 1			1.70 x 10 ⁻⁴	100.0	1.55 x 10 ⁻⁶	1.66 x 10 ⁻⁵	

*Based on yield data of Burris⁷ (see Appendix H).

Number Density of Inclusions[†] (Inclusions/cm³ of Fuel)

Diameter of Inclusion	Average Jeffery Inclusion	Average Jeffery Inclusion + Sb, Sn, In, Nb, Ag
μm	9.68 x 10 ⁷	9.68 x 10 ⁷
1(μm)	1.21 x 10 ⁷	1.21 x 10 ⁷
Calculated Inclusion Density	8.49 gms/cm ³	8.47 gms/cm ³

$$\rho_{\text{calc}} = \frac{\sum_{i=1}^n \frac{w_i}{V_i}}{\sum_{i=1}^n V_i}$$

[†]U not included.

Year	1950	1951	1952	1953	1954	1955	1956	1957	1958	1959	1960
Population	1,000,000	1,050,000	1,100,000	1,150,000	1,200,000	1,250,000	1,300,000	1,350,000	1,400,000	1,450,000	1,500,000
Area	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000
Production	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000
Consumption	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000
Exports	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000
Imports	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000	100,000
Balance	0	0	0	0	0	0	0	0	0	0	0

Table 1. Summary of the results of the investigation.

the fuel and conditions expected in CRBR, and as mentioned previously is included for comparison purposes.

O'Boyle investigated fuel more similar in composition and irradiation history to the hypothesized CRBR fuel pin. The fact that the fuel was initially stoichiometric lowered the weight % of Mo in inclusions, versus what one would expect to find in the hypostoichiometric CRBR fuel. This effect is somewhat compensated for by the fact that CRBR fuel has a larger weight % Pu which has a lower Mo yield and higher Ru yield than U.

Further analysis of O'Boyle's inclusions can be found in Table 4.4. The fission product concentration was calculated using an average O'Boyle inclusion and also by assuming that the other stable elements Sb, Sn, In, Nb, Ag were present in concentrations lower than the detection limit of the microprobe. The calculated density of an inclusion having O'Boyle's weight %, 11.64 g/cm^3 , was much closer to the measured values of Bramman,⁶ 12.2 g/cm^3 , than was Jeffery's.

As mentioned previously, in ANL-7877,³ three different types of metallic inclusions were found. Noble metal inclusions, consisting primarily of Mo, Tc, Ru, Rh, and Pd, were found throughout the columnar region and halfway through the equiaxed-grain region. The second type of inclusions was primarily Pd with small quantities of other fission products and impurities present. The second type of inclusion was found primarily in the equiaxed and unrestructured regions of the fuel. Only a few of the third type of inclusion were found and then

The first condition mentioned in the text is that the reaction must be reversible. This is a necessary condition for the establishment of an equilibrium. The second condition is that the reaction must be exothermic. This is also a necessary condition for the establishment of an equilibrium. The third condition is that the reaction must be homogeneous. This is also a necessary condition for the establishment of an equilibrium. The fourth condition is that the reaction must be elementary. This is also a necessary condition for the establishment of an equilibrium. The fifth condition is that the reaction must be irreversible. This is also a necessary condition for the establishment of an equilibrium. The sixth condition is that the reaction must be reversible. This is also a necessary condition for the establishment of an equilibrium. The seventh condition is that the reaction must be exothermic. This is also a necessary condition for the establishment of an equilibrium. The eighth condition is that the reaction must be homogeneous. This is also a necessary condition for the establishment of an equilibrium. The ninth condition is that the reaction must be elementary. This is also a necessary condition for the establishment of an equilibrium. The tenth condition is that the reaction must be irreversible. This is also a necessary condition for the establishment of an equilibrium.

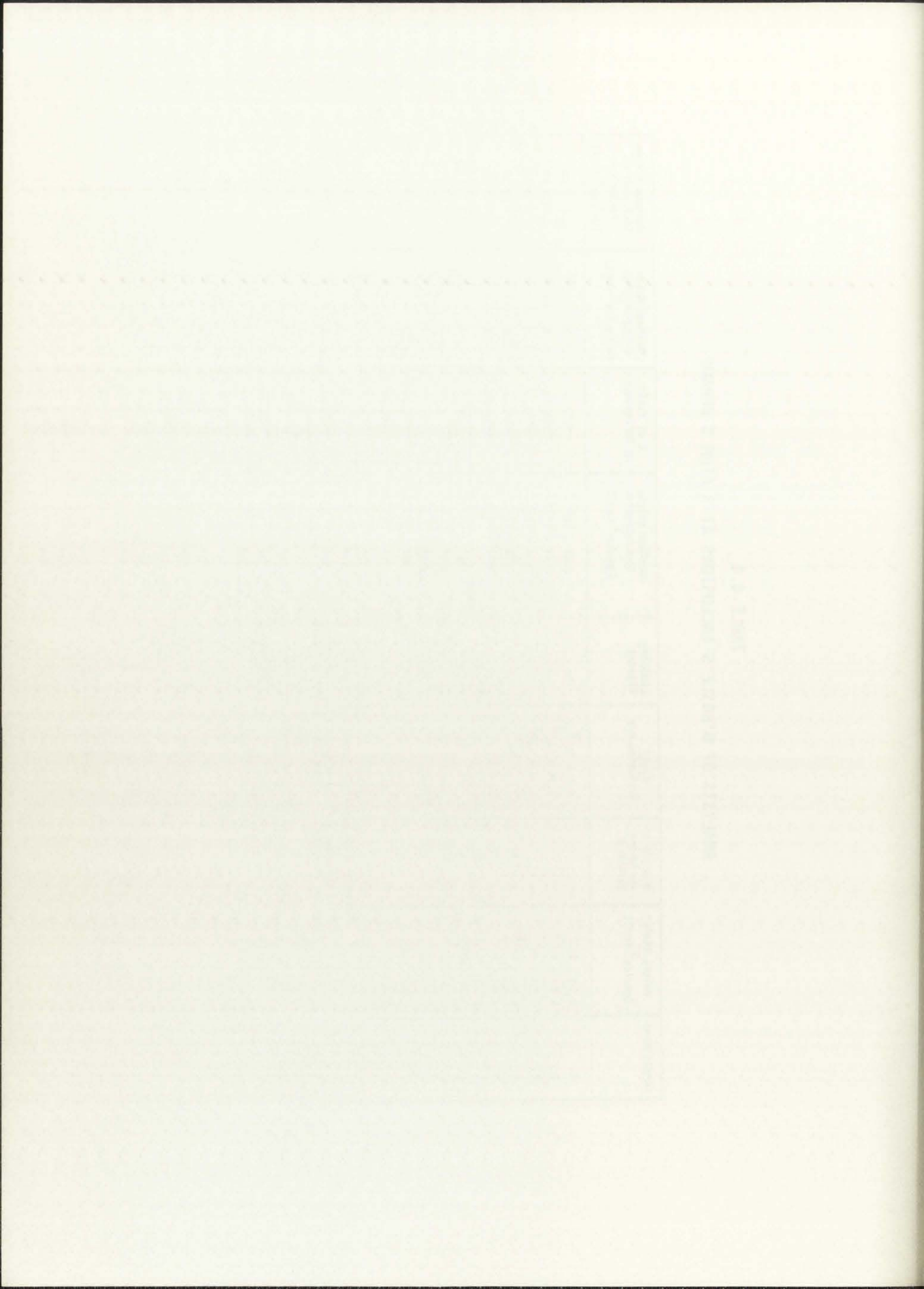
TABLE 4.4
ANALYSIS OF O'BOYLE'S INCLUSIONS AT 3 ATOM % BURNUP

Constituent	Weight Yield* (gms/cm ³ Fuel)	O'Boyle's Inclusion Weight %	Yield Inclusion w/o	Limiting Element	Maximum Weight Concentration (gms/cm ³ Fuel)	% of Yield in Inclusions	Maximum Molar Concentration (Moles/cm ³ Fuel)	Maximum Volume (Alloyed) of Inclusions (cm ³ /cm ³ Fuel)
Mo	2.10 x 10 ⁻²	25.	8.4 x 10 ⁻²	Tc	6.87 x 10 ⁻³	32.7	7.16 x 10 ⁻⁵	6.68 x 10 ⁻⁴
Tc	4.67 x 10 ⁻³	17.	2.75 x 10 ⁻²		4.67 x 10 ⁻³	100.0	4.77 x 10 ⁻⁵	4.09 x 10 ⁻⁴
Ru	2.56 x 10 ⁻²	48.	5.33 x 10 ⁻²		1.32 x 10 ⁻²	51.6	1.31 x 10 ⁻⁴	1.06 x 10 ⁻³
Rh	4.97 x 10 ⁻³	5.**	9.9 x 10 ⁻²		1.37 x 10 ⁻³	27.6	1.33 x 10 ⁻⁵	1.10 x 10 ⁻⁴
Pd	1.68 x 10 ⁻²	5.**	3.36 x 10 ⁻¹		1.37 x 10 ⁻³	8.2	1.30 x 10 ⁻⁵	1.14 x 10 ⁻⁴
Sb	3.75 x 10 ⁻⁴	< 1			2.75 x 10 ⁻⁴	73.3	2.24 x 10 ⁻⁶	2.85 x 10 ⁻⁵
Sn	9.53 x 10 ⁻⁴	< 1			2.75 x 10 ⁻⁴	28.8	2.31 x 10 ⁻⁶	2.68 x 10 ⁻⁵
In	8.84 x 10 ⁻⁵	< 1			8.84 x 10 ⁻⁵	100.0	7.70 x 10 ⁻⁷	8.81 x 10 ⁻⁶
Nb	6.85 x 10 ⁻⁴	< 1			2.75 x 10 ⁻⁴	40.1	2.96 x 10 ⁻⁶	2.89 x 10 ⁻⁵
Ag	1.35 x 10 ⁻³	< 1			2.75 x 10 ⁻⁴	20.4	2.54 x 10 ⁻⁶	2.59 x 10 ⁻⁵

*Based on RIBD⁸ yield data (see Appendix H).

**Used more conservative O'Boyle data. If the RIBD⁸ yield split is used, then the expected weight % would be 7.5% Pd and 2.5% Rh, increasing the weight % of the more volatile Pd.

Diameter of Inclusion	Number Density of Inclusions (Inclusions/cm ³ Fuel)	
	Average O'Boyle Inclusion	Average O'Boyle Inclusion + Sb, Sn, In, Nb, Ag
5 μ m	3.607 x 10 ⁷	3.789 x 10 ⁷
10 μ m	4.509 x 10 ⁶	4.736 x 10 ⁶
Calculated Inclusion Density	11.64 gms/cm ³	11.56 gms/cm ³



always in the unstructured region. These consisted of almost pure Mo with a few percent of other fission products.

Due to the distribution of the three types of inclusions, it will be assumed that the noble metal inclusions are only found to some given radius R, where a step transition occurs to inclusions of the second type. The third type of inclusion will be ignored due to its location, rarity, and composition.

To determine the composition of the inclusions to be input, average values were calculated. These values can be found in Table 4.5. As stated earlier a flat compositional distribution will be initially assumed.

Using these average values of the composition, the maximum concentrations, i.e. molar, weight, and volume, were calculated for the two types of inclusions, using the RIBD yield data. The results can be found in Tables 4.6 and 4.7.

TABLE 4.5
JOHNSON'S³ AVERAGE INCLUSION COMPOSITION

Inclusion Type	Fuel Pin Number	Mo	Tc	Ru	Weight %		Fe	Sn	Sb	Te
					Rh	Pd				
Noble Metal (Type 1)	C-11	19.5	19.0	41.0	15.0	1.0	4.5			
	C-15	9.5	21.1	45.6	20.2	3.2	0.4			
Average (Type 1)		14.5	20.05	43.3	17.6	2.1	2.45			
Palladium (Type 2)	C-15					72.55	22.25	2.8	1.3	1.1

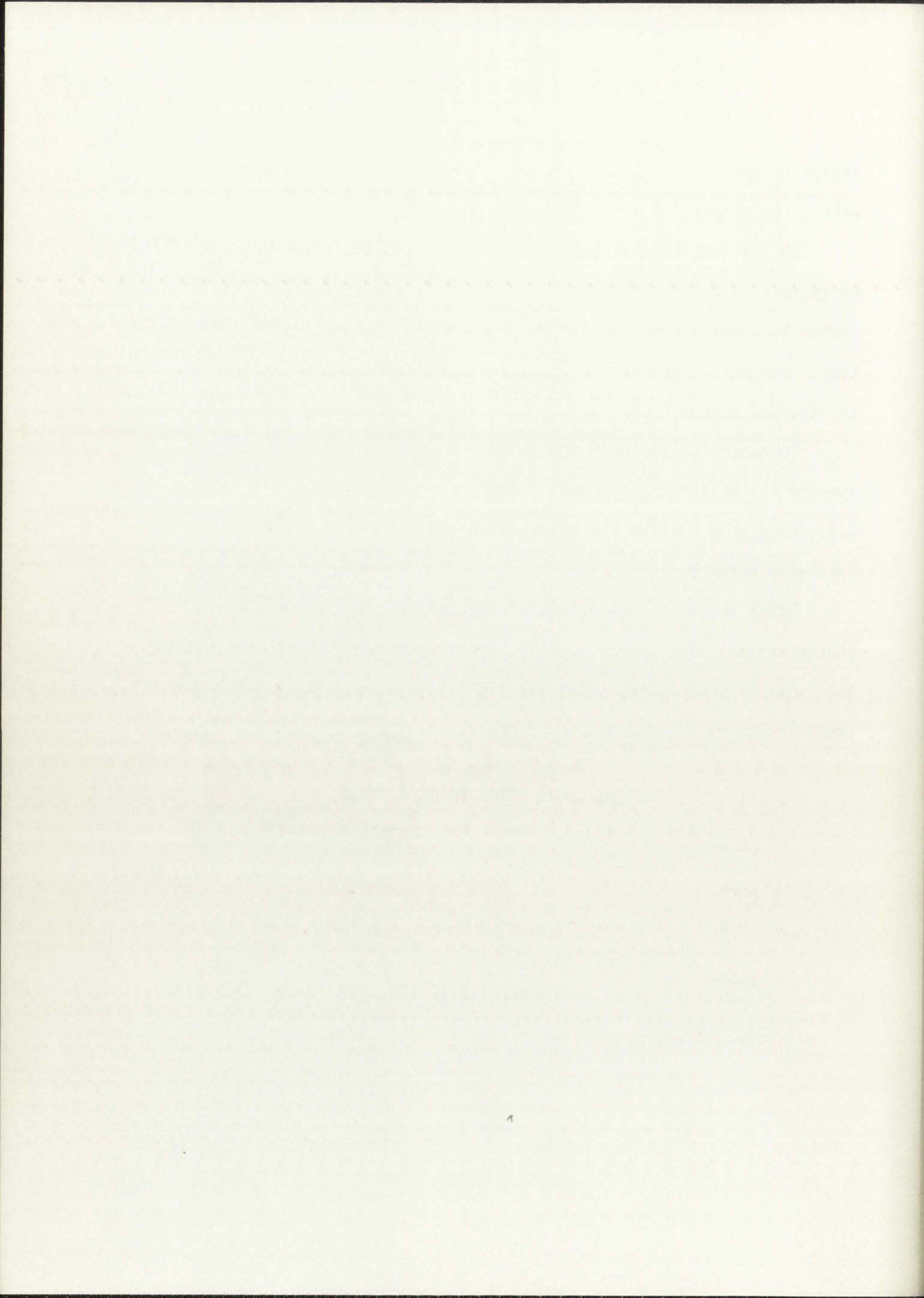


TABLE 4.6
ANALYSIS OF JOHNSON'S INCLUSION (TYPE I) AT 3 ATOM % BURNUP

Constituent	Weight Yield* (gms/cm ³ Fuel)	Type I Inclusion Weight %	Yield Inclusion w/o	Limiting Element	Maximum Weight Concentration (gms/cm ³ Fuel)	% of Yield in Inclusions	Maximum Molar Concentration (Moles/cm ³ Fuel)	Maximum Volume (Alloyed) of Inclusions (cm ³ /cm ³ Fuel)
Mo	2.10 x 10 ⁻²	14.5	1.45 x 10 ⁻¹	Tc	3.38 x 10 ⁻³	16.08	3.52 x 10 ⁻⁵	3.31 x 10 ⁻⁴
Tc	4.67 x 10 ⁻³	20.05	2.33 x 10 ⁻²		4.67 x 10 ⁻³	100.0	4.77 x 10 ⁻⁵	4.09 x 10 ⁻⁴
Ru	2.56 x 10 ⁻²	43.3	5.91 x 10 ⁻²		1.01 x 10 ⁻²	39.40	9.97 x 10 ⁻⁵	8.15 x 10 ⁻⁴
Rh	4.97 x 10 ⁻³	17.6	2.82 x 10 ⁻²		4.10 x 10 ⁻³	82.48	3.98 x 10 ⁻⁵	3.30 x 10 ⁻⁴
Pd	1.68 x 10 ⁻²	2.1	8.0 x 10 ⁻¹		4.89 x 10 ⁻⁴	2.91	4.60 x 10 ⁻⁶	4.10 x 10 ⁻⁵
Fe	-	2.45	-		5.71 x 10 ⁻⁴	-	1.02 x 10 ⁻⁵	7.26 x 10 ⁻⁵
Sn	9.53 x 10 ⁻⁴	< 1			2.33 x 10 ⁻⁴	24.46	1.96 x 10 ⁻⁶	2.27 x 10 ⁻⁵
Sb	3.75 x 10 ⁻⁴	< 1		2.33 x 10 ⁻⁴	62.16	1.91 x 10 ⁻⁶	2.42 x 10 ⁻⁵	
In	8.84 x 10 ⁻⁵	< 1		8.84 x 10 ⁻⁵	100.0	7.70 x 10 ⁻⁷	8.81 x 10 ⁻⁶	
Nb	6.85 x 10 ⁻⁴	< 1		2.33 x 10 ⁻⁴	34.03	2.51 x 10 ⁻⁶	2.45 x 10 ⁻⁵	
Ag	1.35 x 10 ⁻³	< 1		2.33 x 10 ⁻⁴	17.27	2.16 x 10 ⁻⁶	2.19 x 10 ⁻⁵	

*Based on RIBD^B yield data (see Appendix H)

Diameter of Inclusion	Number Density of Inclusions (Inclusions/cm ³ Fuel)	
	Average Johnson (Type I) Inclusion	Average Inclusion + Sn, Sb, In, Nb, Ag
5 μ m	3.05 x 10 ⁷	3.25 x 10 ⁷
10 μ m	3.82 x 10 ⁶	4.06 x 10 ⁶

TABLE 4.7
ANALYSIS OF JOHNSON'S INCLUSIONS (TYPE II) AT 3 ATOM % BURNUP

Constituent	Weight Yield* (gms/cm ³ Fuel)	Type II Inclusion Weight %	Yield Inclusion w/o	Limiting Element	Maximum Weight Concentration (gms/cm ³ Fuel)	% of Yield in Inclusions	Maximum Molar Concentration (Moles/cm ³ Fuel)	Maximum Volume (Alloyed) of Inclusions (cm ³ /cm ³ Fuel)
Pd	1.68×10^{-2}	72.55	2.32×10^{-2}	Pd	1.68×10^{-2}	100.0	1.58×10^{-4}	1.41×10^{-3}
Fe	-	22.25	-		5.15×10^{-3}	-	9.23×10^{-5}	6.56×10^{-4}
Sn	9.53×10^{-4}	2.8	3.40×10^{-2}		6.48×10^{-4}	68.04	5.46×10^{-6}	8.84×10^{-5}
Sb	3.75×10^{-4}	1.3	2.88×10^{-2}		3.01×10^{-4}	80.28	2.47×10^{-6}	4.50×10^{-5}
Te	4.27×10^{-3}	1.1	3.88×10^{-1}		2.55×10^{-4}	5.97	2.00×10^{-6}	4.09×10^{-5}
In	8.84×10^{-5}	< 1			8.84×10^{-5}	100.0	7.70×10^{-7}	8.81×10^{-6}
Nb	6.85×10^{-4}	< 1			2.31×10^{-4}	33.8	2.49×10^{-6}	2.43×10^{-5}
Ag	1.35×10^{-3}	< 1			2.31×10^{-4}	17.2	2.14×10^{-6}	2.18×10^{-5}

*Based on RIBD⁸ yield data (see Appendix H)

Diameter of Inclusion	Number Density of Inclusions (Inclusions/cm ³ Fuel)	
	Average Johnson (Type II) Inclusion	Average Inclusion + In, Nb, Ag
5 μ m	3.42×10^7	3.52×10^7
10 μ m	4.28×10^6	4.40×10^6

1911

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As a comparison to the above data, Table 4.8 contains the number density of inclusions assuming complete segregation of the stable elements for the various yields. As expected Pu with its high noble metal yield has the highest number density with RIBD second and the U yield last.

In the previous calculations, it was assumed that the maximum quantity of fission products, in the appropriate weight %, segregated into inclusions, i.e. a limiting element contributed 100% of its fission yield to the inclusions. Using this principle one would expect to overestimate the inclusion density in the fuel. However, in looking at the micrographs of the inclusions in the fuel matrix by Jeffery,⁴ Bramman,⁶ and Bradbury⁹ it appears that the inclusion volume % (v/o) is >1%. The maximum inclusion v/o calculated, assuming the weight % of the investigators, was on the order of 0.2 - 0.6 v/o. Possible explanations of this small anomaly is (1) the micrographs were taken specifically at high inclusion concentration areas, with migration of fission products occurring, and/or (2) an error existed in the measured composition of the inclusions. Due to independent analysis of composition by the various people, the last explanation probably is not valid. Errors of ± 1 w/o expected by the investigators is not sufficient to substantially increase the v/o of the inclusions.

4.3 Heat Transfer

For the heat transfer calculations, the fuel pin described in Section 4.1 was divided nodally. The pin was divided into 21 axial nodes or 20 equal segments. The plenum temperature was taken as the coolant outlet temperature, and this region was not included in the

The first part of the paper is devoted to the study of the properties of the function $f(x)$ defined by the equation $f(x) = \int_0^x f(t) dt$. It is shown that $f(x)$ is a constant function and that its value is zero. This result is obtained by differentiating the equation with respect to x and using the initial condition $f(0) = 0$.

In the second part of the paper, we consider the problem of finding the maximum value of the function $f(x) = x^2 - 2x + 1$ on the interval $[0, 2]$. The function is a parabola opening downwards with its vertex at $(1, 0)$. Since the vertex lies within the interval, the maximum value of the function is zero, which occurs at $x = 1$.

The third part of the paper deals with the problem of finding the minimum value of the function $f(x) = x^2 + 2x + 1$ on the interval $[0, 2]$. The function is a parabola opening upwards with its vertex at $(-1, 0)$. Since the vertex lies outside the interval, the minimum value of the function on $[0, 2]$ occurs at the left endpoint $x = 0$, where $f(0) = 1$.

In the fourth part of the paper, we study the function $f(x) = \sin(x)$ on the interval $[0, \pi]$. The function starts at $(0, 0)$, reaches a maximum value of 1 at $x = \pi/2$, and ends at $(\pi, 0)$. The derivative of the function is $f'(x) = \cos(x)$, which is zero at $x = \pi/2$.

4.3. Heat Transfer

In the heat transfer problem, we consider a rod of length L with a cross-sectional area A and thermal conductivity k . The temperature distribution $T(x, t)$ in the rod is governed by the heat conduction equation $\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$, where $\alpha = \frac{k}{\rho c}$ is the thermal diffusivity. The initial and boundary conditions are given by $T(x, 0) = T_0(x)$, $T(0, t) = T_1$, and $T(L, t) = T_2$.

TABLE 4.8
INCLUSION NUMBER DENSITY FOR COMPLETE SEGREGATION

Inclusion Diameter	Inclusion Number Density (Inclusions/cm ³ Fuel)							
	Mo, Tc, Ru, Rh, Pd Segregated		Pu ⁷ Yield		RIBD ⁸ Yield		Mo, Tc, Ru, Rh, Pd + Sb, Sn, In, Ag, Nb Segregated	
	RIBD ⁸ Yield	U ⁷ Yield	Pu ⁷ Yield	RIBD ⁸ Yield	U ⁷ Yield	Pu ⁷ Yield	RIBD ⁸ Yield	U ⁷ Yield
5 μ m (Pure) (Alloyed)	9.685 x 10 ⁷	7.04 x 10 ⁷	1.02 x 10 ⁸	1.03 x 10 ⁸	7.50 x 10 ⁷	1.09 x 10 ⁸	1.03 x 10 ⁸	7.50 x 10 ⁷
	9.624 x 10 ⁷	7.02 x 10 ⁷	1.01 x 10 ⁸	1.01 x 10 ⁸	7.44 x 10 ⁷	1.07 x 10 ⁸	1.01 x 10 ⁸	7.44 x 10 ⁷
10 μ m (Pure) (Alloyed)	1.21 x 10 ⁷	8.80 x 10 ⁶	1.27 x 10 ⁷	1.29 x 10 ⁷	9.38 x 10 ⁶	1.36 x 10 ⁷	1.29 x 10 ⁷	9.38 x 10 ⁶
	1.20 x 10 ⁷	8.77 x 10 ⁶	1.27 x 10 ⁷	1.27 x 10 ⁷	9.30 x 10 ⁶	1.34 x 10 ⁷	1.27 x 10 ⁷	9.30 x 10 ⁶

DATE	DESCRIPTION	AMOUNT	BALANCE	INITIALS
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analysis. Radially the fuel contained 11 nodes, or 10 equal Δr segments, with the 11th node at the fuel-bond interface. Additional nodes were at the bond-clad interface, the clad-coolant interface, and within the bulk coolant flow. The number of fuel nodes is variable and is an input quantity to the program.

A. Steady State Temperature. The steady state temperature profile was calculated using the subroutine SSTEMP. The analytical equations used in SSTEMP can be found in Appendix I. These equations were based on the following assumptions:

1. There were constant material properties such as density, heat capacity, and thermal conductivity.
2. There was no axial heat transfer. Since $z/r \gg 1$, this was a realistic assumption.
3. There was no radial dependence for the volumetric heat generation. Since a fast flux was being used, this assumption should be very good.
4. Axially, a chopped cosine volumetric heat generation in the fuel and a flat distribution in the blanket-reflector region was assumed. A maximum of $575.6 \text{ cal/cm}^3\text{-s}^1$ (CRBR) was used with an extrapolation distance of 18.8 cms.¹⁰ A flat $30 \text{ cal/cm}^3\text{-s}$, $\sim 5\%$ of peak value, was assumed in the blanket-reflector regions.
5. The pin dimensions at temperature were equal to those at fabrication; therefore, fuel swelling, thermal expansion, and fuel relocation were ignored.
6. The heat transfer coefficient used for the coolant was for annular flow. The derivation is in Appendix I.
7. The coolant flow rate and the maximum volumetric heat generation was adjusted to give inlet and outlet coolant temperatures close to CRBR. By using the pin pitch to calculate an equivalent annular flow, one ignores the additional coolant flow along the can wall and the possible cross channel heat transfer. Thus, the coolant velocity used, 950 cms/s, was somewhat higher than the projected CRBR flow velocity of $\sim 600 \text{ cms/s}$.

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The steady state temperature profile was generated as a starting point for the transient condition. Plots of representative axial and radial temperature profiles can be seen in Figs. 4.2 and 4.3.

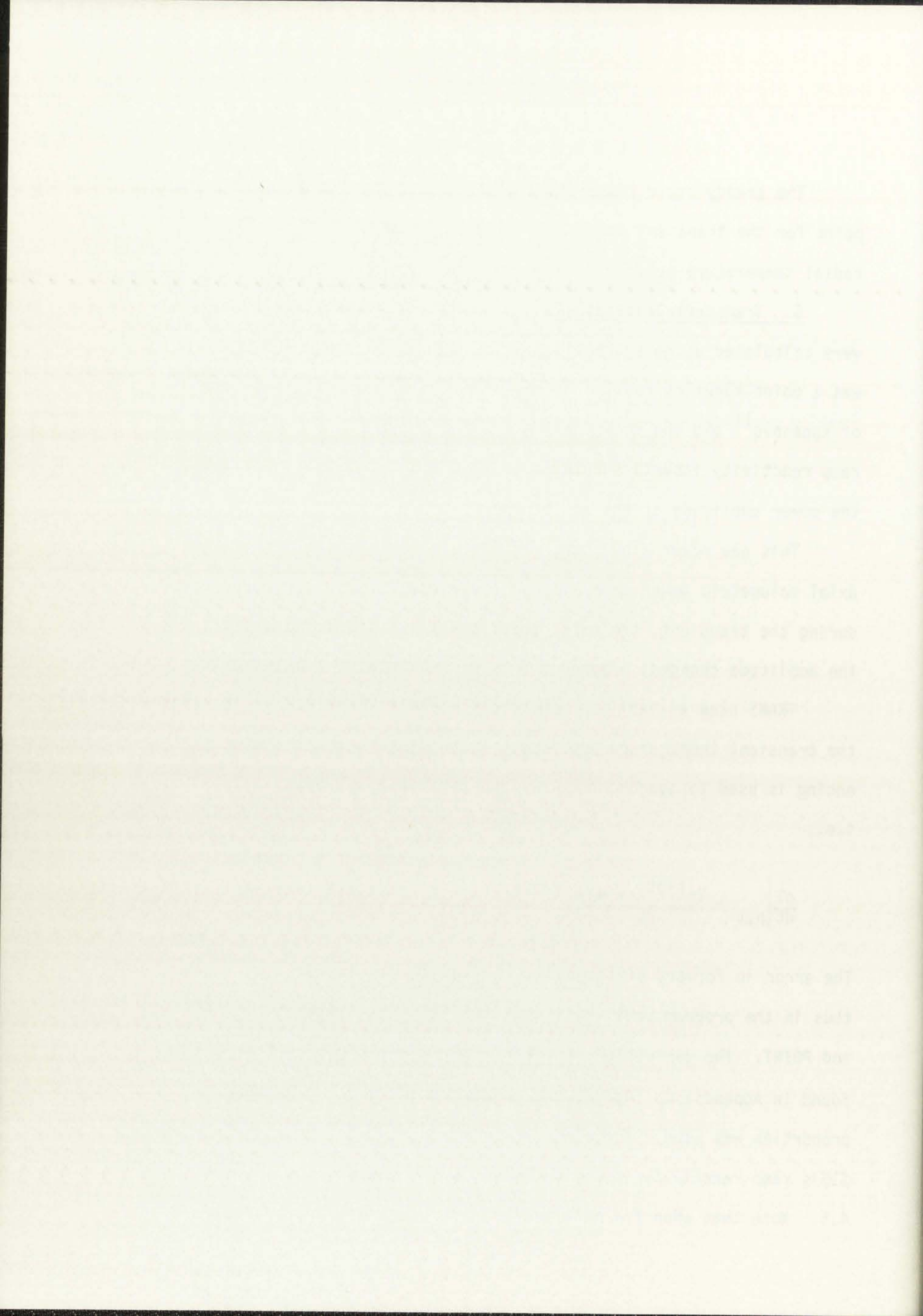
B. Transient Temperature. The transient temperature profiles were calculated using subroutines POINT and TRANS. Subroutine POINT was a point kinetics routine based on the integral solution technique of Kaganove¹¹ and the modifications made by Burns.¹⁰ Inputting a ramp reactivity insertion rate and a time step, Δt , POINT calculates the power amplitude at the end of the time step.

This new power amplitude, P_1 , was used as a multiplier of the axial volumetric power generation. The assumption was thus made that during the transient, the axial power shape remained constant and only the amplitude changed. Appendix J is an expansion of the technique.

TRANS uses an explicit finite-differencing technique to calculate the transient temperature profiles. Euler's method or forward differencing is used to approximate the time derivative of temperature, i.e.,

$$\left. \frac{dT}{dt} \right|_{n,t} = \frac{T_n^{t+\Delta t} - T_n^t}{\Delta t} \quad (4.1)$$

The error in forward differencing is proportional to $(\Delta r)^2$ and to Δt ; thus in the program small Δt 's were used for stability both in TRANS and POINT. The derivation of the finite-differencing equation can be found in Appendix K. Again, the assumption of constant material properties was used. Transient temperature profiles for both \$5/s and \$15/s ramp reactivity insertion rates can be seen in Figs. 4.4 and 4.5. Note that when the melt temperature is reached in a node,



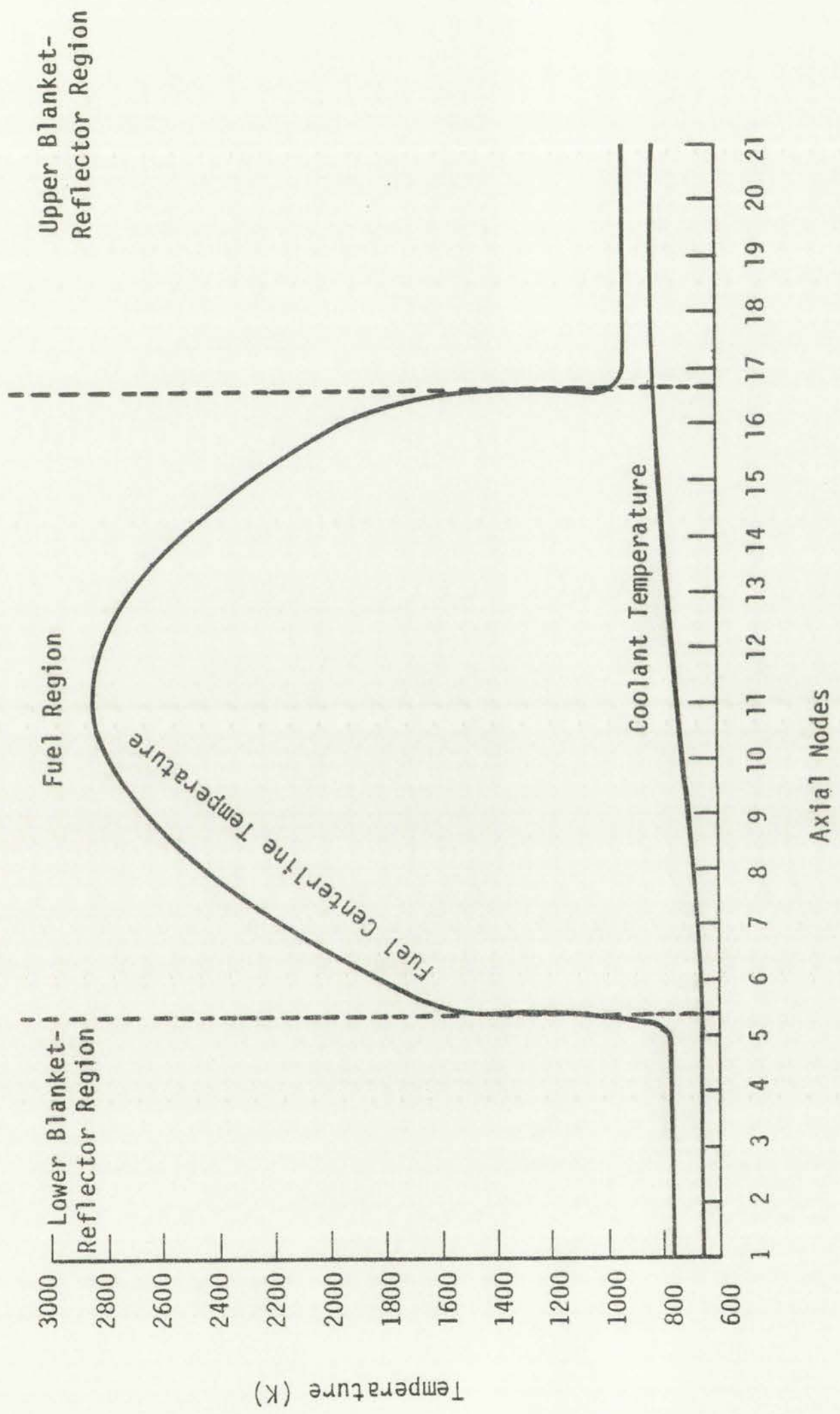


Figure 4.2. Steady state axial temperature profiles.

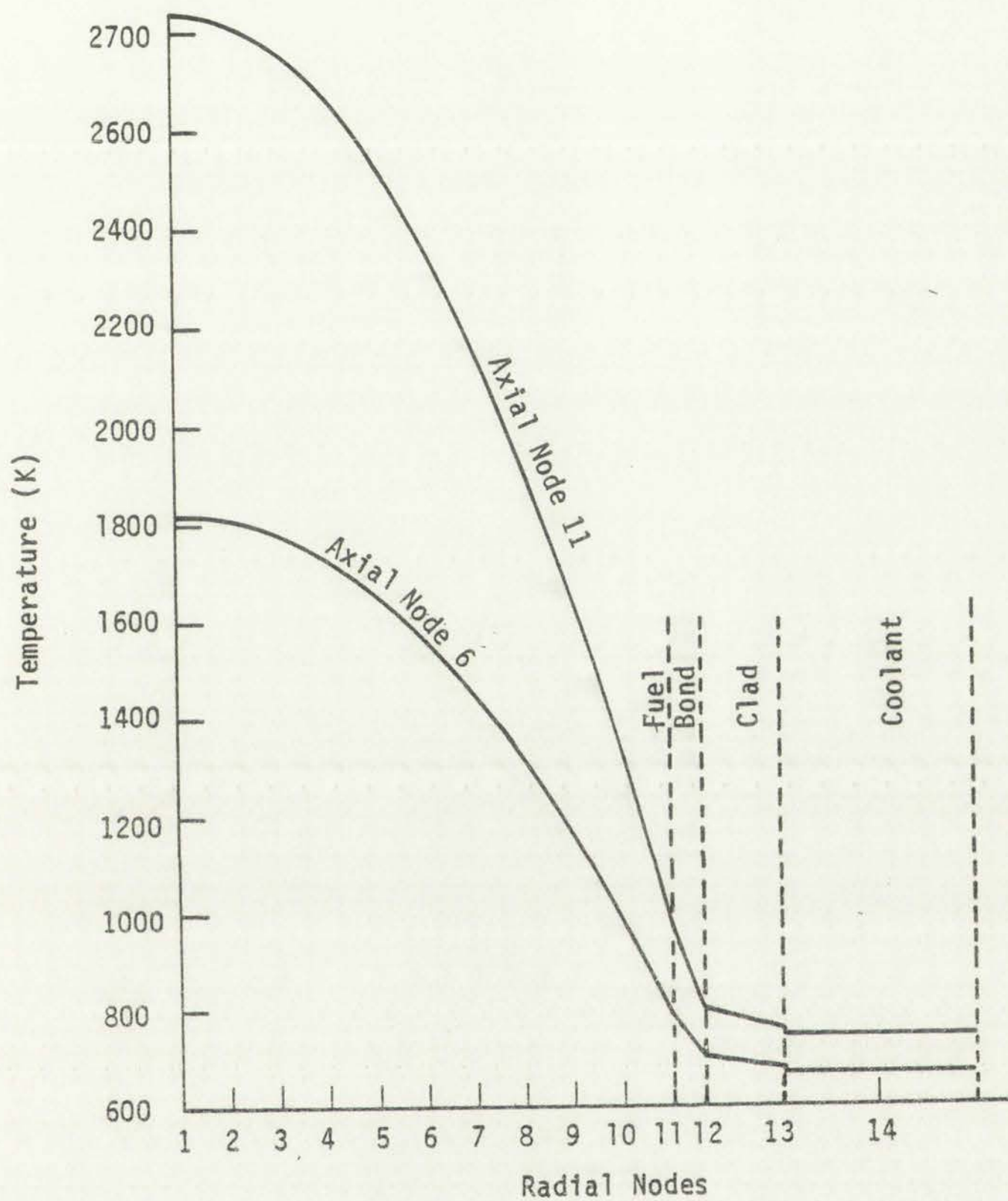


Figure 4.3.
Steady state radial temperature profiles.



Figure 3
 Graph of initial speed vs. temperature

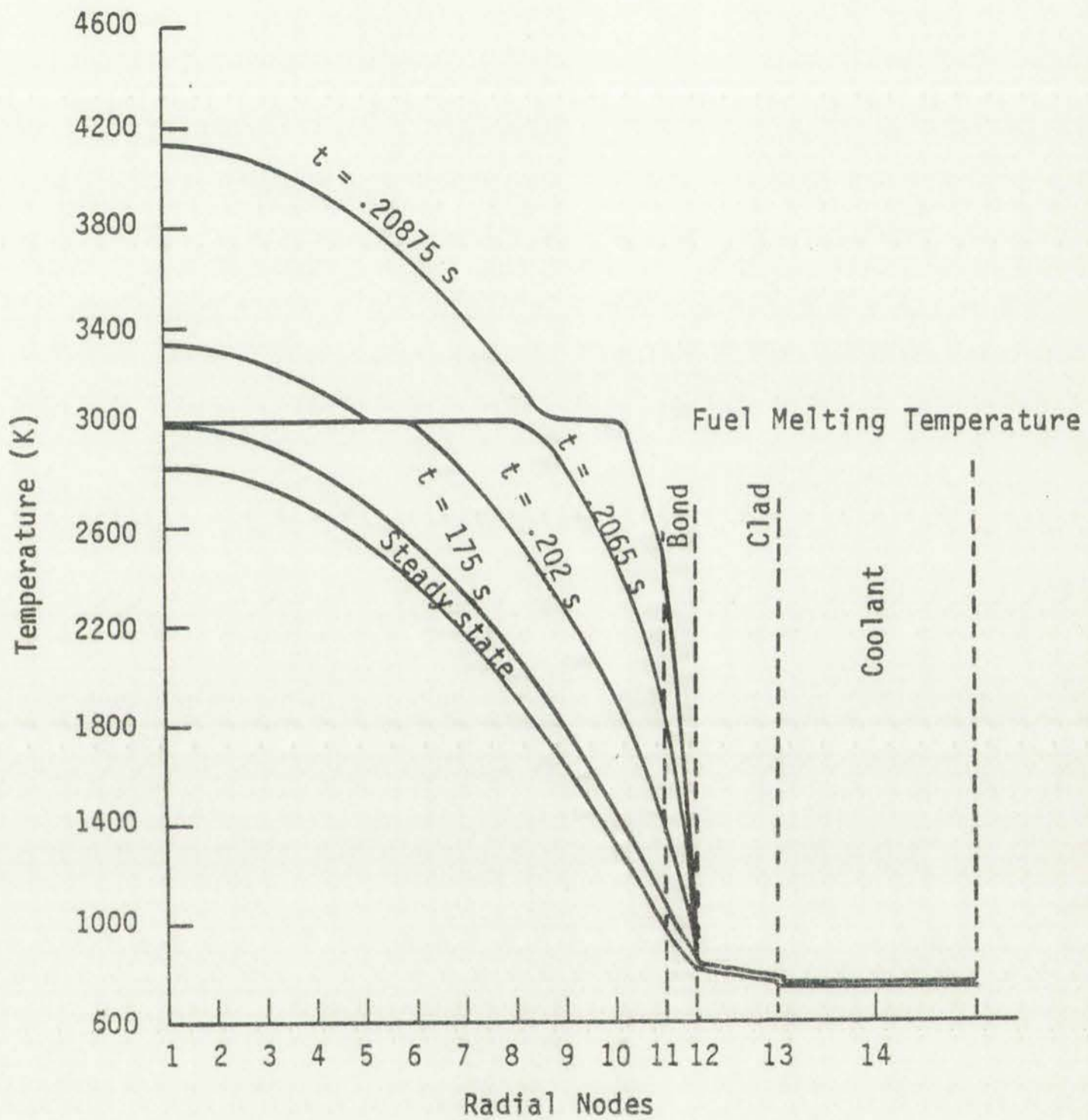


Figure 4.4.
 Transient radial temperature profiles at axial node 11 (hottest) for ramp reactivity insertion of $5/s$.



Figure 3
 Temperature vs. Control Voltage for three different systems (A, B, C)

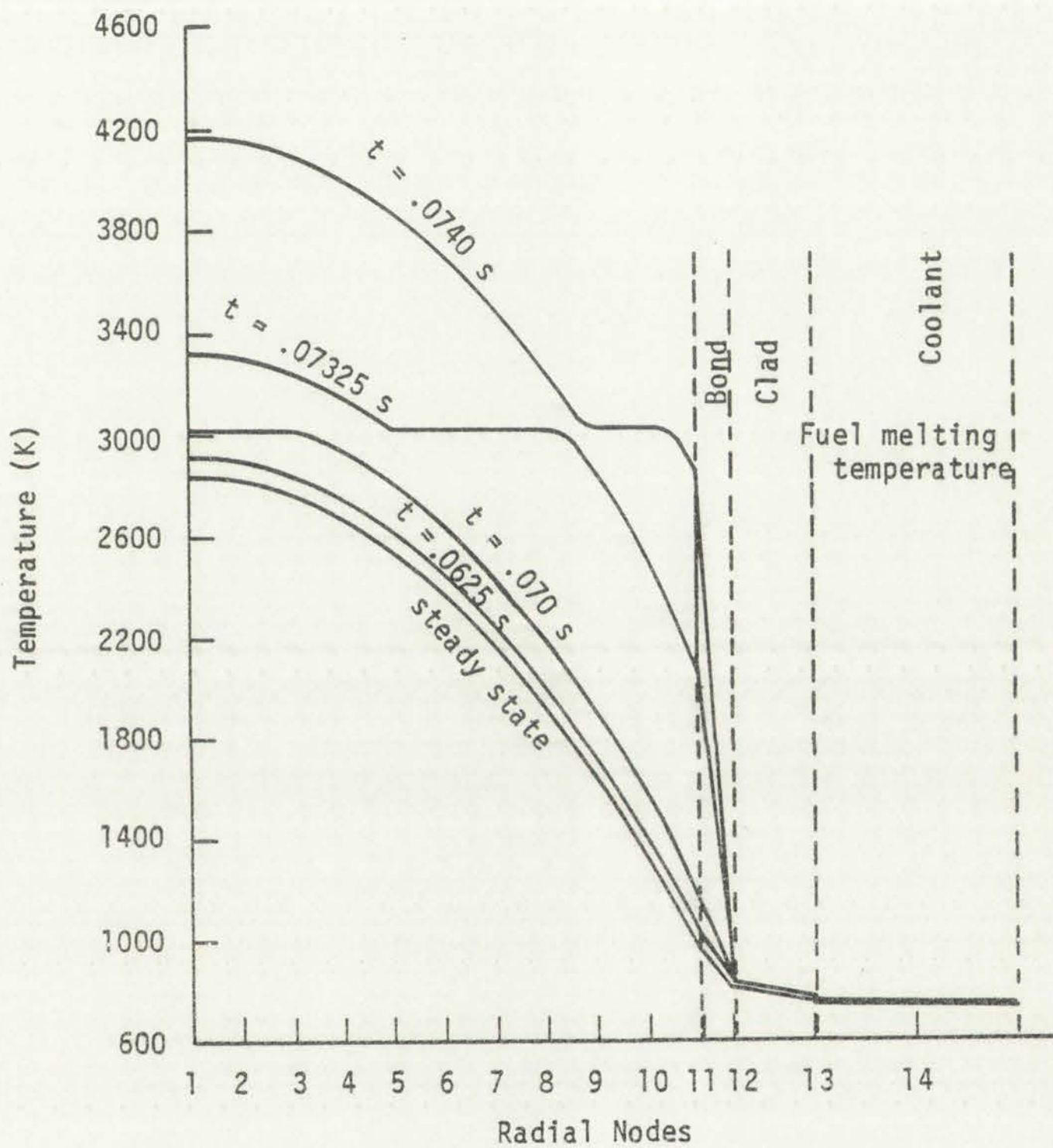


Figure 4.5.
 Transient radial temperature profiles at axial
 node 11 (hottest) for ramp reactivity insertion of $\$15/s$.



Figure 1. Cumulative vs. Temperature for different conditions. The curves represent the cumulative values for different temperatures. The x-axis is Temperature (°C) and the y-axis is Cumulative. The curves are labeled A, B, C, and D.

nodal temperature is kept at the melt temperature until the heat of fusion is acquired for all the mass in that node. Also note that the transient temperature profiles for the \$5/s and \$15/s ramp are almost identical with only the time sequence being different. The fuel edge temperature for the \$5/s ramp is slightly lower since the longer time allows some surface heat removal.

4.4 Inclusion Vaporization

Using the fuel nodal temperatures obtained by the subroutine TRANS, the subroutine VAPOR determines if inclusion vaporization occurs and, if so, the nodal volume expansion and total fuel expansion that can be expected at the end of the transient time step.

Two versions of VAPOR exist. The first version assumes the inclusion compositions are segregated elementally as shown in Fig. 4.6. The second version assumes the inclusion is a homogeneous solution of its constituents. The following assumptions are made by VAPOR:

1. The growth of the bubble upon vaporization is instantaneous. Thus any inertial or heat transfer bubble growth controlling mechanisms were assumed negligible.
2. The various vapors are noninteracting, i.e.,

$$V_T = V_1 + V_2 + \dots$$
3. Free volume expansion exists. Axial fuel-clad drag, solid fuel constraint (pressure bottle), etc., are assumed nonexistent.

Since the first version assumes segregated inclusion composition, species K vaporizes when its vapor pressure exceeds the bulk pressure. In the second version, inclusion vaporization does not occur until the inclusion vapor pressure determined by Raoult's Law, i.e.,

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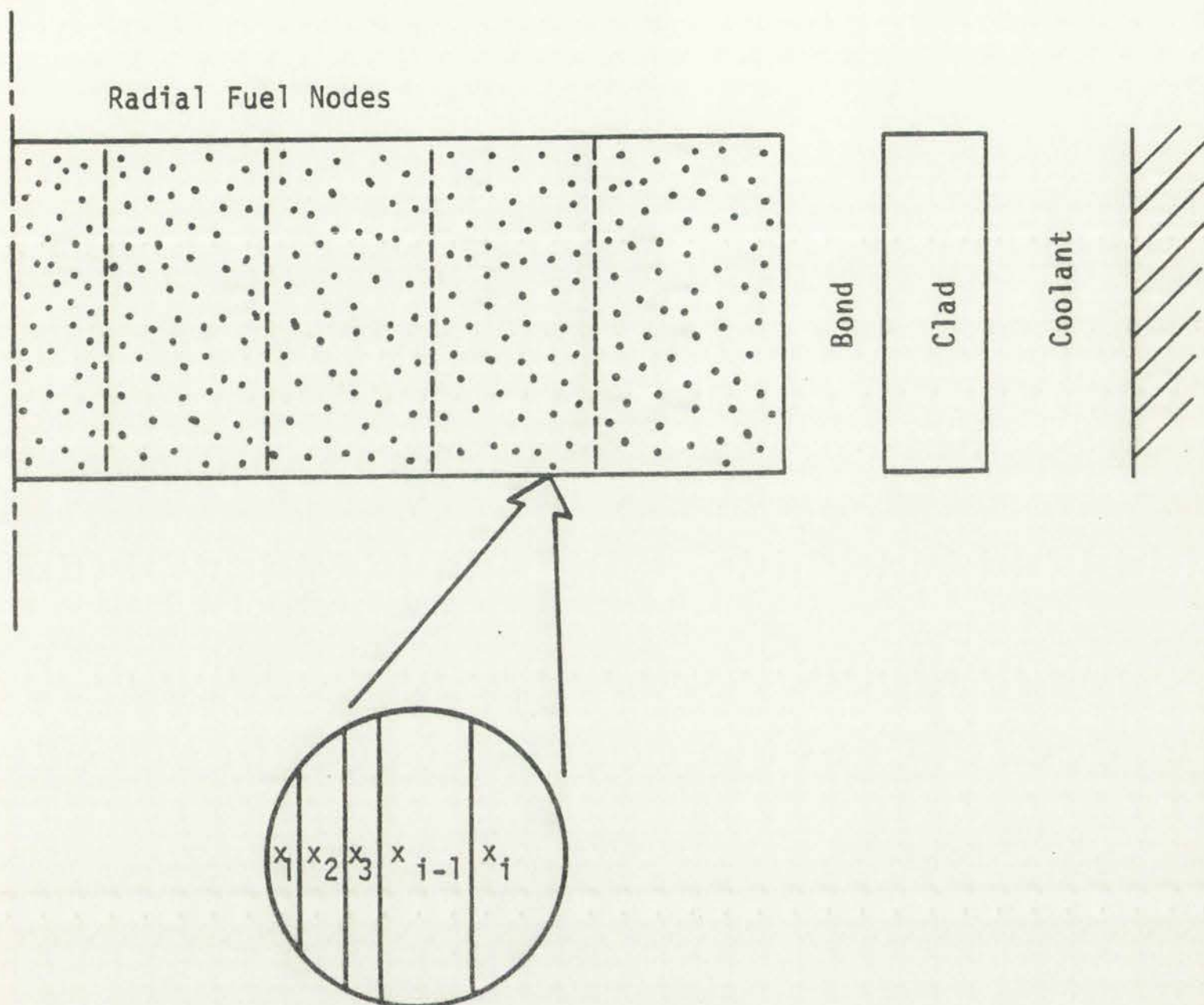
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Compositional Segregated Inclusion Weight Percent for:

O'Boyle Inclusion: Mo-25%, Tc-17%, Ru-48%, Rh-5%
Pd-5%, Sb~1%

Johnson Inclusion (Type I): Mo-14.5%, Tc-20%, Ru-43.3%, Rh-17.6%
Pd-2.1%, Fe-2.45%, Sb~1%

Jeffery Inclusion: Mo-32.3%, Tc-10%, Ru-13.95%, Rh-3.95%,
Pd-2.1%, Ba-6.75%, Zr-3%, Ce-1.65%,
Sr-.9%, Nd-3%, Te-2.1%

Figure 4.6
Segregated inclusions.

Year	1950	1951	1952	1953	1954	1955	1956	1957	1958	1959	1960
...



Figure 2
 Separated fractions

the sum of the partial pressures (see Sec. 5.2), exceeds the bulk pressure.

In the above calculations, saturation vapor pressure curves for the appropriate volatiles must be known. Experimentally and theoretically determined vapor pressure curves can be found in Appendix L. If the data did not exist, it was extrapolated to the pressure range of interest, i.e. 25 to 100 atm. Table 4.9 contains a listing of the saturation pressure-temperature relations for the elements of interest, used in this analysis.

Hornung¹² in extrapolating his data assumes a linear relationship $\text{Log } P \propto \frac{1}{T}$ over a large temperature range. He also states that one must be careful in extrapolating vapor-pressure equations that contain additional phenomenological terms, i.e.,

$$\text{Log } P \propto A - \frac{B}{T} + CT + D \log T \quad , \quad (4.2)$$

since no physical basis exists for these terms. This equation can, however, be derived as shown in Appendix M, if one assumes a temperature dependent latent heat of vaporization, ΔH . Nesmeyanov¹³ uses this equation in his work to represent the saturation vapor pressure curves.

The subroutines along with the driver program can be found in Appendix N.

The first part of the paper is devoted to the study of the properties of the function $f(x)$ defined by the equation $f(x) = \int_0^x f(t) dt$.

In the case of a constant function $f(x) = c$, the equation becomes $c = \int_0^x c dt = cx$, which implies $c = 0$.

For a linear function $f(x) = ax + b$, the equation becomes $ax + b = \int_0^x (at + b) dt = \frac{a}{2}x^2 + bx$, which implies $a = 0$ and $b = 0$.

For a quadratic function $f(x) = ax^2 + bx + c$, the equation becomes $ax^2 + bx + c = \int_0^x (at^2 + bt + c) dt = \frac{a}{3}x^3 + \frac{b}{2}x^2 + cx$, which implies $a = 0$, $b = 0$, and $c = 0$.

For a cubic function $f(x) = ax^3 + bx^2 + cx + d$, the equation becomes $ax^3 + bx^2 + cx + d = \int_0^x (at^3 + bt^2 + ct + d) dt = \frac{a}{4}x^4 + \frac{b}{3}x^3 + \frac{c}{2}x^2 + dx$, which implies $a = 0$, $b = 0$, $c = 0$, and $d = 0$.

For a quartic function $f(x) = ax^4 + bx^3 + cx^2 + dx + e$, the equation becomes $ax^4 + bx^3 + cx^2 + dx + e = \int_0^x (at^4 + bt^3 + ct^2 + dt + e) dt = \frac{a}{5}x^5 + \frac{b}{4}x^4 + \frac{c}{3}x^3 + \frac{d}{2}x^2 + ex$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, and $e = 0$.

For a quintic function $f(x) = ax^5 + bx^4 + cx^3 + dx^2 + ex + f$, the equation becomes $ax^5 + bx^4 + cx^3 + dx^2 + ex + f = \int_0^x (at^5 + bt^4 + ct^3 + dt^2 + et + f) dt = \frac{a}{6}x^6 + \frac{b}{5}x^5 + \frac{c}{4}x^4 + \frac{d}{3}x^3 + \frac{e}{2}x^2 + fx$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, and $f = 0$.

For a sextic function $f(x) = ax^6 + bx^5 + cx^4 + dx^3 + ex^2 + fx + g$, the equation becomes $ax^6 + bx^5 + cx^4 + dx^3 + ex^2 + fx + g = \int_0^x (at^6 + bt^5 + ct^4 + dt^3 + et^2 + ft + g) dt = \frac{a}{7}x^7 + \frac{b}{6}x^6 + \frac{c}{5}x^5 + \frac{d}{4}x^4 + \frac{e}{3}x^3 + \frac{f}{2}x^2 + gx$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, $f = 0$, and $g = 0$.

For a septic function $f(x) = ax^7 + bx^6 + cx^5 + dx^4 + ex^3 + fx^2 + gx + h$, the equation becomes $ax^7 + bx^6 + cx^5 + dx^4 + ex^3 + fx^2 + gx + h = \int_0^x (at^7 + bt^6 + ct^5 + dt^4 + et^3 + ft^2 + gt + h) dt = \frac{a}{8}x^8 + \frac{b}{7}x^7 + \frac{c}{6}x^6 + \frac{d}{5}x^5 + \frac{e}{4}x^4 + \frac{f}{3}x^3 + \frac{g}{2}x^2 + hx$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, $f = 0$, $g = 0$, and $h = 0$.

For an octic function $f(x) = ax^8 + bx^7 + cx^6 + dx^5 + ex^4 + fx^3 + gx^2 + hx + i$, the equation becomes $ax^8 + bx^7 + cx^6 + dx^5 + ex^4 + fx^3 + gx^2 + hx + i = \int_0^x (at^8 + bt^7 + ct^6 + dt^5 + et^4 + ft^3 + gt^2 + ht + i) dt = \frac{a}{9}x^9 + \frac{b}{8}x^8 + \frac{c}{7}x^7 + \frac{d}{6}x^6 + \frac{e}{5}x^5 + \frac{f}{4}x^4 + \frac{g}{3}x^3 + \frac{h}{2}x^2 + ix$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, $f = 0$, $g = 0$, $h = 0$, and $i = 0$.

For a nonic function $f(x) = ax^9 + bx^8 + cx^7 + dx^6 + ex^5 + fx^4 + gx^3 + hx^2 + ix + j$, the equation becomes $ax^9 + bx^8 + cx^7 + dx^6 + ex^5 + fx^4 + gx^3 + hx^2 + ix + j = \int_0^x (at^9 + bt^8 + ct^7 + dt^6 + et^5 + ft^4 + gt^3 + ht^2 + it + j) dt = \frac{a}{10}x^{10} + \frac{b}{9}x^9 + \frac{c}{8}x^8 + \frac{d}{7}x^7 + \frac{e}{6}x^6 + \frac{f}{5}x^5 + \frac{g}{4}x^4 + \frac{h}{3}x^3 + \frac{i}{2}x^2 + jx$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, $f = 0$, $g = 0$, $h = 0$, $i = 0$, and $j = 0$.

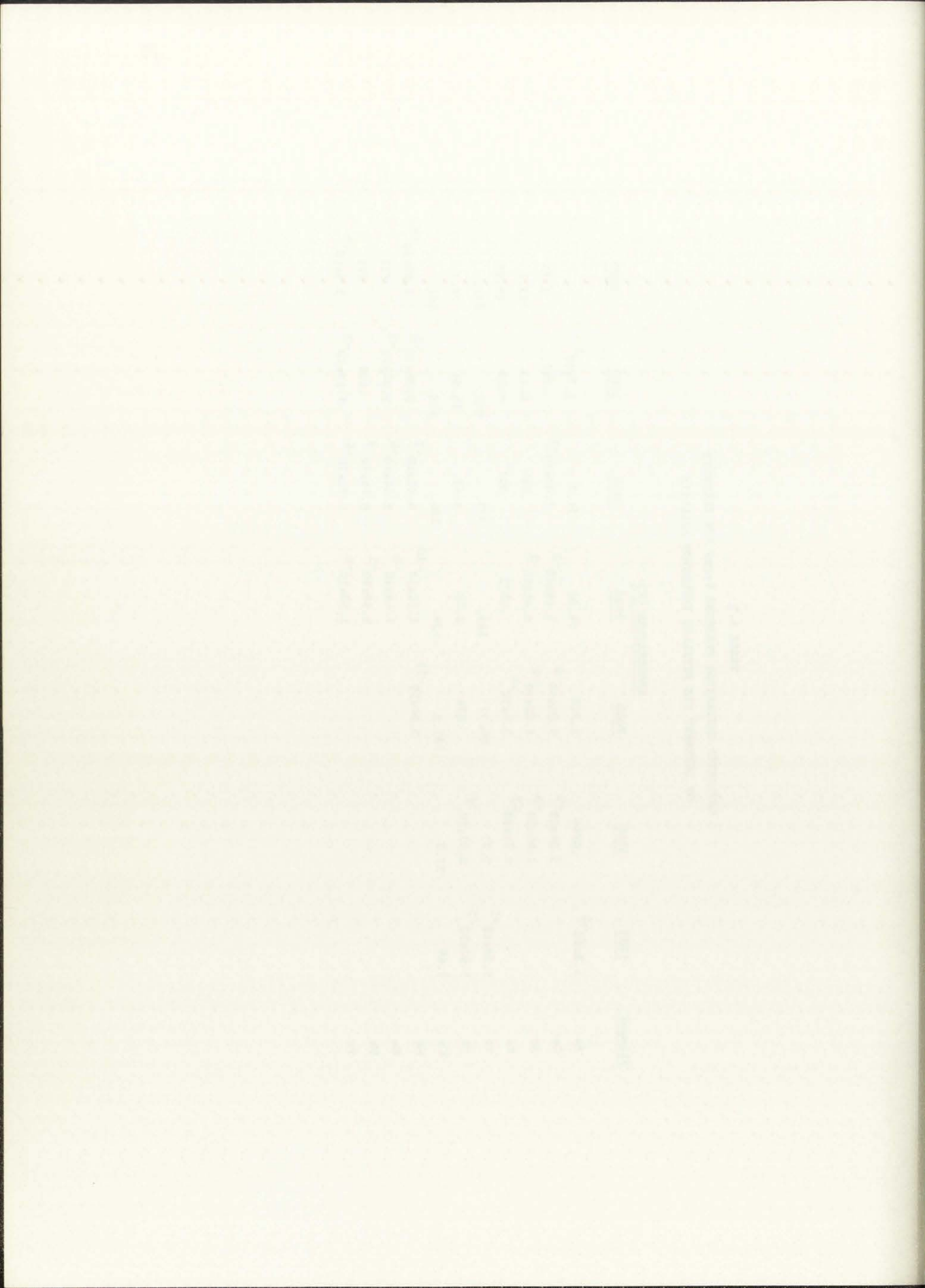
For a decic function $f(x) = ax^{10} + bx^9 + cx^8 + dx^7 + ex^6 + fx^5 + gx^4 + hx^3 + ix^2 + jx + k$, the equation becomes $ax^{10} + bx^9 + cx^8 + dx^7 + ex^6 + fx^5 + gx^4 + hx^3 + ix^2 + jx + k = \int_0^x (at^{10} + bt^9 + ct^8 + dt^7 + et^6 + ft^5 + gt^4 + ht^3 + it^2 + jt + k) dt = \frac{a}{11}x^{11} + \frac{b}{10}x^{10} + \frac{c}{9}x^9 + \frac{d}{8}x^8 + \frac{e}{7}x^7 + \frac{f}{6}x^6 + \frac{g}{5}x^5 + \frac{h}{4}x^4 + \frac{i}{3}x^3 + \frac{j}{2}x^2 + kx$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, $f = 0$, $g = 0$, $h = 0$, $i = 0$, $j = 0$, and $k = 0$.

For an undecimic function $f(x) = ax^{11} + bx^{10} + cx^9 + dx^8 + ex^7 + fx^6 + gx^5 + hx^4 + ix^3 + jx^2 + kx + l$, the equation becomes $ax^{11} + bx^{10} + cx^9 + dx^8 + ex^7 + fx^6 + gx^5 + hx^4 + ix^3 + jx^2 + kx + l = \int_0^x (at^{11} + bt^{10} + ct^9 + dt^8 + et^7 + ft^6 + gt^5 + ht^4 + it^3 + jt^2 + kt + l) dt = \frac{a}{12}x^{12} + \frac{b}{11}x^{11} + \frac{c}{10}x^{10} + \frac{d}{9}x^9 + \frac{e}{8}x^8 + \frac{f}{7}x^7 + \frac{g}{6}x^6 + \frac{h}{5}x^5 + \frac{i}{4}x^4 + \frac{j}{3}x^3 + \frac{k}{2}x^2 + lx$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, $f = 0$, $g = 0$, $h = 0$, $i = 0$, $j = 0$, $k = 0$, and $l = 0$.

For a duodecimic function $f(x) = ax^{12} + bx^{11} + cx^{10} + dx^9 + ex^8 + fx^7 + gx^6 + hx^5 + ix^4 + jx^3 + kx^2 + lx + m$, the equation becomes $ax^{12} + bx^{11} + cx^{10} + dx^9 + ex^8 + fx^7 + gx^6 + hx^5 + ix^4 + jx^3 + kx^2 + lx + m = \int_0^x (at^{12} + bt^{11} + ct^{10} + dt^9 + et^8 + ft^7 + gt^6 + ht^5 + it^4 + jt^3 + kt^2 + lt + m) dt = \frac{a}{13}x^{13} + \frac{b}{12}x^{12} + \frac{c}{11}x^{11} + \frac{d}{10}x^{10} + \frac{e}{9}x^9 + \frac{f}{8}x^8 + \frac{g}{7}x^7 + \frac{h}{6}x^6 + \frac{i}{5}x^5 + \frac{j}{4}x^4 + \frac{k}{3}x^3 + \frac{l}{2}x^2 + mx$, which implies $a = 0$, $b = 0$, $c = 0$, $d = 0$, $e = 0$, $f = 0$, $g = 0$, $h = 0$, $i = 0$, $j = 0$, $k = 0$, $l = 0$, and $m = 0$.

TABLE 4.9
ESTIMATED SATURATION PRESSURE (atm) FOR ELEMENTS
OF INTEREST PIN METALLIC INCLUSION ANALYSIS

Element	TEMPERATURE (K)						
	1000	1500	2000	2500	3000	3500	4000
Ba	1.8×10^{-4}	.0964	2.224	14.62	51.3	2.7×10^4	
Ce		2.84×10^{-9}	9.23×10^{-6}	1.18×10^{-3}	3.00×10^{-2}	.302	1.71
Pd		1.95×10^{-9}	1.68×10^{-6}	6.44×10^{-2}	.944	6.43	27.1
Fe		2.29×10^{-7}	3.4×10^{-4}	.0273	.507	4.09	19.57
Te	5.59×10^{-2}	5.25	46.77	165.	370.	643.	957.
Sb	1.03×10^{-3}	8.92×10^{-2}	.876	3.46	8.65	16.64	27.2
Cs	1.69	27.3	105.2	230.	380.	538.	691.
Mo			5.84×10^{-15}	1.12×10^{-10}	8.06×10^{-8}	8.84×10^{-6}	3.00×10^{-4}
Ru				1.48×10^{-6}	2.44×10^{-4}	9.08×10^{-3}	.131
Rh				9.98×10^{-5}	6.14×10^{-3}	.109	.696
Tc				1.50×10^{-6}	1.31×10^{-4}	3.19×10^{-3}	3.5×10^{-2}



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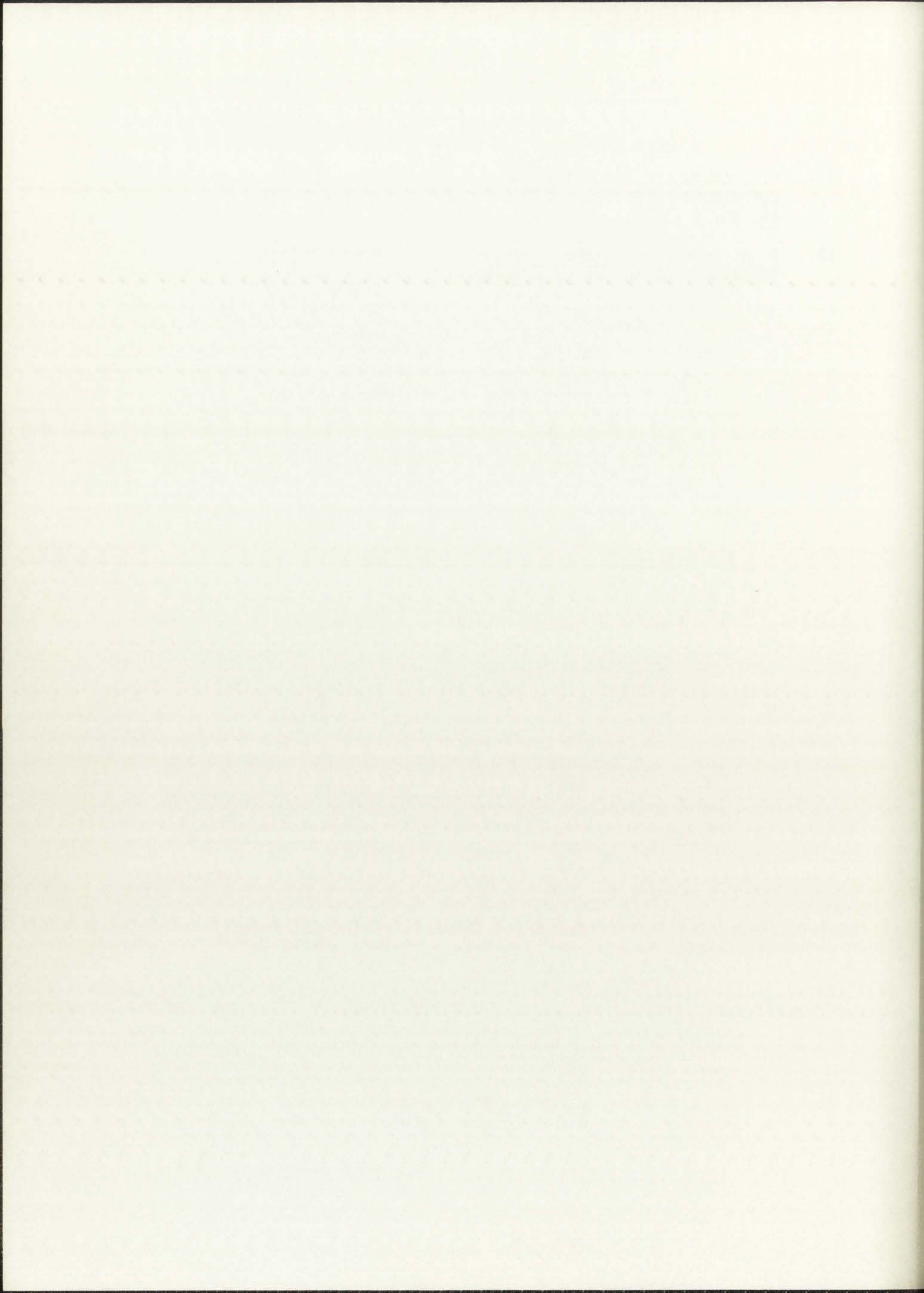
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5. DISCUSSION OF RESULTS

In this section, the local (nodal) and total fuel volume expansion are calculated for a hypothetical transient overpower excursion. The results of the calculations depend strongly on the physical-chemical state of the inclusions. The physical state with respect to the solubility of the inclusion constituents in one another is uncertain. Thus calculations are done assuming: (1) the inclusion constituents are totally segregated from one another (immiscible) and (2) the inclusion constituents are in solid solution with one another (miscible).

5.1 Segregated Inclusions

The nodal and fuel volume expansions are calculated assuming the inclusion constituents are immiscible. This assumption implies that species k vaporizes when its vapor pressure exceeds the local bulk pressure, taken as the plenum pressure in these analyses. In addition, the following assumptions are made:

1. The various vapors are noninteracting, i.e.,
$$V_T(\text{total volume}) = V_1 + V_2 + \dots, V_i$$
2. The growth of the bubbles upon nucleation is instantaneous; thus, inertial and heat transfer controlling mechanisms are ignored.
3. As mentioned previously, the inclusions are considered identical in terms of size and composition, both in the radial and axial direction. The size assumed is $5 \mu\text{m}$ in diameter¹⁻³ and the composition based on O'Boyle³ and Johnson's⁴ average inclusion compositions are used.

Two additional assumptions were made for simplicity in the initial runs. These are:

1. The number density of inclusions is constant in the radial and axial direction. The density assumes total segregation of pertinent fission products.
2. An Ideal Gas equation-of-state is used for the metallic fission product vapor.

In the following calculations the percent volume expansion, $\frac{\Delta V}{V} \times 100\%$, is computed for both the entire fuel pin and for each individual node. Within any given node it is assumed that the temperature profile is flat, and that volatile species k will vaporize when the nodal temperature reaches its vaporization temperature. This leads to step jumps in the nodal volume expansion at the various vaporization temperatures. The contribution of each inclusion constituent is monitored. These calculated volume expansion are then compared to the volume expansion due to the phase change upon fuel melting and the expansion due to fission gas.

Figures 5.1-5.7 show the results using the above assumptions. If one assumes Sb is present in the inclusions at a level of 1 wt%, an additional 3-4% nodal volume expansion can be expected. Consequently the presence of Sb, Nb, Ag, and other stable metallics mentioned previously, in levels under the 0.5 to 1 wt% detection limit of the ion microprobe could substantially increase the expected fuel volume expansion. Future calculations will be done with and without Sb present in order to obtain an order of magnitude approximation to the possible contribution of nondetected metallics. Whether these elements actually

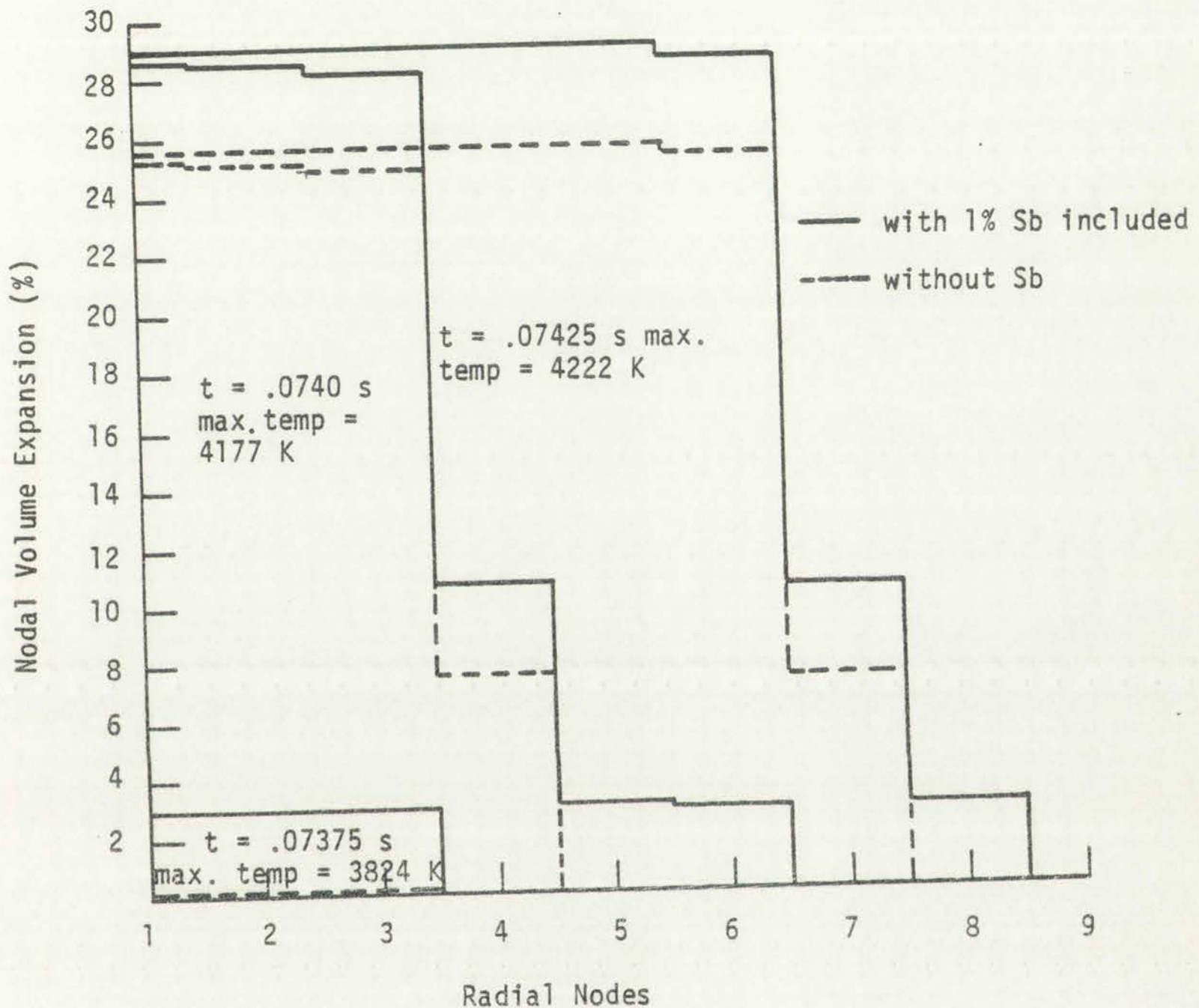


Figure 5.1.
 Nodal volume expansion at axial node II (hottest) for Johnson inclusion using \$15/s ramp insertion, flat inclusion number density profile, and Ideal Gas EOS.



This drawing is a technical drawing of a component, possibly a pipe or a structural member, showing a cross-section or a plan view. The drawing is oriented vertically on the page. It features a rectangular outer boundary with several internal lines and features, including what appears to be a central vertical section and several rectangular cutouts or internal structures. The drawing is very faint and difficult to read, but it shows a complex geometric shape with multiple levels and sections.

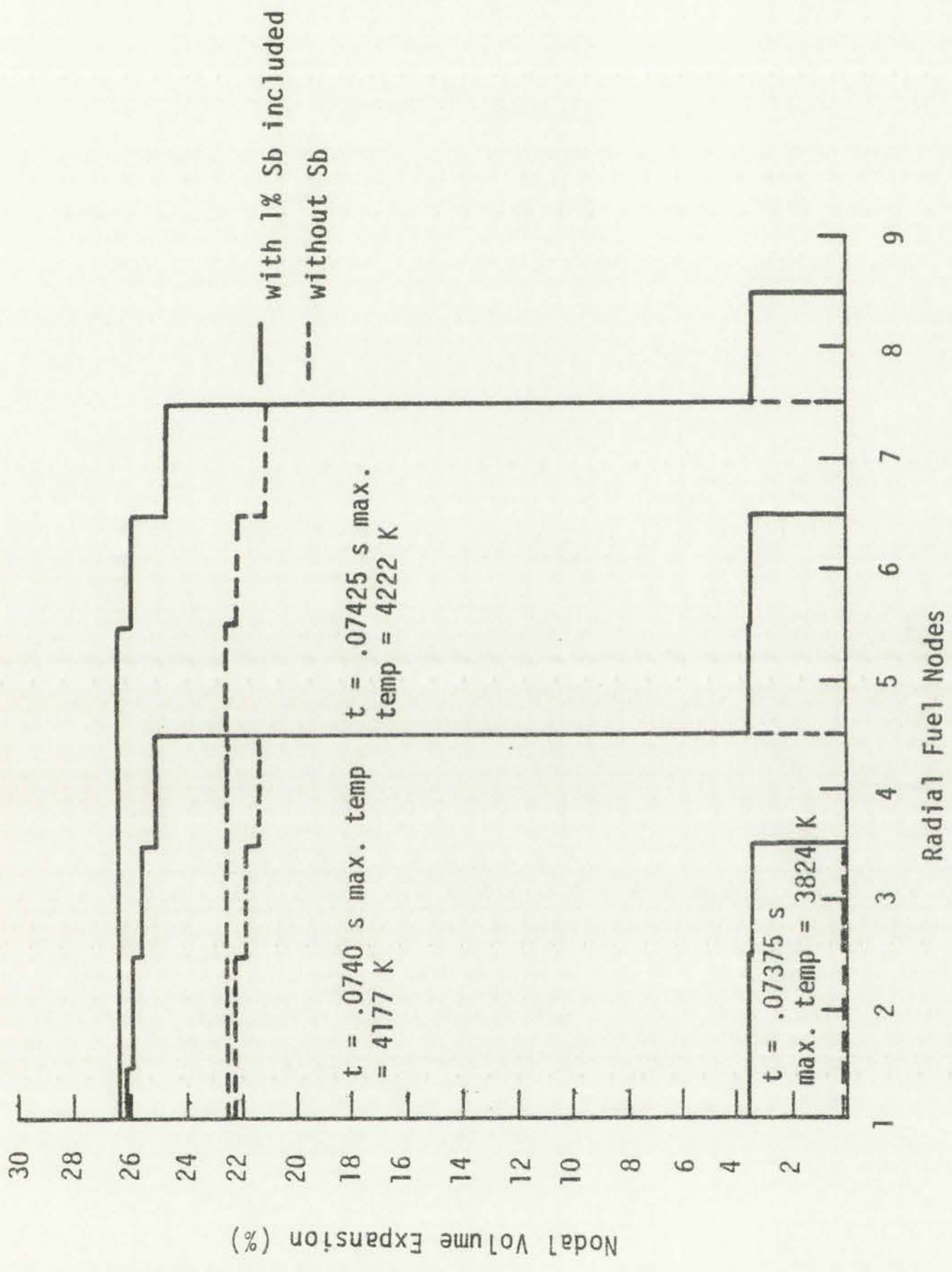


Figure 5.2
Nodal volume expansion at axial node II (hottest) for 0'Boyle inclusions using \$15/s ramp insertion, flat inclusion number density profile, and Ideal Gas EOS.



Figure 10

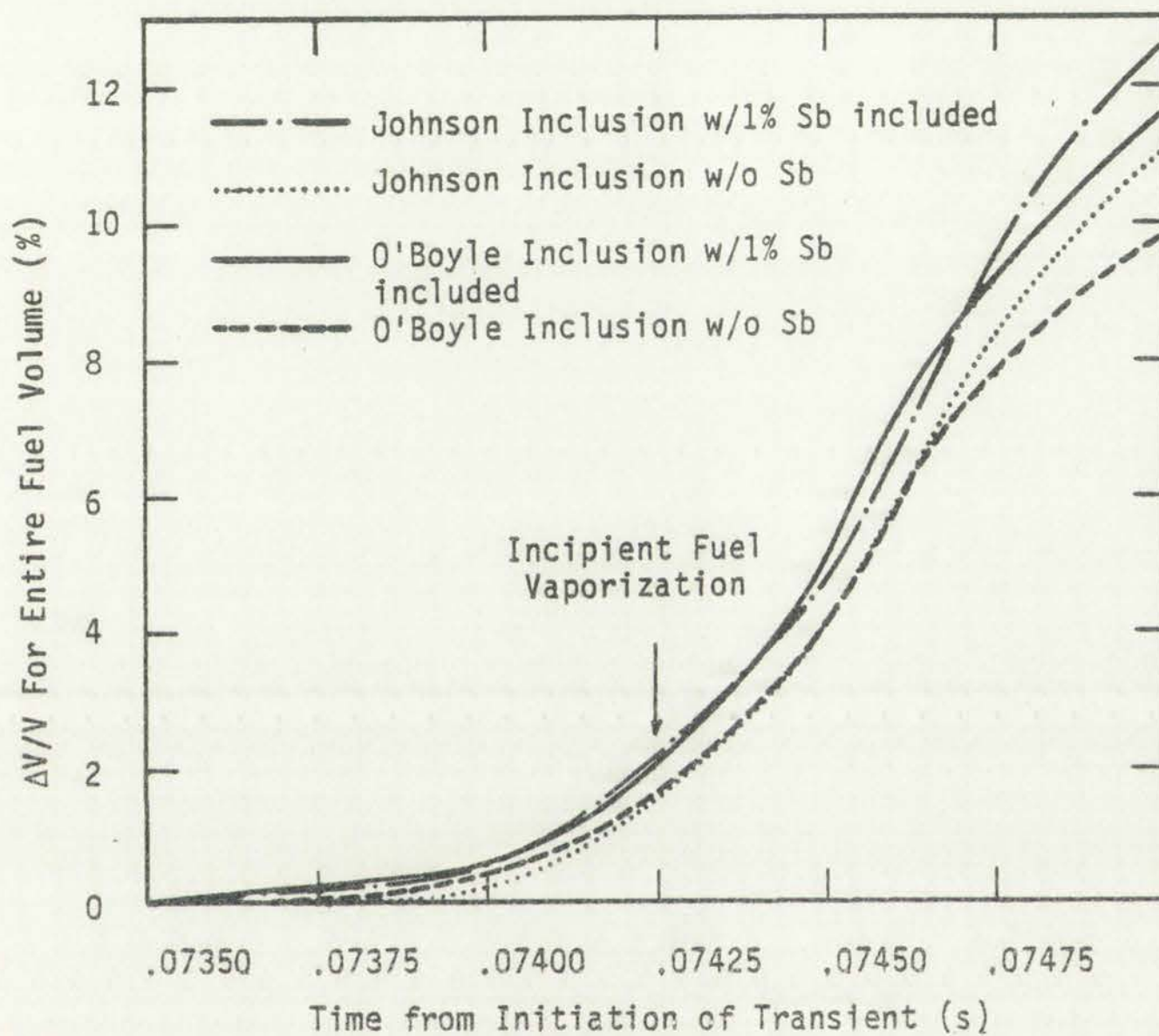


Figure 5.3
 Total fuel volume expansion for \$15/s ramp insertion,
 flat inclusion number density profile, and Ideal Gas EOS.



FIG. 1. Theoretical and experimental curves.

THEORETICAL CURVE (Dotted line)

EXPERIMENTAL CURVE (Solid line)

Wavelength (microns) vs. Frequency (cm⁻¹)

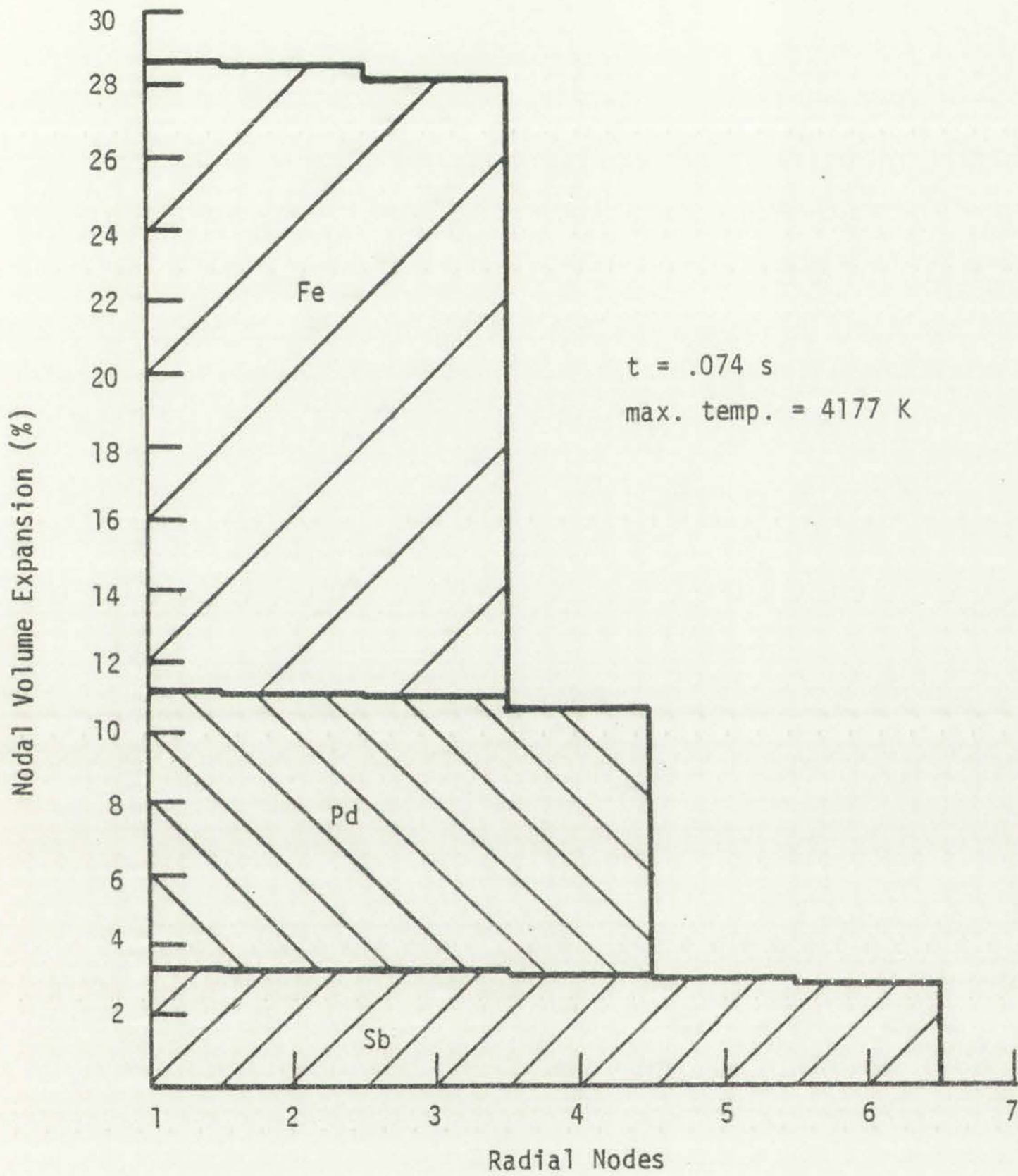


Figure 5.4
 Nodal volume expansion contribution from the various constituents of Johnson's inclusions for \$15/s ramp insertion at axial node 11 (hottest).



Figure 1

The chart displays the results of a statistical analysis. The data shows a clear upward trend across the levels for all categories. The values for category C are consistently higher than those for categories A and B, and the values increase significantly from level 1 to level 3.

The following table provides a summary of the data presented in the chart. The values are rounded to one decimal place.

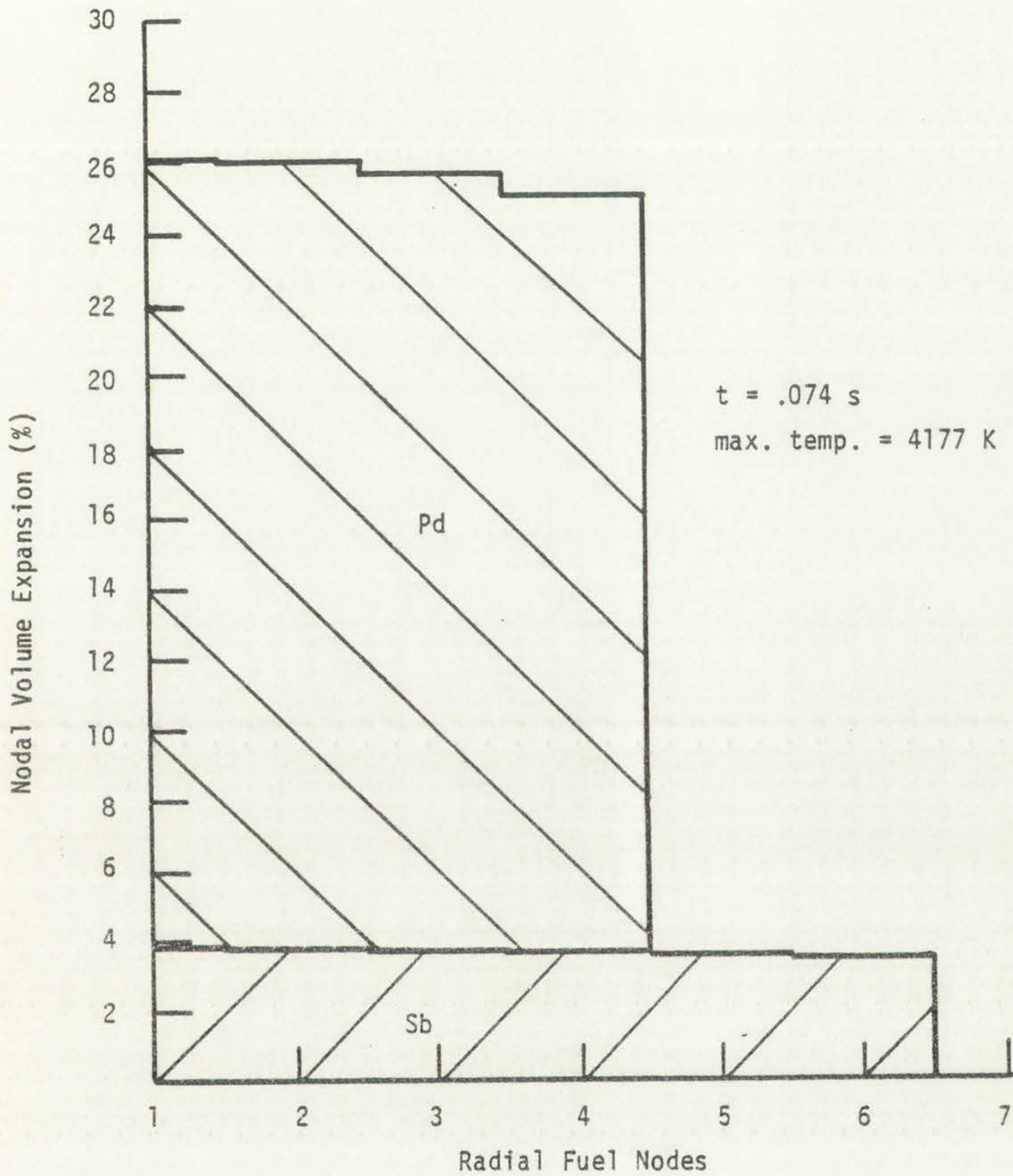
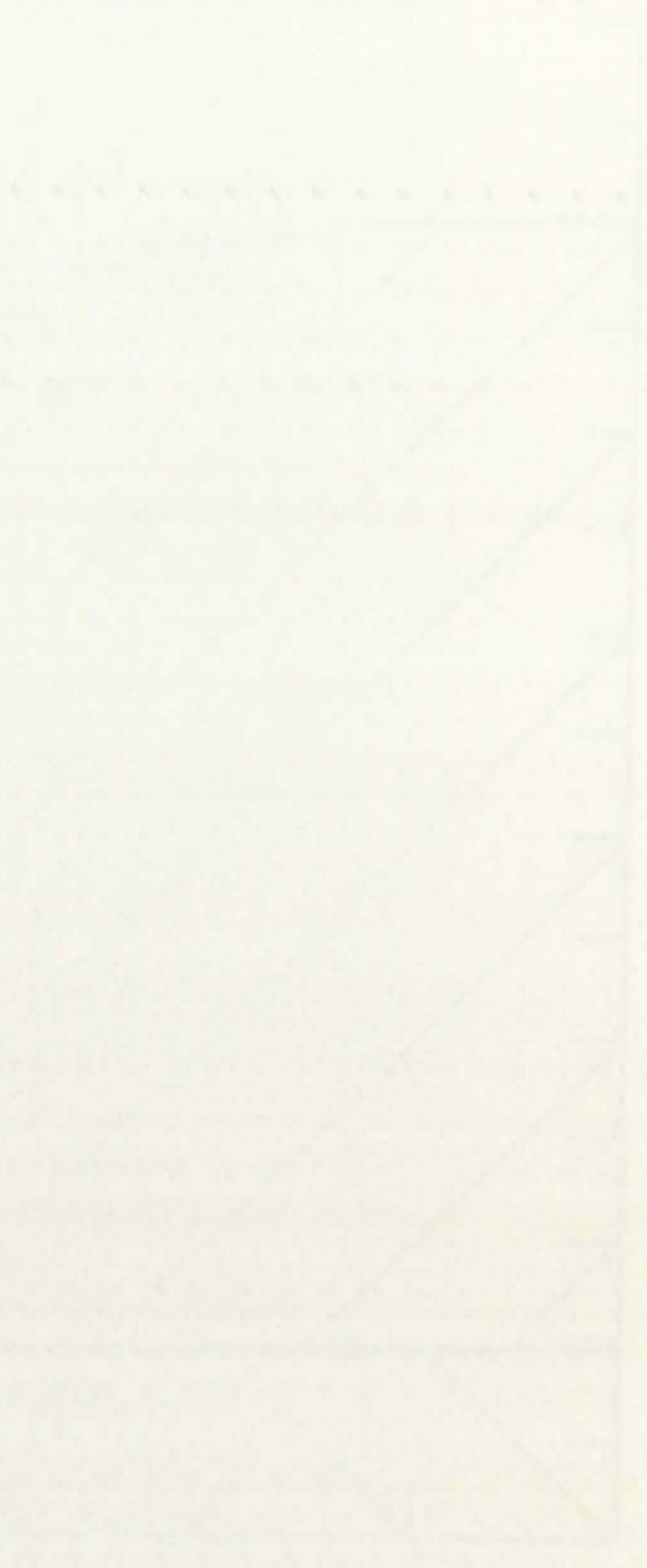


Figure 5.5
 Nodal volume expansion contribution from the various constituents of O'Boyle's inclusions at \$15/s ramp insertion.

(a) Estimated supply of labor



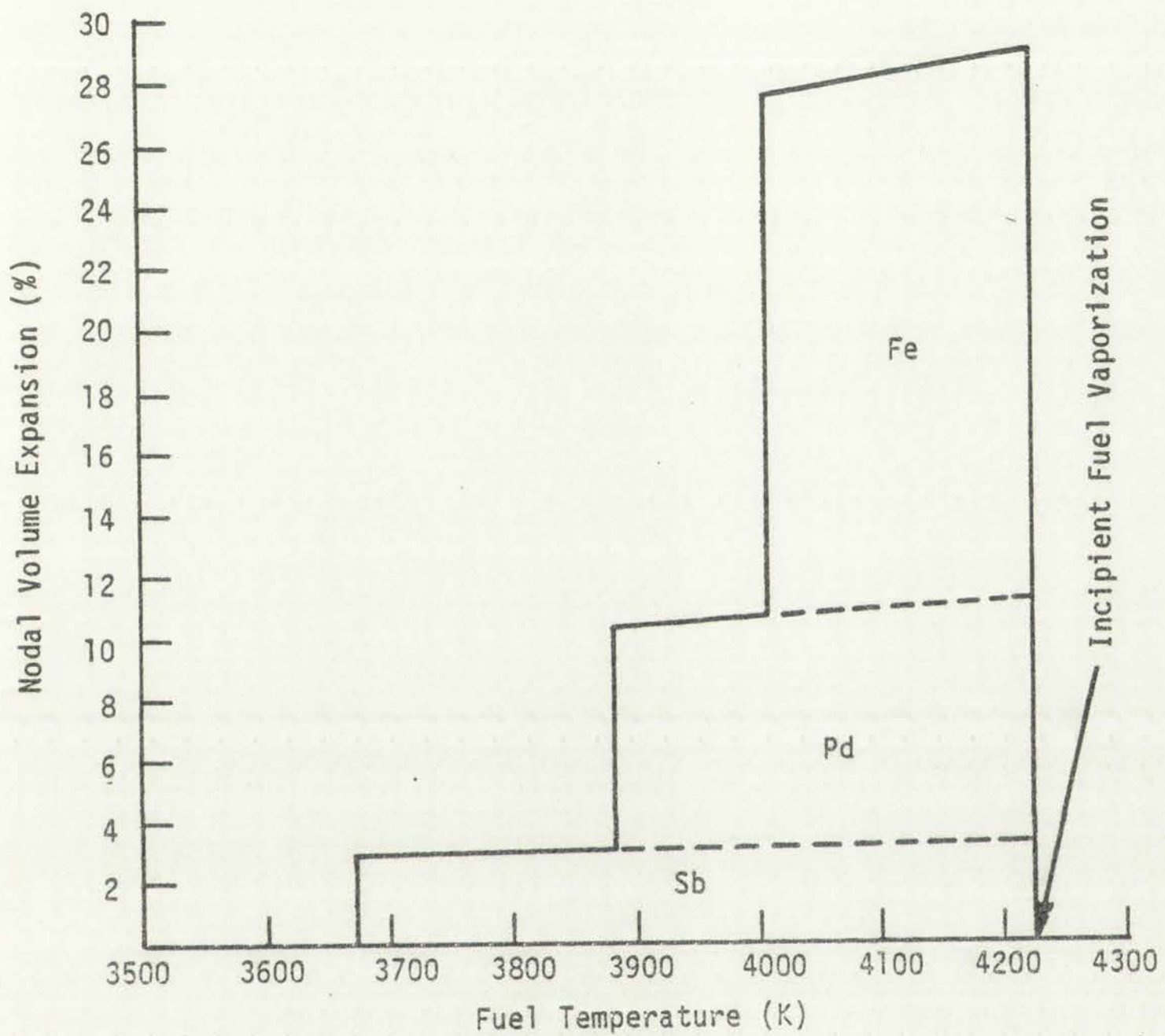


Figure 5.6
 Nodal volume expansion for Johnson inclusions using a flat inclusion number density profile and Ideal Gas EOS.



100 200 300 400 500 600 700 800

10 20 30 40 50 60 70 80

100 200 300 400 500 600 700 800

10 20 30 40 50 60 70 80

100 200 300 400 500 600 700 800

10 20 30 40 50 60 70 80

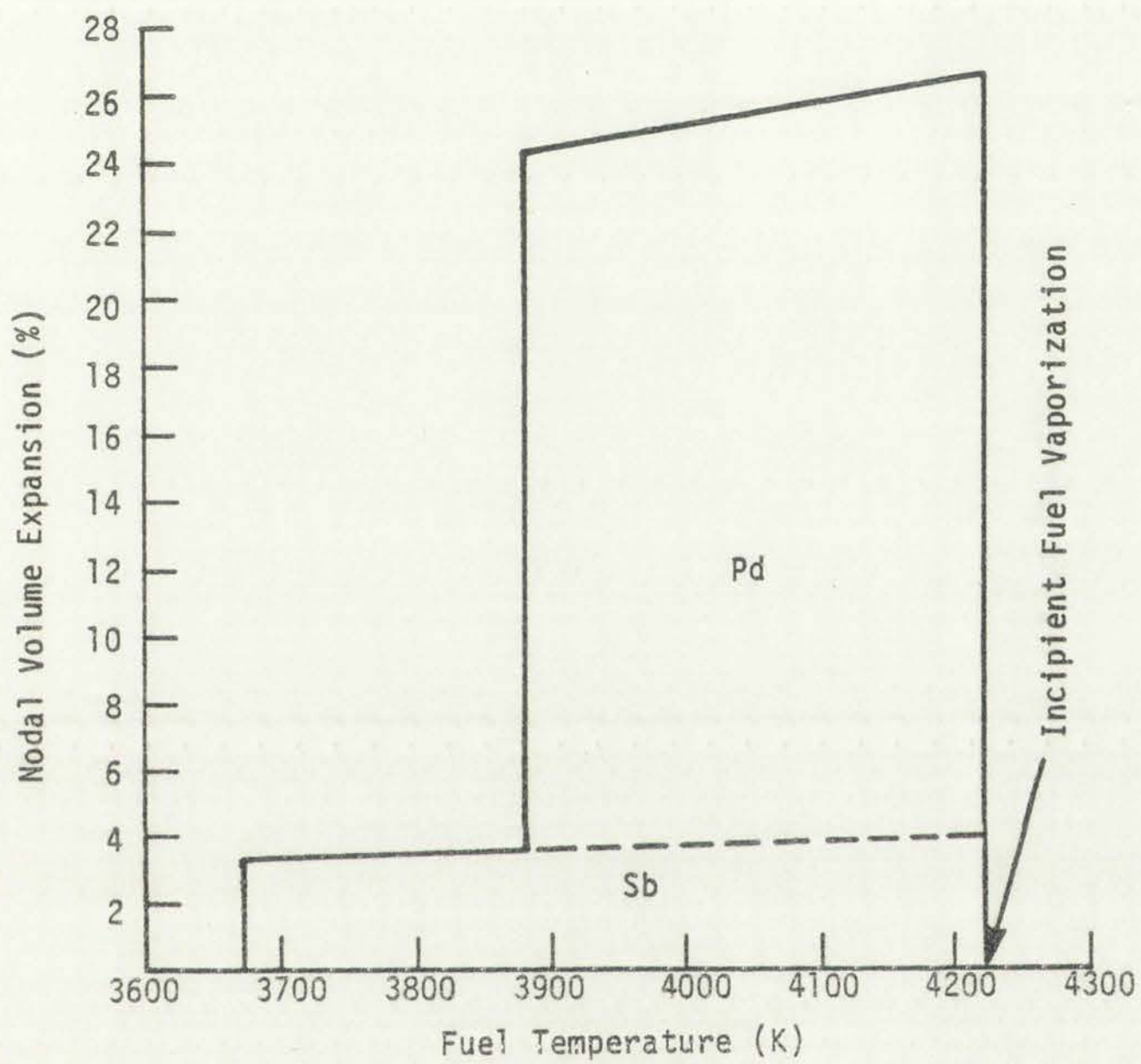


Figure 5.7
Nodal volume expansion for O'Boyle inclusion using a flat inclusion number density profile and Ideal Gas EOS.

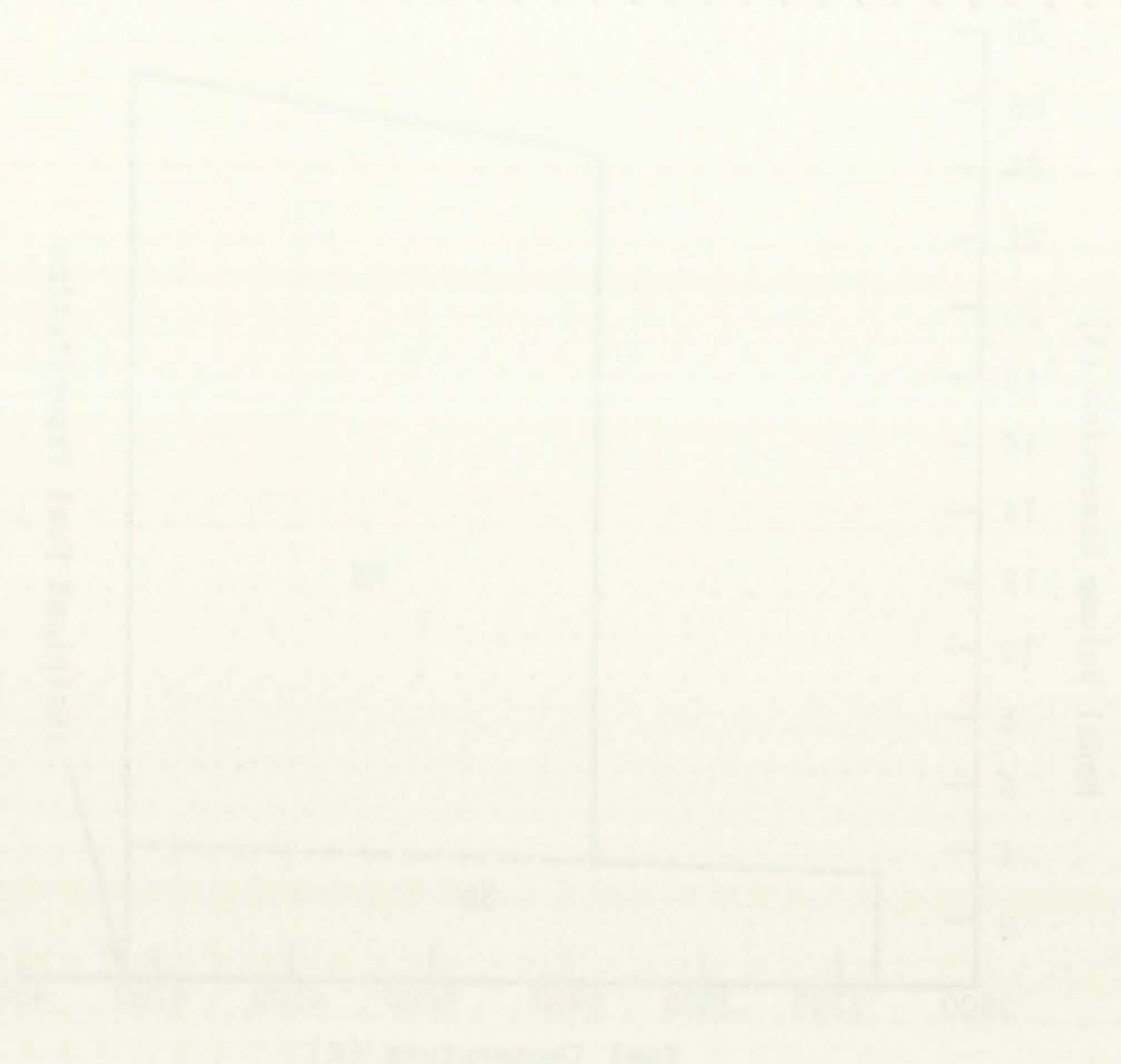
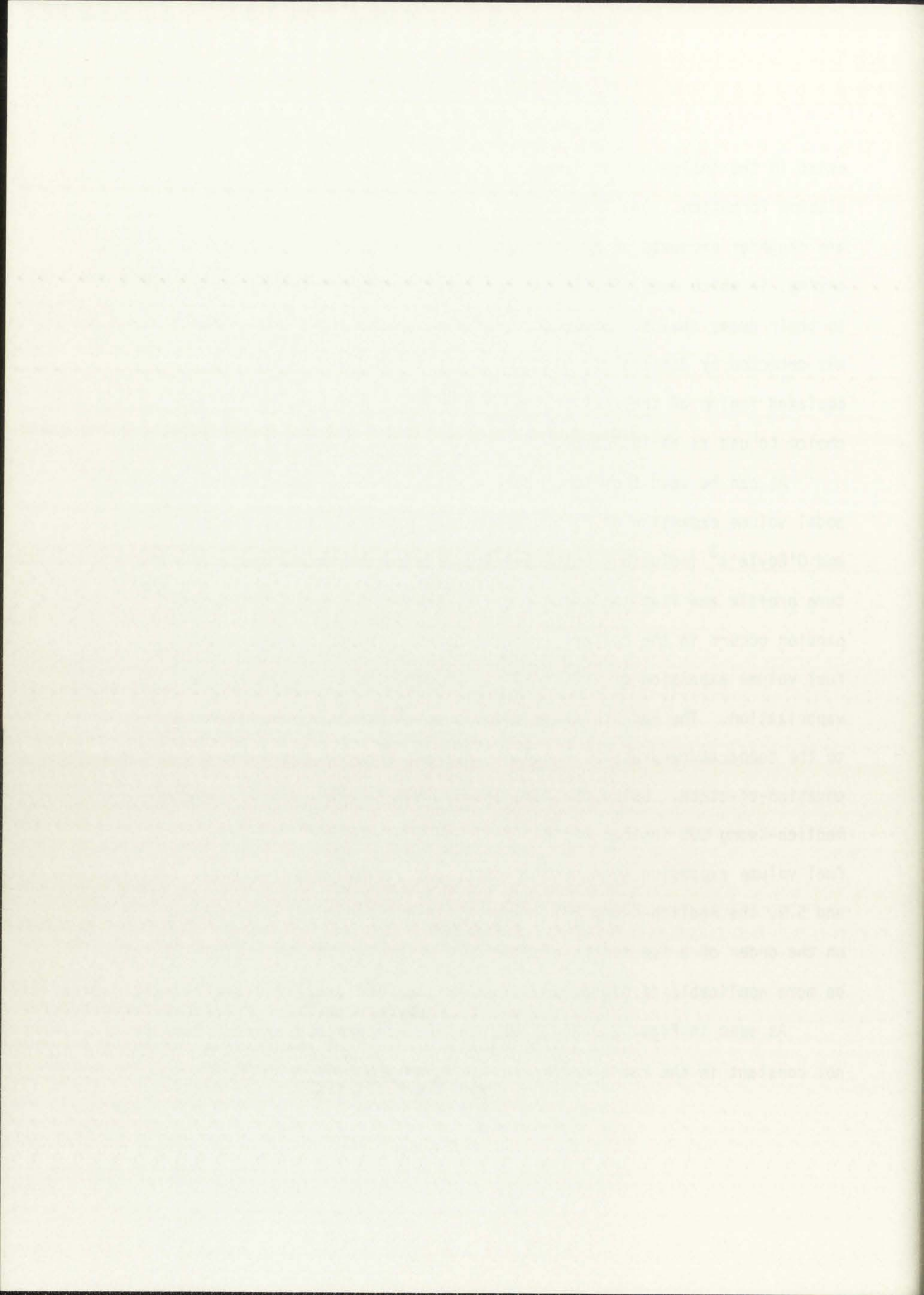


Figure 4.1: Total enthalpy function for air. The total enthalpy is the sum of the static enthalpy and the kinetic energy per unit mass.

exist in the inclusions at levels $< 1\%$ depends on the mechanism of inclusion formation. One investigator⁵ postulated that all elements are daughter products of Mo isotopes which form aggregates before decaying, in which case, Sb, Sn, Ag, Cd, etc., would not be present due to their decay chains. Since the mechanism is not known and since Sb was detected by Johnson⁴ in his type 2 inclusion found in the equiaxed region of the fuel, the potential Sb contribution is a logical choice to use as an indicator.

As can be seen from the figures, without the Sb contribution, a nodal volume expansion of 25 and 22% can be expected for Johnson's⁴ and O'Boyle's³ inclusions respectively. Due to the radial temperature profile and flat inclusion profile, the maximum nodal volume expansion occurs in the hottest (center) nodes. In addition, a total fuel volume expansion of 1.5 to 2% can be expected at incipient fuel vaporization. The Redlich-Kwong equation-of-state is more applicable to the temperature-pressure range of interest than the Ideal Gas equation-of-state. Using the same assumptions as above except with the Redlich-Kwong EOS instead of the Ideal Gas EOS, the nodal and total fuel volume expansion were recalculated. As can be seen from Figs. 5.8 and 5.9, the Redlich-Kwong EOS lowers the predicted nodal volume only on the order of a few tenths of a percent. The Redlich-Kwong EOS will be more applicable if higher pressures are assumed.

As seen in Figs. 2.9 and 2.10, the inclusion number density is not constant in the radial direction as assumed above. A radial



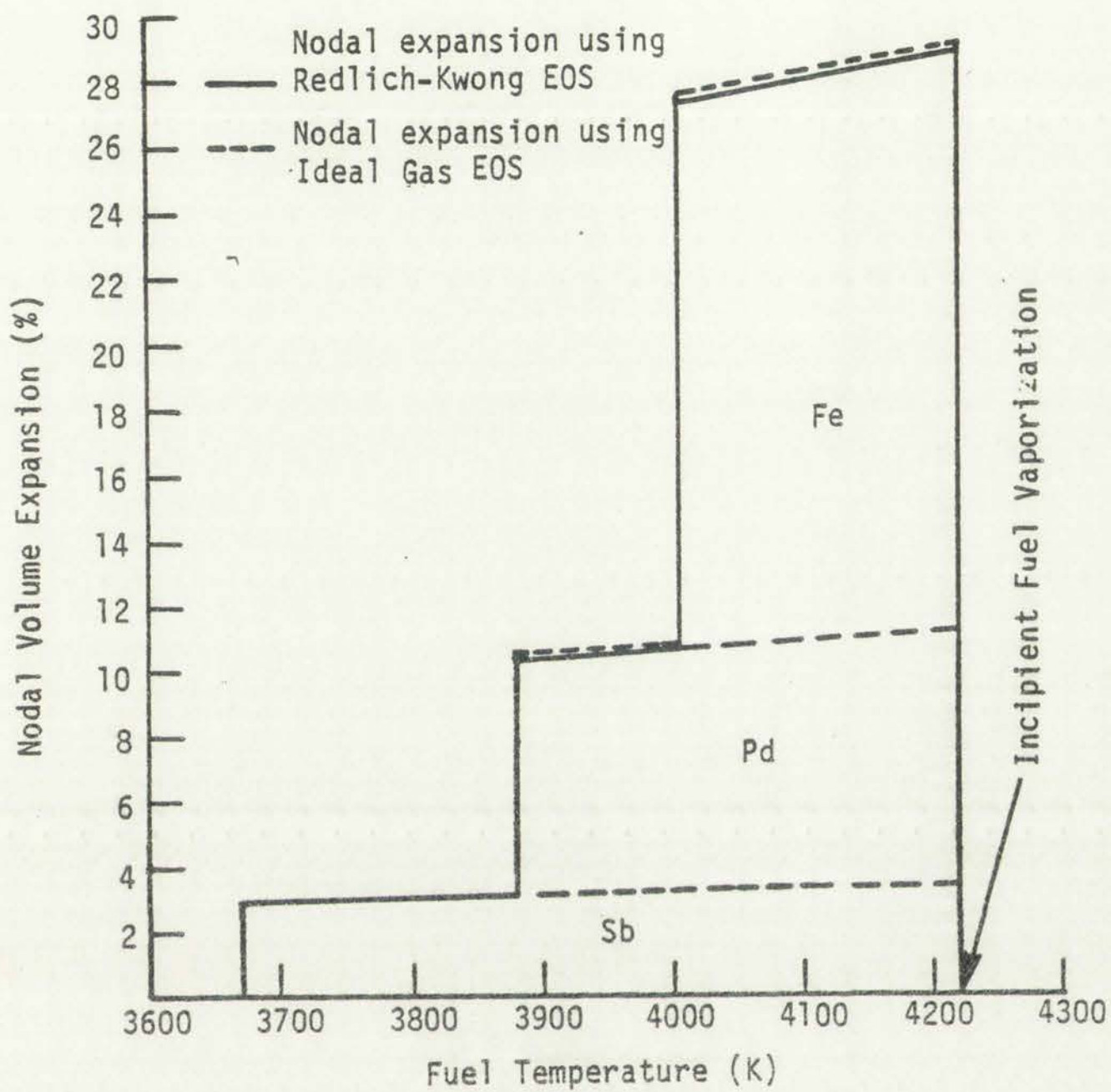


Figure 5.8
 Nodal volume expansion for Johnson inclusions using
 a flat inclusion number density profile
 and Redlich-Kwong EOS.



This drawing shows a stepped shaft with a diameter of 1.5 inches for most of its length and a diameter of 1.0 inch for a section in the middle. The total length of the shaft is 10 inches. The drawing includes a scale bar and various labels indicating dimensions and sections.

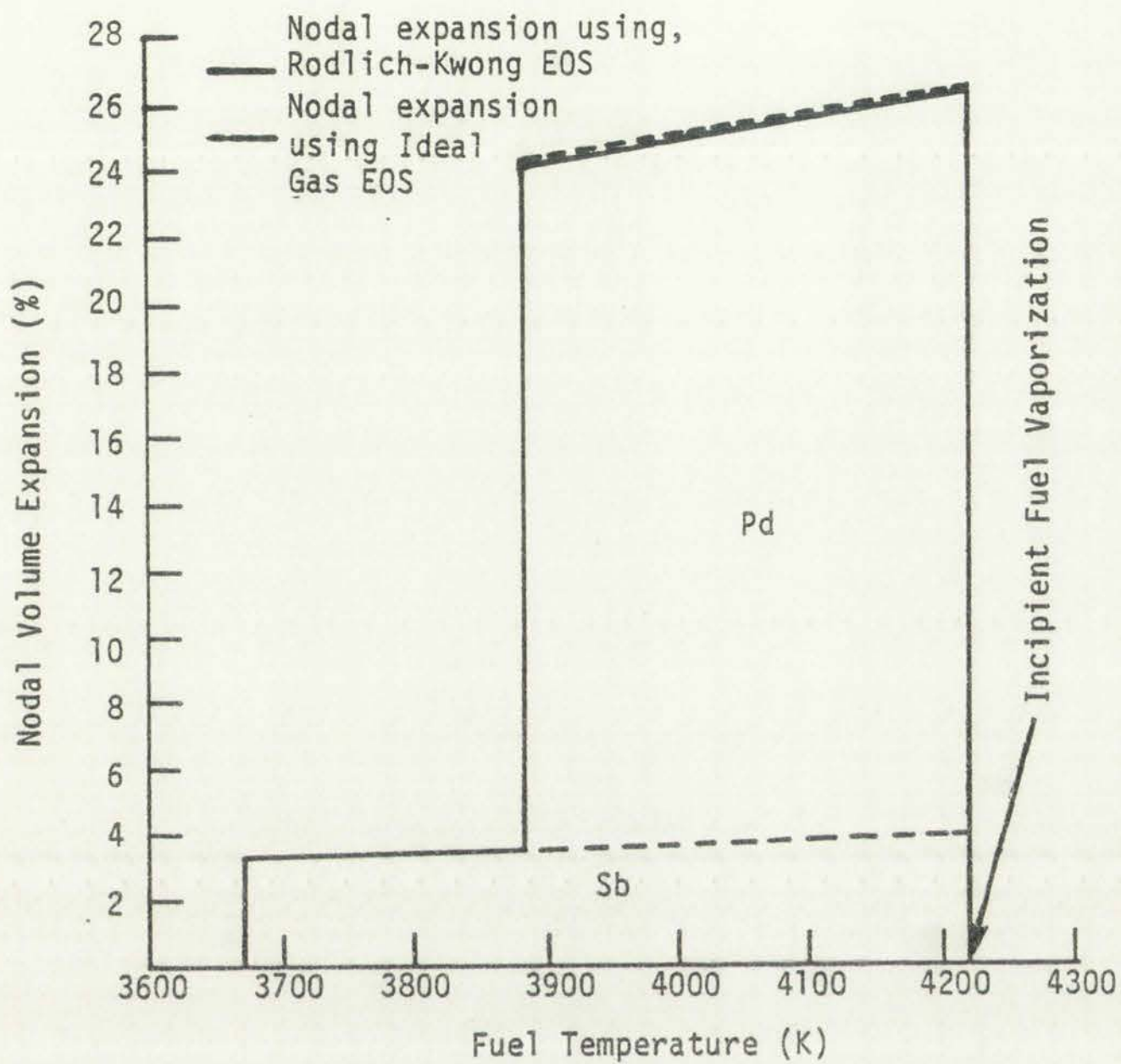


Figure 5.9
 Nodal volume expansion for O'Boyle inclusion
 using a flat inclusion number density
 profile and Redlich-Kwong EOS.

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inclusion density distribution based on work of Baird,⁶ Fig. 2.9, was used to create a normalized inclusion distribution curve found in Fig. 5.10. It should be noted that the inclusion density is zero in the unrestructured region as per experimental evidence. Since, in this analysis a central void is not used, the measured inclusion density at the central void edge was assumed for this region. A multiplication factor is used such that the volume integral of the calculated inclusion density is equal to the volume integral assuming a flat distribution, i.e., for nodal notation:

$$\begin{aligned} \pi \Delta Z \left[\frac{\Delta r}{2} \right]^2 x_1 D + \pi \Delta Z \sum_{i=1}^n \left[\left(r_i + \frac{\Delta r}{2} \right)^2 - \left(r_i - \frac{\Delta r}{2} \right)^2 \right] x_i D \\ = \Delta Z \pi \bar{D} \left(R_n + \frac{\Delta r}{2} \right)^2 \end{aligned} \quad (5.1)$$

where:

- x_i = distribution factors from Fig. 5.10
- \bar{D} = inclusion number density assuming flat distribution
- Δr = radial nodal width
- ΔZ = axial nodal width
- r_i = radius of i th node
- n = outermost node in the equiaxed grain region
- R_n = radius of n th node
- D = $A \cdot \bar{D}$ where A is the multiplication factor

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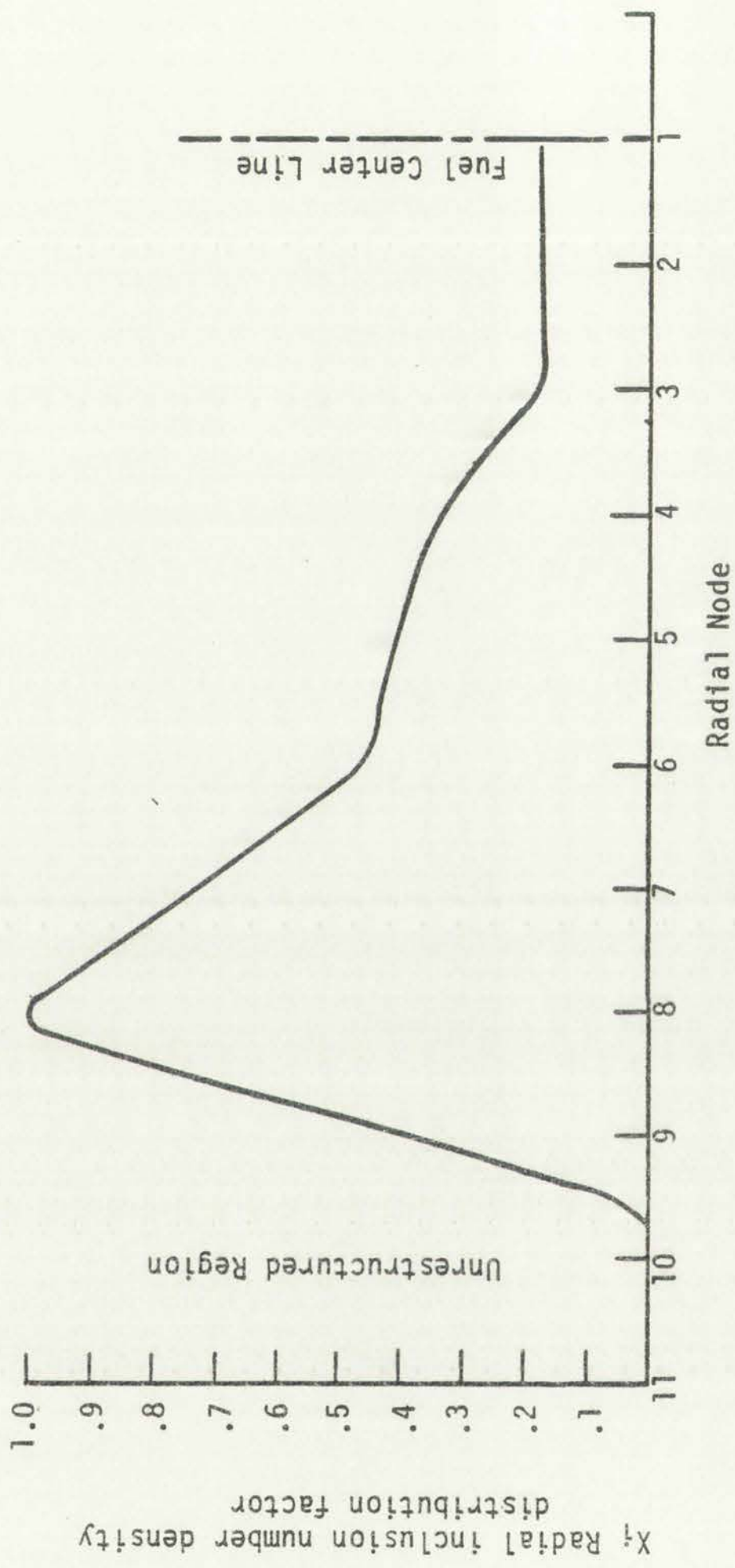


Figure 5.10
Radial inclusion number density profile.



Vertical axis label: $\frac{1}{2} \sin x$

Horizontal axis label: x

Figures 5.11-5.15 show the effect of the radial distribution in inclusion number density. The combination of the cosine shaped radial temperature profile and the number density profile in Fig. 5.10 causes the maximum nodal volume expansion to move outwards, but not to the maximum point in inclusion number density. It actually increases the maximum nodal volume expansion from 26.4% to 28.6% for O'Boyle type inclusion. However, due to the higher vaporization temperature of Fe the maximum nodal volume expansion for Johnson's inclusions decreases from 29% to 20%, both assuming Sb present. The total fuel volume expansion also decreased approximately 0.75-.1% at incipient fuel vaporization. It thus appears that the radial distribution decreases potential fuel motion up to incipient fuel vaporization.

5.2 Homogeneous Inclusions

A more realistic approximation to the physical state of the inclusions is to consider the inclusions as a homogeneous solution of the constituent elements, i.e., miscible and thus in a single phase. This assumption is supported by the experimental work of Bramman⁵ whose X-ray examination found the inclusions to be single phase with a hexagonal structure, i.e. as stated by Bramman, "It was found that insoluble residues contained small particles of the order of 5 μ m in dia., and X-ray examination showed these particles to have a hexagonal structure with $a_0 = 2.756 \pm .001\text{\AA}$, $c_0 = 4.426 \pm .002\text{\AA}$."⁵ No other investigators reported finding more than one phase.

The Hume-Rothery rule⁷ was also used to investigate solubility. This rule states that substitutional solubility is not found if:

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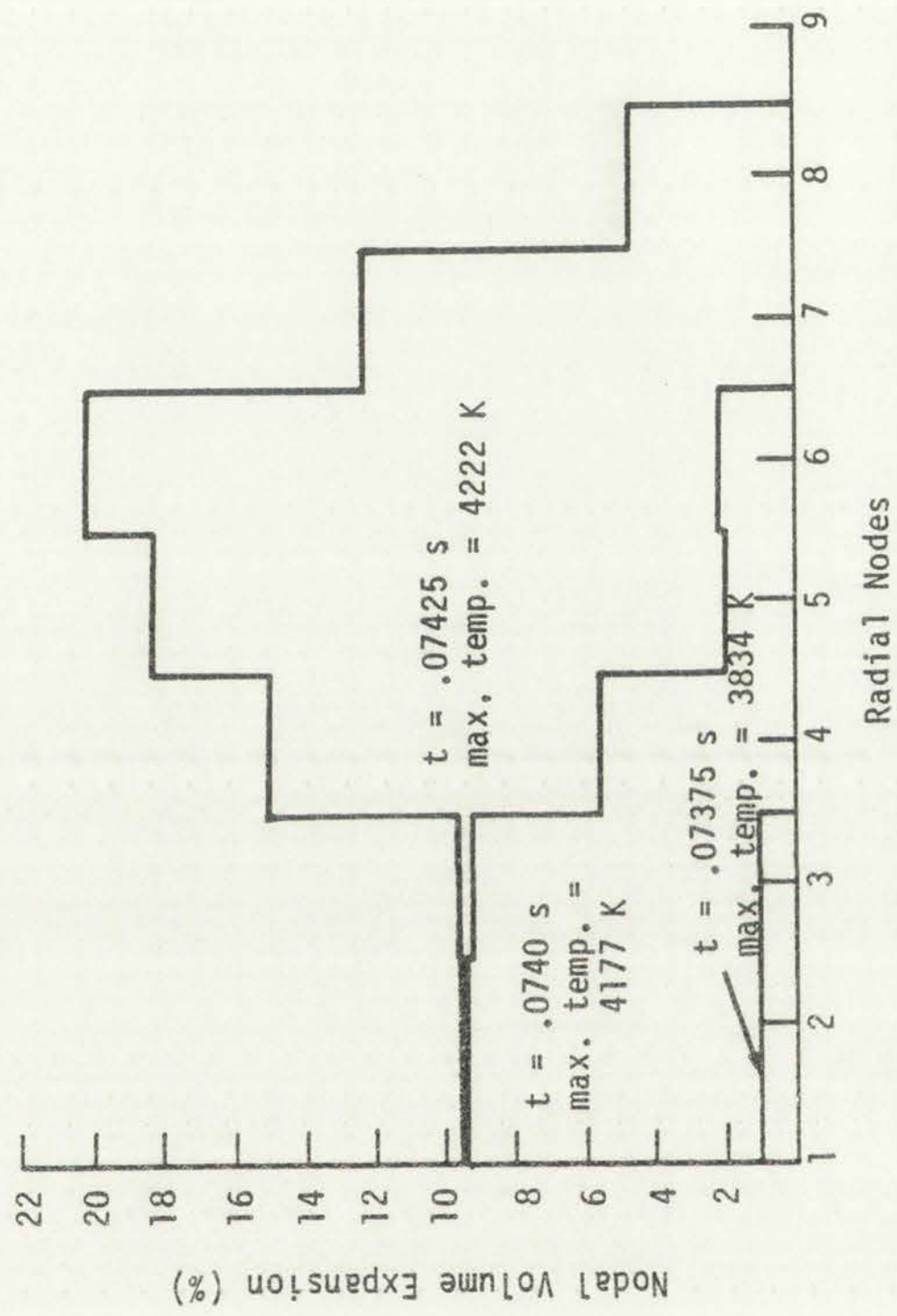


Figure 5.11
 Nodal volume expansion for Johnson inclusions at \$15/s ramp insertion, axial node 11 (Hottest) using radial inclusion distribution.

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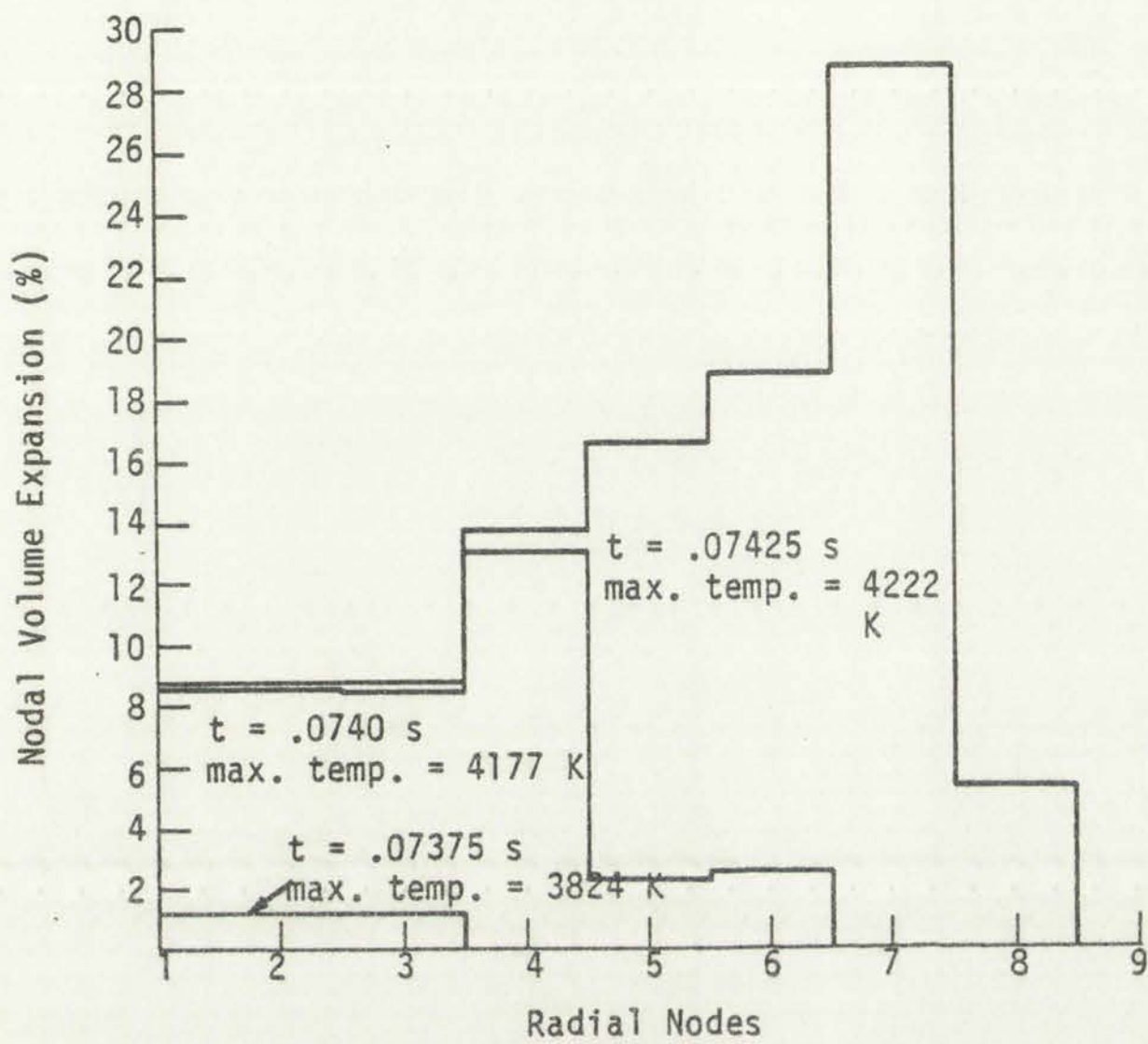


Figure 5.12

Nodal volume expansion for O'Boyle inclusion for \$15/s ramp insertion at axial node 11 (Hottest) using radial inclusion distribution.



Figure 2.12
 Radial nodes
 Total volume calculated for 2100 nodes
 for 2100 nodes (total of 2100 nodes)
 (total) using radial function distribution

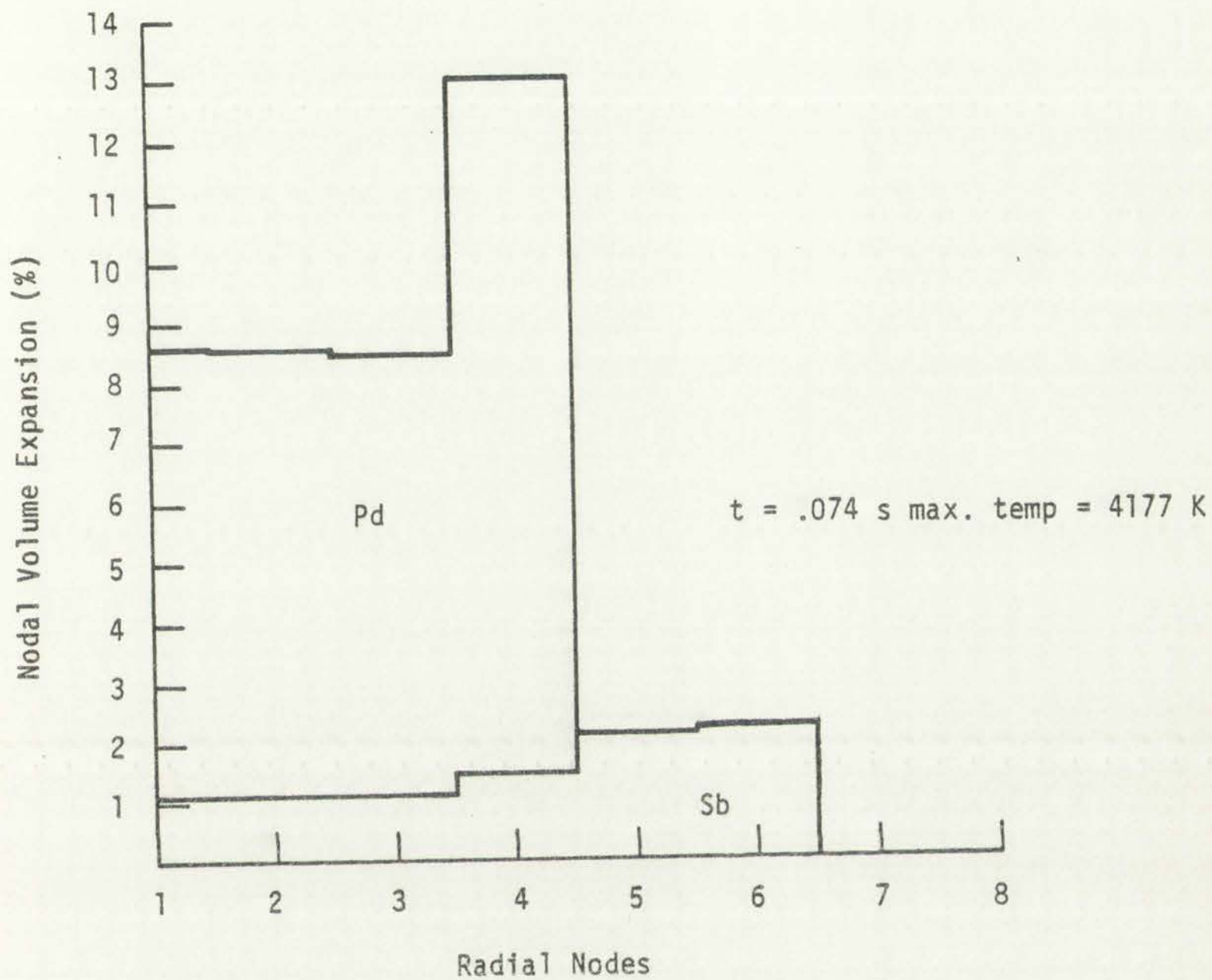


Figure 5.13.
 Nodal volume expansion for $15/s$ ramp insertion at axial node II (hottest) using the radial inclusion distribution in number density in O'Boyle inclusions.

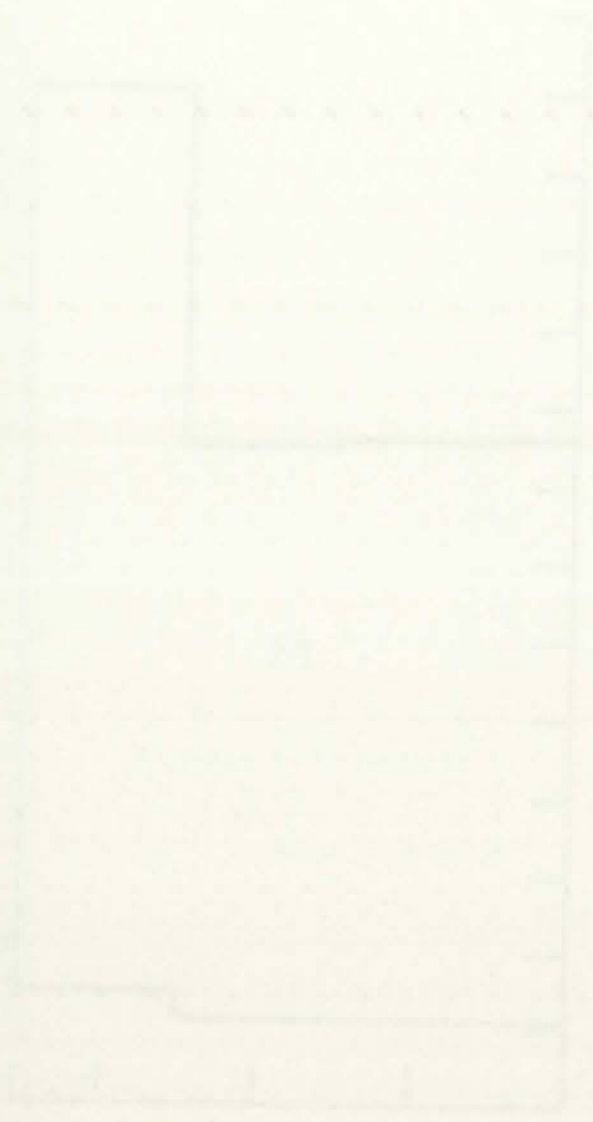


Figure 1: A step function graph.

100% value expansion for
 a 10% (input) value for
 in other words in 0.25

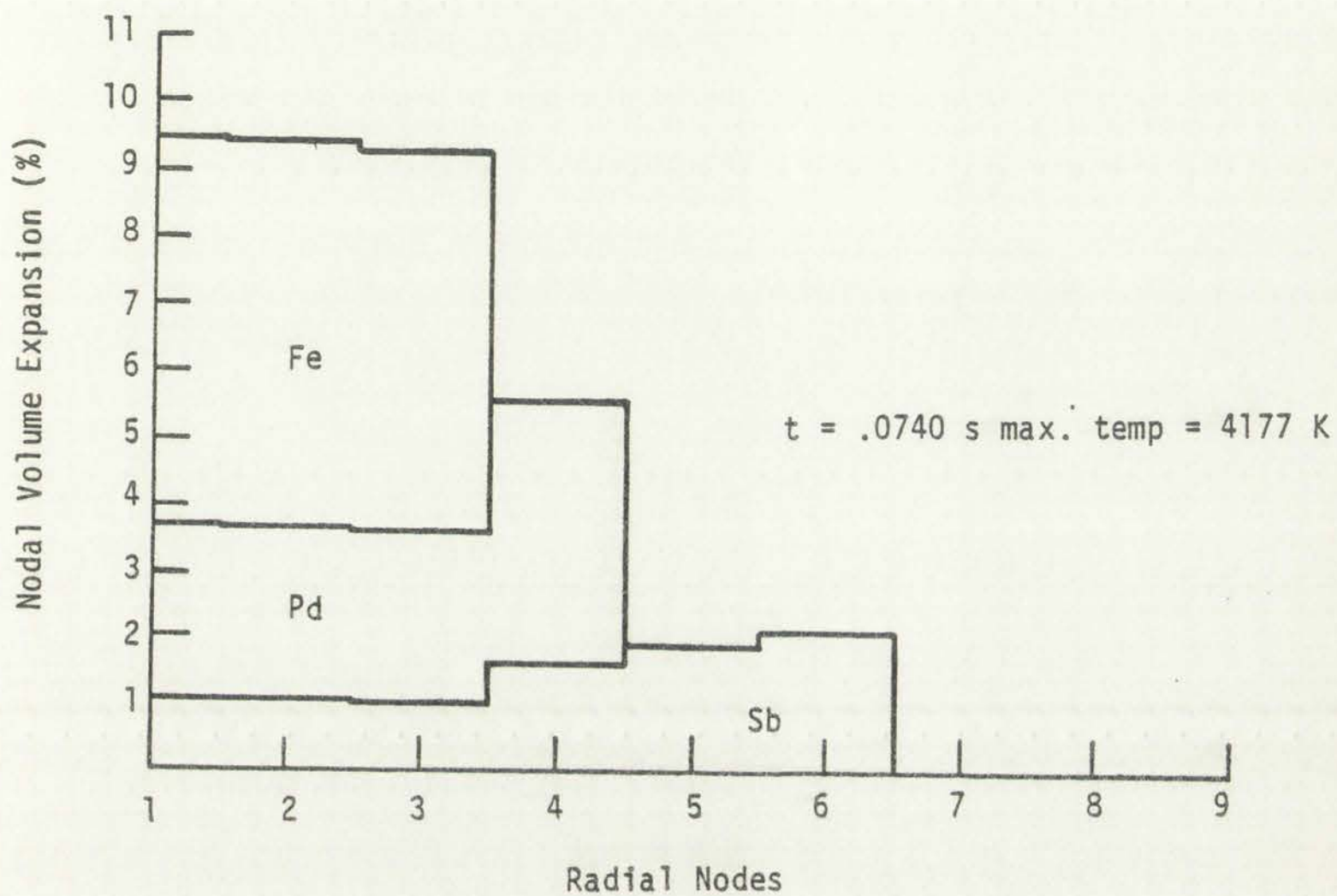


Figure 5.14.

Nodal volume expansion for 15/s ramp insertion at axial node II (hottest) using radial inclusion distribution in number density for Johnson's inclusions.

Figure 1. (a) Plot of $\ln(\frac{1}{1-x})$ vs. $\ln(x)$ for the data of Johnson et al. (1972).



(b) Plot of $\ln(\frac{1}{1-x})$ vs. $\ln(x)$ for the data of Johnson et al. (1972) with a fitted curve. The fitted curve is a smooth, increasing function that passes through the data points.

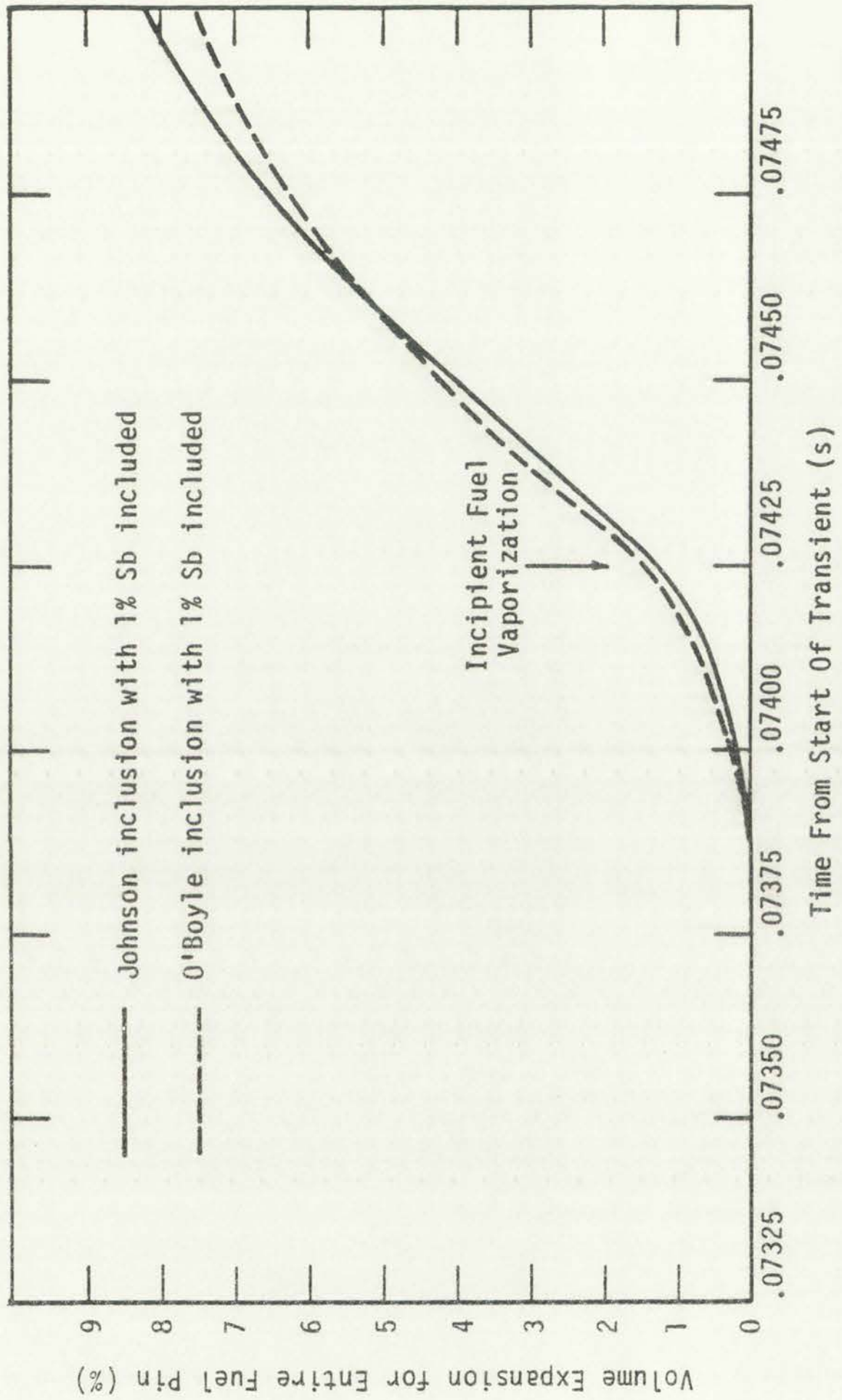


Figure 5.15
Total fuel volume expansion for \$15/s ramp insertion using radial inclusion distribution in number density.

The figure shows the variation of the rate of polymerization with time for the polymerization of styrene in benzene solution at 50°C. The curve shows that the rate of polymerization increases rapidly at first and then gradually approaches a constant value.

Figure 1. Rate of polymerization of styrene in benzene solution at 50°C.



Figure 1. Rate of polymerization of styrene in benzene solution at 50°C.

- a. Atom size difference exceeds 15%.
- b. Large electronegativity difference (ionic compound likely) exists.
- c. Large valence difference exists.
- d. Different in crystal structures.

In Table 5.1 is a comparison of the appropriate variables. It can be seen that rules a. thru c. are not violated. There is, however, different crystalline structure for the various constituents. From this, one cannot infer immiscibility or solubility, but can only say that three Hume-Rothery rules for solubility are satisfied.

Metallic phase diagrams also support the homogeneous inclusion assumption. A ternary phase diagram⁸ of Mo, Ru, and Rh shown in Fig. 5.16 indicates that the Johnson and O'Boyle inclusion compositions are in the single phase, α region, at least at the 1798 K isotherm. By comparing Fig. 5.16 to a ternary phase diagram at 1413 K, it appears that the α phase increases with temperature. This should only be taken as an "in general" assumption since phase diagrams are empirical and cannot be predicted or constructed on a theoretical basis.

In addition, Johnson's and O'Boyle's inclusions contain 17 and 20 wt% (w/o) Tc, and 2 and 5 w/o Pd respectively. Johnson's inclusions also contain 2.5 w/o Fe. It is not known how this affects the Mo, Ru, Rh ternary diagram, since pentary phase diagrams do not exist. However, from binary phase diagrams,⁹⁻¹¹ Tc, Pd, and Fe are soluble at least to some degree in Mo, Ru, and Rh. Tc has a restricted solubility of ≈ 5 atom % (A/o) in Rh but is soluble up to 50 a/o in Mo and

the following results are obtained from the analysis of the data.

The results are presented in Table 1.

The results are presented in Table 1.

Table 1 is a summary of the analysis of the data.

It can be seen that the results are as follows.

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The results are presented in Table 1.

TABLE 5.1
COMPARISON OF PARAMETERS FOR HUME-ROTHERY RULE

<u>Element</u>	<u>Metallic¹³ Radius (Å)</u>	<u>Electronegativity¹⁴</u>	<u>Valency¹³</u>	<u>Crystal Structure¹⁴⁻¹⁶</u>
Mo	1.296	1.8	6	Body centered cubic
Ru	1.246	2.2	6	Hexagonal
Rh	1.252	2.2	6	Face centered cubic
Pd	1.283	2.2	6	Face centered cubic
Tc	1.271	1.9	6	Hexagonal

according to Shunk⁹ and Darby¹², totally in Ru. Pd has restricted solubility, ≈ 5 A/o, in Mo but is totally soluble above 1118 K in Rh, and is soluble to some extent in Ru. It is also soluble in Tc. Fe has restricted solubility in Mo, ≈ 22 A/o at 1813 K, but is totally soluble in Rh and Ru. Thus via phase diagrams there is no basis to assume that Tc, Pd, and Fe are not in solid solution with Mo, Ru, and Rh. Unfortunately one cannot conclude categorically that they are in solid solution; however, this assumption of some degree of solubility seems reasonable and is thus considered here by assessing the upper limit of complete solubility.

The vapor pressure of the homogeneous inclusions was determined from the sum of the constituent partial pressures. The constituent partial pressures were calculated using Raoult's Law¹⁷ as stated in Eq. (5.2)

$$P_i = Y_i P_{oi} \quad (5.2)$$

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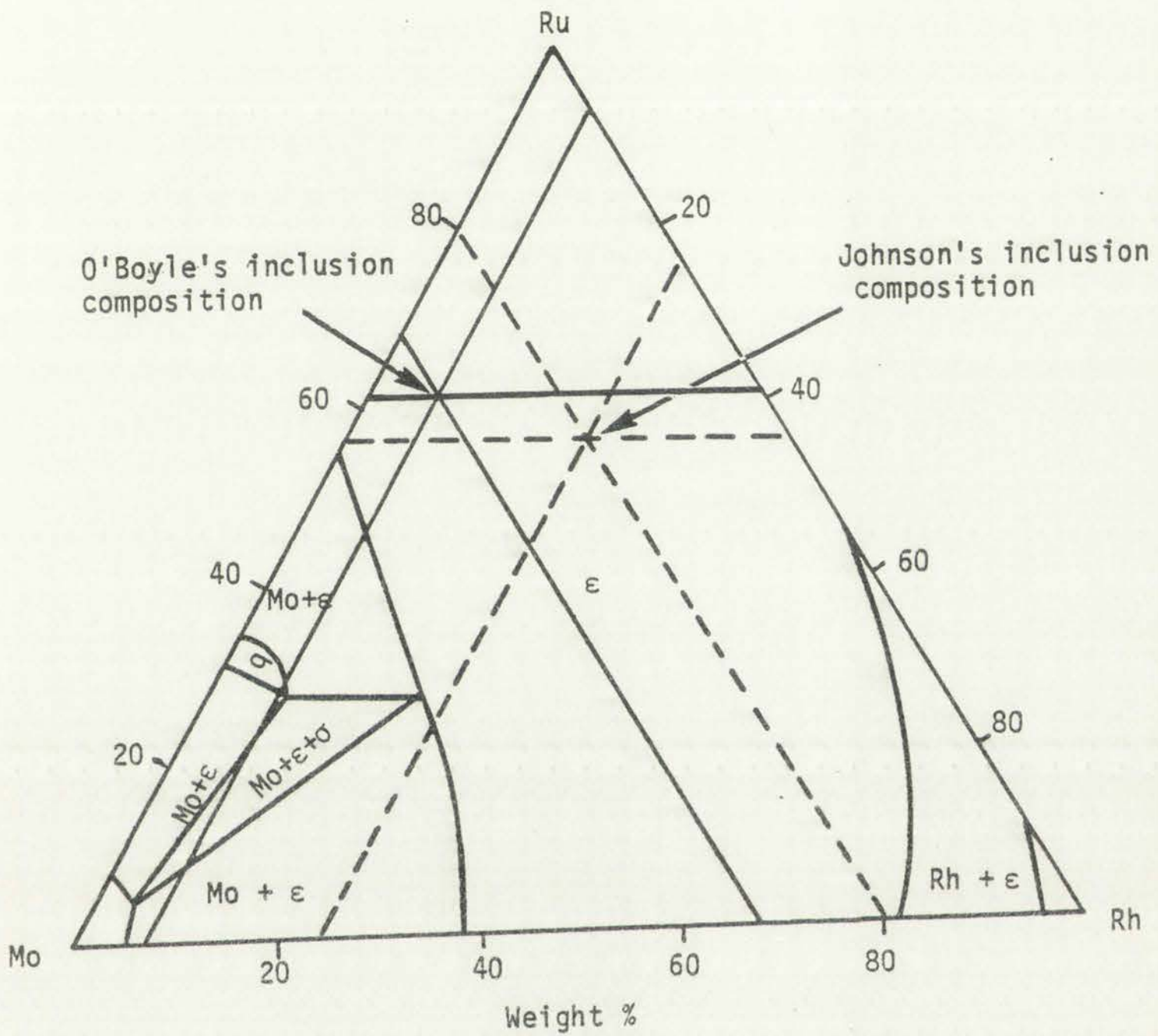


Figure 5.16
1798 K Isotherm of Mo-Ru-Rh ternary phase diagram.



where:

P_i = partial pressure of constituent, i

Y_i = mole fraction of constituent $i = \frac{n_i}{\sum_{i=1}^x n_i}$,

n_i = moles of constituent, i

P_{oi} = vapor pressure of pure constituent, i .

thus

$$P(\text{total inclusion}) = \sum_{i=1}^x \frac{n_i}{\sum_{i=1}^x n_i} P_{oi} \quad (5.3)$$

Raoult's Law is based on an ideal system of liquids, i.e., the presence of molecules of other species has no effect on the intramolecular forces of another species. The species must be completely miscible, and there is no volume or heat change upon mixing. However, if the attraction between molecules of species "B" is much stronger than that between molecules of species "A," and if the intermolecular forces are either repulsive or nonexistent, the effect is to force the molecules of "A" out of the liquid into the vapor. In other words, the vaporization of species "A" is increased by the presence of "B." This results in a positive deviation from Raoult's Law. However, if the intermolecular force between species "A" and "B" are attractive or if

3

of the system

of the system

of the system

of the system

compounds between "A" and "B" are formed in the liquid, negative deviation, i.e. suppression of the total vapor pressure line in Raoult's Law will occur.¹⁸⁻²⁰

The internal pressure for the various inclusion elements was calculated to assess the magnitude of the intramolecular forces. This information can then be used to approximate solubility for metal in the liquid state, as seen in Fig. 5.17 from Hildebrand.²¹ The internal pressure is proportional to σ/v where v is the molar volume and σ is the surface tension which was calculated from the heat of vaporization²² via the equations in Appendix O. Tables 5.2 thru 5.4 contain: (1) the parameters to calculate σ at the melting temperatures; (2) the calculated values of σ ; (3) experimental values of σ ; and (4) the calculated internal pressure.

The internal pressure cannot predict tendencies toward the formation of compounds or abnormally great attractions between atoms of unlike metals. About all that can be said is that insolubility cannot occur unless there is a sufficient difference in internal pressure, and even then it may not occur if compounds are formed. Table 5.5 shows the magnitude of the calculated internal pressures of interest as compared to elements in Fig. 5.2 from Hildebrand.²¹ Looking at Table 5.5, one would expect that only the volatile Fe and possibly Pd would be soluble in Mo, Ru, Rh, and Tc which make up a large weight percent of the inclusion. Hildebrand, however, feels a separation of about 100% difference in internal pressure is required for insolubility. If

The following table shows the results of the calculations for the various cases. The values are given in the columns headed by the appropriate case number. The first column gives the value of the parameter α and the second column gives the value of the parameter β . The third column gives the value of the parameter γ and the fourth column gives the value of the parameter δ . The fifth column gives the value of the parameter ϵ and the sixth column gives the value of the parameter ζ . The seventh column gives the value of the parameter η and the eighth column gives the value of the parameter θ . The ninth column gives the value of the parameter ι and the tenth column gives the value of the parameter κ . The eleventh column gives the value of the parameter λ and the twelfth column gives the value of the parameter μ . The thirteenth column gives the value of the parameter ν and the fourteenth column gives the value of the parameter ξ . The fifteenth column gives the value of the parameter \omicron and the sixteenth column gives the value of the parameter π . The seventeenth column gives the value of the parameter ρ and the eighteenth column gives the value of the parameter σ . The nineteenth column gives the value of the parameter τ and the twentieth column gives the value of the parameter υ . The twenty-first column gives the value of the parameter ϕ and the twenty-second column gives the value of the parameter χ . The twenty-third column gives the value of the parameter ψ and the twenty-fourth column gives the value of the parameter ω . The twenty-fifth column gives the value of the parameter δ and the twenty-sixth column gives the value of the parameter ϵ . The twenty-seventh column gives the value of the parameter ζ and the twenty-eighth column gives the value of the parameter η . The twenty-ninth column gives the value of the parameter θ and the thirtieth column gives the value of the parameter ι . The thirty-first column gives the value of the parameter κ and the thirty-second column gives the value of the parameter λ . The thirty-third column gives the value of the parameter μ and the thirty-fourth column gives the value of the parameter ν . The thirty-fifth column gives the value of the parameter ξ and the thirty-sixth column gives the value of the parameter \omicron . The thirty-seventh column gives the value of the parameter π and the thirty-eighth column gives the value of the parameter ρ . The thirty-ninth column gives the value of the parameter σ and the fortieth column gives the value of the parameter τ . The forty-first column gives the value of the parameter υ and the forty-second column gives the value of the parameter ϕ . The forty-third column gives the value of the parameter χ and the forty-fourth column gives the value of the parameter ψ . The forty-fifth column gives the value of the parameter ω and the forty-sixth column gives the value of the parameter δ . The forty-seventh column gives the value of the parameter ϵ and the forty-eighth column gives the value of the parameter ζ . The forty-ninth column gives the value of the parameter η and the fiftieth column gives the value of the parameter θ . The fifty-first column gives the value of the parameter ι and the fifty-second column gives the value of the parameter κ . The fifty-third column gives the value of the parameter λ and the fifty-fourth column gives the value of the parameter μ . The fifty-fifth column gives the value of the parameter ν and the fifty-sixth column gives the value of the parameter ξ . The fifty-seventh column gives the value of the parameter \omicron and the fifty-eighth column gives the value of the parameter π . The fifty-ninth column gives the value of the parameter ρ and the sixtieth column gives the value of the parameter σ . The sixty-first column gives the value of the parameter τ and the sixty-second column gives the value of the parameter υ . The sixty-third column gives the value of the parameter ϕ and the sixty-fourth column gives the value of the parameter χ . The sixty-fifth column gives the value of the parameter ψ and the sixty-sixth column gives the value of the parameter ω . The sixty-seventh column gives the value of the parameter δ and the sixty-eighth column gives the value of the parameter ϵ . The sixty-ninth column gives the value of the parameter ζ and the seventieth column gives the value of the parameter η . The seventy-first column gives the value of the parameter θ and the seventy-second column gives the value of the parameter ι . The seventy-third column gives the value of the parameter κ and the seventy-fourth column gives the value of the parameter λ . The seventy-fifth column gives the value of the parameter μ and the seventy-sixth column gives the value of the parameter ν . The seventy-seventh column gives the value of the parameter ξ and the seventy-eighth column gives the value of the parameter \omicron . The seventy-ninth column gives the value of the parameter π and the eightieth column gives the value of the parameter ρ . The eighty-first column gives the value of the parameter σ and the eighty-second column gives the value of the parameter τ . The eighty-third column gives the value of the parameter υ and the eighty-fourth column gives the value of the parameter ϕ . The eighty-fifth column gives the value of the parameter χ and the eighty-sixth column gives the value of the parameter ψ . The eighty-seventh column gives the value of the parameter ω and the eighty-eighth column gives the value of the parameter δ . The eighty-ninth column gives the value of the parameter ϵ and the ninetieth column gives the value of the parameter ζ . The ninety-first column gives the value of the parameter η and the ninety-second column gives the value of the parameter θ . The ninety-third column gives the value of the parameter ι and the ninety-fourth column gives the value of the parameter κ . The ninety-fifth column gives the value of the parameter λ and the ninety-sixth column gives the value of the parameter μ . The ninety-seventh column gives the value of the parameter ν and the ninety-eighth column gives the value of the parameter ξ . The ninety-ninth column gives the value of the parameter \omicron and the hundredth column gives the value of the parameter π .

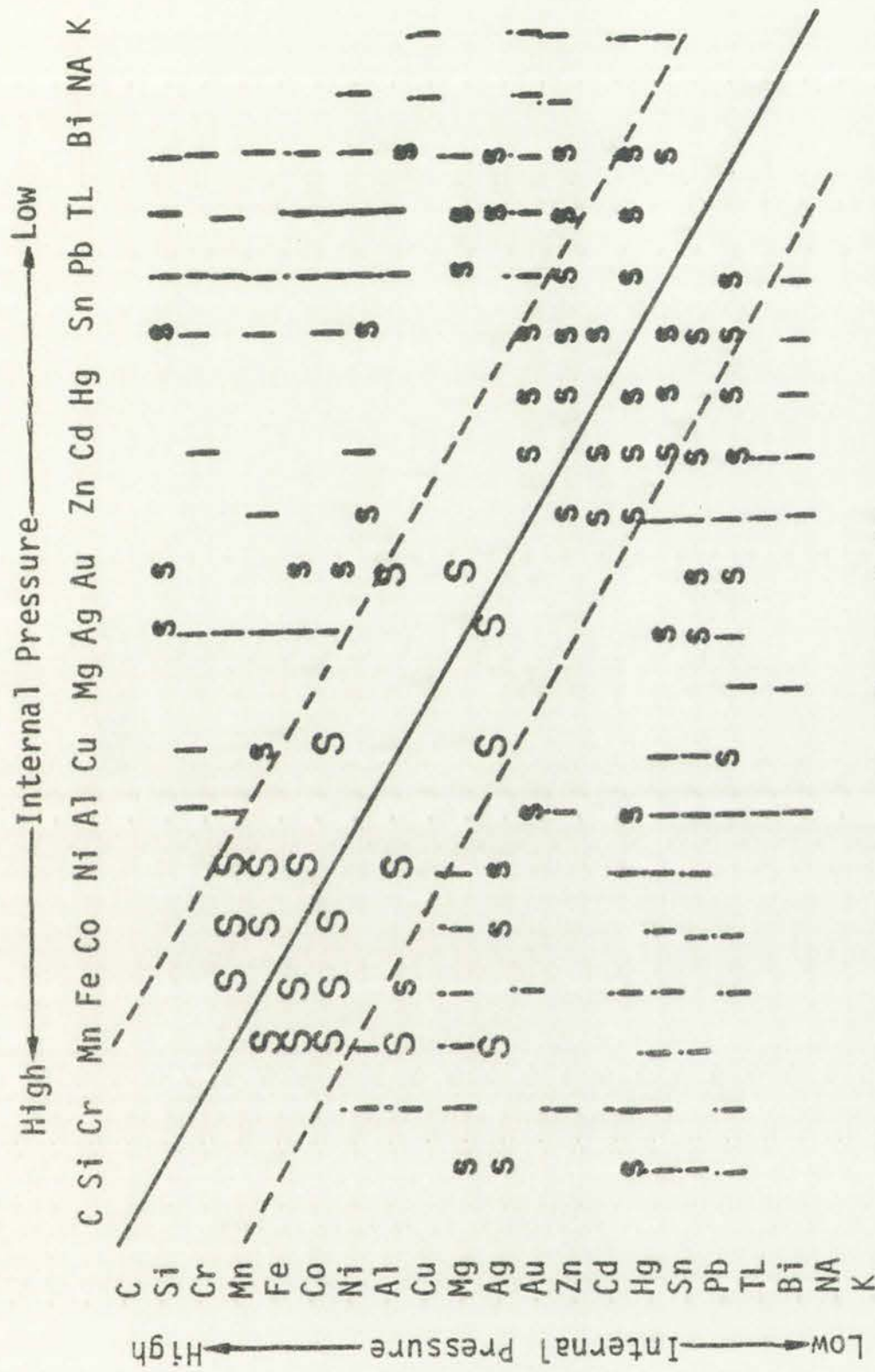
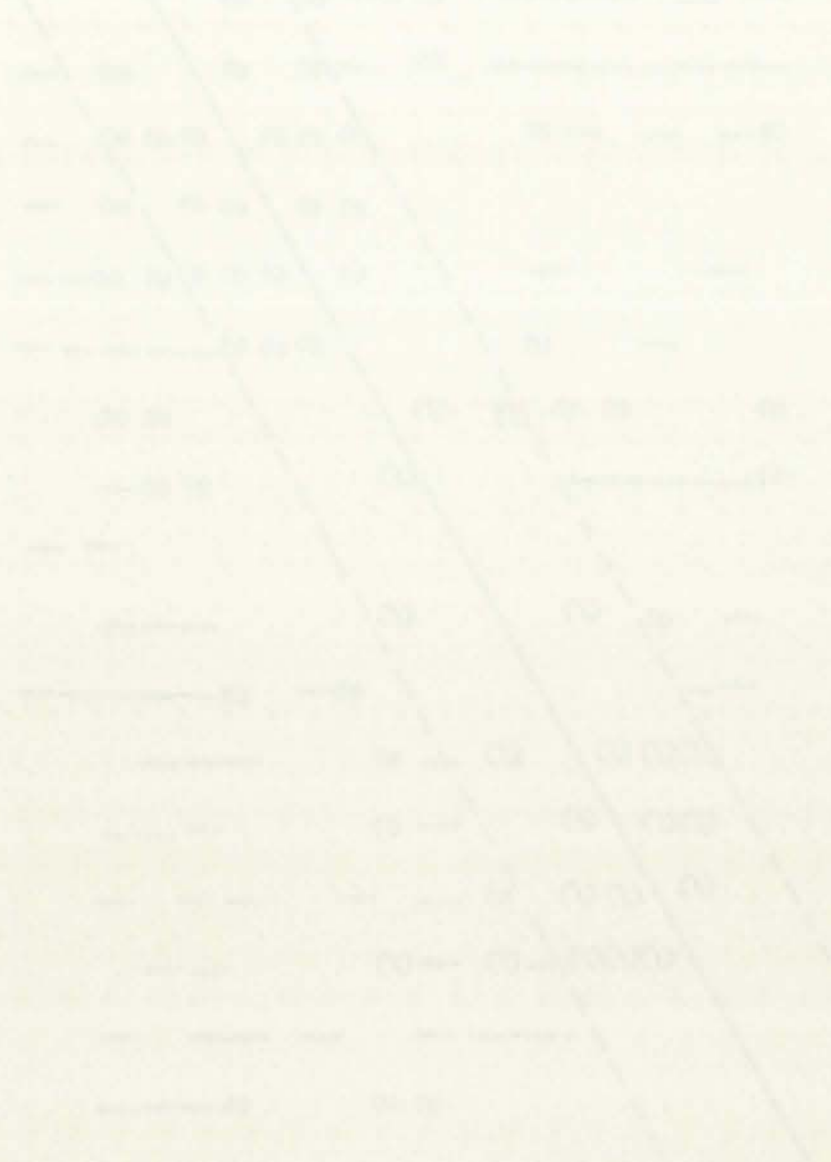


Figure 5.17
Internal pressure series for liquid metals

i: 2 Liquid Phases (immiscible)
S: Complete solubility in the solid state
s: Limited solubility in the solid state

1. The first condition is the existence
of a positive definite matrix P such
that $A^T P + P A < -Q$ for some
positive definite matrix Q .



2. The second condition is the controllability
of the pair (A, B) and the observability
of the pair (A, C) .

3. The third condition is the stability
of the closed-loop system.

TABLE 5.2
PHYSICAL PARAMETERS TO CALCULATE SURFACE TENSION, σ

Element	Molecular Weight	Density, ρ , at Melting Temp. ²³ (g/cm ³)	Crystal Structure ^{24,25}	Heat of Vaporization, ΔH_{vap} (ergs/g-mole)					
				Handbook of Chemistry & Physics ²³	Nesmeyanov ²⁶	Stull ²⁷	Hultgren ²⁸	Hampel ²⁹	Others
Ba	137.34	3.32	BCC	1.49 x 10 ¹²	1.74 x 10 ¹²	1.51 x 10 ¹²	1.54 x 10 ¹²	1.51 x 10 ¹²	
Ce	140.12	≈6.6	BCC	3.06 x 10 ¹²	3.10 x 10 ¹²	3.14 x 10 ¹²	3.89 x 10 ¹²	3.98 x 10 ¹²	
Pd	106.4	10.7	FCC	3.73 x 10 ¹²	3.93 x 10 ¹²	3.93 x 10 ¹²	3.52 x 10 ¹²	3.93 x 10 ¹¹	
Fe	55.847	≈7.04	BCC	3.54 x 10 ¹²	4.05 x 10 ¹²	3.51 x 10 ¹²	4.14 x 10 ¹²	3.54 x 10 ¹²	
Te	127.60	5.77	Hexagonal	4.98 x 10 ¹¹	1.61 x 10 ¹²	5.07 x 10 ¹¹		5.72 x 10 ¹¹	
Sb	121.75	6.49	Rhombohedral	1.95 x 10 ¹²	2.04 x 10 ¹²	6.79 x 10 ¹¹	5.25 x 10 ¹¹ (Sb ₄ only)	1.95 x 10 ¹²	9.28 x 10 ¹¹³⁰
Cs	132.905	1.845	BCC	6.83 x 10 ¹¹	7.71 x 10 ¹¹	6.59 x 10 ¹¹	7.82 x 10 ¹¹	8.12 x 10 ¹¹	
Mo	95.94	9.34	BCC		6.63 x 10 ¹²	5.94 x 10 ¹²	6.63 x 10 ¹²	4.91 x 10 ¹²	
Ru	101.07	≈10.9	Hexagonal		6.68 x 10 ¹²	5.68 x 10 ¹²	6.47 x 10 ¹²	5.67 x 10 ¹²	
Rh	102.905	≈10.7	FCC	5.32 x 10 ¹²	5.54 x 10 ¹²	4.96 x 10 ¹²	5.56 x 10 ¹²	5.78 x 10 ¹²	
Tc	99.0	≈11.5	Hexagonal	≈5.02 x 10 ¹²	6.49 x 10 ¹²	5.78 x 10 ¹²			
Zr	91.22	5.8	BCC	4.19 x 10 ¹²	6.10 x 10 ¹²	5.82 x 10 ¹²	6.09 x 10 ¹²	5.95 x 10 ¹²	
Sr	87.62	2.375	BCC	1.41 x 10 ¹²	1.64 x 10 ¹²	1.39 x 10 ¹²	1.65 x 10 ¹²	1.40 x 10 ¹²	
Nd	144.24	6.8	BCC	≈2.55 x 10 ¹²	3.21 x 10 ¹²	2.84 x 10 ¹²	3.24 x 10 ¹²	2.89 x 10 ¹²	

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WASHINGTON, D.C. 20250

TABLE 5.3
COMPARISON OF CALCULATED AND EXPERIMENTAL
VALUES OF SURFACE TENSION

Element	Range of Heat of Vaporization, ΔH_{vap} (ergs/g-mole)	Corresponding Range of Calculated (Appendix 0) Surface Tension (ergs/cm ²)	Experimentally Determined Surface Tension (ergs/cm ²)
Ba	1.49×10^{12}	197.6	276 ¹⁴ (Tm), 224 ³⁰ (Tm)
	1.74×10^{12}	230.7	
Ce	3.0×10^{12}	620.2	
	3.9×10^{12}	806.3	
Pd	3.9×10^{12}	1384.2	1475 ³¹ (Tm), 1500 ³² (Tm)
	3.5×10^{12}	1233.0	
Fe	3.5×10^{12}	1394.8	1788 ³⁰ (Tm), 1850 ³³ (Tm), 1710 ³⁴
	4.1×10^{12}	1633.9	
Te	5.0×10^{11}	112.7	
	1.6×10^{12}	360.5	
Sb	2.0×10^{12}	573.3	357 ³⁵ (Tm), 383 ³⁰ (Tm), 384 ^{33,36} (Tm)
	6.8×10^{11}	194.4	
Cs	6.6×10^{11}	60.4	69.5 ³⁷ (Tm), 67 ³⁰ (Tm), 68 ³⁶ (Tm)
	7.8×10^{11}	71.4	
Mo	4.9×10^{12}	1643.7	2045 ³⁸ , 2250 ³² (Tm)
	6.6×10^{12}	2213.9	
Ru	5.7×10^{12}	2292.7	2250 ³² (Tm)
	6.6×10^{12}	2654.7	
Rh	5.0×10^{12}	1800.7	2000 ³² (Tm)
	5.5×10^{12}	1980.8	
Tc	5.8×10^{12}	2451.4	
	6.5×10^{12}	2747.2	
Zr	4.2×10^{12}	1060.5	1430 ³² (Tm)
	6.1×10^{12}	1540.3	
Sr	1.4×10^{12}	200.2	
	1.64×10^{12}	234.6	
Nd	2.84×10^{12}	587.5	
	3.2×10^{12}	661.9	

MEMORANDUM FOR THE RECORD
DATE: 10/20/50

TO: SAC, NEW YORK

FROM: SAC, PHOENIX (100-4444)

SUBJECT: [Illegible]

[The remainder of the memorandum text is illegible due to extreme fading.]

TABLE 5.4

CALCULATED INTERNAL PRESSURES

Element	Melting Temperature ²³ T _m (°K)	Surface Tension at T _m ²³ (ergs/cm ²)	Calculated Surface Tension at T _m (ergs/cm ²)	Molar Volume at T _m (cm ³ /g-mole)	Internal Energy (σ/V ^{1/3})
Si	1683	≈725		11.15	324.52
Cr	2130	1700		8.05	847.12
Mn	1517	1030		8.54	503.91
Co	1768	≈1800		7.65	913.52
Ni	1726	1725		7.48	882.04
Al	933	860		11.24	383.92
Cu	1356	≈1300		8.00	650.00
Mg	922	583		15.29	234.89
Ag	1235	920		11.56	405.83
Au	1337	1130		11.40	502.08
Zn	693	760		9.95	353.35
Cd	594	590		14.01	244.74
Hg	234	≈490		14.75	199.80
Sn	505	≈550		16.98	213.99
Pb	601	470		19.37	175.01
Tl	576	465		18.10	177.10
Bi	544	380		20.86	138.04
Na	371	200		24.73	68.65
K	337	110		47.68	30.34
Ba	998	276		41.37	79.80
Ce	1072	---	≈215	21.07	253.44
Pd	1825	1500	≈700	9.94	697.64
Fe	1800	≈1770	≈1310	7.94	887.22
Te	723	180	≈1510	22.0	64.24
Sb	904	380	≈236	18.79	142.94
Cs	301	70	≈383	71.84	16.84
Mo	2890	2250	≈65	10.27	1035.12
Ru	2583	2250	≈1928	9.27	1071.08
Rh	2239	2000	≈2473	9.53	943.34
Tc	2446	---	≈1900	8.61	1268.54
Zr	2125	1400	≈2600	15.73	558.75
Sr	1042	300	≈1300	36.97	90.05
Nd	1294	688	≈220	20.58	251.06
			≈625		

<p>1. 2019年12月31日</p>	<p>2019年12月31日</p>
<p>2. 2020年1月1日</p>	<p>2020年1月1日</p>
<p>3. 2020年12月31日</p>	<p>2020年12月31日</p>
<p>4. 2021年1月1日</p>	<p>2021年1月1日</p>
<p>5. 2021年12月31日</p>	<p>2021年12月31日</p>
<p>6. 2022年1月1日</p>	<p>2022年1月1日</p>

2022年1月1日

2022年1月1日

TABLE 5.5
COMPARISON OF INTERNAL EXERGIES

Elements in Descending Internal Pressure from Fig. 5.16 ²¹	Internal Energy Calculated in Hildebrand ²¹	Internal Energy Calculated in Table 5.3	Placement and Internal Energy of Elements of Interest
Si		324	Tc(1268), Ru(1071), Mo(1035), Rh(943)
Cr		848	
Mn		503	
Fe	490	887	
Co		913	
Ni		882	
Al		384	Pd(700)
Cu	294	650	
Mg		235	Zr(558)
Ag	348	405	
Au	282	502	
Zn	350	353	Ce(253), Nd(251)
Cd	256	245	
Hg	157	200	
Sn	198	214	
Pb	163	175	
Tl		177	Sb(142)
Bi		138	Sr(90), Ba(80), Te(64)
Na		68	
K	114	30	Cs(17)

TABLE 1

CHARACTERISTICS OF STUDENTS

Grade	Number of students	Percentage of total sample	Mean score on test
Elementary	100	100%	75.0
Middle	100	100%	75.0
High	100	100%	75.0
Total	300	100%	75.0

this is the criteria Fe, Pd, and Zr should all be soluble in Mo, Ru, Rh, and Tc.

Using Raoult's Law means that the low vapor pressure elements (Mo, Ru, Rh, Tc) that make up a large portion of the inclusions, are weighted accordingly, depressing the total inclusion vapor pressure.

To determine if the homogeneous inclusions can contribute to fuel swelling and frothing, one must know what the relationship is between the inclusion vapor pressure and that of the fuel. Table 5.6 and Fig. 5.18 contain the vapor pressures of an average Johnson, O'Boyle, and Jeffery homogeneous inclusion based on Raoult's Law. Both Johnson's and O'Boyle's inclusion are assumed to contain 1 w/o Sb, thus maximizing their vapor pressure. Tables 5.7 thru 5.10 contain fuel vapor pressure data from Gabelnick,³⁹ Bogensberger,⁴⁰ and Leibowitz⁴¹ which are plotted on Figs. 5.18 and 5.19. Leibowitz's UO_2 data is based on the work of Gillian⁴² and his mixed oxide work on that of Breitung.⁴³ Above 5000 K Bogensberger's extrapolated curve is used, which deviates greatly from his measured values. It was felt that this deviation may have been caused by a high dynamic pressure preventing free evaporation from the laser heated section.

From Figs. 5.18 and 5.19, it can be seen that the vapor pressures from the homogeneous metallic inclusions for both Johnson and O'Boyle type are less than the oxide and mixed oxide vapor pressure curves. If one of these fuel vapor pressure curves is close to reality in the temperature range of interest, 3000-6000 K, and if Raoult's Law is

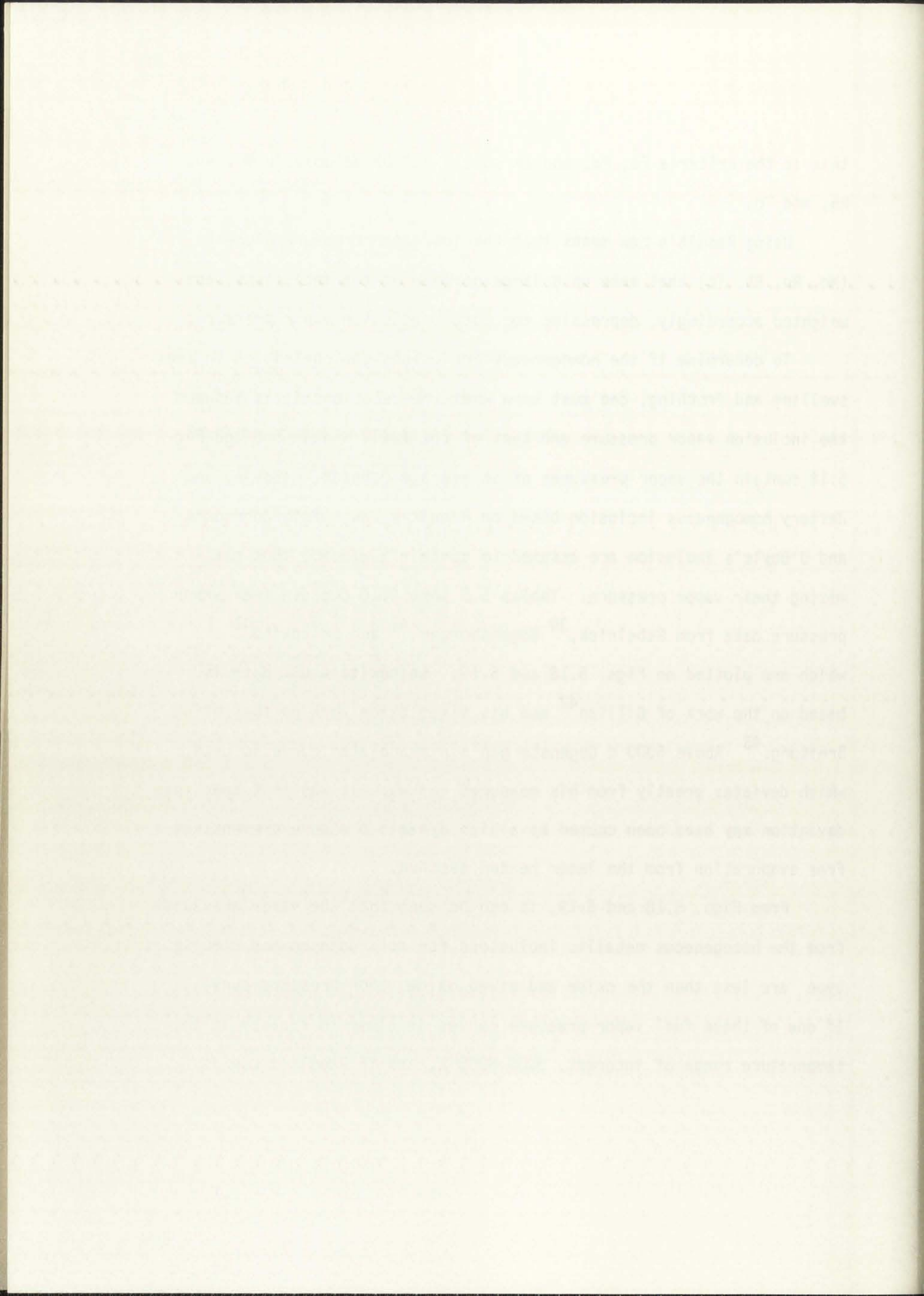


TABLE 5.6
 VAPOR PRESSURE DUE TO INCLUSIONS ASSUMING 100%
 SOLUBILITY OF THE FISSION PRODUCTS

Temperature (K)	Vapor Pressure (atm)		
	Johnson	O'Boyle	Jeffery
10,029.0	2,898.8	5,251.2	
8,490.6	781.4	1,079.6	
6,950.6	180.9	225.1	
5,413.0	26.1	35.1	1,436.8
4,221.6	2.93	4.4	584.5
3,607.8	.73	1.2	320.2
3,015.2	.12	.21	118.4
2,736.3			67.3
2,074.6			9.7
1,690.9			1.6
1,316.3			.107

TABLE 1

MEAN TEMPERATURES OF AIR AND WATER AT STATION 10

TEMPERATURES IN DEGREES FAHRENHEIT

DATE	AIR	WATER	DEPTH
10/10/54	67.5	65.5	0.500, 0.1
10/11/54	67.7	65.5	0.500, 0.1
10/12/54	67.5	65.5	0.500, 0.1
10/13/54	67.5	65.5	0.500, 0.1
10/14/54	67.5	65.5	0.500, 0.1
10/15/54	67.5	65.5	0.500, 0.1
10/16/54	67.5	65.5	0.500, 0.1
10/17/54	67.5	65.5	0.500, 0.1
10/18/54	67.5	65.5	0.500, 0.1
10/19/54	67.5	65.5	0.500, 0.1
10/20/54	67.5	65.5	0.500, 0.1
10/21/54	67.5	65.5	0.500, 0.1
10/22/54	67.5	65.5	0.500, 0.1
10/23/54	67.5	65.5	0.500, 0.1
10/24/54	67.5	65.5	0.500, 0.1
10/25/54	67.5	65.5	0.500, 0.1
10/26/54	67.5	65.5	0.500, 0.1
10/27/54	67.5	65.5	0.500, 0.1
10/28/54	67.5	65.5	0.500, 0.1
10/29/54	67.5	65.5	0.500, 0.1
10/30/54	67.5	65.5	0.500, 0.1
10/31/54	67.5	65.5	0.500, 0.1

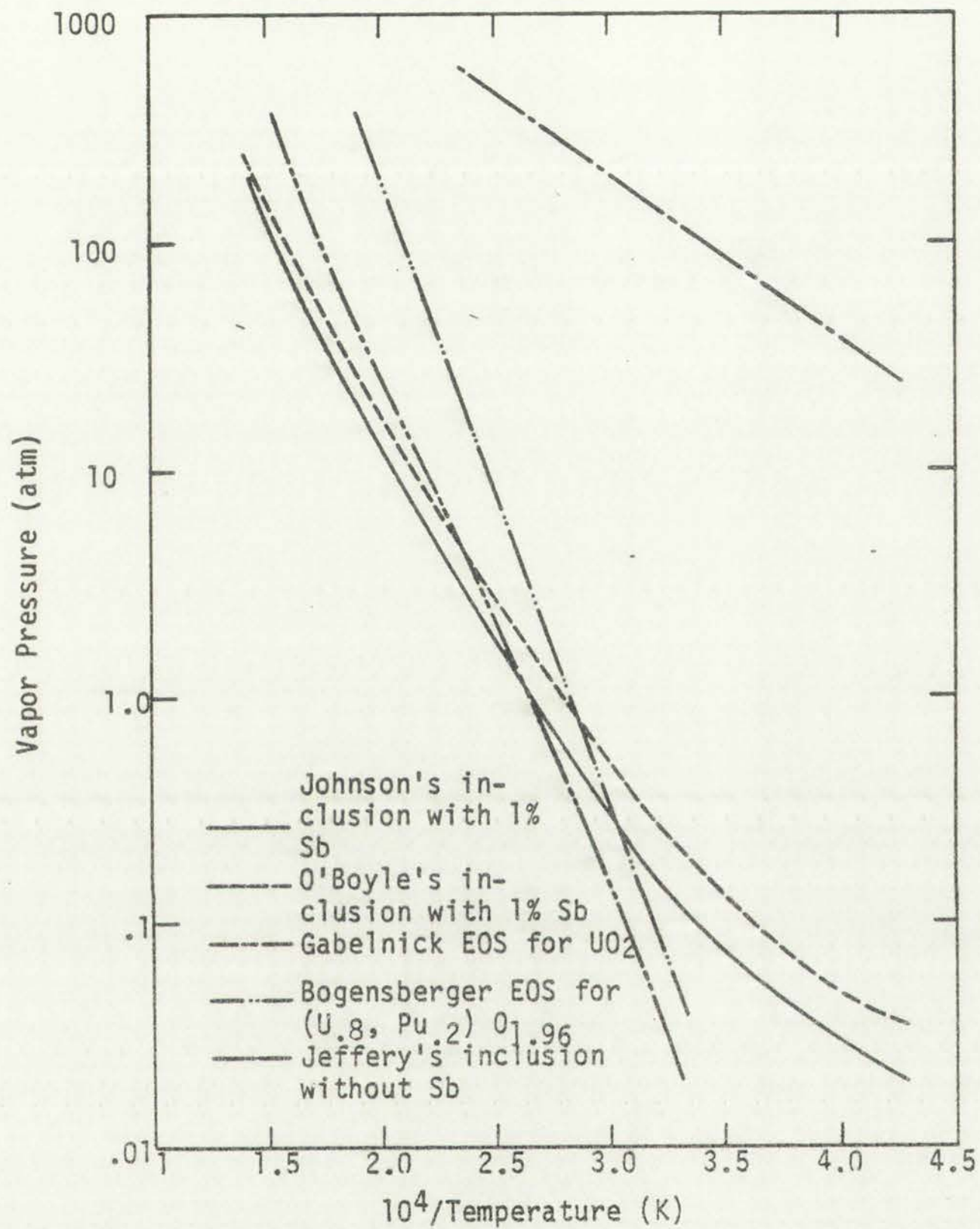


Figure 5.18
Comparison of inclusion and fuel vapor pressures.



Figure 1. Relationship of incision and fuel vector pressure.

TABLE 5.7

GABELNICK³⁹ VAPOR PRESSURE OF UO₂

Temperature (°K)	$\frac{10^4}{T}$	Vapor Pressure (atm)	
		6g/cm ³ Smear Density	7g/cm ³ Smear Density
3000	3.333	.0191	.0191
3500	2.857	.321	
4000	2.500	2.24	2.24
4500	2.222	9.45	
5000	2.000	29.1	29.1
5500	1.818	74.6	
6000	1.667	173.	
6500	1.538	375	

STATISTICAL DATA

Year	Population	Total (1950)	
		Male	Female
1950	100	50	50
1951	101	50.5	50.5
1952	102	51	51
1953	103	51.5	51.5
1954	104	52	52
1955	105	52.5	52.5
1956	106	53	53
1957	107	53.5	53.5
1958	108	54	54
1959	109	54.5	54.5
1960	110	55	55

TABLE 5.8
 VAPOR PRESSURE OF UO_2 AND $(U, Pu)O_2$ BASED
 ON EXPERIMENTAL WORK OF BOGENSBERGER⁴⁰

Temperature (K)	$\frac{10^4}{T}$	Vapor Pressure (atm)	
		UO_2	$(U, Pu)O_2^*$
3000	3.333	.025	.0386
3500	2.857	.535	.845
4000	2.500	5.31	8.546
4600	2.174	43.13	70.67
5000	2.000	131.82 [†]	218.1 [†]
6000	1.667	1122. [†]	1890. [†]
7000	1.429	5179. [†]	8840. [†]

* For 20 atom % Pu and oxygen-to-metal ratio (O/M) of 1.96

[†] Calculated from following empirical formula based on lower temperature experimental points:

For UO_2 above melting temperature

$$P_{(atm)} = 10^{(7.7-27900/T)}$$

For $(U, Pu)O_2$ above melting temperature

$$P_{(atm)} = 10^{(7.966-28137/T)}$$

TABLE I
RESULTS OF THE EXPERIMENTAL INVESTIGATION OF THE
EFFECT OF THE CONCENTRATION OF THE SOLUTION ON THE
RATE OF POLYMERIZATION OF STYRENE

Concentration of solution (%)	Rate of polymerization (g/hr)
0.1	0.001
0.2	0.002
0.5	0.005
1.0	0.010
2.0	0.020
5.0	0.050
10.0	0.100
20.0	0.200
50.0	0.500
100.0	1.000

For 10% solution, the rate of polymerization was found to be 0.100 g/hr. This rate is 10 times greater than that for 1% solution (0.010 g/hr). The results show that the rate of polymerization is directly proportional to the concentration of the solution.

For 20% solution, the rate of polymerization was found to be 0.200 g/hr. This rate is 20 times greater than that for 1% solution (0.010 g/hr). The results show that the rate of polymerization is directly proportional to the concentration of the solution.

For 50% solution, the rate of polymerization was found to be 0.500 g/hr. This rate is 50 times greater than that for 1% solution (0.010 g/hr). The results show that the rate of polymerization is directly proportional to the concentration of the solution.

For 100% solution, the rate of polymerization was found to be 1.000 g/hr. This rate is 100 times greater than that for 1% solution (0.010 g/hr). The results show that the rate of polymerization is directly proportional to the concentration of the solution.

TABLE 5.9
LEIBOWITZ⁴¹ VAPOR PRESSURE FOR UO_2

Temperature (K)	Vapor Pressure (atm)
2000	9.29×10^{-8}
2500	1.25×10^{-4}
3000	1.52×10^{-2}
3500	.344
4000	2.45
4500	10.7
5000	33.1
5500	77.6
6000	151

TABLE I

Properties of the Polymers

Sample	η_{inh} (dl/g)	η_{sp}/c (dl/g)
1	0.15	0.15
2	0.20	0.20
3	0.25	0.25
4	0.30	0.30
5	0.35	0.35
6	0.40	0.40
7	0.45	0.45
8	0.50	0.50
9	0.55	0.55
10	0.60	0.60

TABLE 5.10

LEIBOWITZ⁴¹ VAPOR PRESSURE FOR $(U_{.8}Pu_{.2})O_{1.96}$

Temperature (K)	Vapor Pressure (atm)
2000	1.2×10^{-7}
2500	2.1×10^{-4}
3000	3.6×10^{-2}
3500	.91
4000	9.1
4500	49
5000	170
5500	500*
6000	1000*

*Extrapolated from low temperature data

TABLE 1
 Values of α and β for various γ

γ	α	β
10^{-1}	0.000	0.000
10^{-2}	0.000	0.000
10^{-3}	0.000	0.000
0.001	0.000	0.000
0.01	0.000	0.000
0.1	0.000	0.000
1.0	0.000	0.000
10.0	0.000	0.000
100.0	0.000	0.000
1000.0	0.000	0.000

Values of α and β are given in the table.

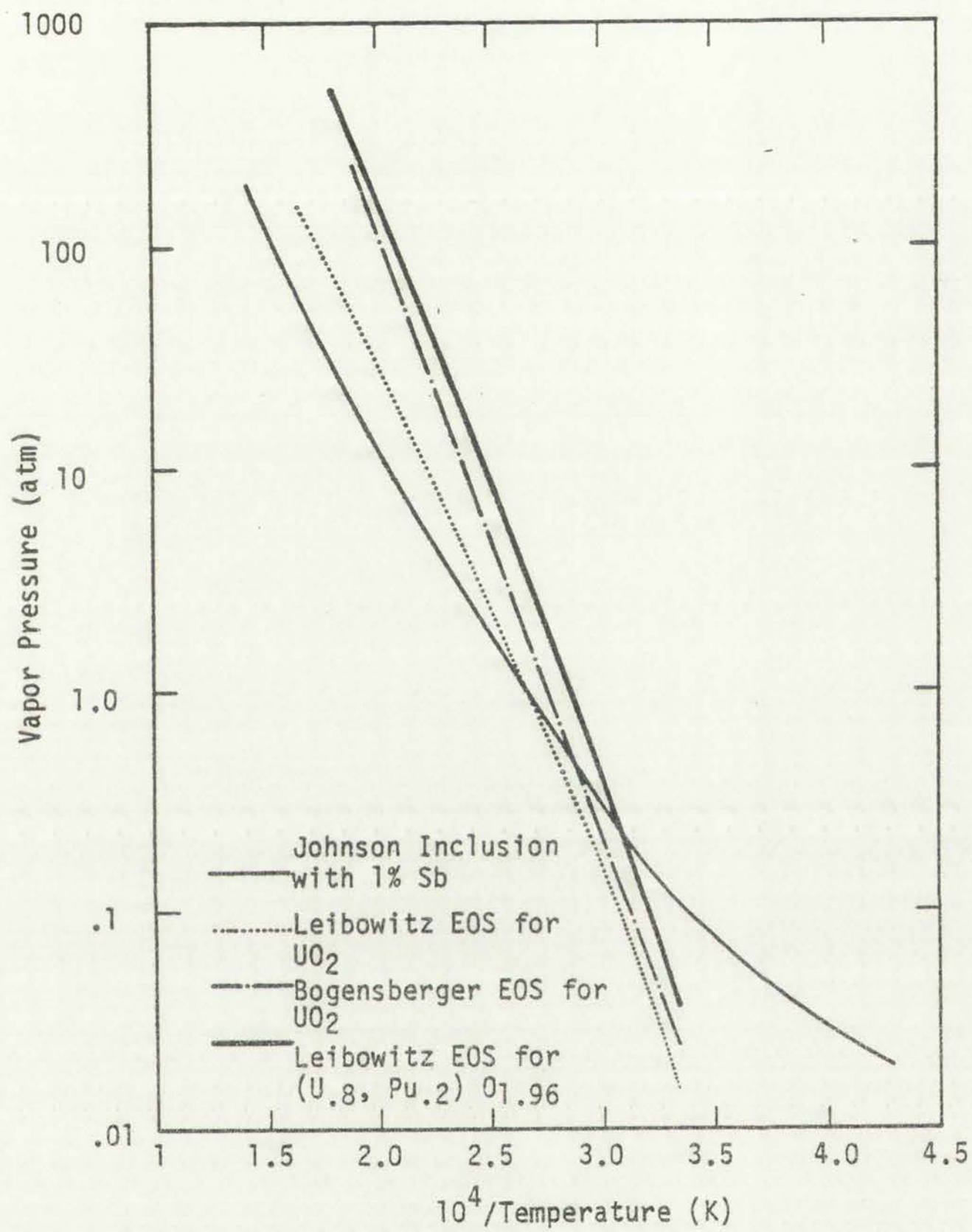


Figure 5.19
Comparison of additional fuel EOS with inclusion vapor pressure.



Graph showing the relationship between the variables.

applicable, the homogeneous metallic inclusions are of no consequence as far as a fuel driving force is concerned. They are still important if one considers their application as decay heat and neutron precursors.

The above two assumptions, total miscibility and total immiscibility, represent limiting conditions on the state of the metallic inclusions. If partial solubility occurs, and occurs in the same molar ratio as the inclusion, it will have a linear effect on the expected nodal expansion.

Table 5.11 contains the fuel vapor pressure, homogeneous inclusion vapor pressure, and the vapor pressure of the segregated volatiles at temperatures from 3000-7000 K. From Fig. 5.20 one additional feature should be noted. Due to the differing slopes of the fuel and individual constituent vapor pressure curves, if the pin internal pressure reaches on the order of hundreds of atmospheres or higher, the fuel may reach incipient vaporization at a lower temperature than some or all of the segregated volatiles depending on the specific local pressure. If this were the case, then even segregated inclusions would not be of importance for prepin failure fuel motion. After pin failure, however, as the pin pressure drops they could still provide a fuel expulsion-foaming force.

5.3 LWR Inclusion

Figure 5.18 also contains the inclusion vapor pressure for a homogeneous, average, Jeffery¹ inclusion. As seen from Table 2.2,

TABLE 5.11
COMPARISON OF THE VAPOR PRESSURES OF SOLUBLE INCLUSIONS, VOLATILE CONSTITUENTS, AND FUEL

Temperature (°K)	Soluble Vapor Pressure (atm)		Individual Constituent Vapor Pressure (atm)			Fuel Vapor Pressure (atm)		
	Raoult's Law		Pd	Sb	Fe	Gabelnick (UO ₂)	Bogensberger	Leibowitz
	Johnson	Boyle						
3000	.115	.2056	.9455	8.647	.507	.0191	.0251 UO ₂	.0152 UO ₂
4000	1.83	2.87	27.133	27.174	19.567	2.24	.0386 (U,Pu)O ₂ 5.31 UO ₂	.036 (U _{.8} Pu _{.2})O _{1.96} 2.45 UO ₂
5000	13.0	17.6	203.3	54.0	175.1	29.1	8.546 (U,Pu)O ₂ 131.8 UO ₂	9.1 (U _{.8} Pu _{.2})O _{1.96} 33.1 UO ₂
6000	57.	77.	778.6	85.4	754.9	173.	218.1 (U,Pu)O ₂ 1122 UO ₂	170. (U _{.8} Pu _{.2})O _{1.96} 151 UO ₂
7000	190	240	2031.7	118.4	2143.5	740 .	1890 (U,Pu)O ₂ 5179 UO ₂	1000 (U _{.8} Pu _{.2})O _{1.96} 325 UO ₂ 2200 (U _{.8} Pu _{.2})O _{1.96}

1	2	3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50
51	52	53	54	55	56	57	58	59	60
61	62	63	64	65	66	67	68	69	70
71	72	73	74	75	76	77	78	79	80
81	82	83	84	85	86	87	88	89	90
91	92	93	94	95	96	97	98	99	100

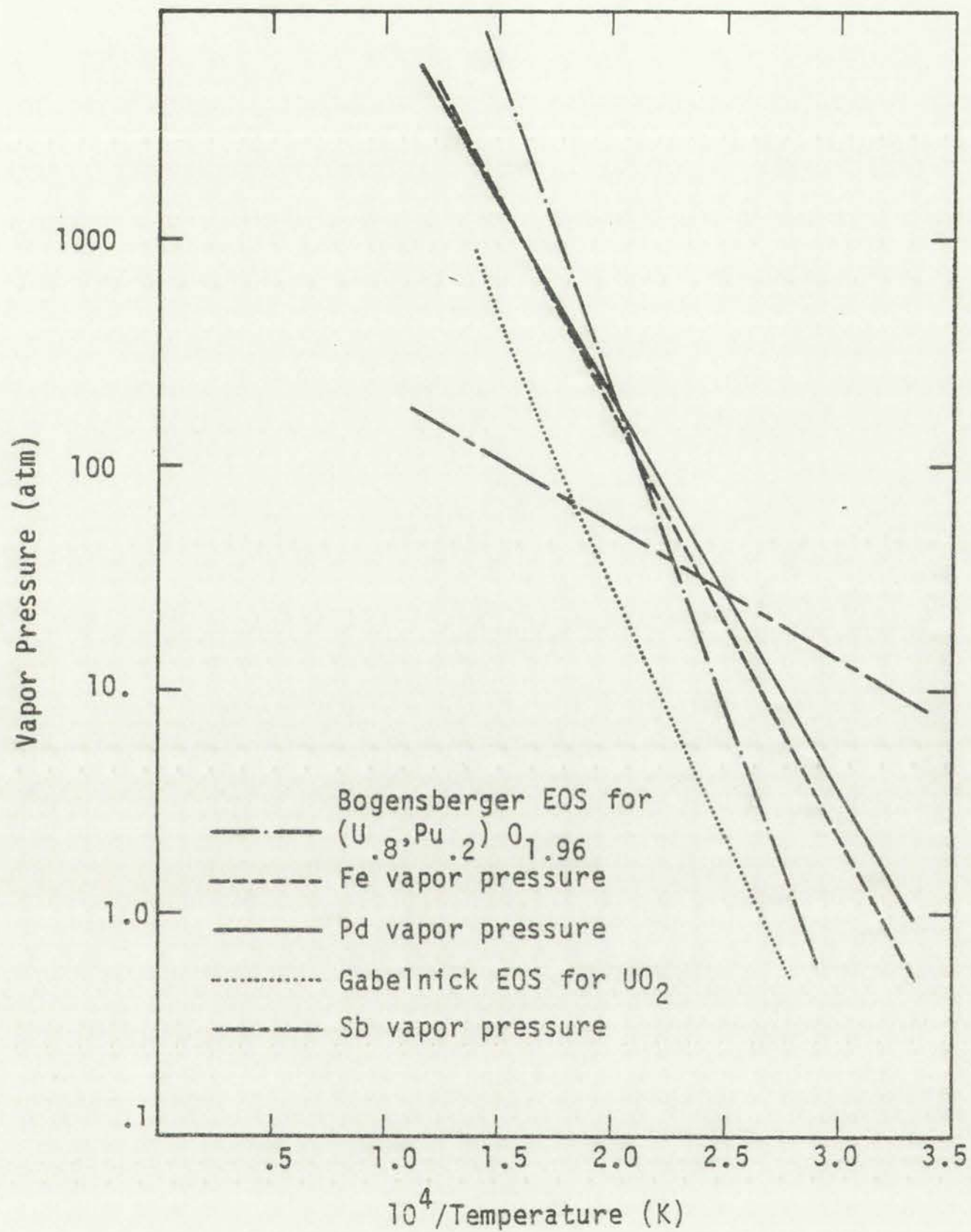


Figure 5.20
 Comparison of fuel EOS and vapor
 pressures of individual constituents.



Figure 1: Relationship between Dose and Area Under the Curve (AUC)

the UO_2 fuel was irradiated in a thermal spectrum and the inclusion composition differed substantially from the mixed oxide, fast spectrum inclusions of Johnson⁴ and O'Boyle.³ From Figs. 5.18 and 5.19, it appears that thermal reactor fuel analysis may have to consider possible contribution to accident scenerios from the metallic inclusions. The homogeneous inclusion vapor pressure is much higher than the EOS for UO_2 , leading to a large, i.e. 40% $\Delta V/V$, for the entire fuel pin at 20 atm. and peak temperature of 2800 K. Using a β 15/s ramp insertion of reactivity, the total fuel volume expansion increases to 360% at incipient fuel vaporization. From Figs. 5.21 and 5.22, it can be seen that if one assumes Jeffery's inclusions to be in the segregated form vs homogeneous form, a nodal volume expansion on the order of 100% and a total fuel pin volume expansion of 37% can be expected at incipient fuel vaporization. This is assuming a flat distribution in the inclusion number density and using the Ideal Gas EOS. Tellurium, strontium, and barium are constituents not found in the fast reactor fuel metallic inclusions. These three elements are more volatile than the palladium, iron, and antimony and contributes a minimum of 75% of the nodal volume expansion. The high volatility also causes expansion to occur much earlier in the transient. It thus appears that thermal reactor fuel may swell due to volatilization during a transient if either segregated or homogeneous inclusions are assumed.

Two questions, however, must be addressed before a definitive statement to that effect can be made. First, the electron microprobe

the first part of the paper, the authors discuss the
theoretical background of the problem and the
experimental method used. In the second part, the
results of the measurements are presented and
discussed. It is shown that the results are
in good agreement with the theoretical predictions.
The authors conclude that the experimental method
is reliable and that the theoretical model is
valid. The authors thank the National Science
Foundation for the support of this work.

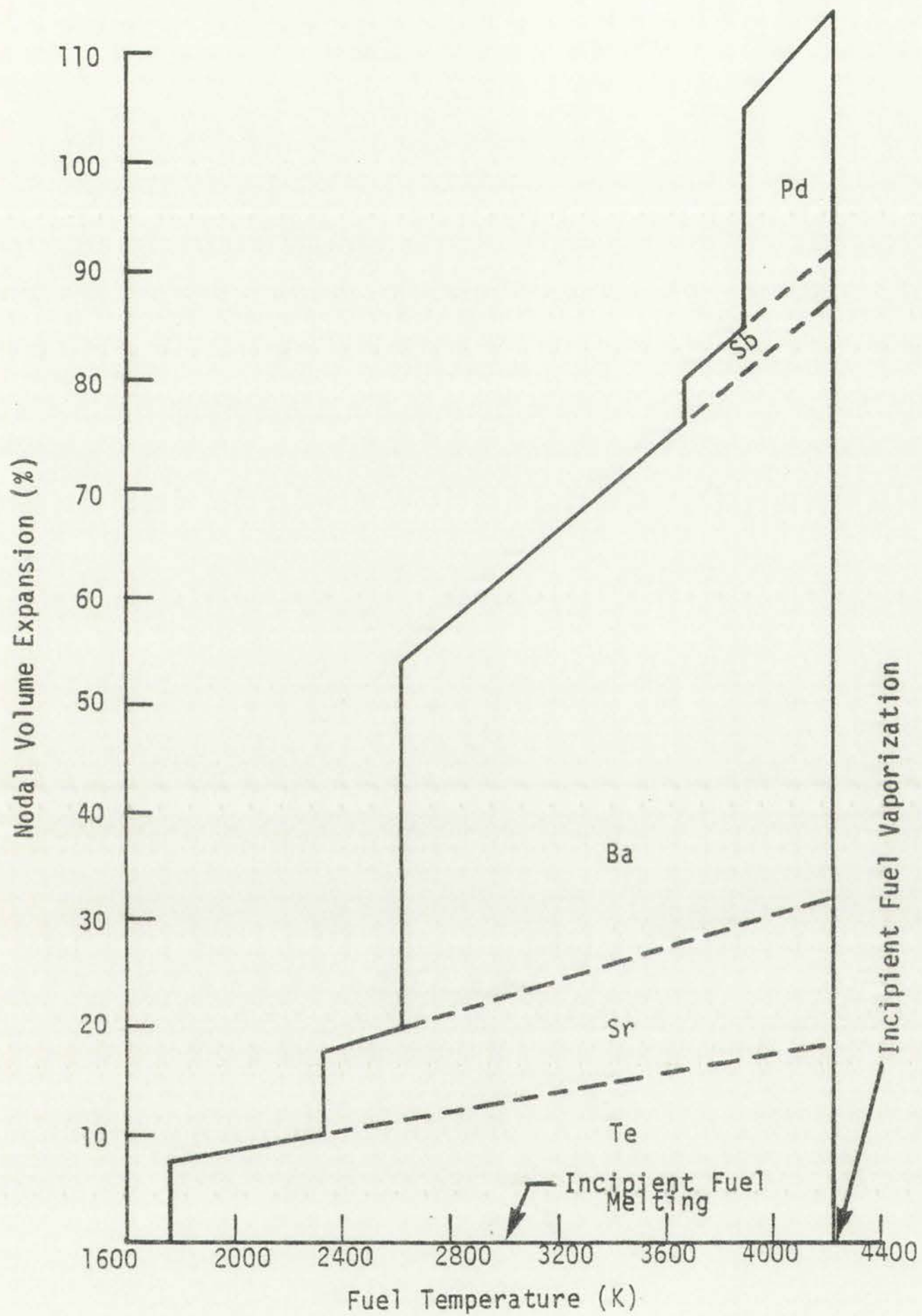


Figure 5.21
 Nodal volume expansion for Jeffery inclusions using
 a flat inclusion number density profile and Ideal Gas EOS.



11) 11/12/1957 10:00 AM

11/12/1957 10:00 AM
 11/12/1957 10:00 AM
 11/12/1957 10:00 AM

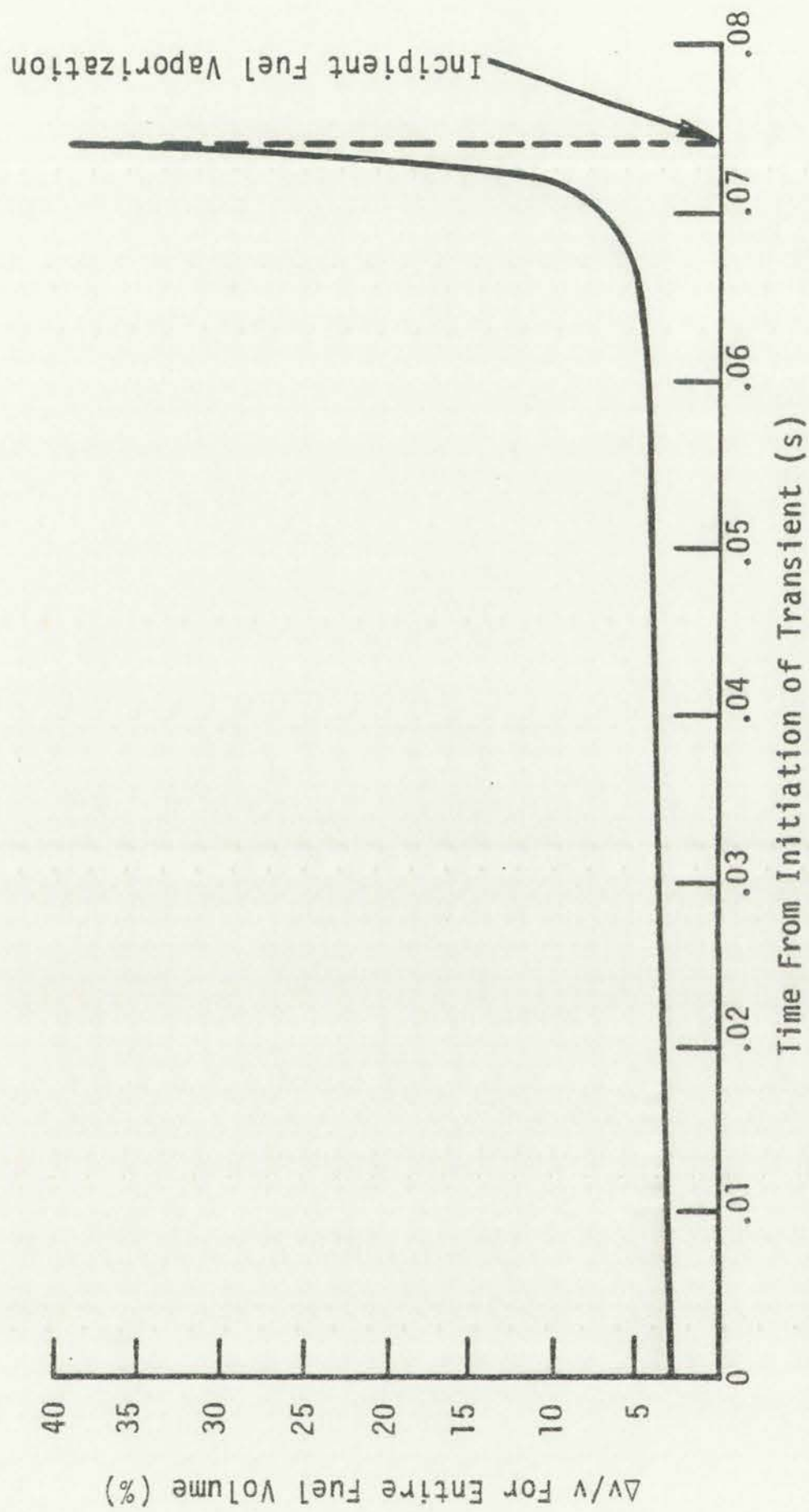


Figure 5.22

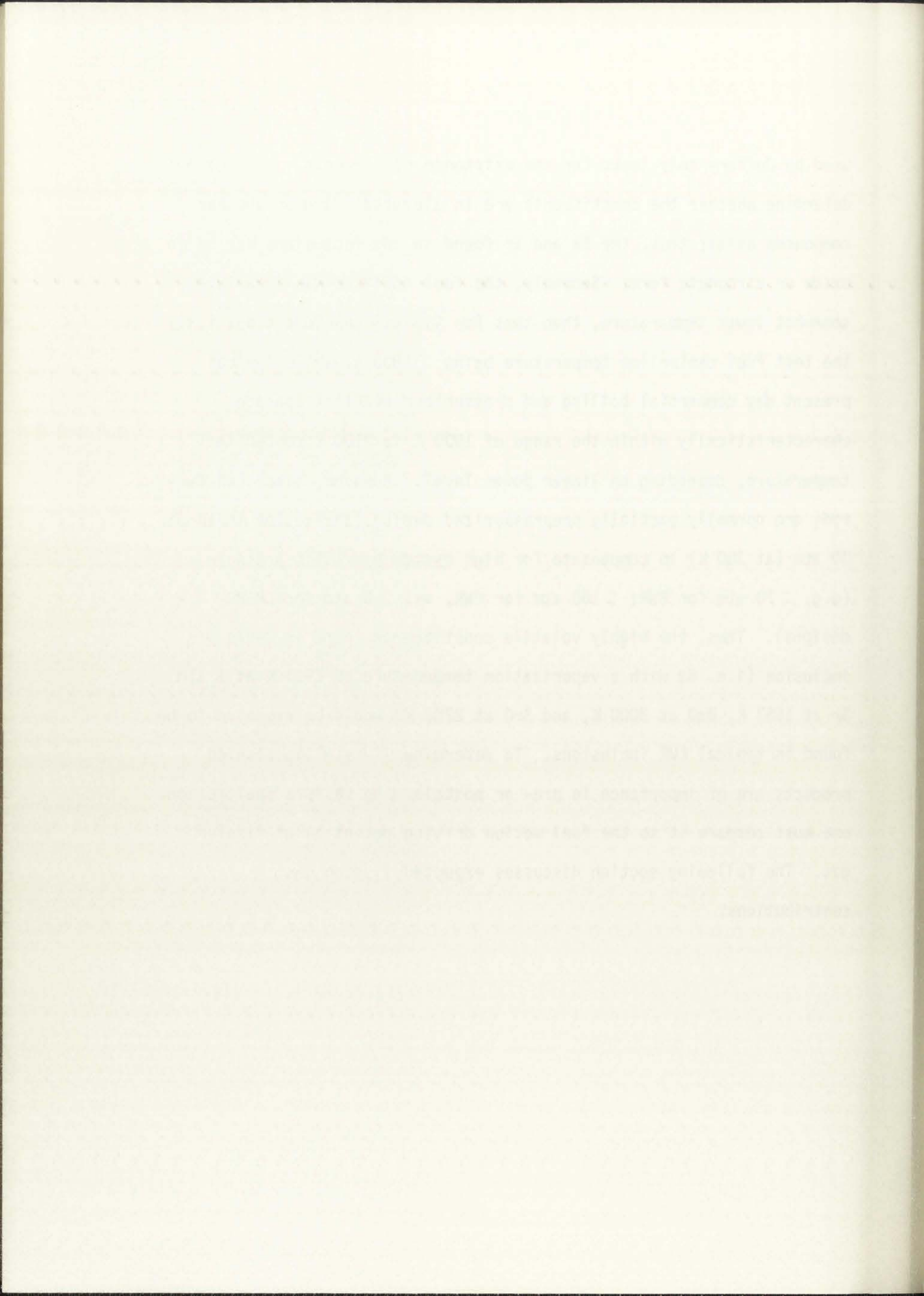
Total fuel volume expansion for Jeffery inclusion using $15/s$ ramp insertion, flat inclusion number density profile, and Ideal Gas EOS.

(a) $\log_{10} \frac{1}{1 - \frac{1}{2} \left(\frac{1}{2} \right)^{t-1}}$
 (b) $\log_{10} \frac{1}{1 - \frac{1}{2} \left(\frac{1}{2} \right)^{t-1}}$

(c) $\log_{10} \frac{1}{1 - \frac{1}{2} \left(\frac{1}{2} \right)^{t-1}}$



used by Jeffery only looks for the existence of elements. It does not determine whether the constituents are in elemental form or whether compounds exist; thus, the Ba and Sr found in the inclusions may be in oxide or zirconate form. Secondly, the fuel analyzed was irradiated at somewhat lower temperature, than that for typical LWR condition, i.e., the test fuel centerline temperature being ≈ 1800 K, while typical present day commercial boiling and pressurized reactors operate characteristically within the range of 1900 K to 2100 K centerline temperature, depending on linear power level. However, since LWR fuel rods are normally partially prepressurized during fabrication to about 30 atm (at 300 K) to compensate for high system hydraulic pressure (e.g. ≈ 70 atm for BWR; ≈ 160 atm for PWR, vs. 2-5 atm for LMFBR designs). Thus, the highly volatile constituents found in Jeffery's inclusion (i.e. Ba with a vaporization temperature of 1913 K at 1 atm Sr at 1657 K, BaO at 3000 K, and SrO at 2703 K) would be expected to be found in typical LWR inclusions. To determine if metallic fission products are of importance in pre- or postcladding failure fuel motion, one must compare it to the fuel motion driving potential of fission gas. The following section discusses expected fission gas contributions.



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1. The first part of the paper discusses the general theory of the subject and its importance in the field of research.

2. The second part of the paper discusses the experimental methods used in the study and the results obtained.

3. The third part of the paper discusses the theoretical aspects of the study and the implications of the results.

4. The fourth part of the paper discusses the conclusions of the study and the suggestions for further research.

5. The fifth part of the paper discusses the references and the sources used in the study.

6. FISSION GAS

To determine whether the metallic inclusion contribution to fuel motion and expansion is of importance, one can compare to the expected range of volume expansion from fission gas.

Fission gas retention is temperature dependent and thus varies radially across the fuel pin. In Fig. 6.1,¹ the radial distribution for a mixed oxide fuel pin irradiated in EBR-II at a peak power level of ≈ 10 kW/ft to an average burnup of ≈ 3.2 atom % is shown. This distribution was determined by measuring the activity of Kr-85. The fission gas retention varies from 4% in the columnar region to 64% in the unstructured region yielding a volume average fission gas retention of 42.2%. Due to the low irradiation power, these gas retention numbers should be at the high end of expected values.

Table 6.1 contains the yield data for 3 atom % burnup for Xe, Kr, and I based on Burris.² The totals in Table 6.1 are close to the $\approx 1.99 \times 10^{20}$ atoms/cm³ fuel, value obtained from Stahl.¹ The gas exists in solution or in small (unresolvable) bubbles within the matrix, in intragranular bubbles ($\approx 650 \text{ \AA}$ ⁰ in diameter), and at the grain boundaries (intergranular bubbles). Intragranular bubble size seems to decrease with increase in fission rate, i.e. 300 \AA ⁰ diameter for 17 kW/ft. and 1000-1800 \AA ⁰ diameter for ≈ 8.9 kW/ft.

In the hand calculations presented here, to obtain the maximum fuel volume expansion due to fission gas, it was assumed that during a

The first part of the paper is devoted to a description of the experimental method and the results obtained. The second part is devoted to a discussion of the results and to a comparison with the results obtained by other workers. The third part is devoted to a discussion of the results obtained in the present work and to a comparison with the results obtained by other workers. The fourth part is devoted to a discussion of the results obtained in the present work and to a comparison with the results obtained by other workers.

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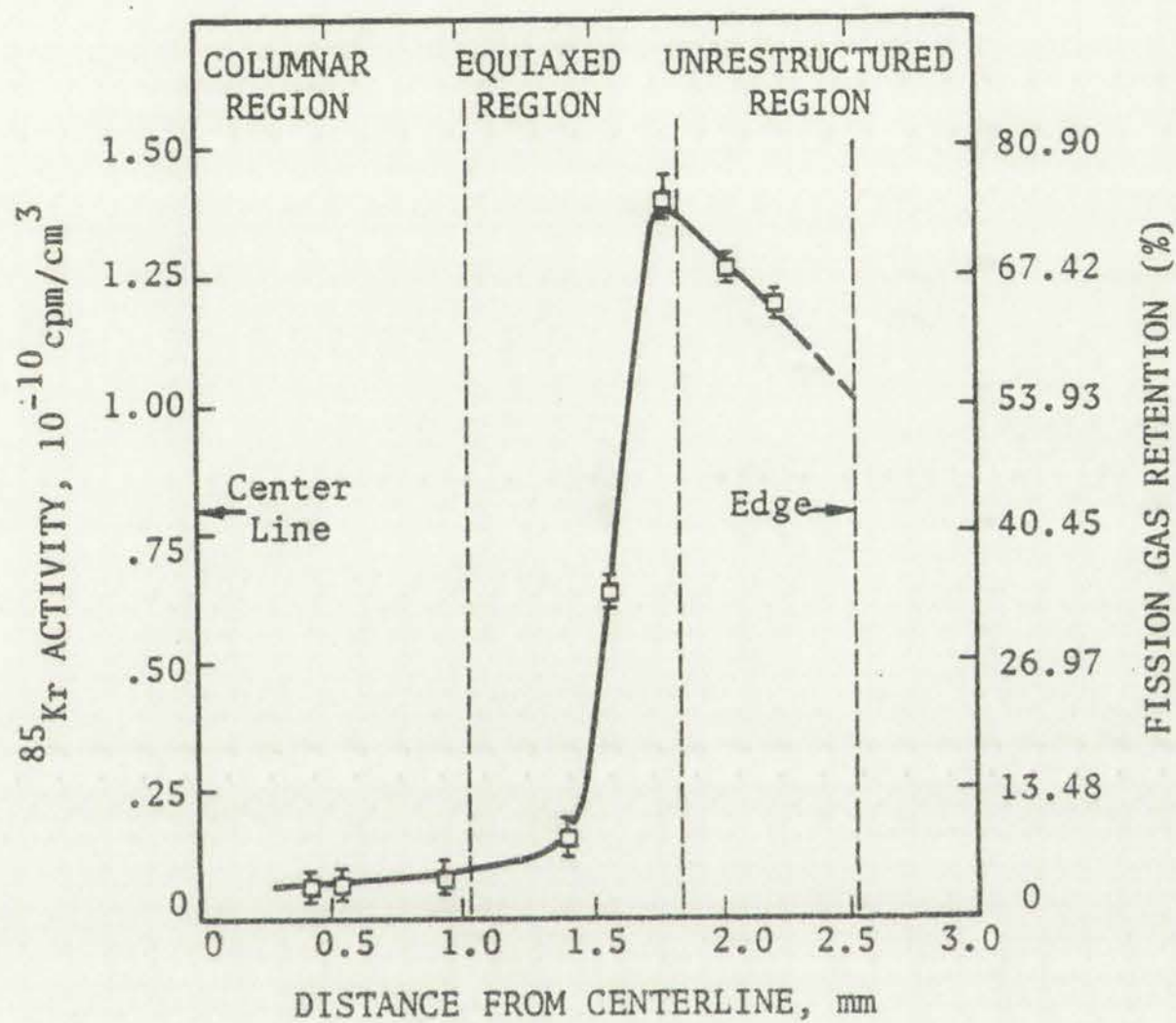


Figure 6.1
Fission gas retention.

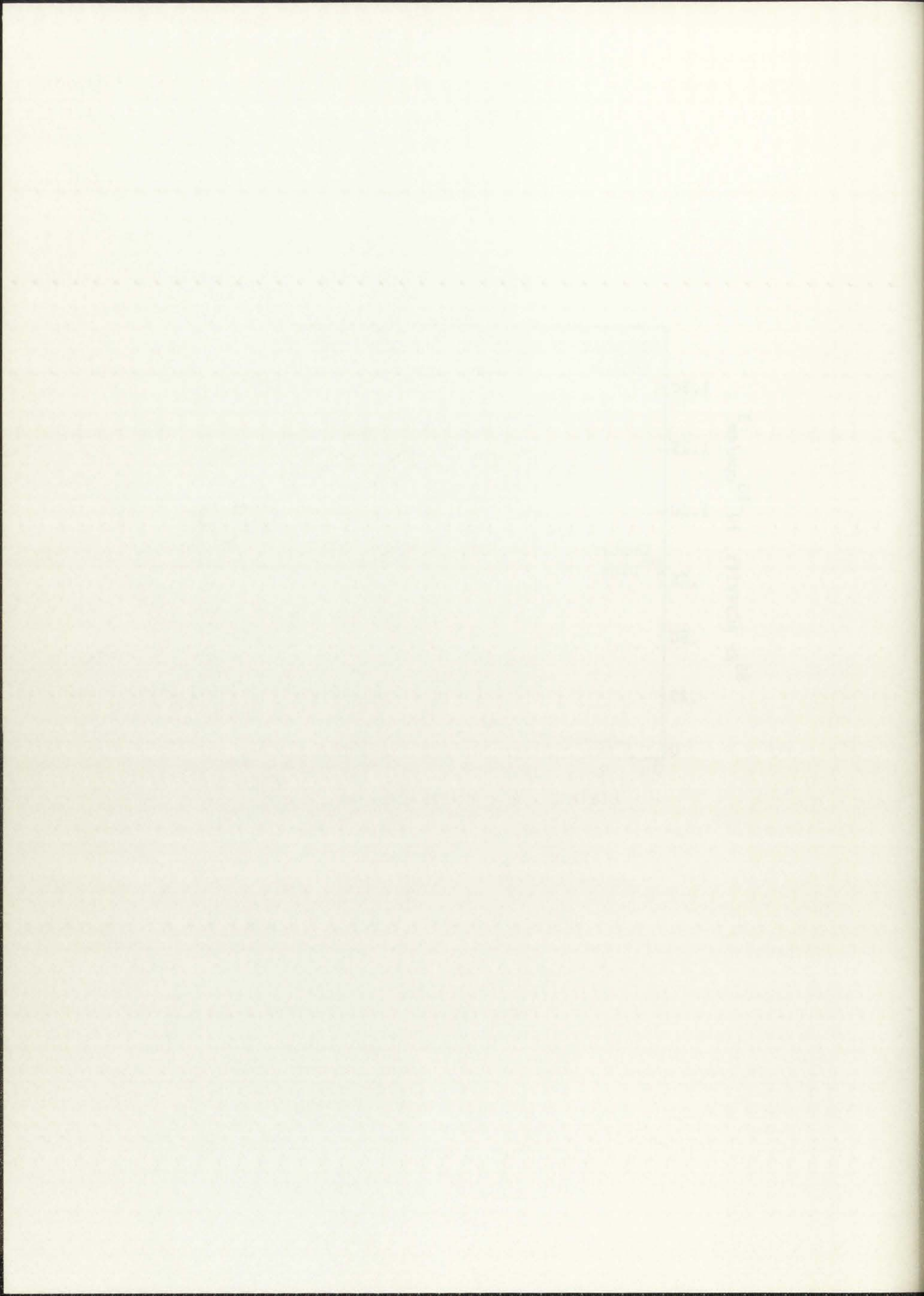


TABLE 6.1
 FISSION GAS YIELD FOR 3 ATOM % BURNUP
 ($\approx 6.624 \times 10^{20}$ FISSION/ cm^2 FUEL) BASED ON BURRIS

<u>Fuel Species</u>	<u>Yield (Atoms/cm^3 Fuel)</u>			<u>I</u>	<u>Total</u> (Atoms/ cm^3 Fuel)	<u>(Moles/cm^3 Fuel)</u>
	<u>Kr</u>	<u>Xe</u>				
U^{235}	1.97×10^{19}	1.441×10^{20}		8.737×10^{18}	1.7254×10^{20}	2.865×10^{-4}
Pu^{239}	6.001×10^{18}	1.566×10^{20}		1.796×10^{19}	1.806×10^{20}	2.999×10^{-4}

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transient no further fission gas release occurred and all existing gas is precipitated into large bubbles (i.e. ignoring surface tension effects). Using the Ideal Gas EOS (Eq. (6.1)) and a bulk pressure of 20 atm. the volume % occupied by fission gas in the various grain regions was calculated.

$$V = \frac{nRT}{P}, \quad V_2 - V_1 = nR \left(\frac{T_2}{P_2} - \frac{T_1}{P_1} \right) \quad (6.1)$$

These results can be found in Table 6.2 and Fig. 6.2. They indicate that the maximum fission gas contribution to fuel expansion varies from 10% in the columnar region to 260% near the radius of maximum fission gas retention.

As mentioned above, in actuality the fission gas is in solution, in intragranular bubbles, and in intergranular bubbles. During a fast transient (15/s ramp insertion) intragranular bubble coalescence and diffusion due to temperature gradients has little effect. Even if coalescence occurs, pressure equilibration does not occur in very short time frames. The rate of bubble migration is on the order of 4 $\mu\text{m/s}$,^{1,3} and the diffusion coefficient for a single atom at 1773 K is $\approx 1.3 \times 10^{-15} \text{ cm}^2/\text{s}$.^{4,5} Also gas in solution precipitates into extremely small intragranular bubbles which do not significantly contribute to fuel expansion due to the large internal bubble pressure from surface tension effects. Stahl¹ in his experimental work determined the quantity of gas in inter- and intragranular bubbles. To

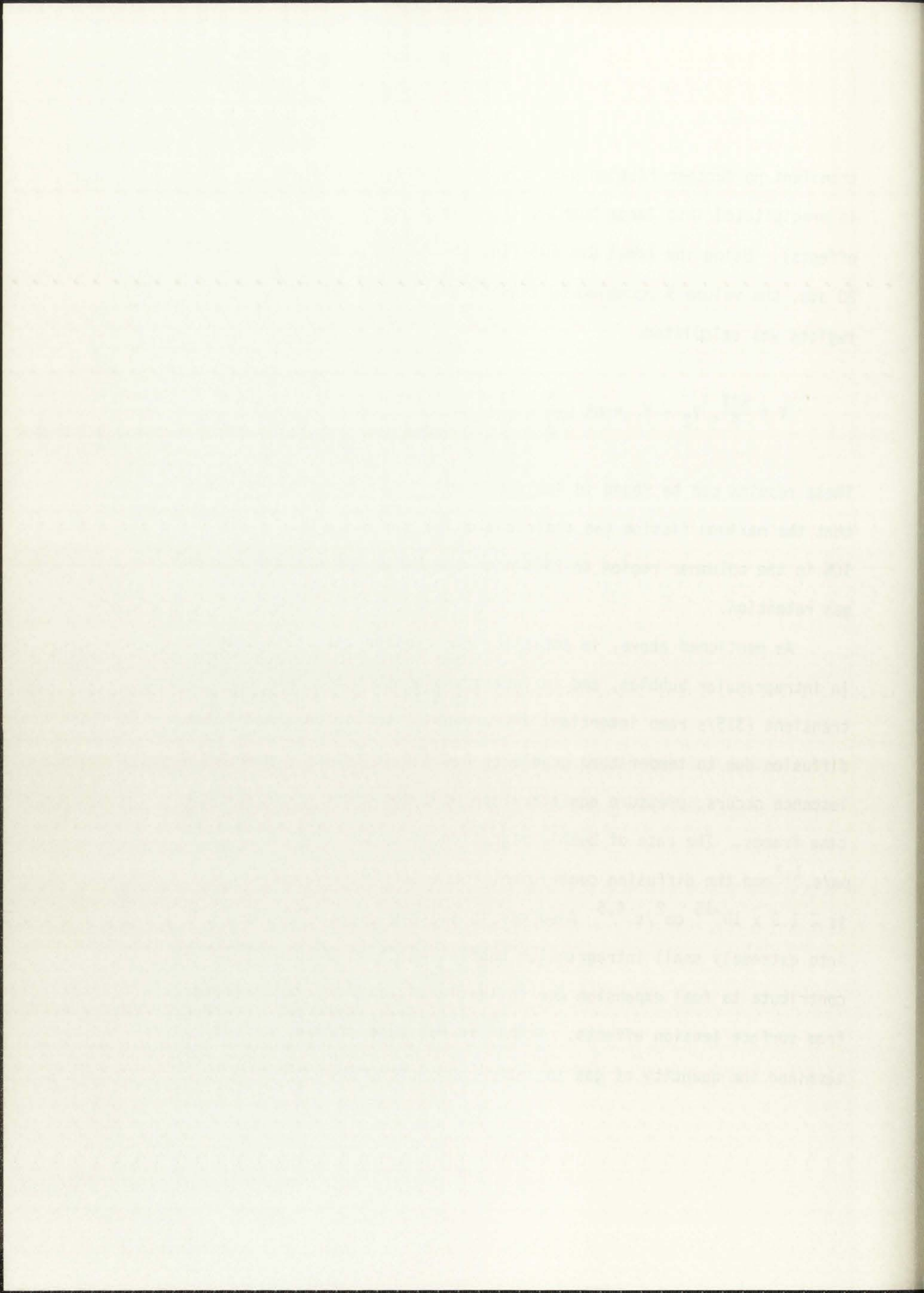
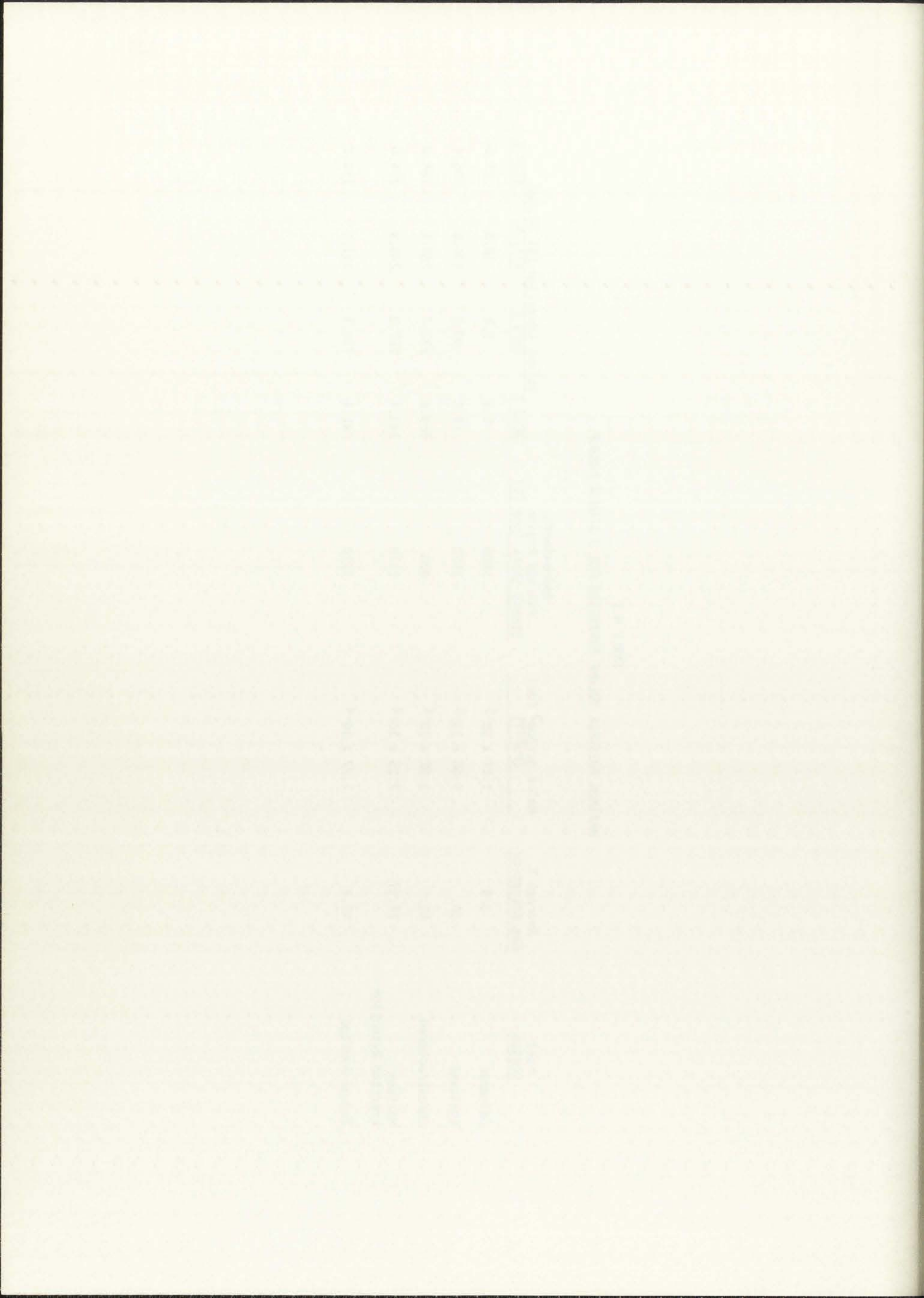


TABLE 6.2
 MAXIMUM POSSIBLE VOLUME EXPANSION FOR 3 ATOM % BURNUP

Fuel Region	Average % Gas Retention	Moles gas/cm ³ Fuel (Pu ²³⁹)	Approximate Average Region Steady State Temp (K)		Volume Expansion (%)		
			3023 K	3824 K	4177 K	20 Atm	4222 K
Columnar	3.9	1.17 x 10 ⁻⁵	5.3	9.1	10.8	11.0	
Equiaxed	32.	9.60 x 10 ⁻⁵	59.2	90.7	104.6	106.4	
Unrestructured	64.	1.92 x 10 ⁻⁴	169.6	232.7	260.5	264.0	
Maximum Expected Retention	74.97	2.25 x 10 ⁻⁴	143.4	217.3	249.9	254.0	
Volume Average	42.2	1.27 x 10 ⁻⁴	91.3	133.1	151.5	153.8	



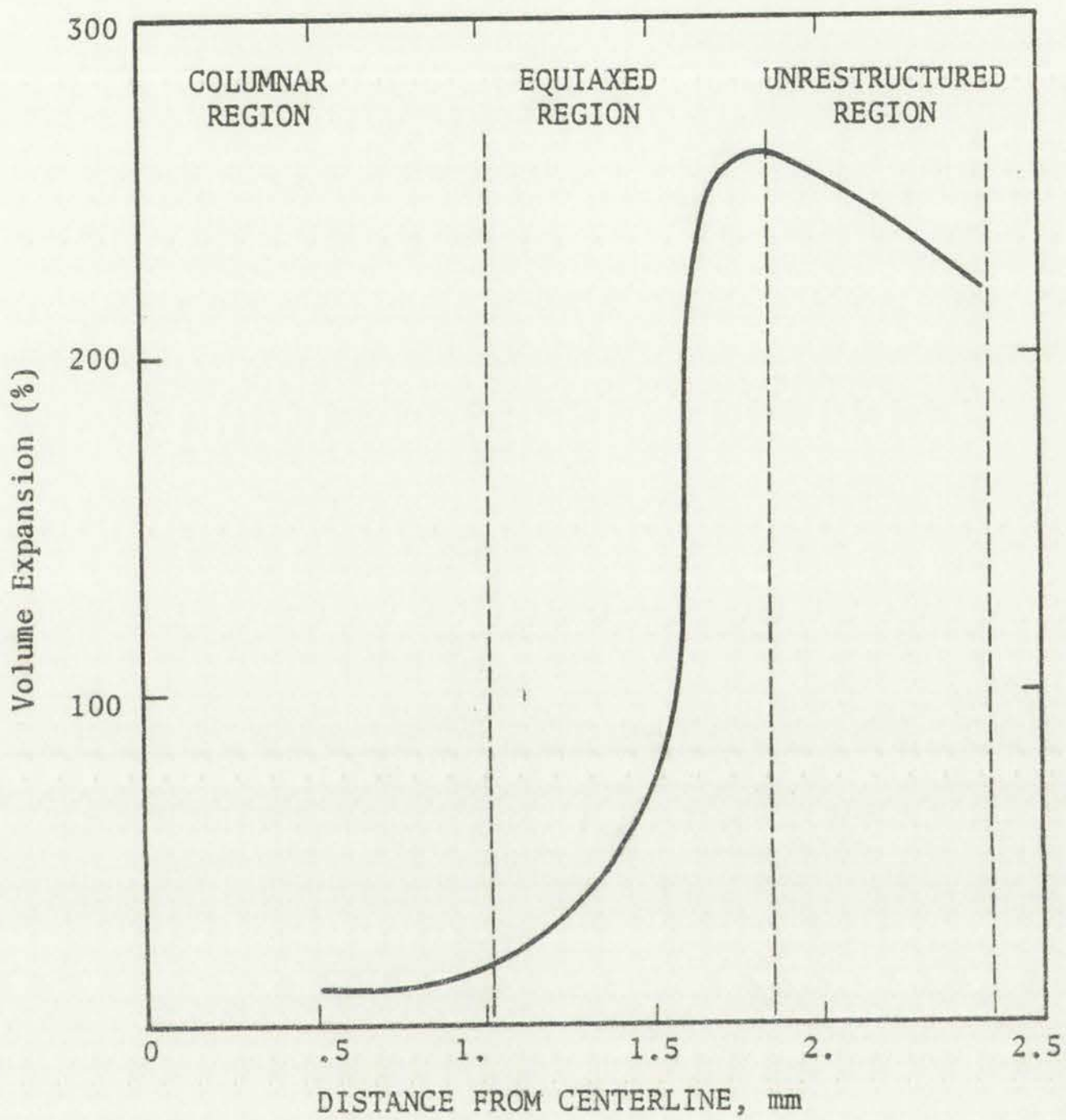


Figure 6.2
Maximum fuel volume expansion due to
fission gas at $P = 20$ atms, $T = 4222$ K



as illustrated in the graph

By this illustration we can see that
 the courage of a scientist is much greater than that of a professor or a military man.

obtain the possible contributions from the various grain regions, the maximum fission gas expansions are calculated via Eq. (6.1) and the results listed in Table 6.3. Again this maximum possible contribution ignores surface tension and the usual transient gas release of 8%¹ - 16%.⁶ Transient gas release is usually associated with intergranular gas and the interlinking of bubbles, forming paths to the central void. The degree of linkage is a function of burnup, power, and the transient conditions, but is not considered here except to say that a substantial portion of intergranular gas can be expected to be released, especially in a slow transient.

As seen in Table 6.3, the majority of the fission gas in the columnar and equiaxed region is in bubble form. In the unrestructured region, however, the major portion of the gas is in solution or unresolvable intragranular bubbles. For the unrestructured region Ronchi and Matzke⁷ calculated that 0.8% of the fission gas was in intragranular bubbles, 3-17% in grain boundaries, and 97-75% in solution, which is not much different than the results of Stahl.¹ The volume expansion calculations in Tables 6.2 and 6.3 were done using the Ideal Gas EOS. This tends to underestimate the volume expansion as can be seen in Table 6.4 which compares the Ideal Gas EOS to Harrison's tabular EOS⁸ for Xe, for temperature-pressure ranges as close as can be found to those of interest. Thus the fuel swelling due to existing bubbles is only on the order of 2 to probably 40% if the transient is rapid enough that coalescence and precipitation have a negligible effect.

The text on this page is extremely faint and illegible. It appears to be a technical or scientific document, possibly containing a list of items or a detailed description. The content is too light to transcribe accurately.

TABLE 6.3
VOLUME EXPANSION FOR 3 ATOM % BURNUP FROM EXISTING FISSION GAS BUBBLES

Fission Gas Description	Fuel Region	Approximate Ave. Region Steady State Temp (K)	Gas Density (Atoms/cm ³ Fuel)	% of Gas in Region	Volume Expansion (%)		
					3023 K	3824 K	4222 K
Intergranular (.5-5 μ m dia.)	Columnar	1920	1.8 x 10 ¹⁸	25.6	1.4	2.3	2.8
	Equiaxed	1520	3.01 x 10 ¹⁹	52.5	31.1	47.6	55.9
	Columnar	1920	4.5 x 10 ¹⁸	63.9	3.4	5.8	7.1
Intragranular (.065 μ m dia.)	Equiaxed	1520	1.01 x 10 ¹⁹	17.5	10.4	15.9	18.6
	Unstructured	870	3.75 x 10 ¹⁸	3.2	5.5	7.5	8.6

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TABLE 6.4
COMPARISON OF IDEAL GAS EOS AND HARRISON'S EOS FOR XENON

<u>T(K)</u>	<u>P(atm)</u>	<u>Harrison v (cm³/mole)</u>	<u>Ideal Gas v (cm³/mole)</u>
2028	306.6	597.3	542.7
2028	660.9	298.7	251.8
2028	1075.	199.1	154.8
1160	170.1	597.3	559.5
1160	357.8	298.7	266.0
1160	570.5	199.1	166.8
1160	818.7	149.3	116.3
1160	1116.	199.5	85.3

The surface tension of the fuel will affect the fuel swelling. Using a solid UO₂ surface tension of 750 ergs/cm²,^{9,3} one can calculate the internal pressure of the bubble using:

$$P_{\text{int}} - P_{\text{bulk}} = \frac{2\sigma}{r} \quad , \quad (6.2)$$

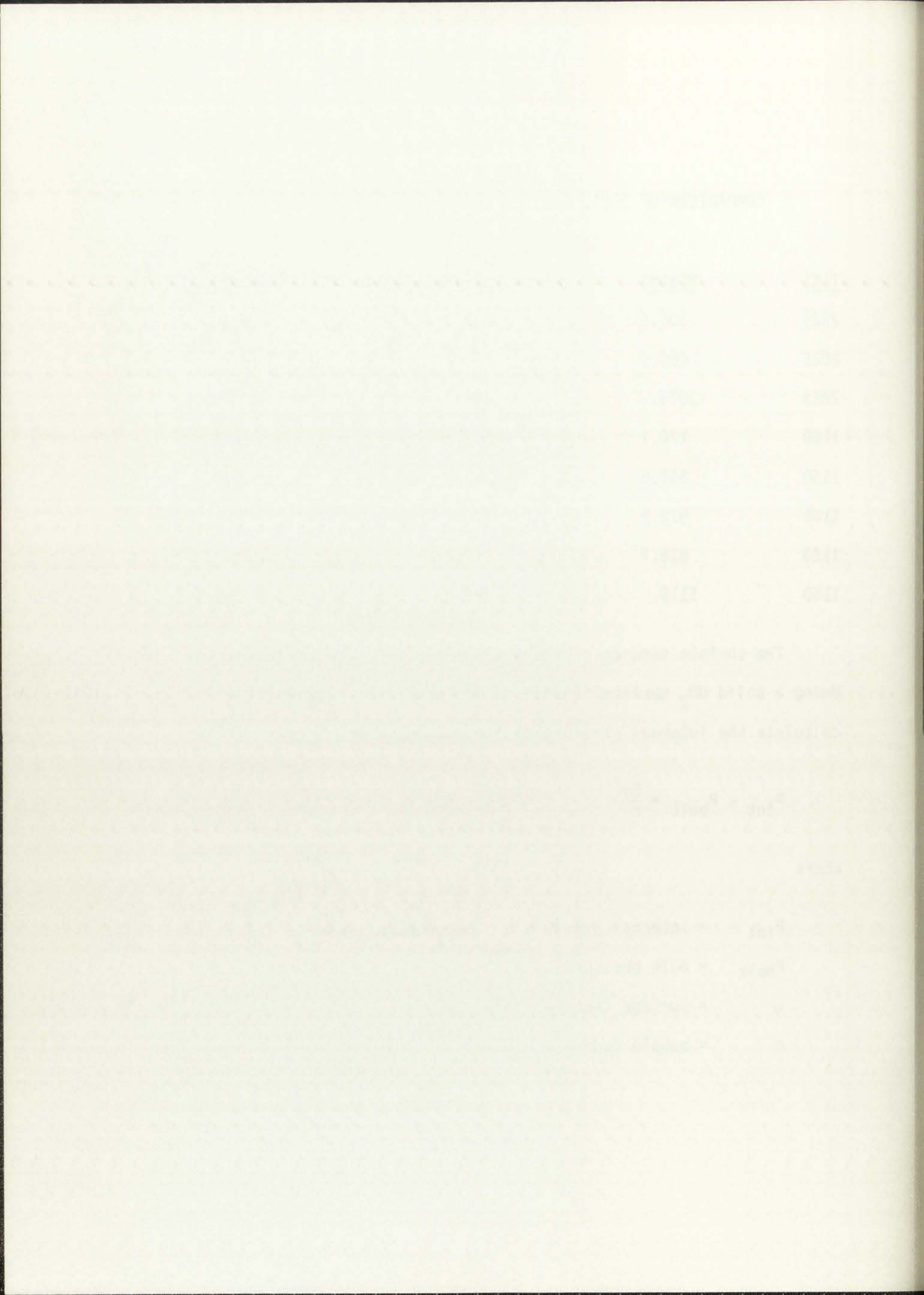
where

P_{int} = internal pressure of the bubbles,

P_{bulk} = bulk pressure,

σ = surface tension (≈ 750 ergs/cm²), and

r = bubble radius ($\approx 325 \text{ \AA}$).



One obtains $P_{int} = P_{bulk} + 455.5$ atms, for an intragranular bubble. In molten UO_2 , the surface tension has a value of only 450 ergs/cm².^{9,3} Thus upon the change of phase the surface tension pressure (thus the bubble internal pressure) will drop to 273 atm + P_{bulk} , leading to a 30%¹⁰ increase in the gas volume due to surface tension effects only. To demonstrate, however, the overall effect of surface tension, the intragranular, equiaxed volume expansion (10.4%) is recalculated using Eq. (1) with $P_1 = 475.5$ atm, $T_1 = 1520$ K, $P_2 = 293$ atm, and $T_2 = 3023$ K, obtaining a volume expansion of only 1%.

Experimentally a 3.6 volume % expansion⁶ was attributed to fission gas during an overpower transient in TREAT. The 25% PuO_2 mixed oxide fuel was irradiated at 9 kW/ft to a burnup of 8250 MWd/MTM (≈ 1 atom %) in EBR-II. The transient irradiation produced a peak pin power of 75 kW/ft with a pulse duration measured at half-peak of .97 s resulting in the inner 50 areal percent of the fuel being within 270 K of fuel melting temperature. Approximately 8% of the fission gas generated was released during steady state with an additional 16% released during the transient. The intragranular bubble size was 1000 Å compared to 650 Å found by Stahl.¹ Calculated maximum expected swelling in the unrestructured region was done by Stahl¹ yielding a volumetric swelling of 1%. GRASS calculations by Dias⁴ for a hypothetical FFTF fuel pin at 6 atom % burnup undergoing a $\$5/s$ ramp insertion of reactivity lead only to a .05% volume expansion if hydrostatic pressure (fuel constraint, cladding constraint, etc.) is

included. However, if hydrostatic pressure is ignored and the calculation done with a constant 10 atm bulk pressure, a swelling of 3.17% occurs at incipient fuel melting. Calculations done by Makenas and Poeppel reported by Dias⁴ for the same transient conditions gave an unrestrained (10 atm.) fission gas swelling of 34.8% and a restrained swelling of 3.4%.

Further parametric work by Dias⁴ indicates that for short transients, as investigated in this work, re-solution of fission gas, thermal gradients, and initial bubble-size distribution have little effect on the final swelling.

Gruber¹¹ also calculated intragranular fission gas swelling for 50, 500, and 5000 K/s fuel temperature rises using FRAS2 and obtained swelling of 6.8%, 10.6%, and 10.9% respectively. At the even higher rates, expected for \$15/s ramp insertion, the volume expansion is expected to be lower. The gas in solution precipitates into extremely small bubbles, thus with very high internal pressure due to surface tension effects, and does not contribute substantially to volume expansion. Also the fast transient does not allow time for bubble coalescence to occur.

Prediction of fission gas swelling is very difficult. Parameters such as burnup, irradiation power and temperature, initial porosity, etc., effect the quantity and form of gas retention. The transient preheat, time and power scale, hydrostatic forces (such as cladding and solid fuel), fuel temperature and thus surface tension, irradiation time, axial and radial restraints, etc., all effect gas release, bubble

The first part of the paper is devoted to a review of the literature on the subject of the effect of the concentration of the solution on the rate of the reaction.

It is shown that the rate of the reaction increases with the concentration of the solution.

The second part of the paper is devoted to a study of the effect of the temperature on the rate of the reaction.

It is shown that the rate of the reaction increases with the temperature.

The third part of the paper is devoted to a study of the effect of the pH of the solution on the rate of the reaction.

It is shown that the rate of the reaction increases with the pH of the solution.

The fourth part of the paper is devoted to a study of the effect of the ionic strength of the solution on the rate of the reaction.

It is shown that the rate of the reaction increases with the ionic strength of the solution.

The fifth part of the paper is devoted to a study of the effect of the dielectric constant of the solvent on the rate of the reaction.

It is shown that the rate of the reaction increases with the dielectric constant of the solvent.

The sixth part of the paper is devoted to a study of the effect of the viscosity of the solution on the rate of the reaction.

It is shown that the rate of the reaction increases with the viscosity of the solution.

The seventh part of the paper is devoted to a study of the effect of the surface area of the reactants on the rate of the reaction.

It is shown that the rate of the reaction increases with the surface area of the reactants.

The eighth part of the paper is devoted to a study of the effect of the nature of the reactants on the rate of the reaction.

It is shown that the rate of the reaction increases with the nature of the reactants.

The ninth part of the paper is devoted to a study of the effect of the nature of the products on the rate of the reaction.

It is shown that the rate of the reaction increases with the nature of the products.

The tenth part of the paper is devoted to a study of the effect of the nature of the catalyst on the rate of the reaction.

It is shown that the rate of the reaction increases with the nature of the catalyst.

The eleventh part of the paper is devoted to a study of the effect of the nature of the solvent on the rate of the reaction.

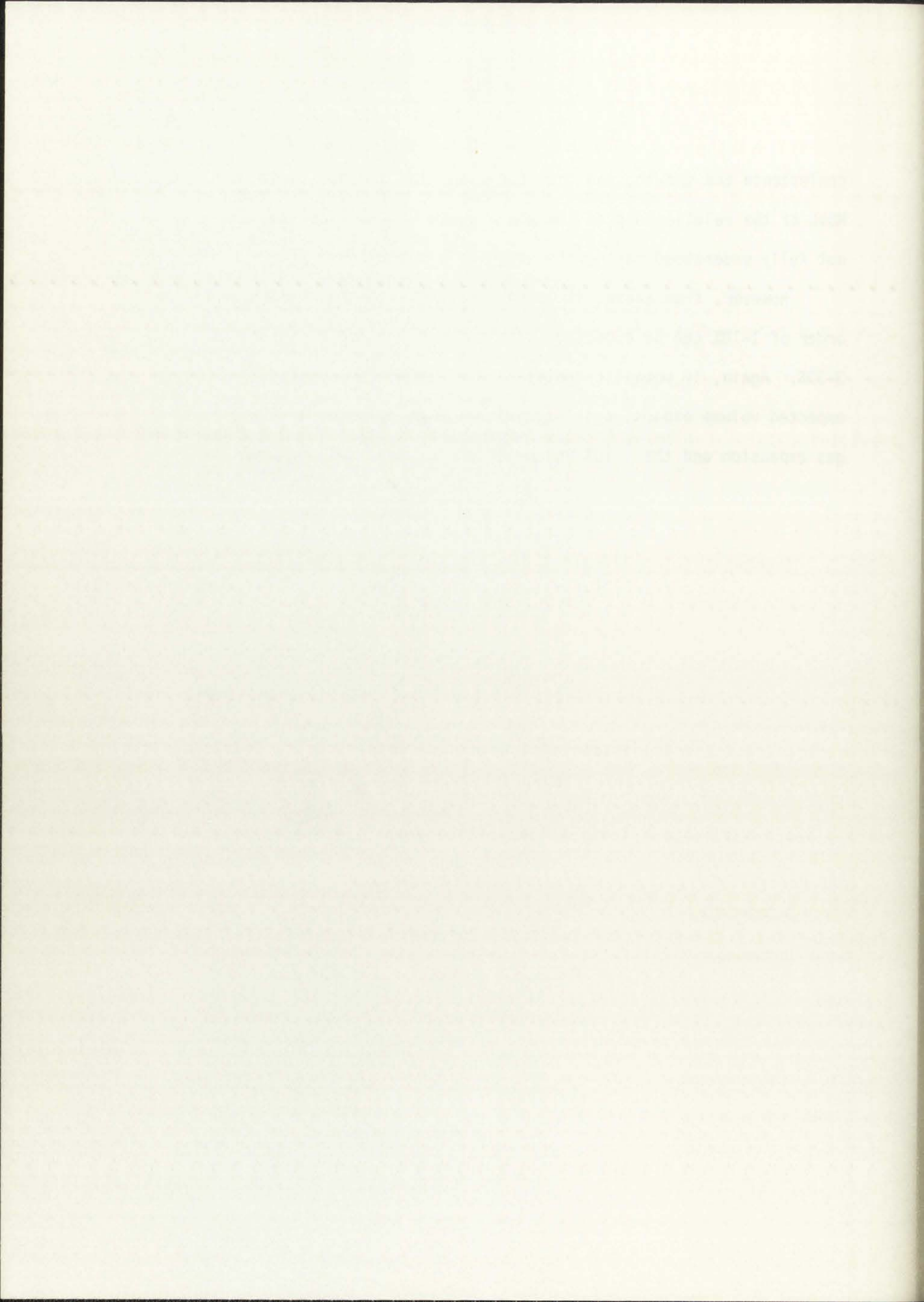
It is shown that the rate of the reaction increases with the nature of the solvent.

The twelfth part of the paper is devoted to a study of the effect of the nature of the reaction medium on the rate of the reaction.

It is shown that the rate of the reaction increases with the nature of the reaction medium.

coalescence and growth, and thus fuel swelling due to fission gas. Most of the relationship of the above parameters to fuel swelling are not fully understood making the swelling predictions difficult.

However, from above, it appears that fission gas expansion on the order of 1-10% can be expected, with an unrestrained expansion of 3-30%. Again, if metallic inclusion are assumed segregated, its expected volume expansion is significant when compared to the fission gas expansion and the $\sim 10\%$ volume expansion upon fuel melting.



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1. The first part of the report deals with the general situation of the country and the progress of the work done during the year. It is a summary of the work done by the various departments and is intended to give a general impression of the work done during the year.

2. The second part of the report deals with the work done by the various departments during the year. It is a detailed account of the work done by each department and is intended to give a detailed impression of the work done during the year.

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10. The tenth part of the report deals with the work done by the various departments during the year. It is a detailed account of the work done by each department and is intended to give a detailed impression of the work done during the year.

7. EXPERIMENTAL COMPARISON

In order to determine possible contributions to pre- and postclad failure fuel motion from metallic fission products and/or fission gases, a number of experiments on fuel motion were investigated. Both transient overpower and undercooling tests have been performed using fresh and preirradiated fuel. From such experiments only qualitative results could be drawn due to the difficulty of transient instrumentation and the resolution of hodoscope and other current techniques.

7.1 E and H Series

In the Argonne National Laboratory (ANL) E and H transient overpower test series,¹⁻³ both fresh and preirradiated fuel rods were subject to 50¢-\$1/s and \$3-\$5/s reactivity ramp insertions respectively. The H-series was largely intended to determine the failure threshold for FTR-type fuel pins with energy input not much in excess of the failure energy for 50¢-\$1/s ramp reactivity transients. The E-series was intended to examine not only the failure threshold, but events subsequent to failure, including fuel motion. Tests H4, E6, and E7 used high-power-preirradiated (10-11.6 kW/ft) pins with a burnup of ≈ 4.5 atom %. Tests H3 and H5 used intermediate-power-irradiated fuel with a burnup of ≈ 3.4 atom %. Table 7.1 summarizes fuel rod descriptions for the various tests.

The first step in the synthesis of the polymer was the preparation of the monomer.

The monomer was prepared by the reaction of the starting materials in the presence of a catalyst.

The reaction was carried out in a round-bottomed flask equipped with a magnetic stirrer.

The reaction mixture was stirred at room temperature for a period of 24 hours.

The resulting polymer was then purified by reprecipitation from a solution in a non-solvent.

The purified polymer was dried under vacuum at room temperature for 48 hours.

The final product was a white, crystalline solid.

3.1.1. Synthesis of the monomer

In the first step, the starting materials were weighed and placed in a round-bottomed flask.

The flask was equipped with a magnetic stirrer and a reflux condenser.

The reaction mixture was stirred at room temperature for a period of 24 hours.

The resulting polymer was then purified by reprecipitation from a solution in a non-solvent.

The purified polymer was dried under vacuum at room temperature for 48 hours.

The final product was a white, crystalline solid.

The yield of the monomer was approximately 85%.

The monomer was then used in the synthesis of the polymer.

The polymer was prepared by the reaction of the monomer in the presence of a catalyst.

The reaction was carried out in a round-bottomed flask equipped with a magnetic stirrer.

The reaction mixture was stirred at room temperature for a period of 24 hours.

TABLE 7.1
SUMMARY OF TRANSIENT TESTS

<u>Test</u>	<u>Fuel Description</u>	<u>Fuel Motion Restraints (Axial)</u>	<u>Transient Description</u>	<u>Results</u>
E1	Fresh UO ₂	None	Transient overpower; no preheat TREAT high heating rate, burst max. 1800 (MW) total energy 500 (MW-s), rise period .064 (s).	Prefailure fuel motion.
H2	Fresh (U.75, Pu.25) O ₂	½" insulator pellet.	Transient overpower; no preheat, TREAT low heating rate, burst max. 1518 (MW), total energy 490 (MW-s), rise period .080 (s).	Prefailure fuel motion.
E4	Fresh (U.75, Pu.25) O ₂	½" insulator pellet.	Transient overpower; no preheat, TREAT high heating rate, burst max. 2584 (MW), total energy 700 (MW-s), rise period .066 (s).	Possible prefailure fuel motion.
E2	Fresh UO ₂	½" depleted UO ₂ 2" stainless steel	Transient overpower; no preheat, TREAT high heating rate, burst max. 2865 (MW), total energy 750 (MW-s), rise period .050 (s).	Compressed spring .3 in. before failure, no other significant prefailure axial motion.
H3	(U.75 Pu.25) O ₂ Irradiated in EBR-II (fast), 3.4 atom % burnup at intermediate power.	½" insulator pellet	Transient overpower; preheat 160 (MW) for 3 (s), TREAT (50¢-\$1/s ramp) burst max. 425 (MW), total energy 810 (MW-s), rise period .9 (s).	No clad failure. No transient fuel or clad swelling. No fuel melting.

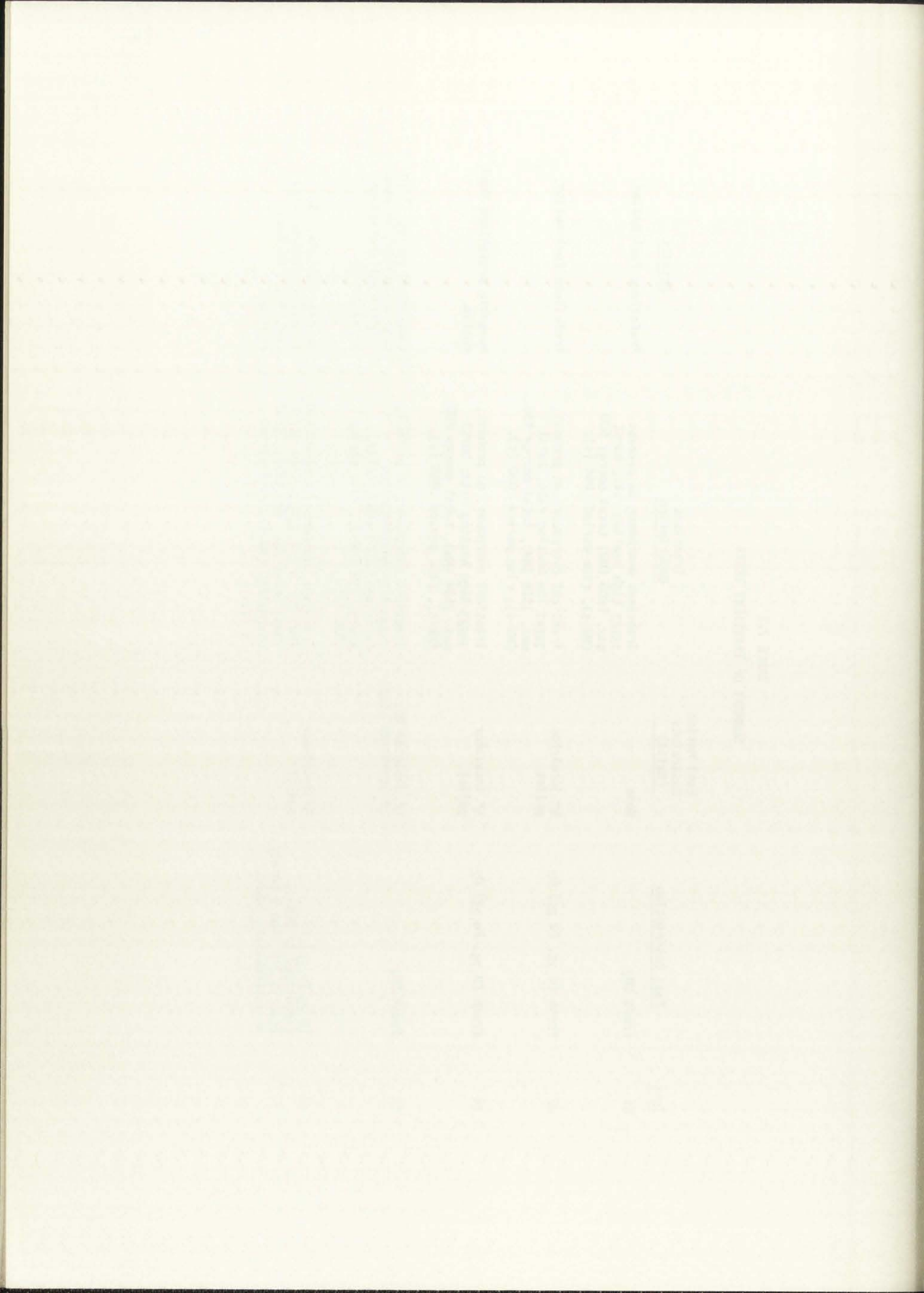


TABLE 7.1 (cont)

<u>Test</u>	<u>Fuel Description</u>	<u>Fuel Motion Restraints (Axial)</u>	<u>Transient Description</u>	<u>Results</u>
H4	(U.75, Pu.25) O ₂ irradiated in EBR-II 4.5 atom % burnup at high power	7" insulator pellets 5" inconel reflector.	Transient overpower; preheat 235 (MW) for 2.5 (s), TREAT (50¢/s ramp), burst max. 650 (MW), total energy 1250 (MW-s), rise period .96 (s).	No prefailure fuel motion.
H5	(U.75, Pu.25) O ₂ irradiated in EBR-II 3.4 atom % burnup at intermediate power.	½" insulator pellet	Transient overpower; preheat 115 (MW) for 3 (s), TREAT (50¢/s ramp), burst max. 650 (MW), total energy 1090 (MW-s), rise period 1.1 (s).	No prefailure fuel motion.
E6	(U.75, Pu.25) O ₂ irradiated in EBR-II 4.5 atom % burnup at high power.	7" insulator pellets 5" inconel reflector.	Transient overpower; preheat 167 (MW) for 3 (s), TREAT (3¢/s ramp), burst max. 2250 (MW), total energy 1211 (MW-s), rise period .188 (s).	No prefailure fuel motion (preliminary, neutron radiography only).
E7	(U.75, Pu.25) O ₂ irradiated in EBR-II 4.5 atom % burnup at high power.	7" insulator pellets 5" inconel reflector.	Transient overpower; preheat 142 (MW) for 2.4 (s), TREAT (3¢/s ramp), burst max. 2468 (MW), total energy 1450 (MW-s), rise period .180 (s).	No prefailure fuel motion.
E3	UO ₂ irradiated in MTR (thermal) 4.82-6.33 atom % burnup.	No axial restraint.	Transient overpower; no preheat, TREAT (3¢-5¢/s ramp), burst max. 6500 (MW), total energy 1250 (MW-s), rise period (.035 s).	Pin failure prior to fuel melting.
F1	(U.75, Pu.25) O ₂ irradiated in EBR-II at 12 kW/ft to 2.55 atom % burnup.	6.7" depleted UO ₂ insulator pellets 5" inconel reflector. No coolant channel restraint.	Loss-of-flow treat at pin design power level. Axial peak flat topped at 11-12 kW/ft. duration 11 s.	Clad melting and drainage, fuel swelling and axial fuel drainage through central region.

General Abstracts

1. The first part of the book is devoted to a general survey of the history of the subject.

2. The second part of the book is devoted to a detailed study of the various methods of the subject.

3. The third part of the book is devoted to a study of the various applications of the subject.

4. The fourth part of the book is devoted to a study of the various theoretical aspects of the subject.

5. The fifth part of the book is devoted to a study of the various practical aspects of the subject.

6. The sixth part of the book is devoted to a study of the various historical aspects of the subject.

7. The seventh part of the book is devoted to a study of the various philosophical aspects of the subject.

8. The eighth part of the book is devoted to a study of the various social aspects of the subject.

9. The ninth part of the book is devoted to a study of the various political aspects of the subject.

Part I

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7. The seventh part of the book is devoted to a study of the various philosophical aspects of the subject.

8. The eighth part of the book is devoted to a study of the various social aspects of the subject.

9. The ninth part of the book is devoted to a study of the various political aspects of the subject.

Part II

1. The first part of the book is devoted to a general survey of the history of the subject.

2. The second part of the book is devoted to a detailed study of the various methods of the subject.

3. The third part of the book is devoted to a study of the various applications of the subject.

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TABLE 7.1 (cont)

<u>Test</u>	<u>Fuel Description</u>	<u>Fuel Motion Restraints (Axial)</u>	<u>Transient Description</u>	<u>Results</u>
F2	(U.75, Pu.25) O ₂ irradiated in EBR-II at 11.6 kW/ft to .35 atom % burnup.	5.4" natural UO ₂ insulator pellets. No coolant channel restraint.	Loss-of-flow; TREAT at design level to 10 times design level. Axial peak linear power generation of 12.5 kW/ft for 6.5 s, followed by power burst of 135 kW/ft (11 x) over 1 s.	Early clad melting and drainage. Fuel dispersal during burst portion of transient believed driven by fuel vaporization.
EOS-1	(U.75, Pu.25) O ₂ Fresh	.5" Boron nitride insulator pellets. No coolant channel Axial constraint.	No preheat Burst max. power 1302 kw/ft, duration .25 s (100 x nominal design).	Fuel dispersal Believed stainless steel driven.
EOS-2	(U.75, Pu.25) O ₂ irradiated in EBR-II at 11.3 kW/ft to .85 atom %	Same as EOS-1.	No preheat. Burst max. 1236 kW/ft, duration .25 s (100 x nominal design).	Fuel Dispersal. Earlier in transient than EOS-1. Believe fission gas effect.
EOS-3	(U.75, Pu.25) O ₂ irradiated in EBR-II at 8.12 kW/ft to .81 atom % burnup.	Same as EOS-1.	No preheat. Burst max. 978 kW/ft, duration .3 s.	Fuel dispersal. Slightly earlier in transient than EOS-2. Believe fission gas effect.
C5A	UO ₂ irradiated in General Electric test reactor (thermal) at low power (12 kW/ft peak) to 2 atom % burnup.	14.25" natural uranium blanket (solid).	Preheat fuel to 500 K, TREAT transient initial period .131 s, reactivity insertion 1.37%, duration 1 s, peak power 160 kW/ft intergrated power 338 MW/s.	Clad failure post axial fuel motion in coolant channel.

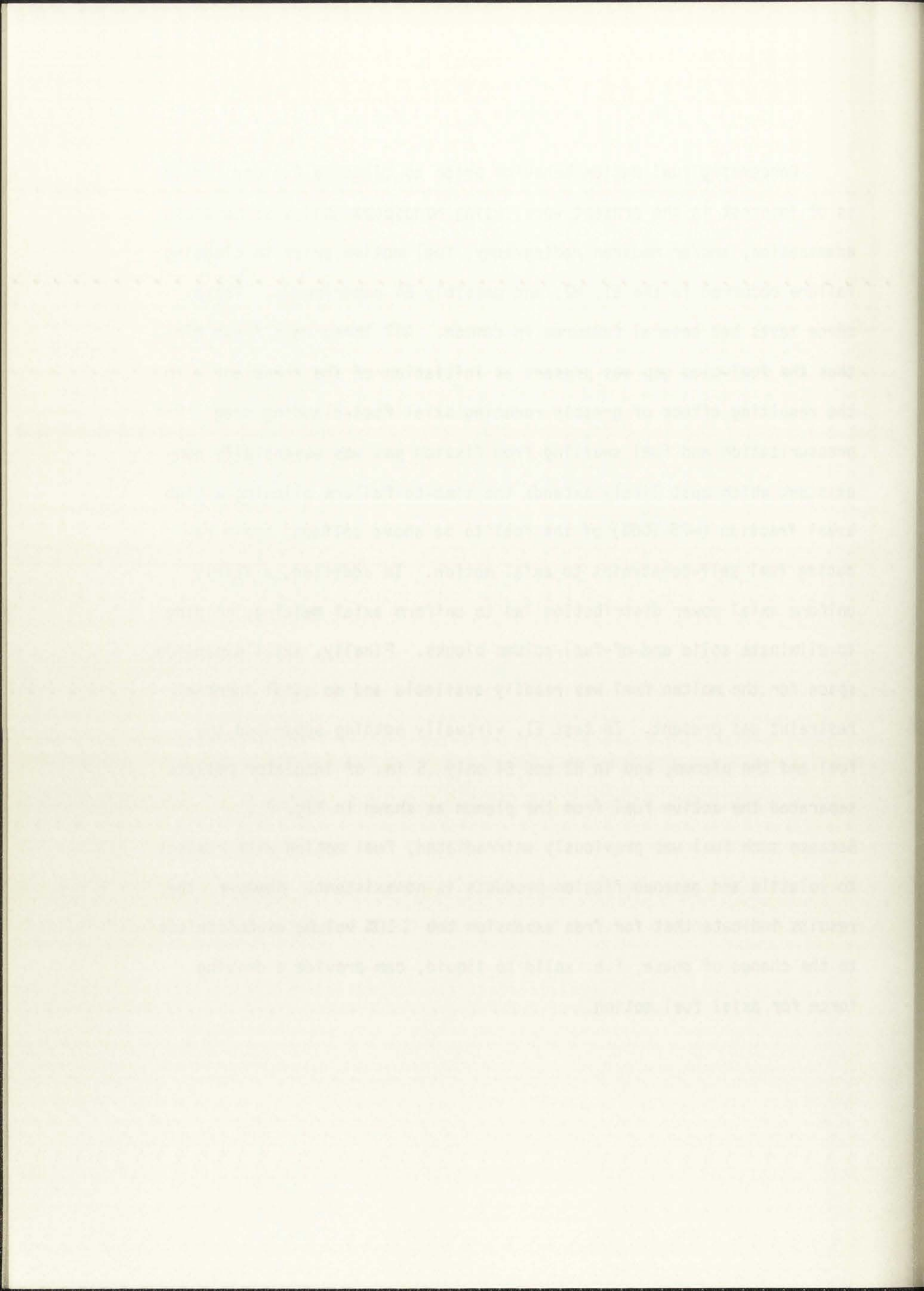
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TABLE 7.1 (cont)

<u>Test</u>	<u>Fuel Description</u>	<u>Fuel Motion Restraints (Axial)</u>	<u>Transient Description</u>	<u>Results</u>
C5B	UO ₂ irradiation same as C5A.	14.25" natural uranium annular blanket (.07" i.d.).	preheat fuel to 500 K, TREAT transient initial period .136 s, reactivity insertion 1.35% duration 1 s, peak power 155 kw/ft integrated power 339 MW/s.	no clad failure axial expulsion of fuel (10") into annular blanket pellets.
L5	(U.75, Pu 25) O ₂ in General Electric test reactor (thermal) at 12.2 kw/ft to 8 atom % burnup.	.5" UO ₂ insulator pellets, 3" inconel reflector, no coolant channel restraint.	TREAT transient 1) 9 s at nominal power (11 kw/ft) 2) followed by burst peak power 66 kw/ft (6x) rise period 835 ms.	Sodium voiding, clad failure, mild fuel dispersal at or after scram.



Concerning fuel motion behavior prior to cladding failure, which is of interest in the present work, using hodoscope analysis, posttest examination, and/or neutron radiography, fuel motion prior to cladding failure occurred in the E1, H2, and possibly E4 experiments. These three tests had several features in common. All three were fresh pins, thus the fuel-clad gap was present at initiation of the transient with the resulting effect of greatly reducing axial fuel-cladding drag. Pin pressurization and fuel swelling from fission gas was essentially nonexistent which most likely extends the time-to-failure allowing a high areal fraction ($\approx 75-100\%$) of the fuel to be above solidus, again reducing fuel self-constraint to axial motion. In addition, a fairly uniform axial power distribution led to uniform axial melting, helping to eliminate solid end-of-fuel-column blocks. Finally, axial expansion space for the molten fuel was readily available and no axial inertial restraint was present. In test E1, virtually nothing separated the fuel and the plenum, and in H2 and E4 only .5 in. of insulator pellets separated the active fuel from the plenum as shown in Fig. 7.1. Because such fuel was previously unirradiated, fuel motion with respect to volatile and gaseous fission products is nonexistent. However, the results indicate that for free expansion the $\approx 10\%$ volume expansion due to the change of phase, i.e. solid to liquid, can provide a driving force for axial fuel motion.



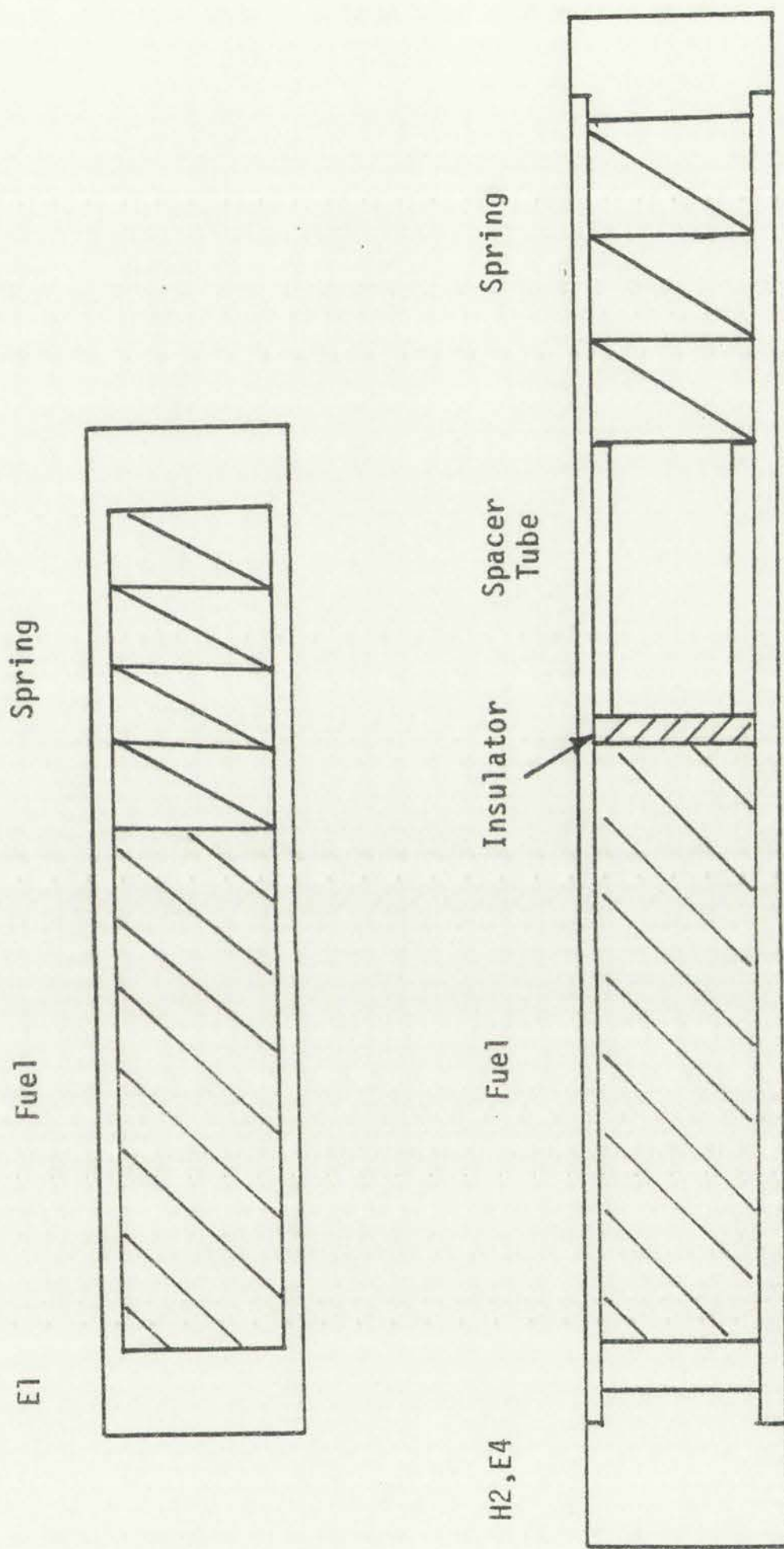


Figure 7.1.
Schematic of E1, H2, and E4 fuel rods.

RESPECTIVE OF THE WALL AND THE WALL JOINT



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In the remaining tests (pre-irradiated fuel), H3, H4, H5, E3, E6, E7, and E8, hodoscope analysis, posttest examination, and/or neutron radiography suggest that prefailure axial fuel motion did not occur. However in some cases the results were inconclusive. Again as seen in the summary Table 7.1, this includes intermediate and high power irradiated fuel subjected to transients both in the 50¢-\$1/s and \$3-\$5/s ramp ranges. The power distribution was more cosine-shaped leading to less melting at the end of the pins, with the consequence of additional mechanical constraint at the fuel column extremities. In addition pre-irradiation leads to fuel swelling and fuel-cladding gap closure, thus increasing the potential for drag effects. Three out of the four test in this preirradiated group that experienced fuel melting and clad failure had thick insulator pellets and reflectors with hold down springs providing additional inertial and mechanical restraints to axial fuel motion. The melt fraction upon cladding failure was $\approx 20\%$ for H4 and $\approx 25\%$ for H5, corresponding to the situation where the melt front reaches the area of large fission gas retention as can be seen in Fig. 6.1. Gas release could contribute to pin pressurization and cladding failure or could coincide with the cladding stress due to differential thermal expansion of the fuel and cladding. Since more prototypic (inertial and axial constraints) fresh fuel pins, run with the preirradiated fuel pin tests, did not exhibit prefailure fuel motion,

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it thus appears for the E- and H-series tests, that prefailure fuel motion only occurs for unrestrained fuel. Fission gas and other volatile fission products appear not to be able to overcome the axial mechanical constraints for fuel motion prior to clad failure as seen in Fig. 7.2. They may however, contribute to radial swelling, clad failure, and possible postfailure fuel movement. The spring compression force, F_s , is probably minimal. After only hours in the irradiation environment, the spring anneals and loses much of its compressive force. However, due to fuel restructuring and swelling and fuel-cladding gap closure, the frictional forces, F_f and F_g , become significant. Unfortunately, the magnitude of this force is not known, but it will depend on initial fuel conditions the steady state irradiation, and the transient conditions. Due to differential thermal expansion between the fuel and cladding during a TOP accident this force will become very large and as mentioned above the resulting cladding stress could lead to cladding failure.

7.2 F-Series

The TREAT F-series tests were simulated loss-of-flow (LOF) or transient undercooling accidents to provide data for possible LMFBR fuel motion. The LOF test condition is achieved by surrounding a single fuel element with an annular nuclear heated wall in a dry (no sodium) test capsule (Mark-II loop as seen in Fig. 7.3). The F1

1. The object of the test is to determine the effect of the test on the test results.

2. The test is conducted in a controlled environment.

3. The test results are compared with the results of the control test.

4. The test results are compared with the results of the control test.

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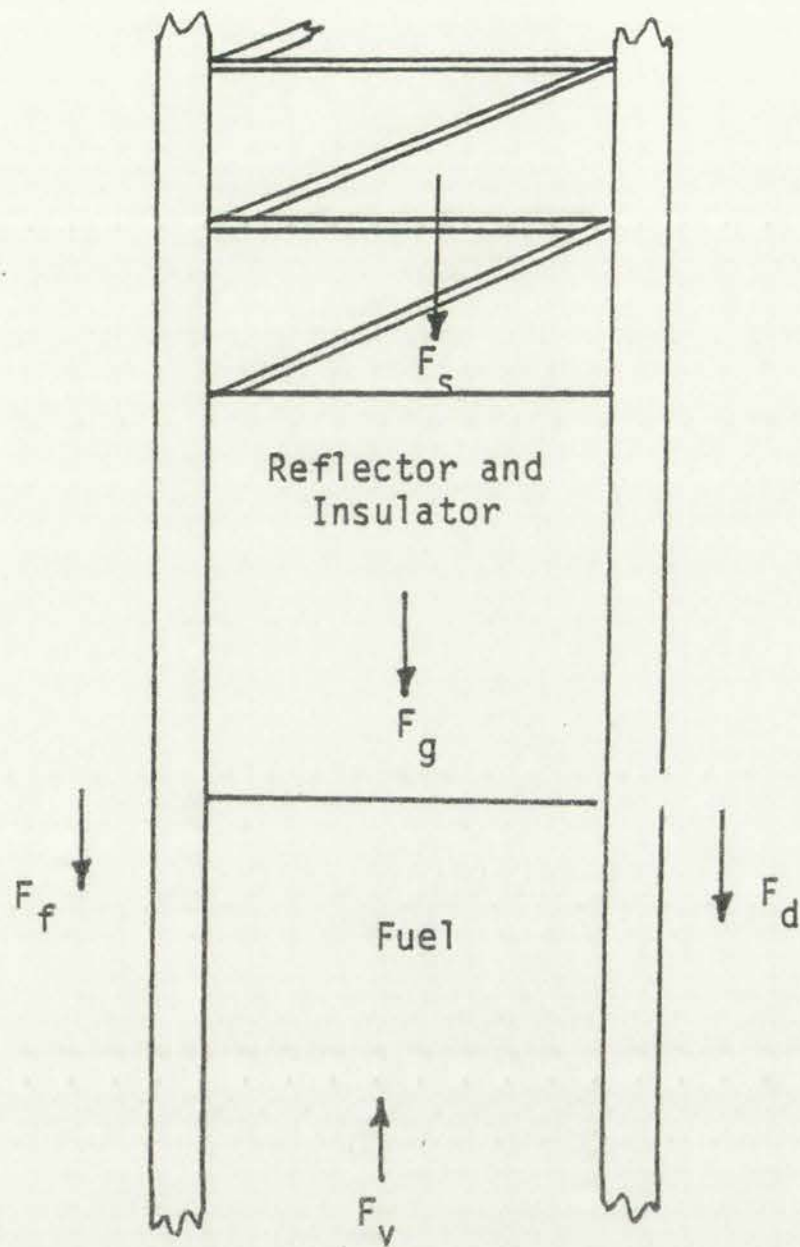
26. The test results are compared with the results of the control test.

27. The test results are compared with the results of the control test.

28. The test results are compared with the results of the control test.

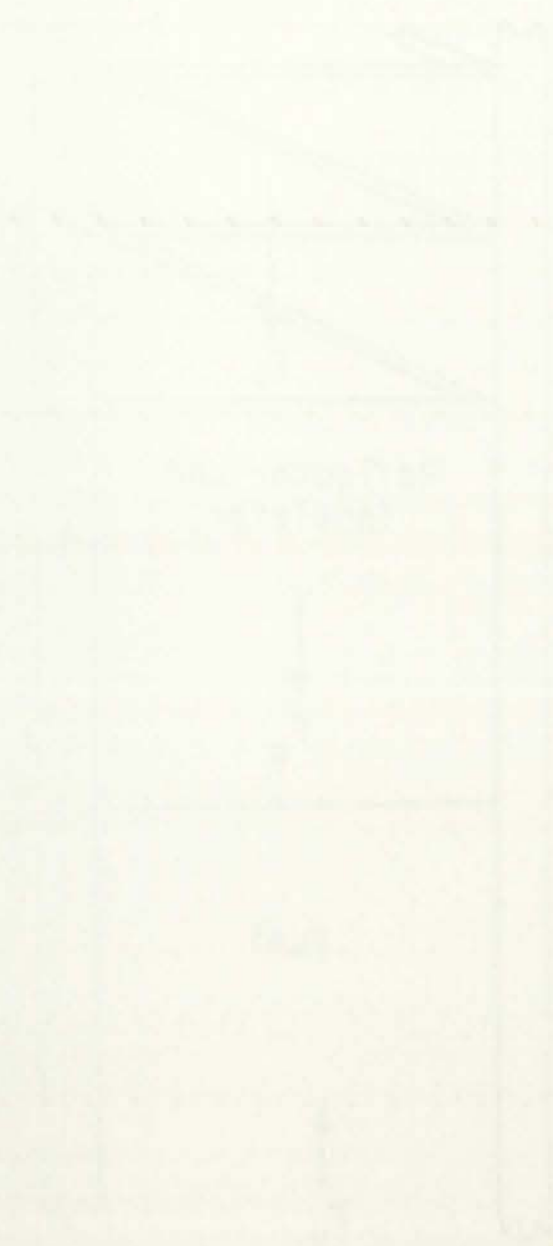
29. The test results are compared with the results of the control test.

30. The test results are compared with the results of the control test.



- F_s = force due to spring compression,
 F_g = gravitational force due to mass of reflector and insulator,
 F_d = drag force (=0 for zero velocity)
 F_f = static friction force due to fuel swelling and closure of fuel-cladding gap,
 F_v = force due to fission gas, volatiles, and fuel = $P_v A$,
 A = cross-sectional area, and
 P_v = total vapor pressure of fission gas, volatiles, and fuel.

Figure 7.2.
Forces affecting fuel motion prior to cladding failure.



The force due to gravity is $F_g = mg$
 The normal force is $F_n = F_g \cos \theta$
 The friction force is $F_f = \mu F_n$
 The net force is $F_{net} = F_g \sin \theta - F_f$
 The acceleration is $a = \frac{F_{net}}{m}$
 The final velocity is $v = at$
 The distance traveled is $d = \frac{1}{2}at^2$

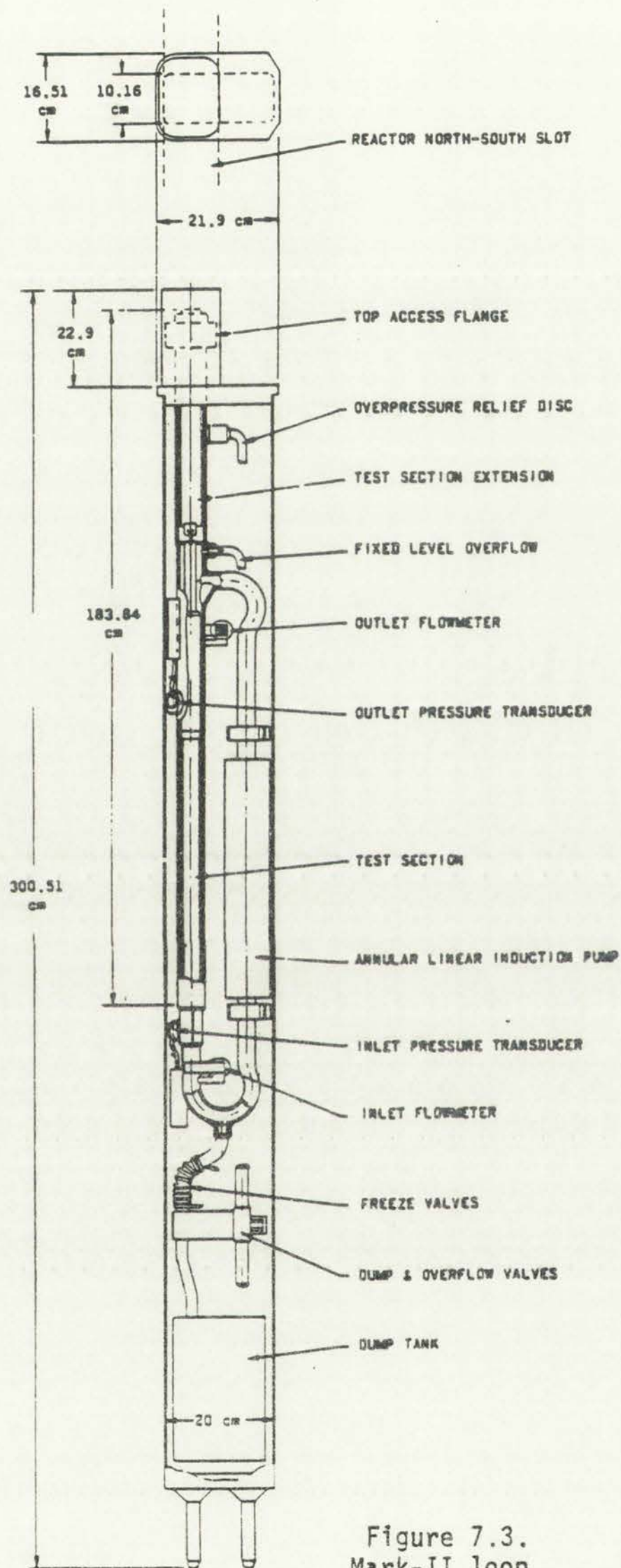


Figure 7.3.
Mark-II loop.



test^{4,5} was performed to investigate the effect of fission gas on fuel motion at design power levels following clad melt and drainage. The F1 test fuel contained (U_{.75}, Pu_{.25}) O₂ irradiated at 12 kW/ft to 2.55 atom % burnup and was fully restructured. Axial motion of the entire fuel pin was constrained by a tungsten pin through the lower fuel pin and plug, and a fuel pin retainer on the top end plug which restricted downward but allowed upward movement of the top end plug. Internal to the cladding, 6.7 in. of insulator pellets and 5 in. of Inconel reflector was above the active fuel column as seen in Fig. 7.3. However, these axial constraints were not important as far as axial fuel motion was concerned since cladding melting and drainage occurred prior to fuel melting.

The TREAT transient, at the test pin axial peak power, was approximately flat-topped at 11 to 12 kW/ft (design power levels) and lasted \approx 11 s. The TREAT reactor can be seen in Fig. 7.4. Hodoscope, neutron radiography, and posttest examination showed that only downward fuel motion was experienced, with no upward fuel motion detected at any time. Fission gas and volatiles did cause axial and radial fuel swelling to occur, as evidenced by posttest photomicrographs,⁴ however, bubble release to the central void region allowed fuel drainage to occur versus a "foaming" axial driving situation. It was concluded that retained fission gas and volatiles did not prevent an axial

The first part of the paper is devoted to a review of the literature on the topic.

The second part of the paper is devoted to a description of the experimental design.

The third part of the paper is devoted to a description of the results of the experiment.

The fourth part of the paper is devoted to a discussion of the results of the experiment.

The fifth part of the paper is devoted to a conclusion.

The sixth part of the paper is devoted to a list of references.

The seventh part of the paper is devoted to an appendix.

The eighth part of the paper is devoted to a list of figures.

The ninth part of the paper is devoted to a list of tables.

The tenth part of the paper is devoted to a list of equations.

The eleventh part of the paper is devoted to a list of symbols.

The twelfth part of the paper is devoted to a list of abbreviations.

The thirteenth part of the paper is devoted to a list of acronyms.

The fourteenth part of the paper is devoted to a list of definitions.

The fifteenth part of the paper is devoted to a list of terms.

The sixteenth part of the paper is devoted to a list of phrases.

The seventeenth part of the paper is devoted to a list of sentences.

The eighteenth part of the paper is devoted to a list of paragraphs.

The nineteenth part of the paper is devoted to a list of sections.

The twentieth part of the paper is devoted to a list of chapters.

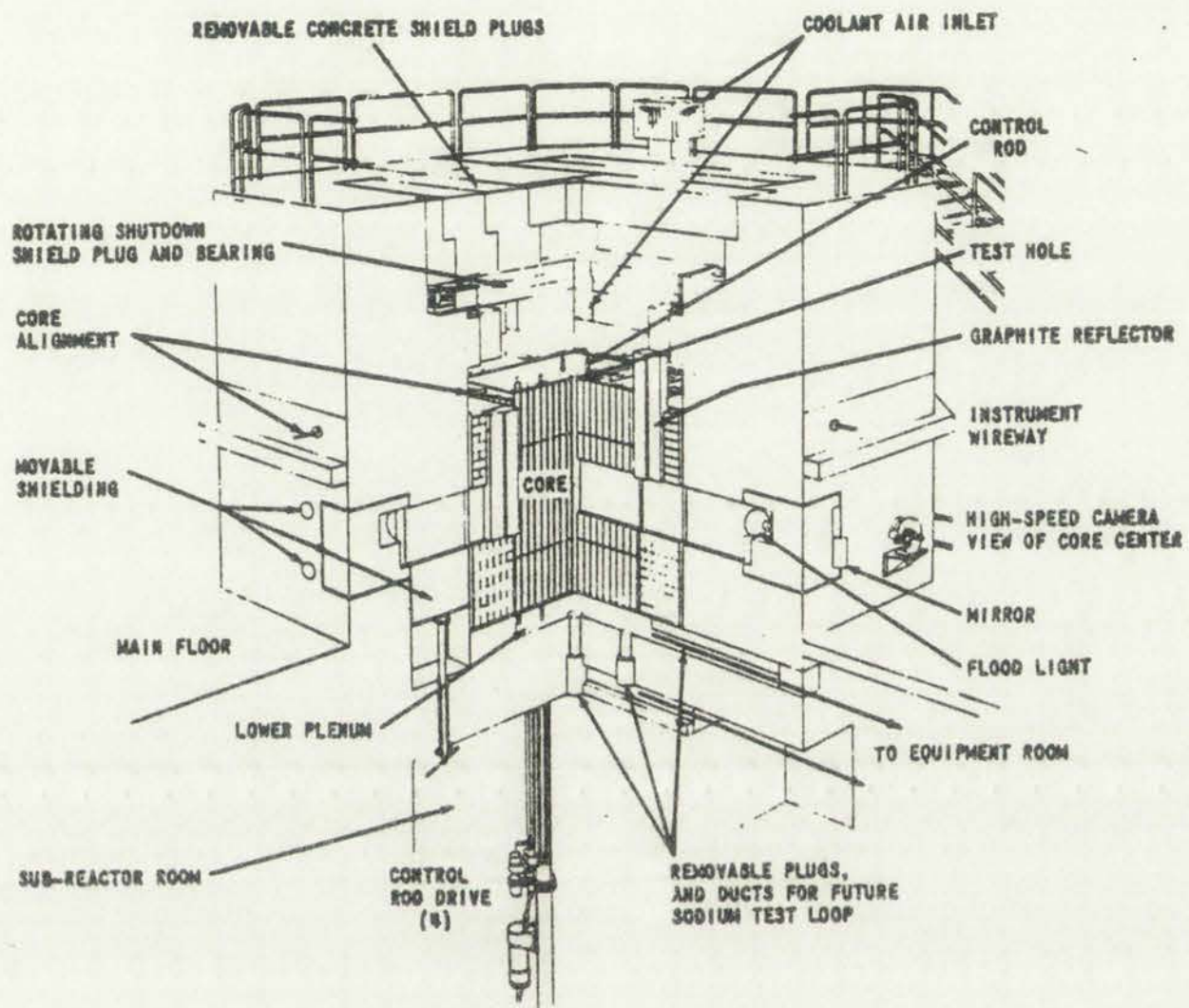


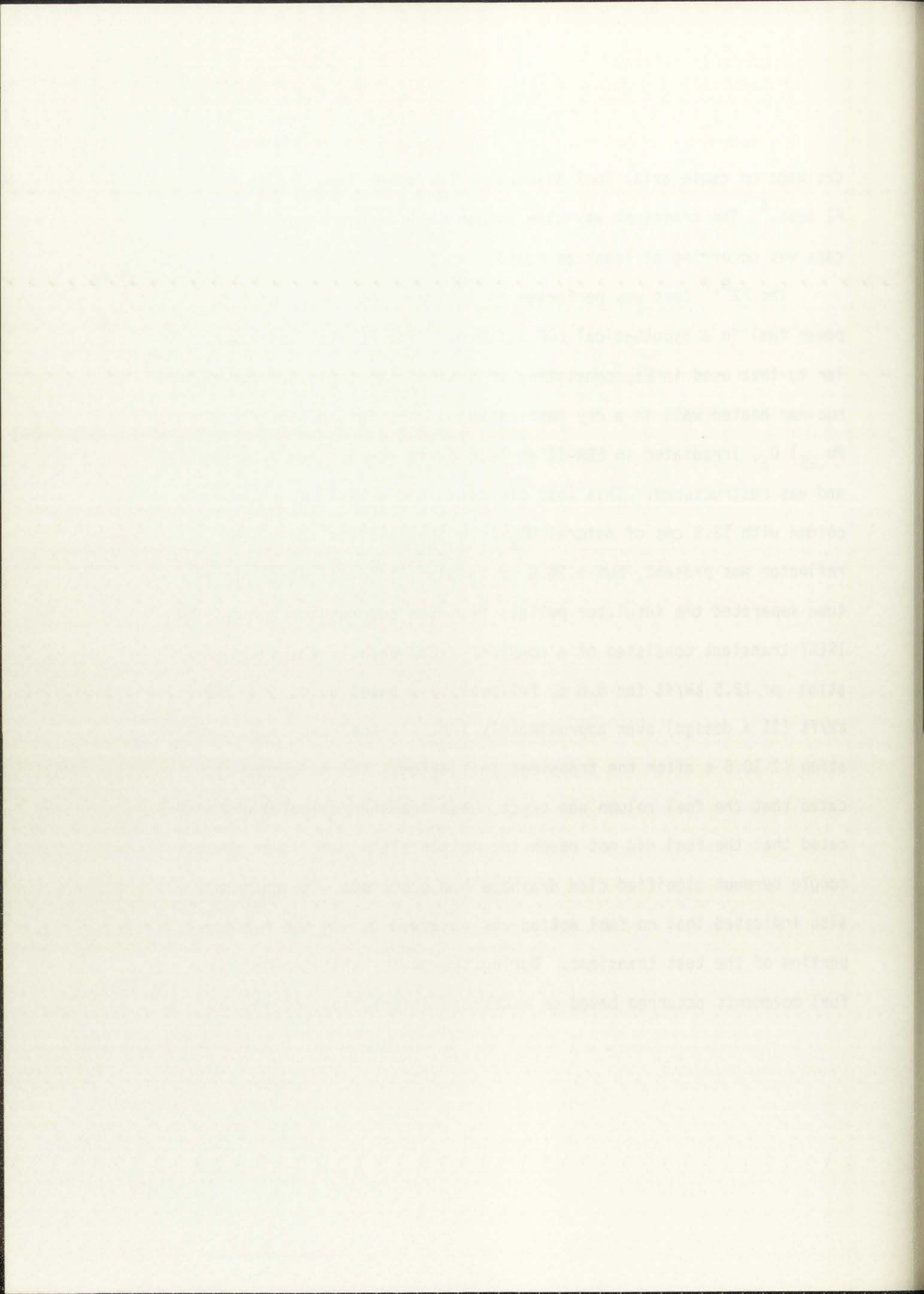
Figure 7.4.
TREAT reactor.



FIG. 1. TURBINE SECTION
FIG. 2. COMBUSTOR SECTION
FIG. 3. REDUCER SECTION
FIG. 4. SHAFT SECTION

drainage or cause axial fuel dispersion for power-time scales as in the F1 test.⁴ The transient was slow enough that fission gas bubble escape was occurring at least as rapidly as bubble growth.

The F2^{6,7} test was performed to evaluate the motion of high power fuel in a hypothetical LOF accident. The F2 test train was similar to that used in F1, consisting of a single test pin surrounded by a nuclear heated wall in a dry test capsule. The fuel pin was (U_{.75} Pu_{.25}) O₂, irradiated in EBR-II at 11.6 kW/ft to .35 atom % burnup and was restructured. This test pin contained a 34.4 cm active fuel column with 13.8 cms of natural UO₂ insulator pellets above. No reflector was present, but a 26.8 cm annular stainless steel spacer tube separated the insulator pellets from the compression spring. The TREAT transient consisted of a constant axial peak linear power generation of 12.5 kW/ft for 6.5 s, followed by a power burst of \approx 135 kW/ft (11 x design) over approximately 1 s. At the power burst initiation (\approx 10.5 s after the transient initiation), the hodoscope indicated that the fuel column was erect, heat transfer calculations indicated that the fuel did not reach the molten state, and lower thermocouple burnout signified clad drainage had occurred. The hodoscope also indicated that no fuel motion was observed during the flattop portion of the test transient. During the power burst two major upward fuel movements occurred based on hodoscope information, moving fuel to



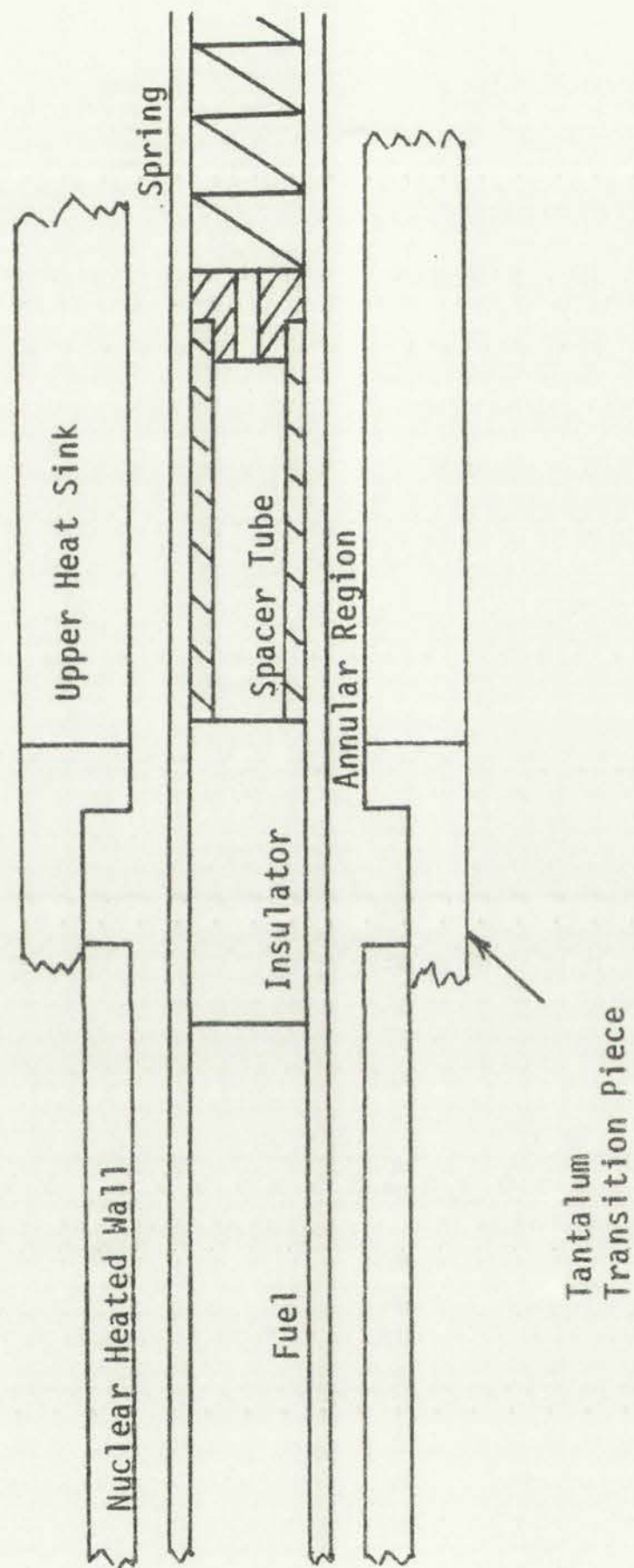


Figure 7.5.
Test F2 annular region.



a maximum of 19 cms above the active fuel column into the annular region formed by the upper insulator and spacer portion of the fuel pin and the upper heat sink as shown in Fig. 7.5. The first upward dispersal occurred at 11.04 s into the transient and consisted of the top ≈ 10 cm portion of the fuel pin. The hodoscope indicated the second dispersion occurred at 11.18 s into the transient and was located at the center of the active fuel column, moving an additional 5-8 cms of fuel upward. About 17 grams of fuel froze in the cool annular region, but the remaining fuel drained back into the lower half of the fuel pin. At fuel ejection, all the fuel was calculated to be at or above the solidus temperature.

To determine the driving species for this upward fuel dispersal, the maximum fuel temperature and the pressure required to overcome the head pressure and frictional loss were calculated.⁶ A pressure of 1.5 atm. (22 psi) at a maximum temperature of 3273 K was obtained. As demonstrated in Table 7.2 under these temperature conditions, fission gas, cladding, volatile fission products, and fuel species could be responsible for the dispersion. The inclusion of the fuel species assumes the maximum temperature is not well defined but may be off by as much as 300 K. Also from Table 7.2, it can be seen that the homogeneous inclusion composition of O'Boyle⁸ and Johnson⁹ could not have driven the dispersal. Their individual volatile constituents (segregated compositionally) as well as Jeffery's¹⁰ homogeneous inclusion

TABLE 7.2
 DETERMINATION OF POSSIBLE F2 FUEL DISPERSAL DRIVING SPECIES

<u>Species Description</u>	<u>Temperature (K)</u>	<u>Pressure (atm)</u>
<u>A. Inclusions</u>		
Johnson inclusion composition (Homogenous)	3273	.26
O'Boyle inclusion composition (Homogenous)	3273	.45
Jeffery inclusion composition (Homogeneous)	3273	180
<u>B. Segregated Inclusion Volatiles</u>		
Sb	3273	13
Ba	3273	97
Te	3273	512
Pd	3273	3
<u>C. Cladding</u>		
Fe	3273	1.8
<u>D. Gases</u>		
Noble gases (Xe, Kr)	3273	100

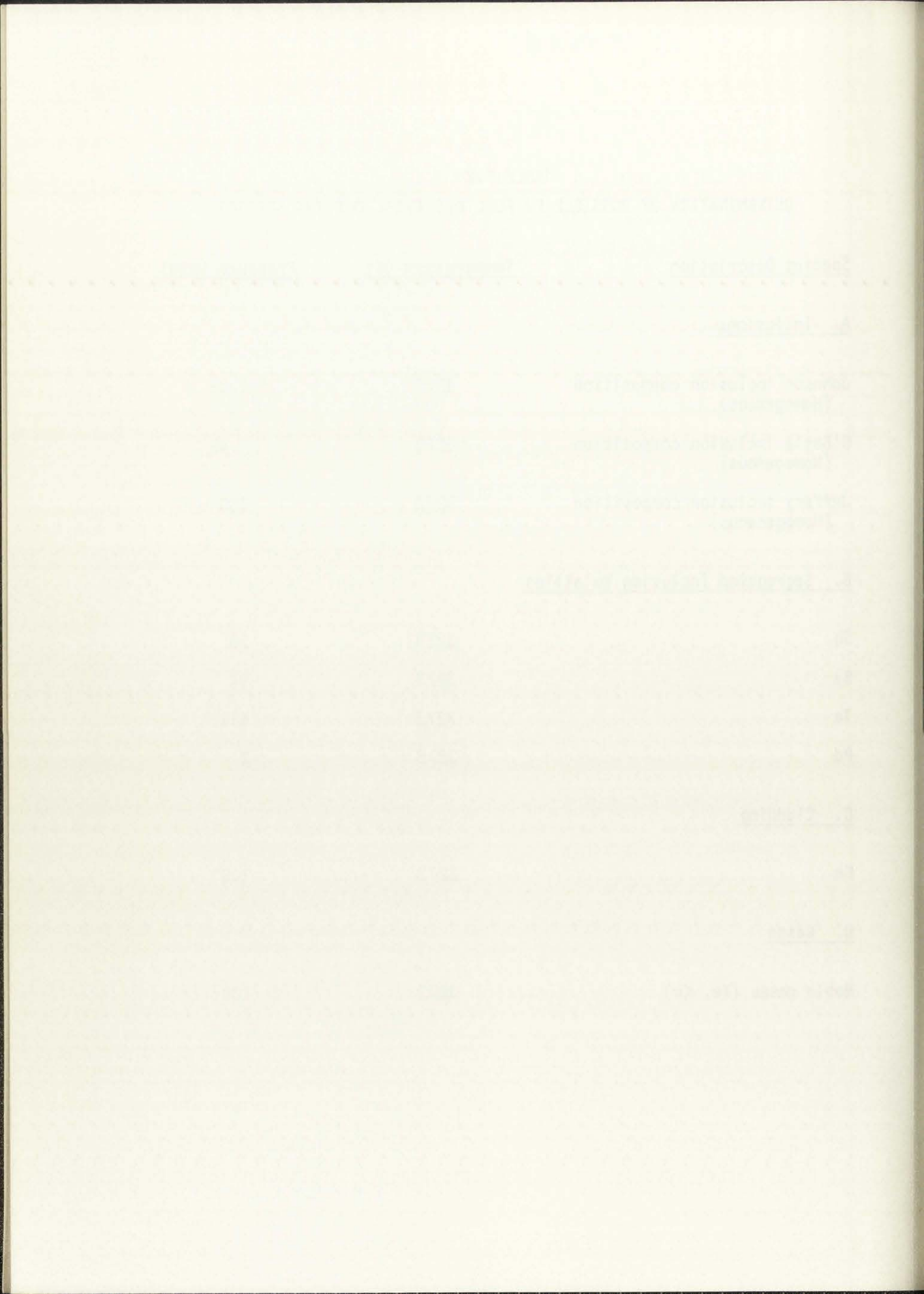


TABLE 7.2 (cont)

<u>Species Description</u>	<u>Temperature (K)</u>	<u>Pressure (atm)</u>
<u>E. Fuel EOS</u>		
Bogensberger EOS (U.8, Pu.2) 01.96	3600	1.5
Bogensberger EOS UO ₂	3700	1.5
Gabelnick EOS UO ₂	3900	1.5
Leibowitz EOS UO ₂	3800	1.5
Leibowitz EOS (U.8, Pu.2) 01.96	3570	1.5

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composition, however, have a high enough vapor pressure to cause ejection. The authors believe that the stainless steel clad probably would not have been intimately mixed in the fuel at the ejection time. Thus fission product pressurization and fuel vapor pressure are considered the primary causes for fuel dispersal. From Sec. 5, evidence supports homogeneous inclusion composition, leaving fission gas and fuel species as the most probable driving forces. From the results in Sec. 6, at .35 atom % burnup and assuming a radial average fission gas retention of 42%, approximately 1.47×10^{-5} moles of gas/cm³ of fuel exists. Using the Ideal Gas Law, a $\Delta T = 3273 \text{ K} - 1270 \text{ K}$ (average steady state temperature), and ignoring the surface tension, one could expect a 160% volume expansion at the peak temperature location due to fission gas. Since the F2 transient radial temperature profiles are very flat, not much gas release is expected, i.e. no driving potential, except from interlinking porosity and cracks (8-16% as discussed in Sec. 6). However, a minimum of 40% of the gas in the various fuel regions is in solution versus existing intra- and intergranular bubbles. Also surface tension effects on the fission gas bubble increase the pressure felt by the gas from 1.5 atm. to 1.5 +273 atm.* If one considers these factors the expected volume expansion

*As shown in Sec. 6, the liquid fuel surface tension increases the fission gas intragranular bubble (650 Å dia.) pressure by 273 atms.

concentration of the solution.

It is found that the rate of

reaction is not affected by

the concentration of the

reactants. This is because

the reaction is zero order

with respect to the reactants.

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at the peak fuel temperature is approximately .5%; far less than that needed for fuel dispersal. Even if the expected volume expansion at fuel melting due to surface tension effects is taken into account, the volume expansion is still only a few percent. It thus appears that the unknowns in the transient and heat transfer calculations were sufficient to encompass the required fuel temperature, and that the fuel vapor was the driving species. The fission gas pressure was high enough, it just appears that not enough gas is available to cause the fuel dispersion.

7.3 EOS Test Series

TREAT tests EOS-1, EOS-2, and EOS-3¹¹ were performed to determine LMFBR irradiated fuel behavior to a rapid energetic power burst following coolant voiding and clad relocation (LOF driven TOP). The fuel was of the mixed oxide type, $(U_{.75} Pu_{.25}) O_2$, with EOS-1 being fresh fuel, EOS-2 preirradiated at high power (11.3 kW/ft) in EBR-II to a burnup of .85 atom %, and EOS-3 preirradiated at intermediate power (8.12 kW/ft) to a burnup of .81 atom %. The active fuel column had a .5 in. boron nitride insulator pellet separating it from the hold down spring. The test train consisted of the test pin mounted in a dry capsule with 1.7 mm between the clad (5.33 mm O.D. for EOS-1 and EOS-2, 5.79 mm O.D. for EOS-3) and a boron nitride crucible. Room thus existed for radial expansion. Also, once cladding failure or

melting occurred, axial expansion into an upper test train plenum region was possible. The temperature limited TREAT transient was similar for the EOS-1 and EOS-2 tests. In the EOS-1 test, the transient consisted of a step reactivity insertion of 4.66% $\Delta K/K$ with an initial period of 22.9 ms. This led to a power burst of ≈ 0.25 s with a maximum of 1302 kW/ft. The EOS-2 transient consisted of a step reactivity insertion of 4.42% $\Delta K/K$ with an initial period of 24.3 ms, leading to a power burst of ≈ 0.25 s with a maximum of 1236 kW/ft. Both tests thus reached the desired level of ≈ 100 x nominal design. The EOS-3 transient also was similar except the initial period was slightly longer (26.8 ms) and the peak power was lower, 978 kW/ft.

In the transient test of EOS-1 upward fuel dispersal occurred, based on preliminary hodoscope data and pressure and thermocouple traces. Such upward fuel motion was believed to have been driven by stainless steel vapor pressure. The shortness of the test fuel, 4 in. active fuel length and 5.8 in. total test pin length, and the fact that the boron nitride crucible enclosed the bottom portion of the test volume, indicates that the drained cladding was in intimate contact with the hot fuel. In the F-series, the drained cladding settled around the bottom cooler fuel pellets and thus was not considered the principal dispersed species. The vapor pressure of iron is ≈ 1 atm. at the fuel melting temperature (3023 K) and is ≈ 4 atms. at 3500 K, sufficient to cause fuel dispersal.

The first experiment was designed to determine the effect of the concentration of the solution on the rate of reaction. The temperature of the solution was kept constant at 25°C. The reaction was carried out in a 250 ml beaker. The reactants were 10 ml of 0.1 M potassium persulfate and 10 ml of 0.1 M potassium iodide. The reaction was started by the addition of 10 ml of 0.1 M sodium bisulfite. The time taken for the color to appear was recorded. The experiment was repeated five times and the average time was calculated. The results are shown in Table 1.

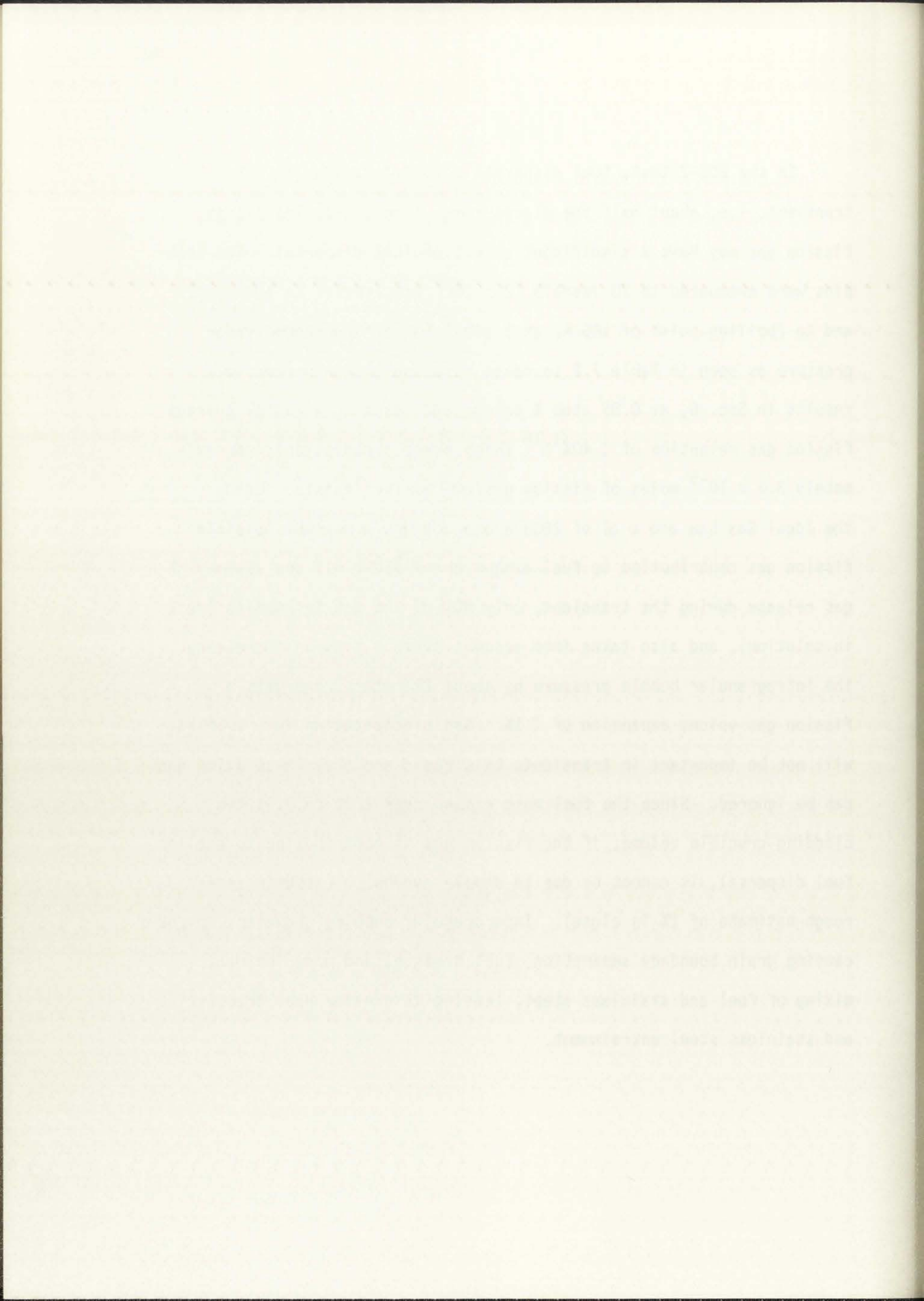
The second experiment was designed to determine the effect of the concentration of the potassium persulfate on the rate of reaction. The temperature of the solution was kept constant at 25°C. The reaction was carried out in a 250 ml beaker. The reactants were 10 ml of 0.1 M potassium iodide and 10 ml of 0.1 M sodium bisulfite. The concentration of the potassium persulfate was varied from 0.05 M to 0.2 M. The time taken for the color to appear was recorded. The experiment was repeated five times and the average time was calculated. The results are shown in Table 2.

The third experiment was designed to determine the effect of the concentration of the potassium iodide on the rate of reaction. The temperature of the solution was kept constant at 25°C. The reaction was carried out in a 250 ml beaker. The reactants were 10 ml of 0.1 M potassium persulfate and 10 ml of 0.1 M sodium bisulfite. The concentration of the potassium iodide was varied from 0.05 M to 0.2 M. The time taken for the color to appear was recorded. The experiment was repeated five times and the average time was calculated. The results are shown in Table 3.

The fourth experiment was designed to determine the effect of the concentration of the sodium bisulfite on the rate of reaction. The temperature of the solution was kept constant at 25°C. The reaction was carried out in a 250 ml beaker. The reactants were 10 ml of 0.1 M potassium persulfate and 10 ml of 0.1 M potassium iodide. The concentration of the sodium bisulfite was varied from 0.05 M to 0.2 M. The time taken for the color to appear was recorded. The experiment was repeated five times and the average time was calculated. The results are shown in Table 4.

The fifth experiment was designed to determine the effect of the concentration of the sodium bisulfite on the rate of reaction. The temperature of the solution was kept constant at 25°C. The reaction was carried out in a 250 ml beaker. The reactants were 10 ml of 0.1 M potassium persulfate and 10 ml of 0.1 M potassium iodide. The concentration of the sodium bisulfite was varied from 0.05 M to 0.2 M. The time taken for the color to appear was recorded. The experiment was repeated five times and the average time was calculated. The results are shown in Table 5.

In the EOS-2 test, fuel dispersal occurred earlier in the transient, i.e. about half the elapse time, than EOS-1, indicating fission gas may have a significant effect on fuel dispersal. The test pins were evacuated to 20 Pascals (2×10^{-4} atm.) prior to the test, and Xe (boiling point of 166 K, at 1 atm.) has a high enough vapor pressure as seen in Table 7.2 to cause dispersal. Again from the results in Sec. 6, at 0.85 atom % burnup and assuming a radial average fission gas retention of $\approx 40\%$ ^{1,12} (high power irradiation), approximately 3.4×10^{-5} moles of fission gas/cm³ of fuel exists. Using the Ideal Gas Law and a ΔT of 2000 K one obtains a maximum possible fission gas contribution to fuel expansion of 550%. If one assumes 8% gas release during the transient, only 60% of the gas in bubbles (rest in solution), and also takes into account surface tension increasing the intragranular bubble pressure by about 273 atms., one gets a fission gas volume expansion of $\approx 1\%$. Gas precipitation into bubbles will not be important in transients this rapid and thus in-solution gas can be ignored. Since the fuel must expand over 100% to fill the cladding-crucible volume, if the fission gas is contributing to earlier fuel dispersal, it cannot be due to simple expansion (assuming the rough estimate of 1% is close). Intergranular bubbles, however, may be causing grain boundary separation, fuel breakup, and more intimate mixing of fuel and stainless steel, leading to greater heat transfer and stainless steel entrainment.



In the EOS-3 transient, which was at lower power than EOS-2, fuel dispersal appeared to occur slightly sooner in the transient than the EOS-2 test. This may be attributed to the larger fission gas retention in the intermediate power preirradiated test pin. From these tests it appears that for LOF and LOF driven TOP accidents with relatively low burnup fuel, fission gas and other volatiles potential for fuel motion appears to be in the form of fuel breakup for very rapid transients and for some fuel swelling (< 10%) for slower transients. Little potential appears to exist, however, for axial dispersal, since for LOF accidents clad melt allows expansion into the coolant channel.

7.4 Series V Tests

The General Electric Series V tests¹³ were designed to investigate the effects of molten fuel movement, fission product gases, and fuel and blanket length, on transient failure thresholds and mechanisms. Two test pins, C5A and C5B, consisted of UO₂ fuel irradiated at low power (12 kW/ft peak) in the General Electric Test Reactor (GETR) to a burnup of $\approx 20,000$ Mwd/Te (≈ 2 atom %). Both pins had an active fuel length of 24 in. with a 14.25 in. natural uranium blanket between the fuel and the gas plenum (He at 1 atm.). The test pins in this series were identical except the C5A blanket was composed of solid pellets, and the C5B blanket had annular pellets with a .07 in. I.D. (see Fig. 7.6). Due to the low power steady state irradiation (≈ 1840

In the first experiment, a solution of 10% sodium hydroxide was prepared in distilled water. The solution was then diluted to a concentration of 1% and used for the experiment. The results showed that the rate of reaction was directly proportional to the concentration of the reactants. This is in agreement with the law of mass action.

4.1. Results

The results of the experiment are shown in Table 1. The rate of reaction was measured by the volume of gas evolved per unit time. The rate of reaction was found to be directly proportional to the concentration of the reactants. This is in agreement with the law of mass action. The rate of reaction was also found to be directly proportional to the surface area of the reactants. This is in agreement with the law of mass action. The rate of reaction was also found to be directly proportional to the temperature of the reactants. This is in agreement with the law of mass action.

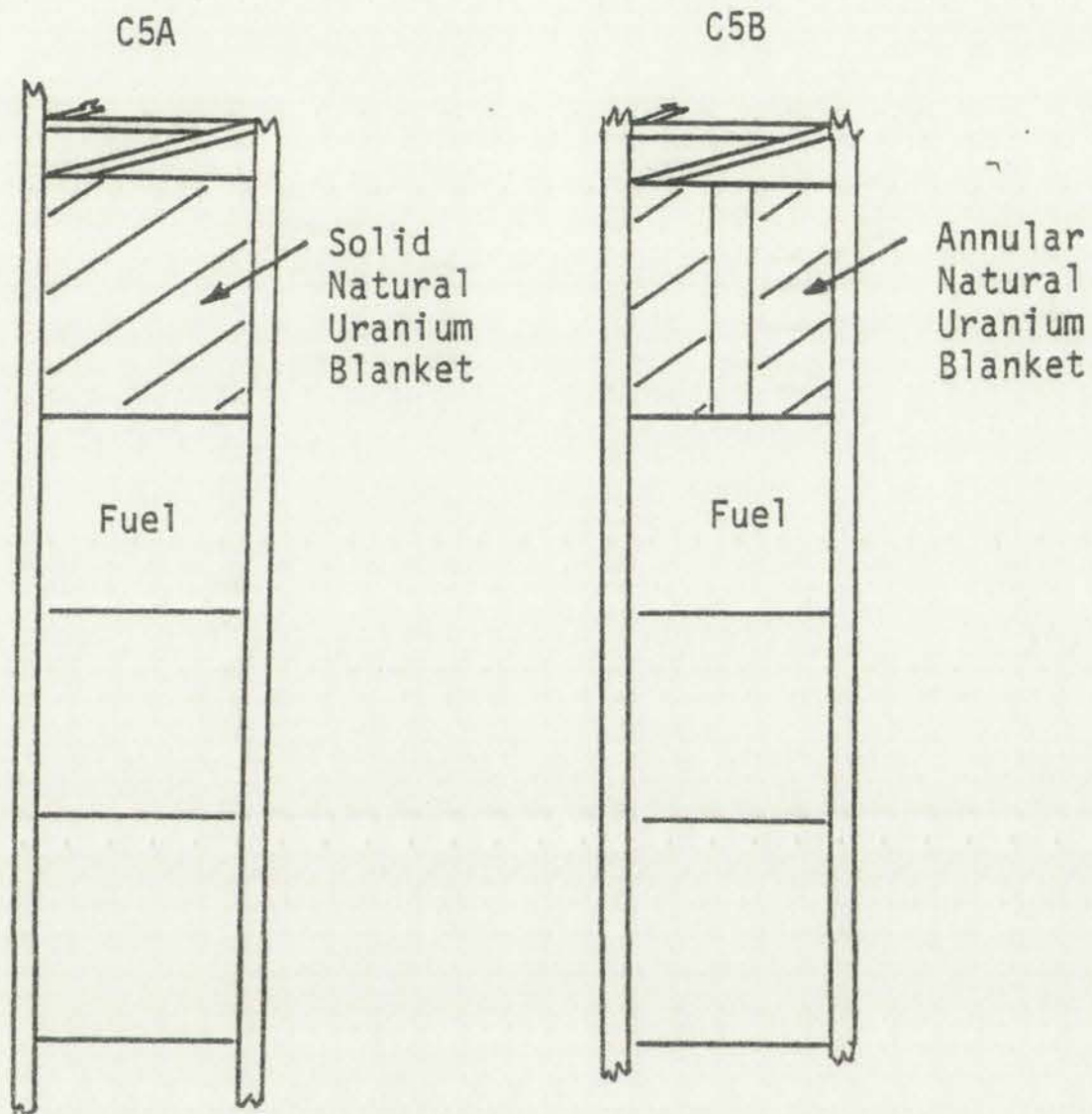


Figure 7.6.
Comparison of fuel rods C5A and C5B.

Fig. 1

Fig. 2

Fig. 1
Fig. 2
Fig. 3

Fig. 1
Fig. 2
Fig. 3

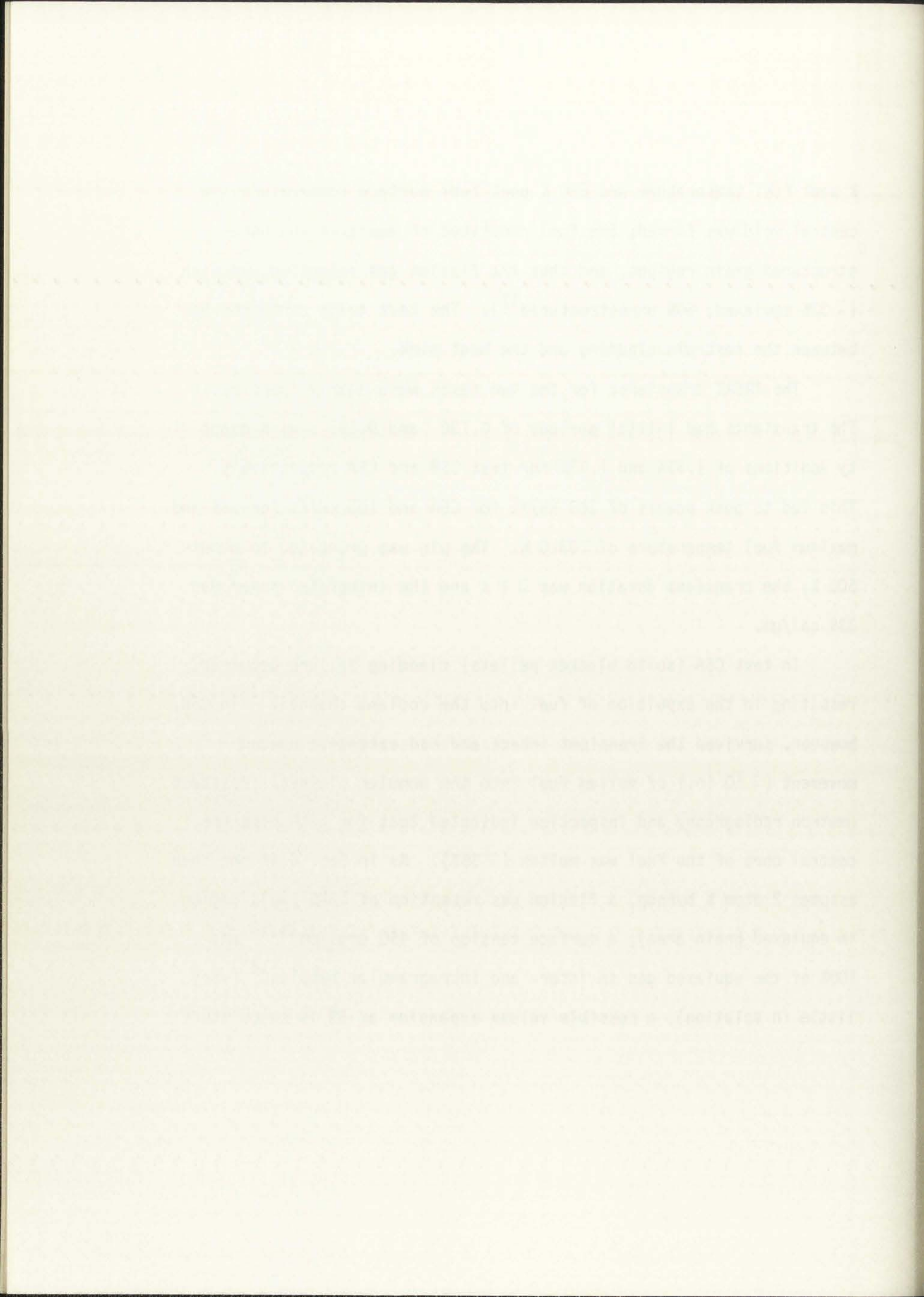


Fig. 1 Fig. 2 Fig. 3

K peak fuel temperature and 850 K peak fuel surface temperature) no central void was formed; the fuel consisted of equiaxed and unstructured grain regions, and thus the fission gas retention was high ($\sim 32\%$ equiaxed, 64% unstructured¹²). The test train contained NaK between the test pin cladding and the heat sink.

The TREAT transients for the two tests were nearly identical. The transients had initial periods of 0.136 and 0.131 s with reactivity additions of 1.35% and 1.37% for test C5B and C5A respectively. This led to peak powers of 160 kW/ft for C5A and 155 kW/ft for C5B and maximum fuel temperature of ~ 3310 K. The pin was preheated to about 500 K, the transient duration was ~ 1 s and the integrated power was 339 cal/gm.

In test C5A (solid blanket pellets) cladding failure occurred, resulting in the expulsion of fuel into the coolant channel. Pin C5B, however, survived the transient intact and had extensive upward movement (~ 10 in.) of molten fuel into the annular blanket. Posttest neutron radiography and inspection indicated that for both pins the central core of the fuel was molten ($\sim 35\%$). As in Sec. 6 if one then assumes 2 atom % burnup, a fission gas retention of $\sim 32\%$ (melt region in equiaxed grain area), a surface tension of 450 ergs/cm^{14,15} and 100% of the equiaxed gas in inter- and intragranular bubbles¹² (very little in solution), a possible volume expansion of 6% is calculated.



This is also assuming no bubble coalescence or release. Release is very possible since $\approx 90\%$ of the equiaxed gas is intergranular, however since no central void was initially present, it can be assumed that the gas remained trapped in the molten fuel volume. If one uses the higher surface tension (750 ergs/cm^2) of solid fuel and recalculate the volume expansion at fuel melting, taking into account the drop in surface tension, i.e. from 750 ergs/cm^2 for solid fuel to 450 ergs/cm^2 for liquid fuel with a corresponding drop in bubble pressure and corresponding increase in bubble radius, an additional increase of only a few percent can be expected. The fission gas expansion along with the expected 10% volume expansion upon fuel change of phase could be the driving force for the axial fuel motion. The annular blanket accommodated $\approx 11\%$ of the molten fuel volume ($\approx 4\%$ of the total fuel volume) which apparently was sufficient to prevent clad failure. In this test it appears that fission gas is the most probable cause of axial fuel motion.

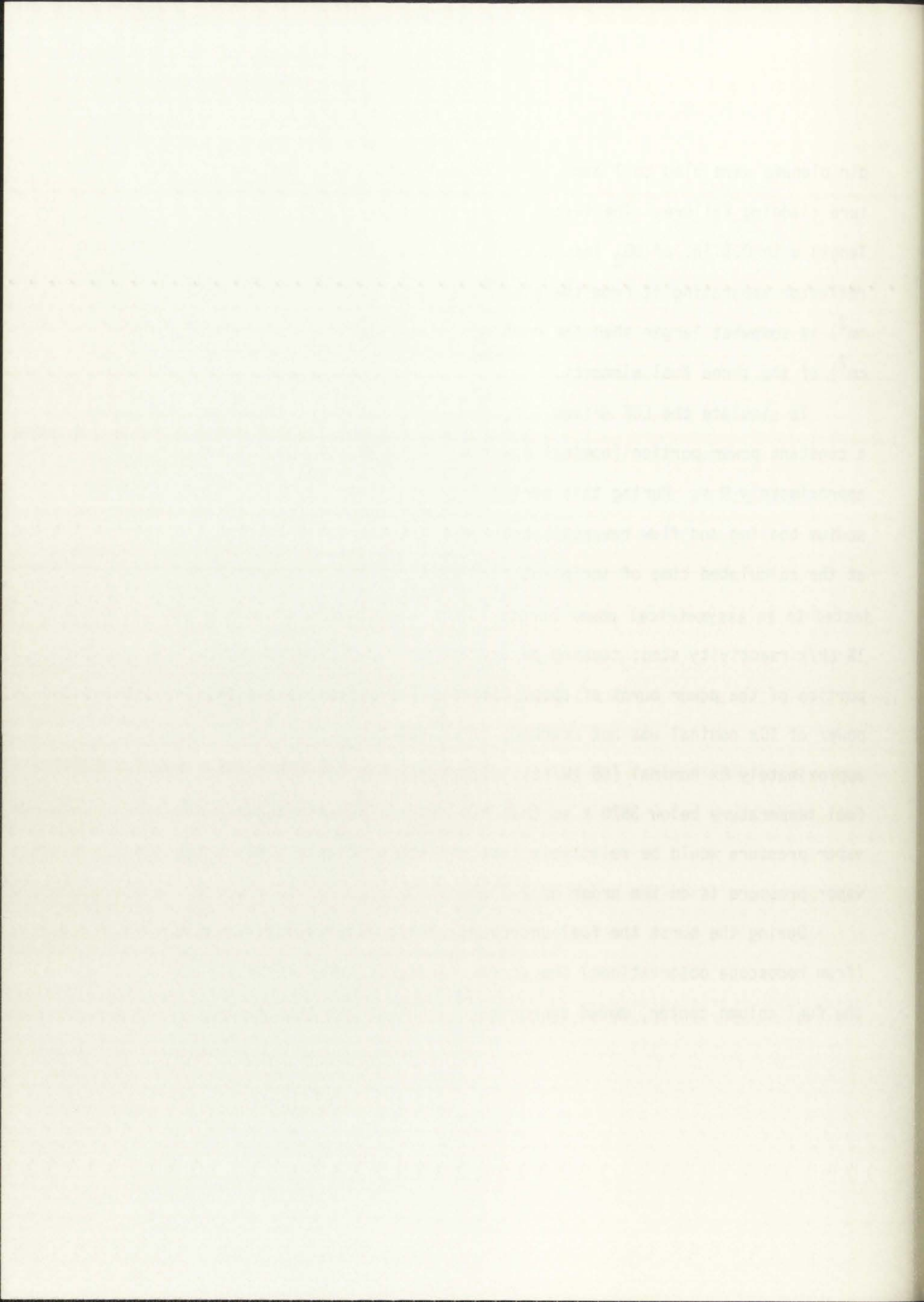
7.5 Test L5

The L5 test¹⁶ was performed to simulate the behavior of moderate power fuel subjected to a hypothetical loss-of-flow driven transient overpower accident in an LMFBR. Three ($\text{U}_{.75}, \text{Pu}_{.25}$) O_2 fueled test elements irradiated in the General Electric Test Reactor (thermal) at 12.2 kW/ft to 8 atom % burnup were arranged in a triangular pattern in a closed sodium loop test train (MARK-II C). The test

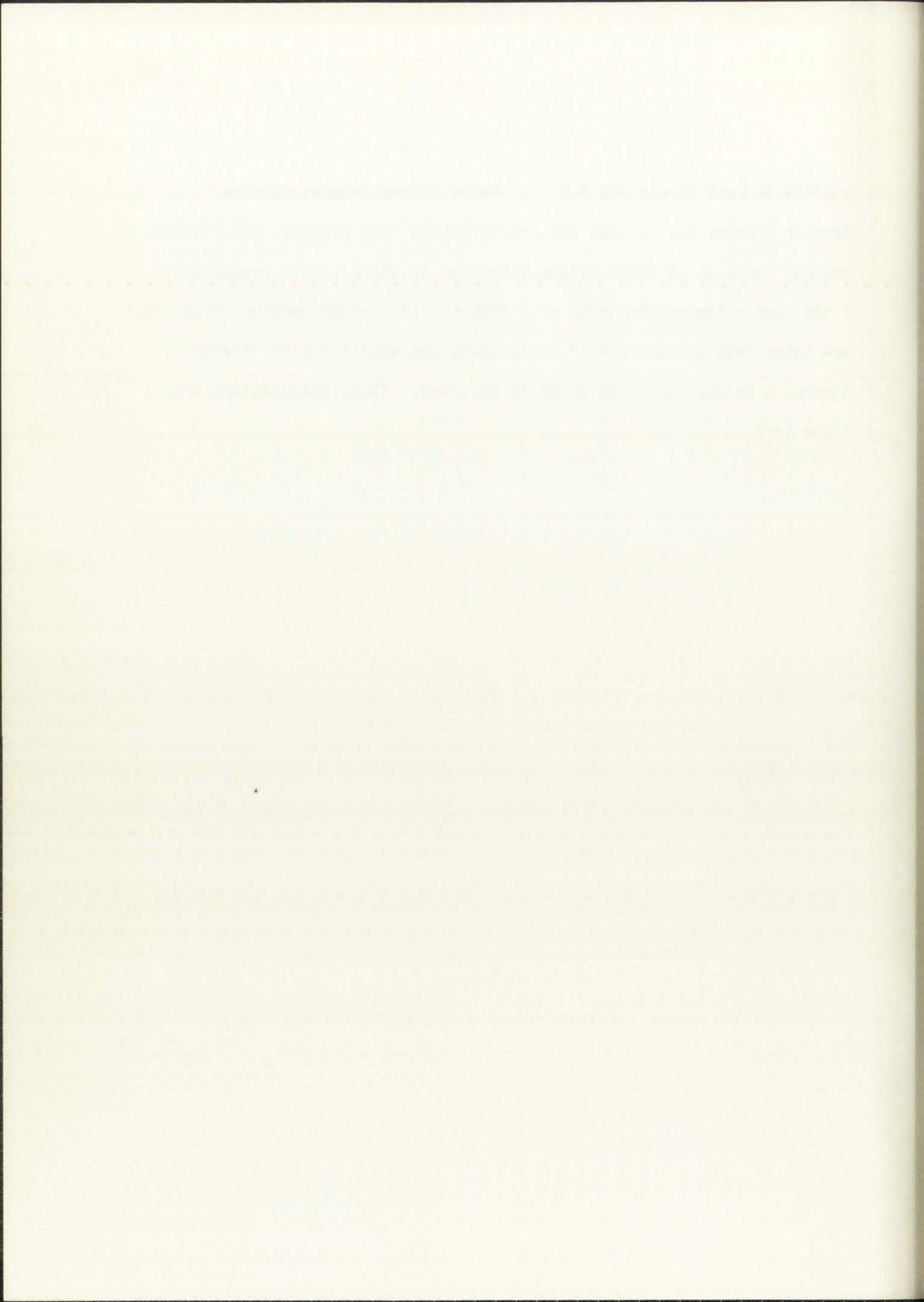
pin plenums were bled to 1 atm. pressure and resealed to prevent premature cladding failure. The test pins consisted of a 34 in. active fuel length with 0.5 in. of UO_2 insulator pellets, and 3 in. of Incone 1 reflector separating it from the plenum. The sodium flow area (0.63 cm^2) is somewhat larger than the combined cross-sectional area (0.57 cm^2) of the three fuel elements.

To simulate the LOF driven TOP, the TREAT transient consisted of a constant power portion (nominal power of $\approx 11 \text{ kW/ft}$) that lasted approximately 9 s. During this period flow coastdown was initiated and sodium boiling and flow reversal occurred. After channel voiding and at the calculated time of incipient clad melting, the pins were subjected to an asymmetrical power burst. This was equivalent to about a $1\% \Delta k/k$ reactivity step, causing an average period in the rising portion of the power burst of about 835 ms. The target peak burst power of 10x nominal was not reached; in actuality the peak power was approximately 6x nominal (66 kW/ft). The burst was planned to keep the fuel temperature below 3870 K so that the dispersive effects of fuel vapor pressure would be relatively insignificant. Even at 3870 K the vapor pressure is on the order of 2-3 atms.

During the burst the fuel underwent a mild dispersal at or after (from hodoscope observations) the scram. This dispersal centered at the fuel column center, moved approximately 15% of the test fuel



axially in both directions 4-8 in. Again if one ignores surface tension effects and assumes 25% precipitation into bubbles, the fission gas may cause up to 1400% volume expansion assuming a bulk pressure of 1 atm. and a temperature rise of ≈ 2000 K. If surface tension effects and are taken into account and if coalescence and equilibration effects ignored a volume expansion of 6% is obtained. These calculations are shown here.



From Eq. (6.1)

$$V_2 - V_1 = nR \left(\frac{T_2}{P_2} - \frac{T_1}{P_1} \right) .$$

At 8 atom % burnup (Table 6.1) assuming 42.2% average fission gas retention, assuming conservative 25%¹² of available gas in bubbles, ignoring surface tension effects, and assuming a bulk pressure of 1 atm.,

$$n = (2.999 \times 10^{-4} \text{ moles gas/cm}^3) \left(\frac{8}{3} \right) (.42) (.25) .$$

Assume

$$T_2 = 3023 \text{ K (Fuel melting temperature)}$$

$$T_1 = 1000 \text{ K.}$$

Then

$$\begin{aligned} V &= (2.999 \times 10^{-4}) \left(\frac{8}{3} \right) (.422) (.25) (82.05 \frac{\text{cm}^3 \text{ atm}}{\text{K}}) \left(\frac{2023 \text{ K}}{1 \text{ atm}} \right) \times 100\% \\ &= 1400\% \end{aligned}$$

Using same assumptions, except taking into account surface tension effects, i.e. from Sec. 6,

$$y = 2x^2 + 3x - 5$$

At a fixed interest rate (Table 1) we find that the average return on capital is 12% of the total value of the capital stock. This is a very low return on capital, and it is likely that the return on capital is even lower in other countries.

$$r = 0.12 \times 10^6 \text{ (total value of capital)} = 12,000,000$$

Table 1

$$I = 1000 \times (1 + r)^t$$

$$I = 1000 \times (1 + 0.12)^t$$

$$y = 2x^2 + 3x - 5 \quad \text{and} \quad r = 0.12 \times 10^6 \text{ (total value of capital)}$$

Table 2

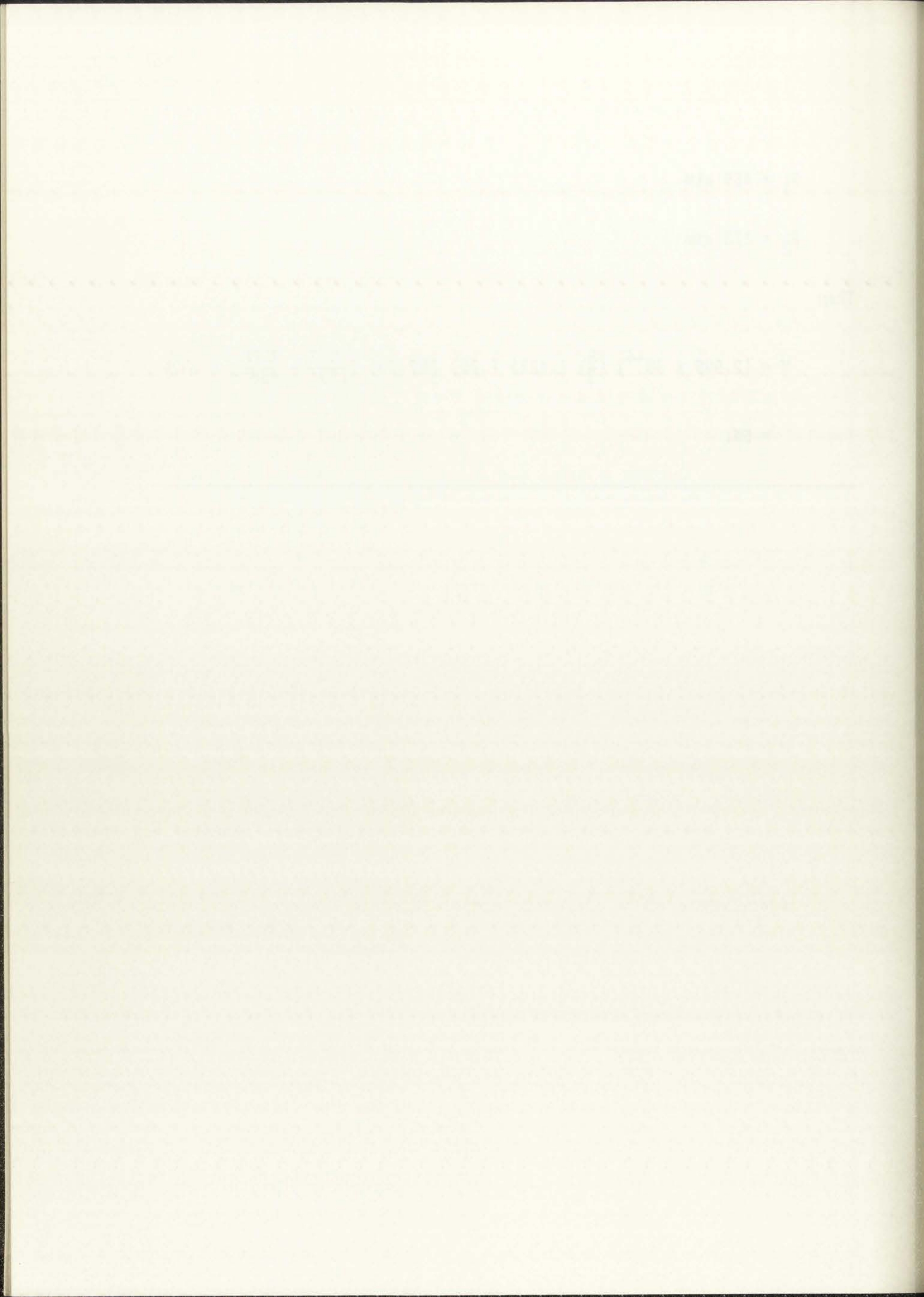
Table 2 shows the results of the simulation. The return on capital is 12% of the total value of the capital stock. This is a very low return on capital, and it is likely that the return on capital is even lower in other countries.

$$P_1 = 455 \text{ atm}$$

$$P_2 = 273 \text{ atm}$$

Then

$$V = (2.999 \times 10^{-4}) \left(\frac{8}{3}\right) (.422) (.25) (82.05) \left(\frac{3023}{273} - \frac{1000}{455}\right) \times 100\%$$
$$= 6\%.$$



For a transient such as this where the temperature rise is rapid, coalescence and precipitation probably can be ignored in the initial short time span. However, since the transient analysis continues past scram and the fuel remains at elevated temperatures, coalescence, bubble growth, precipitation, etc. become important and may lead to substantial swelling in later stages of the transient as observed in this test. Since the fuel vapor pressure was deliberately kept low and since the dispersal seems to have occurred after peak power, it appears that fission gas was the mild dispersing force. The bubble pressure equilibration time of .1 to 1 s¹⁷ for the coalescence of 2, 100 nm dia. bubbles at 3070 K is the right time frame for the dispersal experienced in this test. Microanalysis of the L5 fuel indicates that precipitation and growth of intragranular bubbles occur.

The vapor pressure of the fuel as well as that of the mixed oxide homogeneous metallic inclusions discussed previously, are both on the order of 1-2 atm. As stated in Sec. 2, the fuel composition and irradiation temperature affect the final inclusion composition more than the irradiation spectrum. One thus would not expect the LWR inclusions found by Jeffery.¹⁰ If Jeffery's type of inclusion were present, their high vapor pressure (see Fig. 5.18) and the high burnup would have led to a rapid and large fuel dispersal which was not experienced in this test.

The above experimental analyses is summarized in Table 7.3 and support the fact that fission gas and other highly volatile fission products (Cs, etc.) may contribute to fuel dispersal. However, in tests C5B, F1, E7, and H4 metallic inclusions were present in the post-test metallographic examination. No microprobe analysis was done to assure that the inclusions were in fact solid fission products of roughly the same composition as found in "as irradiated" fuel. Their size, i.e. microns in diameter, support solid fission product inclusions rather than dispersed clad and their posttransient presence supports the homogeneous inclusion state.

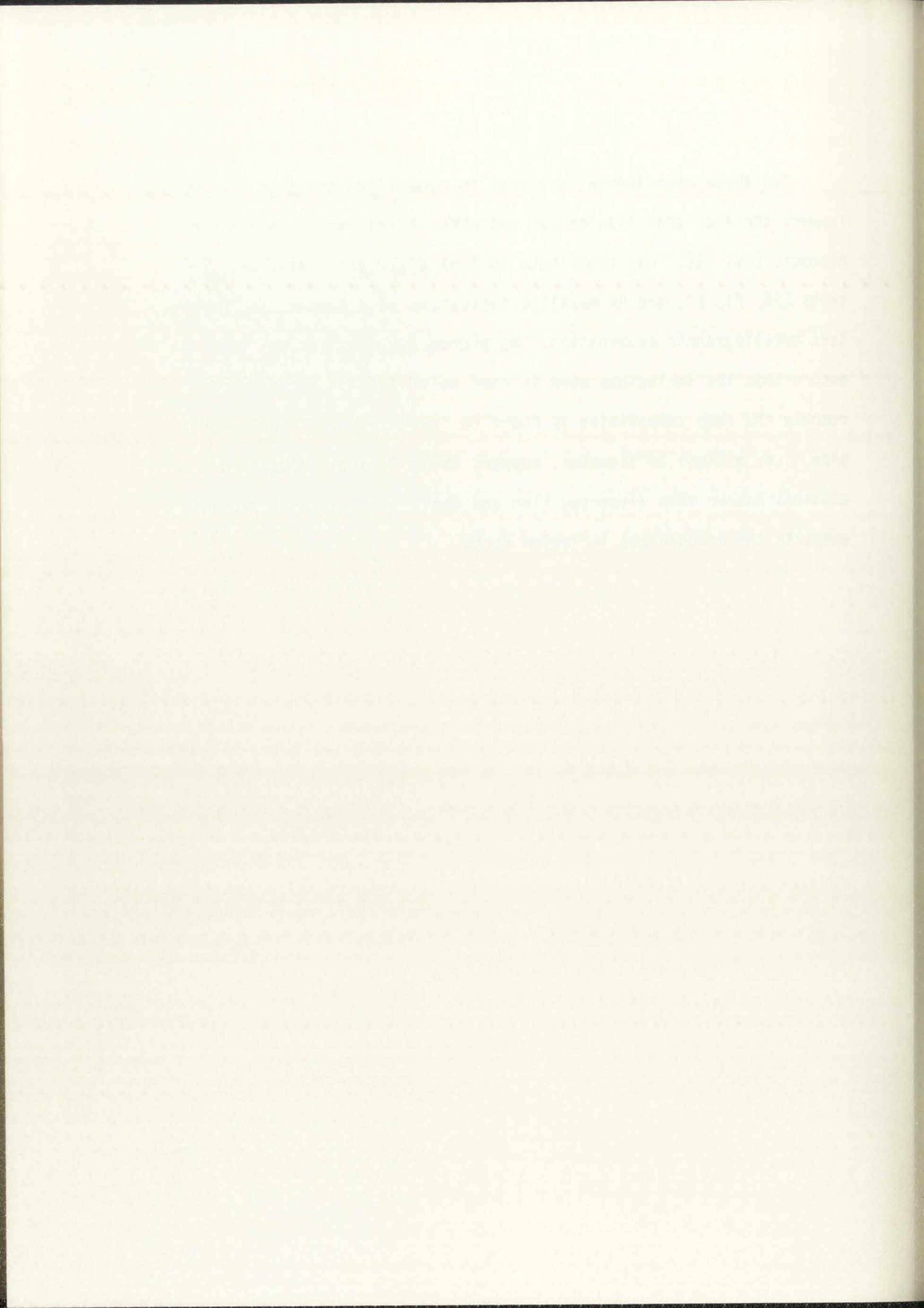


TABLE 7.3
SUMMARY OF EXPERIMENTAL FUEL MOTION

<u>Test</u>	<u>Pre- or Postfailure Motion</u>	<u>Postulated Mechanisms</u>
E1	Prefailure	~10% volume expansion due to fuel change of phase, possibly fuel vapor pressure.
H2	Prefailure	Same as E1.
E4	Prefailure	Same as E1.
F2	Postfailure (LOF)	Fuel vapor pressure.
E0S-1	Postfailure (LOF)	Stainless steel vapor pressure.
E0S-2	Postfailure (LOF)	Fission gas fuel breakup, stainless steel vapor pressure.
E0S-3	Postfailure (LOF)	Fission gas fuel breakup stainless steel vapor pressure.
C5B	Prefailure	Fission gas.
L5	Postfailure (LOF)	Fission gas.

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1. The first part of the report deals with the general situation of the country and the position of the various groups. It is a very general and superficial treatment of the subject, but it is useful as a starting point for a more detailed study.

2. The second part of the report is devoted to a study of the economic situation. It is a very detailed and thorough study, and it is one of the best of its kind. It is a very valuable contribution to the knowledge of the economic situation of the country.

3. The third part of the report is devoted to a study of the social situation. It is a very detailed and thorough study, and it is one of the best of its kind. It is a very valuable contribution to the knowledge of the social situation of the country.

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10. The tenth part of the report is devoted to a study of the energy situation. It is a very detailed and thorough study, and it is one of the best of its kind. It is a very valuable contribution to the knowledge of the energy situation of the country.

8. SUMMARY

In analyzing the free energy of formation of the various fission products of UO_2 and $(Pu, U)O_2$, their general chemical state can be determined. The fission products can be broken into four general categories:

1. stable gases,
2. stable oxides,
3. stable metallics, and
4. molybdenum, which has an oxygen potential very close to that of the fuel.

Of interest here are metallic fission products which exist as aggregate inclusions throughout the fuel, and which upon heating can vaporize, providing a possible driving force for fuel motion. Fission products that exist as gases during normal reactor operating temperatures such as xenon and krypton, are swept out of the columnar and equiaxed fuel regions and are analyzed as a comparison contribution to fuel swelling. The stable oxides in general, are present in solution form within the fuel matrix and thus, cannot volatilize preferentially. However, in the metallurgical analysis of irradiated nuclear reactor fuel rods, fission product inclusions, approximately 5 microns in diameter, consisting mainly of molybdenum and stable metallic elements, have been found both in LMFBR (mixed oxide) and LWR (uranium

The first step in the analysis of the reaction is to determine the rate of reaction.

The rate of reaction is defined as the change in concentration of a reactant or product per unit time.

Mathematically, the rate of reaction can be expressed as follows:

$$Rate = -\frac{1}{\nu} \frac{d[A]}{dt} = \frac{1}{\nu} \frac{d[B]}{dt}$$

where ν is the stoichiometric coefficient of the reactant or product, $[A]$ and $[B]$ are the concentrations of the reactant and product respectively, and t is time.

For example,



the rate of reaction is given by:

$$Rate = -\frac{1}{2} \frac{d[A]}{dt} = -\frac{d[B]}{dt} = \frac{d[C]}{dt} = \frac{d[D]}{dt}$$

or the rate

of reaction is the same for all reactants and products when divided by their stoichiometric coefficients.

One method for determining the rate of reaction is to measure the change in concentration of a reactant or product over a known period of time.

For example, if the concentration of a reactant decreases from 1.0 M to 0.5 M in 10 minutes, the rate of reaction is 0.05 M/min.

Another method for determining the rate of reaction is to measure the change in volume of a gas produced or consumed over a known period of time.

For example, if the volume of a gas produced increases from 0 to 100 ml in 10 minutes, the rate of reaction is 10 ml/min.

The rate of reaction can also be determined by measuring the change in pressure of a gas in a closed system over a known period of time.

For example, if the pressure of a gas in a closed system increases from 1.0 atm to 1.5 atm in 10 minutes, the rate of reaction is 0.05 atm/min.

It is important to note that the rate of reaction is always a positive quantity, and it is independent of the direction of the reaction.

For example, the rate of reaction for the reaction $A \rightarrow B$ is the same as the rate of reaction for the reaction $B \rightarrow A$.

The rate of reaction is also dependent on the concentration of the reactants and products, and it is affected by temperature and the presence of a catalyst.

In general, the rate of reaction increases with increasing concentration of the reactants and with increasing temperature.

A catalyst is a substance that increases the rate of reaction without being consumed in the process.

dioxide) fuels. since some metallic fission products have lower vaporization temperatures than the fuel itself, such metallic inclusions have the potential to volatilize during overheating events. An assessment of the potential contribution of such metallic inclusions to fuel motion, during postulated accident overheating events, was assessed for the first time in this work.

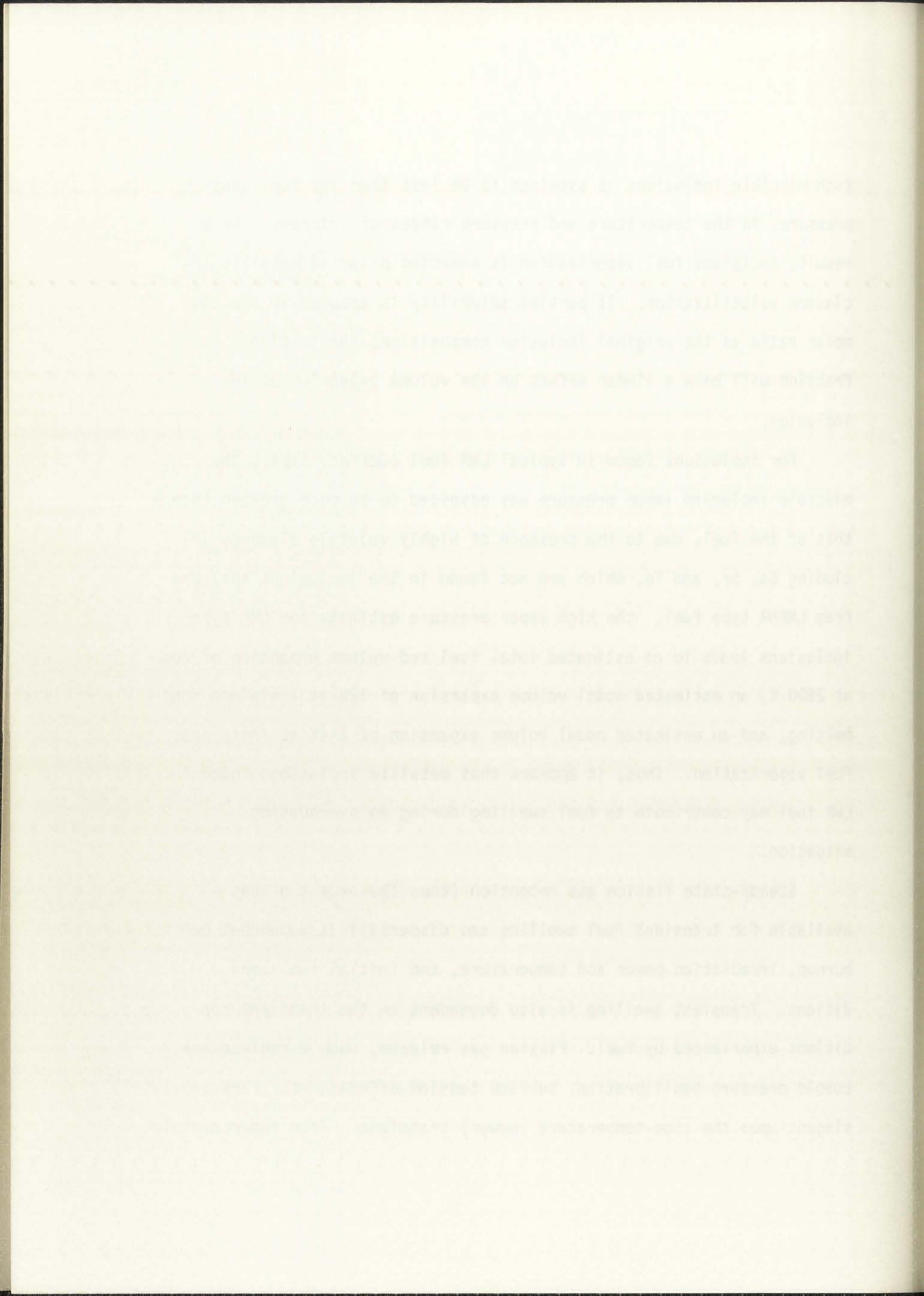
For an LMFBR inclusion (Johnson type), if the metallic constituents are assumed completely immiscible and for a bulk fuel rod internal pressure of 20 atm a maximum inclusion nodal volume expansion of $\sim 26\%$ and a total fuel column volume expansion of $\sim 1-1/2\%$ was calculated at incipient fuel vaporization. This is based on an assumption of a flat distribution profile in the number density of inclusions and the Ideal Gas EOS for the vapor. The Redlich-Kwong EOS, which appears more applicable than the Ideal Gas, van der Waals, or the modified hard-sphere EOS, did not change the results significantly. However, when a representative radial distribution in the inclusion number density is incorporated, a maximum nodal volume expansion of $\sim 11.5\%$ can be expected. If the radial inclusion number density profile is used, the total fuel pin volume expansion also drops from 1.5 to 1% at incipient fuel vaporization.

If the inclusion constituents are assumed to be completely miscible in one another, the vapor pressure of the such single-phase inclusions are calculated using Raoult's Law of Partial Pressure. This assumption is supported by thermodynamic solution consideration and by established binary and ternary phase diagrams. The vapor pressure for

such miscible inclusions is assessed to be less than the fuel vapor pressure, in the temperature and pressure ranges of interest. As a result, incipient fuel vaporization is expected prior to metallic inclusion volatilization. If partial solubility is assumed in the same molar ratio as the original inclusion composition, the insoluble fraction will have a linear effect on the volume expansion of the inclusion.

For inclusions found in typical LWR fuel (Jeffery type), the miscible inclusion vapor pressure was assessed to be much greater than that of the fuel, due to the presence of highly volatile elements including Ba, Sr, and Te, which are not found in the inclusions analyzed from LMFBR type fuel. The high vapor pressure estimate for LWR type inclusions leads to an estimated total fuel rod volume expansion of 40% at 2800 K, an estimated nodal volume expansion of 62% at incipient fuel melting, and an estimated nodal volume expansion of 114% at incipient fuel vaporization. Thus, it appears that metallic inclusions found in LWR fuel may contribute to fuel swelling during an overheating situation.

Steady-state fission gas retention (thus the amount of gas available for transient fuel swelling and dispersal) is dependent on burnup, irradiation power and temperature, and initial fuel conditions. Transient swelling is also dependent on the transient conditions experienced by fuel. Fission gas release, bubble coalescence, bubble pressure equilibration, surface tension effects, etc., are contingent upon the time-temperature (power) transient. From experimental



evidence it appears that for very slow transients (i.e. seconds, at or near design power), fission gas release from the fuel is greater than bubble growth, with the net result of slumping and drainage versus fuel swelling. However, for extremely rapid transients (i.e. milliseconds, at high powers 10 to 100 times design levels) it appears that intergranular fission gas may contribute to fuel breakup (dependent on steady-state irradiation history) but that coalescence and pressure equilibration of intragranular bubbles does not have time to occur during the transient itself. After scram, however, coalescence and equilibration may cause a mild dispersal or foaming of the fuel. As demonstrated by Deitrich¹ and equilibration time for the coalescence of 2 bubbles of 100 nm radius is assessed to be approximately 0.3 s. It thus appears that neither fission gas bubble growth or thermal expansion due to change-of-phase from solid to molten fuel will dominate the possible volume expansion effects from vaporization of homogeneous metallic inclusions found to occur in UO_2 fuel irradiated at thermal neutron energies. Thus, serious consideration should be given to the modeling of metallic inclusions for incorporation into LWR fuel behavior codes for accident analysis. However, this would not be the case for LMFBR fuels based on the analysis presented in this work. This is due to the fact that metals with rather high vaporization temperature are characteristically found in LMFBR type inclusion, indicating that fuel expansion by volatilization of homogeneous LMFBR type inclusions would be negligible.

The text on this page is extremely faint and illegible. It appears to be a technical or scientific document, possibly discussing topics like "analysis", "reaction", and "product". The text is organized into several paragraphs, but the specific details are unreadable due to the low contrast and blurriness of the scan.

REFERENCE

1. L. W. Deitrich and R. W. Ostensen, "An Assessment of Fission-Gas-Driven Fuel Disruption and Dispersal in a Hypothetical LMFBR Loss-of-Flow Accident," Argonne National Laboratory report ANL/RAS 77-4 (February 1977).

1. The following information was obtained from the
files of the Bureau of the Census, Department of
Commerce, Washington, D. C., on the subject of
the above-captioned company, and is being furnished
to you for your information.

2. The company was organized in the State of
California on the 15th day of January, 1954, and
has since that time operated as a corporation
under the laws of that State.

3. The principal office of the company is located
at 1234 Main Street, Los Angeles, California.
The company has no other offices or branches
anywhere.

4. The company is engaged in the business of
selling and distributing various types of
merchandise, and has a net worth of approximately
\$100,000.

5. The company is a wholly owned subsidiary
of the parent company, and is not a public
utility, and is not a corporation of the
United States.

6. The company is not a member of any
national, state, or local association,
and is not a member of any labor union.

7. The company is not a member of any
other organization, and is not a member
of any other association.

9. CONCLUSIONS AND RECOMMENDATIONS

The question of assessing the effect of metallic inclusions, found to occur in irradiated fuel, on fuel motion during an overpower transient depends upon an accurate understanding of constituent solubility. The question of whether the various metal species found within the inclusions of irradiated nuclear fuel elements are either segregated or in a homogeneous solution cannot be answered theoretically, since an analytical basis does not exist to construct multicomponent phase diagrams from first principles. Thus, such a question must be resolved experimentally if one is to be able to accurately assess with assurance the role metallic inclusion volatilization has on fuel behavior phenomena for high temperature overheating reactor transients. It is suggested that a metallurgical sample be prepared of the same metal species composition as found to occur for the inclusion of typical irradiated fuel rods. This sample could be heated to in situ temperatures and analyze to determine its metallographic structure, i.e. its phases and transition temperatures, as well as the total vapor pressure vs. temperature characteristics.

Based upon existing information an educated guess can be made that the metallic inclusions will not contribute to fuel motion for LMFBR type inclusions. The assumption that the inclusions are single-phase, i.e. totally miscible, is strongly supported not conclusively proven. However, fuel behavior assessment for LWR accident analysis

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may have to consider the metallic inclusion contribution to fuel swelling during an accident transient. Large fuel volume expansion due to the vaporization of the inclusions, both assuming the inclusion constituents are totally miscible and immiscible, can be expected, due to the presence of the highly volatile species of Barium, Strontium, and Tellurium found to exist in LWR type inclusions (which are not found in LMFB type inclusions). Further investigation, however, should be done in the area of inclusion composition assessment. Comparison of expected volume expansion due to LWR type inclusion vaporization with fission gas bubble expansion and volume expansion due to UO_2 change-of-phase from solid to melt, indicates that inclusion volatilization may be as great or greater than these two effects, thus, metallic LWR type inclusions may provide a substantial fuel motion driving force during a transient overheating situation.

Other factors which were not included in this analysis, but should be considered in future work in this area are:

1. Separate oxide inclusion contribution.
2. Bubble growth dynamics at inclusion vaporization.
3. More realistic fuel pin geometry, i.e., central void, fuel swelling and closure of bond gap, fuel cracking and thus possible communication of central void and outer fuel surface.
4. Differential thermal expansion of fuel and clad and thus differing geometry.
5. Fuel-clad shear drag opposing free expansion of fuel nodes.
6. Temperature dependence of physical parameters, i.e., heat capacity, density, thermal conductivity, etc.
7. Time (temperature) dependence of bulk and local pressures.
8. Inclusion volatilization analysis for such advanced concept fuels as UC, which have higher fission product retention characteristics.

The first part of the paper is devoted to a general discussion of the problem of the existence of a solution of the boundary value problem for the Laplace equation in a domain bounded by a piecewise smooth surface. It is shown that the necessary and sufficient conditions for the existence of a solution are the vanishing of the integrals of the normal derivatives of the unknown function over the boundary of the domain. The second part of the paper is devoted to the construction of the Green's function for the Laplace equation in a domain bounded by a piecewise smooth surface. It is shown that the Green's function can be constructed in explicit form if the boundary of the domain is a sphere or a cylinder. The third part of the paper is devoted to the construction of the Green's function for the Laplace equation in a domain bounded by a piecewise smooth surface. It is shown that the Green's function can be constructed in explicit form if the boundary of the domain is a sphere or a cylinder. The fourth part of the paper is devoted to the construction of the Green's function for the Laplace equation in a domain bounded by a piecewise smooth surface. It is shown that the Green's function can be constructed in explicit form if the boundary of the domain is a sphere or a cylinder.

APPENDIX A
DERIVATION OF THE FREE ENERGY OF FORMATION (Eq. 2.1)

From Gibb's free energy,

$$\Delta F = \Delta H - T\Delta S \quad , \quad (A-1)$$

where

ΔF = free energy,

ΔH = enthalpy,

T = temperature,

ΔS = entropy.

Let heat capacity, C_p , be represented in the form of a power series

$$C_p = f(T) = \Delta a + (\Delta b \times 10^{-3}) T + (\Delta c \times 10^{-6}) T^2 + \frac{\Delta d \times 10^5}{T^2} \quad , \quad (A-2)$$

where Δa , Δb , Δc , Δd are empirical coefficients. Thus,

$$\begin{aligned} \Delta H &= \Delta H_T - \Delta H_{298} = \int_{298}^T C_p dt = \Delta a (T - 298) + \frac{1}{2} (\Delta b \times 10^{-3}) (T^2 - 298^2) \\ &\quad + \frac{1}{3} (\Delta c \times 10^{-6}) (T^3 - 298^3) - (\Delta d \times 10^5) \left(\frac{1}{T} - \frac{1}{298} \right) \quad , \\ &= (\Delta a)T + \frac{1}{2} (\Delta b \times 10^{-3}) T^2 + \frac{1}{3} (\Delta c \times 10^{-6}) T^3 - \frac{\Delta d \times 10^5}{T} + \Delta A \quad , \quad (A-3) \end{aligned}$$

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$$(4.5) \quad \dots = \dots + \dots + \dots + \dots + \dots$$

$$\dots = \dots + \dots + \dots + \dots + \dots$$

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where

$$\Delta A = -298 \Delta a - \frac{1}{2} (\Delta b \times 10^{-3}) (298^2) - \frac{1}{3} (\Delta c \times 10^{-6}) (298^3) + \frac{\Delta d \times 10^5}{298} , \quad (A-4)$$

$$\begin{aligned} \Delta S &= \Delta S_T - \Delta S_{298} = \int_{298}^T \frac{c_p}{T} dT , \\ &= \Delta a \ln \left(\frac{T}{298} \right) + (\Delta b \times 10^{-3}) (T - 298) + \frac{1}{2} (\Delta c \times 10^{-6}) (T^2 - 298^2) \\ &\quad - \frac{1}{2} (\Delta d \times 10^5) \left(\frac{1}{T^2} - \frac{1}{298^2} \right) , \\ &= \Delta a \ln T + (\Delta b \times 10^{-3}) T + \frac{1}{2} (\Delta c \times 10^{-6}) T^2 - \frac{\frac{1}{2} (\Delta d \times 10^5)}{T^2} - B' \quad (A-5) \end{aligned}$$

$$\begin{aligned} B' &= \Delta a \ln (298) + (\Delta b \times 10^{-3}) (298) + \frac{1}{2} (\Delta c \times 10^{-6}) (298^2) \\ &\quad - \frac{1}{2} (\Delta d \times 10^5) \left(\frac{1}{298^2} \right) , \quad (A-6) \end{aligned}$$

$$\begin{aligned} \Delta S_T &= 2.303 \Delta a \log T + (\Delta b \times 10^{-3}) T + \frac{1}{2} (\Delta c \times 10^{-6}) T^2 \\ &\quad - \frac{\frac{1}{2} (\Delta d \times 10^5)}{T^2} - B , \quad (A-7) \end{aligned}$$

where

$$B = B' - \Delta S_{298} ,$$

$$(1000 + 100 \times 10) \times \frac{1}{2} + (1000 + 100 \times 10) \times \frac{1}{2} = 10000$$

20000

$$10000 \times \frac{1}{2} + 10000 \times \frac{1}{2} = 10000$$

$$(1000 + 100 \times 10) \times \frac{1}{2} + (1000 + 100 \times 10) \times \frac{1}{2} = 10000$$

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since

$$\Delta F_T = \Delta H_T - T\Delta S_T,$$

$$\begin{aligned} \Delta F_T - \Delta H_{298} &= (\Delta H_T - \Delta H_{298}) - T\Delta S_T = -(2.303 \Delta a) T \log T \\ &\quad - \frac{1}{2} (\Delta b \times 10^{-3}) T^2 - \frac{1}{6} (\Delta c \times 10^{-6}) T^3 \quad (\text{A-8}) \\ &\quad - \frac{\frac{1}{2} (\Delta d \times 10^5)}{T} - T\Delta (B - a) + \Delta A . \end{aligned}$$

(10) 4 1/2 x 6 1/2 = 27 1/4

10 - 27 1/4 = -17 1/4

APPENDIX B
CALCULATION OF CRITICAL POINT OF METALS

From Young and Alder¹

$$V_C = 2.417 \times 10^{24} \sigma^3 \qquad T_C = .7232 a/RV_C,$$

$$P_C = .2596 a/V_C^2 \qquad Z_C = P_C V_C / RT_C = .3590,$$

$$a = - E_0 V_0,$$

where

R = gas constant = .08205 l-atm/K mole,

σ = diameter of metal atoms*,

E_0 = molar cohesive energy in solid state,

V_0 = molar volume of the metal in solid state,

*Young and Alder¹ calculated σ by fitting the first peak of the Percus-Yevick Hard-sphere structure factor $S(K)$ to the experimental curves for liquid metals,² finding

$$v \approx .45 = \frac{1}{6} \pi N_0 \sigma^3 / V_L .$$

The molar volume V_L of the metal must be known at the melting point to find σ . It was found that the metallic diameters given in Ref. 3 were very close to those calculated by Young and Alder and thus were used.

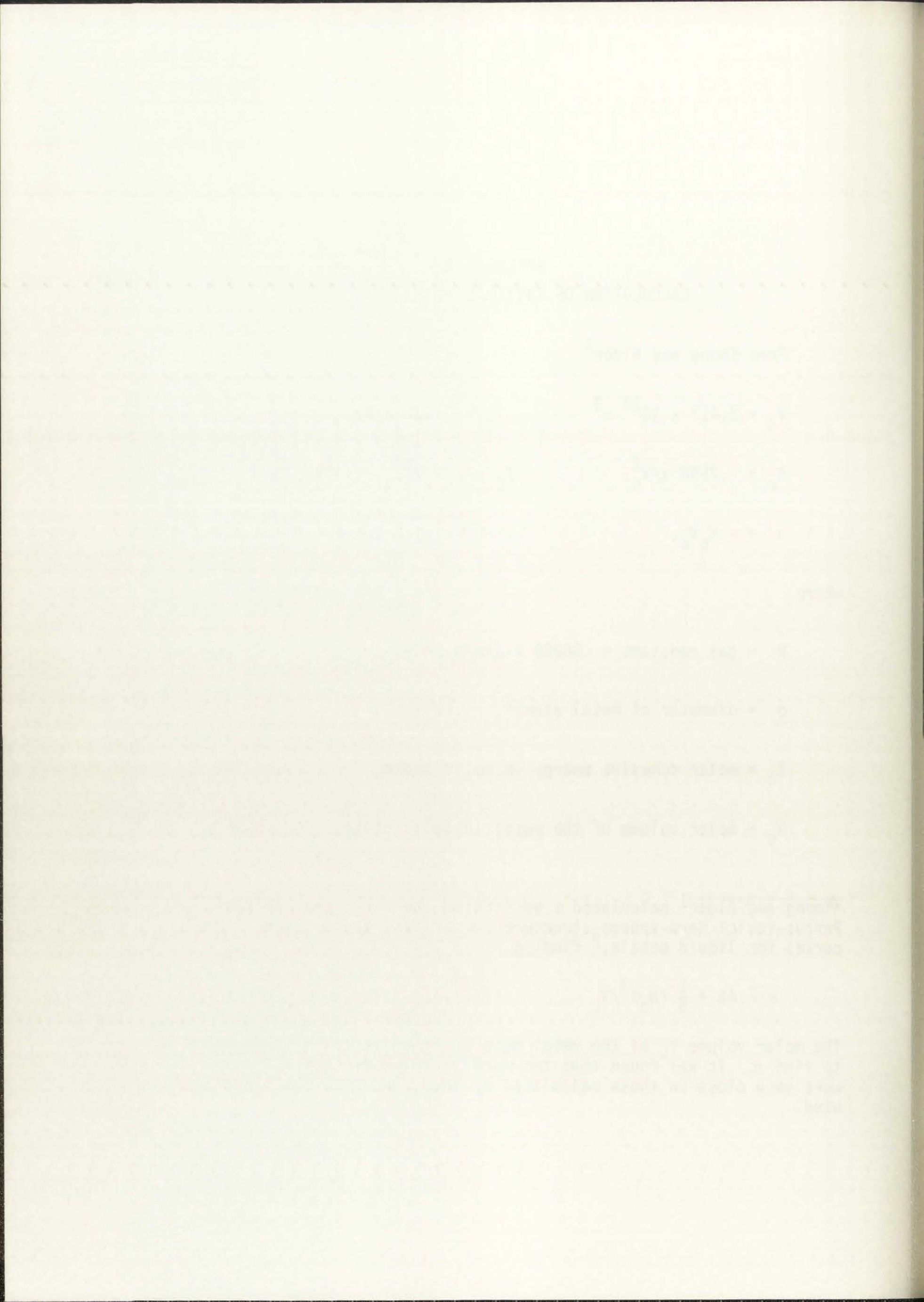
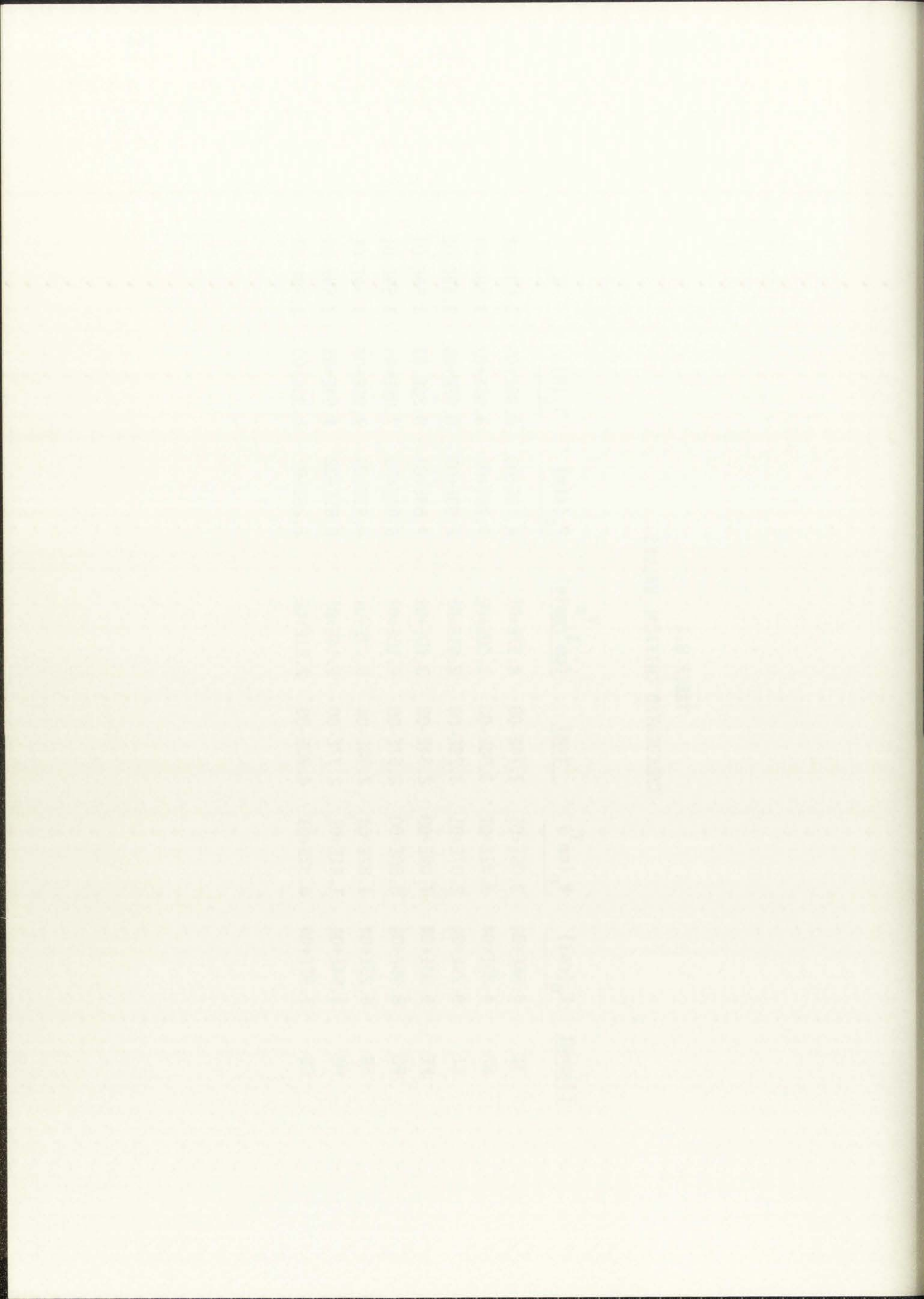


TABLE B.1
CALCULATED CRITICAL VALUES

<u>Element</u>	<u>E_0 (cal)</u>	<u>V_0 (cm³)</u>	<u>(cm)</u>	<u>V_C (cm³/mole)</u>	<u>P_C (atm)</u>	<u>T_C (K)</u>	<u>Z_C</u>
TE	4.66E+04	2.05E+01	2.74E-08	4.97E+01	4.13E+03	6.98E+03	3.59E-01
BA	4.28E+04	3.81E+01	3.96E-08	1.50E+02	7.76E+02	3.95E+03	3.59E-01
CE	9.79E+04	2.07E+01	3.29E-08	8.61E+01	2.93E+03	8.57E+03	3.59E-01
FE	9.94E+04	7.09E+00	2.34E-08	3.10E+01	7.88E+03	8.28E+03	3.59E-01
PD	8.99E+04	8.88E+00	2.57E-08	4.10E+01	5.08E+03	7.08E+03	3.59E-01
SB	6.23E+04	1.82E+01	2.78E-08	5.19E+01	4.51E+03	7.95E+03	3.59E-01
HG	1.54E+04	1.41E+01	2.77E-08	5.14E+01	8.81E+02	1.54E+03	3.59E-01
CS	1.92E+04	6.92E+01	4.70E-08	2.51E+02	2.26E+02	1.93E+03	3.59E-01



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1. D. A. Young and B. J. Alder, "Critical Point of Metals from the van der Waals Model," *Physical Review A*, Vol. 3, No. 1, (January 1971) pp. 364-371.
2. N. W. Ashcroft and J. Lekner, "Structure and Resistivity of Liquid Metals," *Physical Review*, Vol. 145, No. 1, (May 1966) pp. 83-90.
3. L. Pauling, The Nature of the Chemical Bond (Cornell U. P., Ithica, New York, 1960) third edition.

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APPENDIX C
VAN DER WAALS EQUATION-OF-STATE

The van der Waals equation-of-state takes into account the attractive force between molecules as well as the finite size of the molecules. The pressure exerted by a gas is due to molecular collision with the boundary. The attractive force, however, pulls molecules away from the boundary, due to the nonisotropic conditions which exist at the boundary and is proportional to n , molecules/unit volume. The number of molecules striking the boundary is also proportional to n , thus the total force $\propto n^2 \propto \frac{1}{v^2}$, where v is the molar volume. Thus,

$$\text{corrected ideal pressure} = P \text{ (observed pressure)} + \frac{a}{v^2} \quad (\text{C-1})$$

Also, to take into account the finite volume of the molecules,

$$\text{corrected ideal volume} = V \text{ (total molar volume)} - b \text{ (correction term due to the volume of the molecules)} \quad (\text{C-2})$$

Using Ideal Gas equation:

$$\text{(ideal volume)} \text{ (ideal pressure)} = RT, \quad (\text{C-3})$$

one obtains the van der Waals equation

APPENDIX I
THE EQUATION OF STATE

The van der Waals equation of state is written in the form
$$\left(p + \frac{a}{v^2}\right)(v - b) = RT$$

where p is the pressure, v is the volume per molecule, R is the gas constant, and T is the absolute temperature. The constants a and b are determined by the critical constants of the gas. The critical constants are the pressure, volume, and temperature at which the gas and liquid phases are in equilibrium. The critical constants are denoted by p_c , v_c , and T_c respectively. The constants a and b are given by the following equations:
$$a = \frac{27}{64} \frac{R^2 T_c^2}{p_c}$$

$$b = \frac{R T_c}{8 p_c}$$

Also, the critical constants are related to the van der Waals constants a and b by the following equations:
$$p_c = \frac{a}{27 b^2}$$

$$v_c = 3b$$

$$T_c = \frac{8a}{27Rb}$$

The equation of state can be written in the form of a cubic equation in v . The cubic equation is given by:
$$v^3 - \left(\frac{RT}{p} + b\right)v^2 + \frac{a}{p}v - \frac{ab}{p} = 0$$

$$(v - b) \left(P + \frac{a}{v^2} \right) = RT \quad , \quad (C-4)$$

or

$$P = \frac{RT}{v - b} - \frac{a}{v^2} \quad . \quad (C-5)$$

The critical isotherm passes through a point of inflection at the critical point, where the slope is zero; thus from Eq. (C-5)

$$\left(\frac{\partial P}{\partial v} \right)_T = \frac{-RT}{(v - b)^2} + \frac{2a}{v^3} = 0 \quad , \quad (C-6)$$

$$\left(\frac{\partial^2 P}{\partial v^2} \right)_T = \frac{2RT}{(v - b)^3} - \frac{6a}{v^4} = 0 \quad . \quad (C-7)$$

Also from Eq. (C-5), at the critical point

$$P_c = \frac{RT_c}{(v_c - b)} - \frac{a}{v_c^2} \quad . \quad (C-8)$$

Using Eqs. (C-6), (C-7), and (C-8) solve for a and b

$$a = \frac{27 RbT_c}{8} \quad , \quad (C-9)$$

$$b = \frac{v_c}{3} \quad . \quad (C-10)$$

critical point, where the slope is zero, then the function

$$f(x) = \frac{1}{2}x^2 - \frac{1}{3}x^3$$

$$f'(x) = x - x^2 = 0$$

At the point $(0, 0)$ of the critical point

$$f''(0) = 1 - 2(0) = 1 > 0$$

Using the first derivative test, we see that

$$f(x) \text{ has a local minimum at } x = 0$$

$$f(0) = 0$$

In a rearrangement of the equations, one obtains

$$\frac{RT_c}{P_c V_c} = \frac{8}{3} = 2.67 \quad , \quad (C-11)$$

thus if the van der Waals EOS is accurate, $\frac{RT_c}{P_c V_c}$ is approximately constant irrespective of the nature of the substance. However, values of 3.18 for He,¹ 3.42 for oxygen,¹ and 2.79 for Pd (using the critical values calculated previously) have been found, indicating that a more complicated function for the attractive-repulsive forces between molecules is required. The van der Waals EOS is more appropriate for higher pressures than the Ideal Gas EOS, but still its error is significant far below the critical point conditions.

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10. The Reaction of Ethylmagnesium Chloride with Ethyl Acrylate
by J. H. Goldstein and J. H. Goldstein

REFERENCE

1. S. Glasstone and D. Lewis, Elements of Physical Chemistry (D. Van Nostrand Co., Inc., Princeton, New Jersey, 1960) second edition.



APPENDIX D
 EOS CALCULATION USING HARD-SPHERE PRESSURE MODIFIED BY
 VAN DER WAALS MEAN-FIELD APPROXIMATION TO COHESIVE ENERGY

The mean field approximation of the cohesive energy used in the classical van der Waals model is:

$$E = -a/ac \quad , \quad (D-1)$$

where

a = positive constant.

The free electron theory for the cohesive energy generally assumed for a dense metallic phase, is of the form:

$$E = \frac{A}{v^{1/3}} + \frac{B}{v^{2/3}} + \frac{C}{ac} + D \quad , \quad (D-2)$$

and provides a fairly accurate description at high fluid density. At lower densities, substantial deviation of the theoretical and experimental values occur since the electrons attach themselves to the ions. There is evidence that this metal-nonmetal transition occurs near the critical density. At metal vapor densities lower than the critical density, which will be the expected range of interest in this study, the vapor will behave like a normal imperfect gas and at very low

RESULTS
THE CALCULATION OF THE ELECTRON ENERGY SPECTRUM BY
THE NEW METHOD AND ITS APPLICATION TO THE THEORY OF
THE ELECTRON ENERGY SPECTRUM

The new method of calculation of the electron energy spectrum is

$$E = \frac{1}{2}mv^2 + \dots$$

where λ is a positive constant.

The first electron theory for the electron energy spectrum
is based on the assumption that the electron energy spectrum
is a function of the electron energy E and the electron
density n .

$$E = \frac{1}{2}mv^2 + \dots$$

and provides a fairly accurate description of the electron energy spectrum.

The new method, which is based on the assumption that the electron energy spectrum

is a function of the electron energy E and the electron density n , provides

a more accurate description of the electron energy spectrum than the old method.

At the present time, the electron energy spectrum is calculated by the old method.

It is shown that the new method provides a more accurate description of the electron energy spectrum.

The new method is based on the assumption that the electron energy spectrum is a function of the electron energy E and the electron density n .

densities the energy will vary as V^{-1} rather than $V^{-1/3}$, thus supporting the use of the mean-field approximation.

A refined equation for the energy, based on the free electron theory,

$$E = \frac{A}{V^{1/3}} + \frac{B}{(V - V_i)^{2/3}} \quad , \quad (D-3)$$

includes the volume, V_i , excluded from the electrons by the ion cores. It represents a more realistic behavior at the energy minimum but still fails at low density.

Due to the uncertainty in the validity of the free-electron theory and the lack of experimental data in the critical region, the use of the mean-field approximation to the cohesive energy appears justified. The mean-field approximation yields a pressure, using Eq. (D-1) of

$$\frac{-\partial E}{\partial V} = \frac{-a}{V^2} \quad , \quad (D-4)$$

so that the first-order perturbation theory is

$$P = P_0 - a/V^2 \quad , \quad (D-5)$$

where

$$P_0 = \text{hard-sphere pressure,}$$

... the energy will vary as $\frac{1}{r^2}$...
... the use of the mean-field approximation ...
... a method similar to the one used in the first chapter ...

...

$$\psi = \frac{1}{\sqrt{2\pi}} e^{ikx} \quad (10-1)$$

... includes the volume V ...
... the energy E ...
... the first part of the theory ...

... Due to the uncertainty in the velocity of the free electron ...
... theory and the fact of experimental data in the critical region ...
... use of the mean-field approximation in the present theory ...
... justified. The mean-field approximation yields a ...

...

$$\psi = \frac{1}{\sqrt{2\pi}} e^{ikx} \quad (10-2)$$

... to that the first-order perturbation theory is ...

...

...

$$P_0 = \frac{RT}{V} \frac{1 + v + v^2 - v^3}{(1 - v)^3}, \quad (D-6)$$

where

$$v = \frac{\pi N_0 \sigma^3}{6V},$$

where

σ = hard-sphere diameter,

N_0 = avogadro's number,

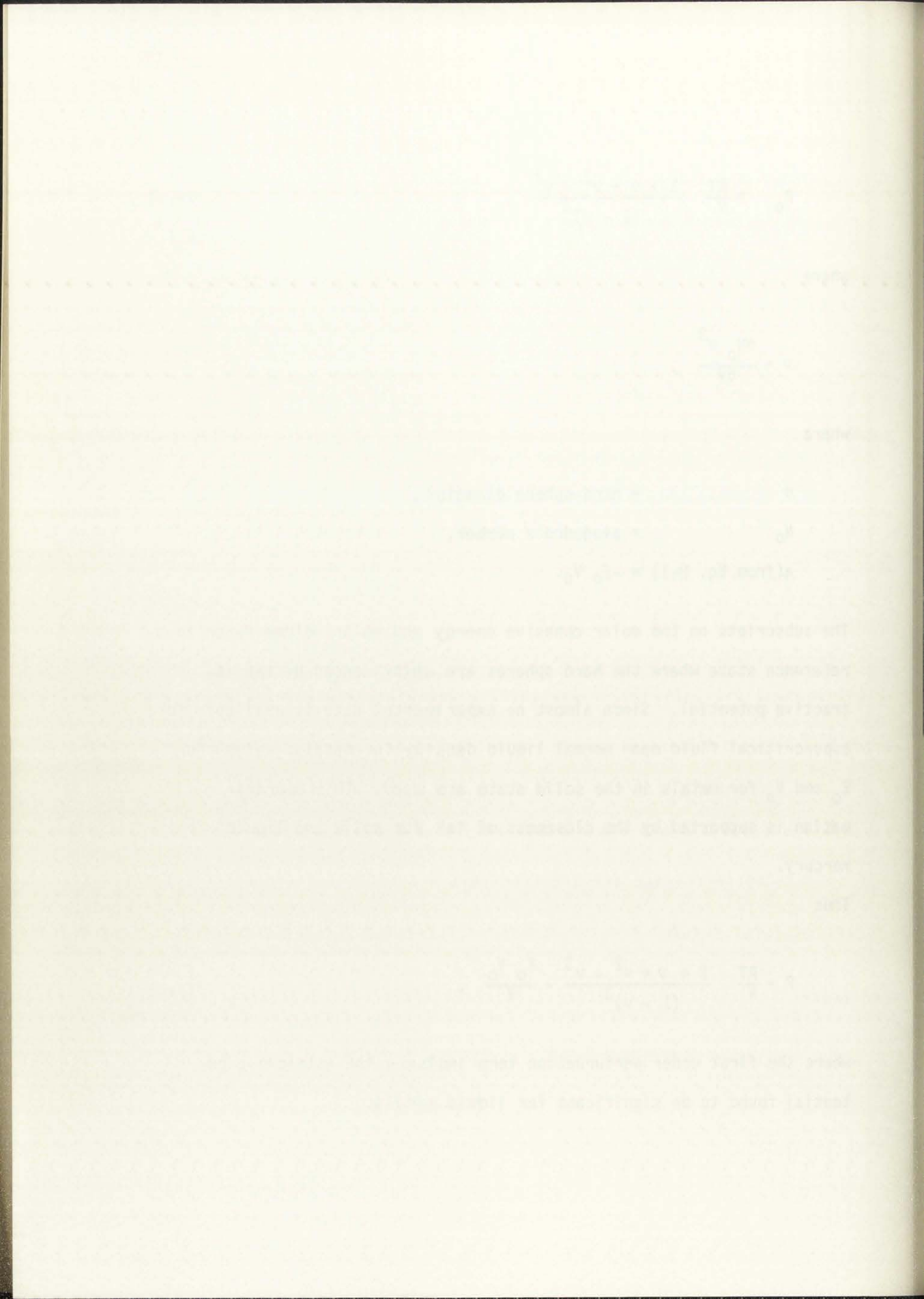
a (from Eq. D-1) = $-E_0 V_0$.

The subscripts on the molar cohesive energy and molar volume refer to a reference state where the hard spheres are uninfluenced by the attractive potential. Since almost no experimental data is available for supercritical fluid near normal liquid density for metals, values for E_0 and V_0 for metals in the solid state are used. This approximation is supported by the closeness of "a" for solid and liquid mercury.

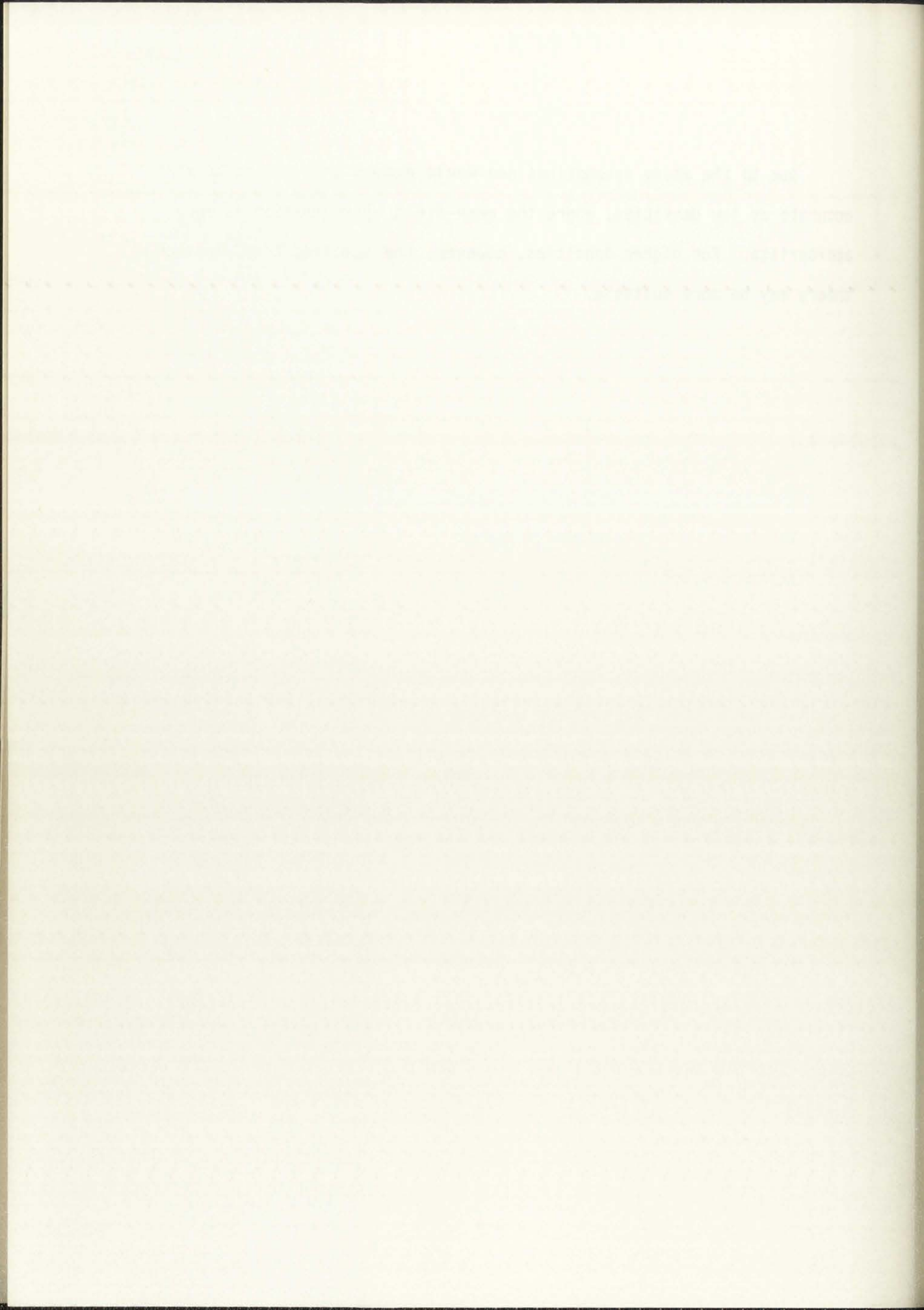
Thus

$$P = \frac{RT}{V} \frac{1 + v + v^2 - v^3}{(1 - v)^3} - \frac{E_0 V_0}{V},$$

where the first order perturbation term includes the attractive potential found to be significant for liquid metals.



Due to the above assumptions one would expect this EOS to be more accurate at low densities, where the mean-field approximation is more appropriate. For higher densities, however, the modified free electron theory may be more suitable.



APPENDIX E
REDLICH-KWONG EQUATION-OF-STATE

The Redlich-Kwong is a generalized equation-of-state, Eq. (1) that is more accurate than the van der Waals EOS.

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b) T^{1/2}}, \quad (\text{E-1})$$

where

$$a = .4275 \frac{R^2 T_c^{5/2}}{P_c},$$

$$b = .0866 \frac{RT_c}{P_c},$$

and subscripts denote critical value. The numerical values have been determined empirically to give a good fit at moderate densities.

Expanding Eq. (1) in terms of v :

$$(P)v^3 + (-RT)v^2 + \left(\frac{a}{T^{1/2}} - Pb^2 - RTb\right)v + \left(-\frac{ab}{T^{1/2}}\right) = 0. \quad (\text{E-2})$$

This EOS has been used frequently for hydrocarbons and mixture calculations.

PROBLEM 1

Let $f(x) = x^2 + 2x + 1$ and $g(x) = x^2 - 2x + 1$. Find $(f+g)(x)$.

$(f+g)(x) = (x^2 + 2x + 1) + (x^2 - 2x + 1)$
 $= x^2 + 2x + 1 + x^2 - 2x + 1$
 $= 2x^2 + 2$

$$\frac{1}{\sqrt{1-x^2}} = \frac{1}{\sqrt{1-x^2}}$$

Find the derivative of $f(x) = \frac{1}{\sqrt{1-x^2}}$.

$$f(x) = (1-x^2)^{-1/2}$$
$$f'(x) = -\frac{1}{2}(1-x^2)^{-3/2} \cdot (-2x)$$
$$= \frac{x}{(1-x^2)^{3/2}}$$

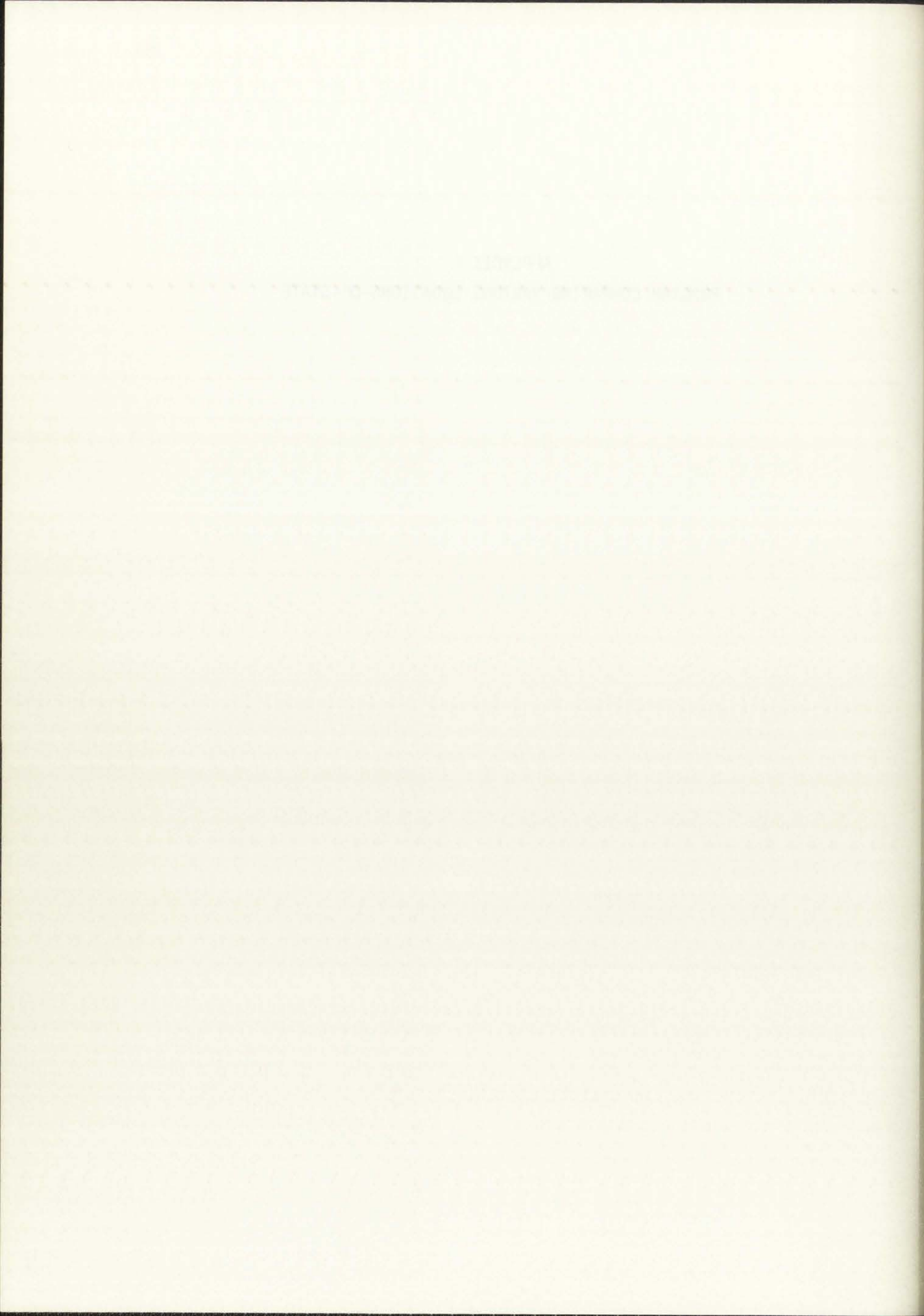
Find the derivative of $f(x) = \frac{1}{\sqrt{1-x^2}}$ using the quotient rule.

Let $f(x) = \frac{1}{\sqrt{1-x^2}}$. Then $f(x) = (1-x^2)^{-1/2}$.
Using the chain rule, $f'(x) = -\frac{1}{2}(1-x^2)^{-3/2} \cdot (-2x)$
 $= \frac{x}{(1-x^2)^{3/2}}$

Find the derivative of $f(x) = \frac{1}{\sqrt{1-x^2}}$ using the quotient rule.

Let $f(x) = \frac{1}{\sqrt{1-x^2}}$. Then $f(x) = (1-x^2)^{-1/2}$.
Using the chain rule, $f'(x) = -\frac{1}{2}(1-x^2)^{-3/2} \cdot (-2x)$
 $= \frac{x}{(1-x^2)^{3/2}}$

APPENDIX F
PROGRAM COMPARING VARIOUS EQUATIONS-OF-STATE




```

PROGRAM SKI (INPUT,TAPE11)
DIMENSION EO(12),VO(12),SIG(12),ELEM(12),A(12),VC(12),TC(12),
PC(12),ZC(12),RB(12),AA(12),PCHK(12),C(4),E(6),VM(3),PCALC(3),
IZERO(3),CRK(4),ERK(5)

```

```
CALL CHANGE(2R+8)
```

```
C NN=NUMBER OF ELEM. IN INPUT
```

```
NN=8
```

```
AV=6.023E23
```

```
PI=3.14159
```

```
SM=1.E-4
```

```
R=82.05
```

```
C C UNITS:V IN CMS**3, P IN ATM, T IN DEG. K
```

```
C C READ INPUT, CALC. CRIT. VALUES, AND VAN DE WAALS CONSTS.  
C E IN CAL., VO IN CMS**3, SIG IN CMS.
```

```
10 DO 15 I=1,NN
READ(2,210) ELEM(I),EO(I),VO(I),SIG(I)
A(I)=EO(I)*VO(I)
VC(I)=2.417E24*SIG(I)**3
TC(I)=.7232*A(I)/(1.987*VC(I))
PC(I)=.2546*A(I)*82.05/(1.987*VC(I)**2)
ZC(I)=PC(I)*VC(I)/(TC(I)*82.05)
RB(I)=VC(I)/3.0
AA(I)=276.92*RB(I)*TC(I)
PCHK(I)=AA(I)/(27.*RB(I)**2)
15 CONTINUE
WRITE(11,215)
```

```
C C INPUT P , T-START, T-END, AND STEP SIZE OF T.  
C C IF P SET LE 0., PROG. WILL CALL NEXT ELEM.  
C C IF T2(TEND) IS SET LE 0., WILL PRINT CRIT VALUES AND END  
C C PROG. WILL END AUTO. AFTER LAST ELEM. HAS BEEN CALC AND P SET 0.
```

```
N=0
```

```
5 N=N+1
IF(N.GT.NN) GO TO 40
WRITE(11,220) ELEM(N)
WRITE(11,225)
WRITE(11,230)
WRITE(11,235)
20 WRITE(59,220) ELEM(N)
WRITE(59,240)
READ(59,245) P
IF(P.LE.0.) GO TO 5
WRITE(59,250)
READ(59,255) T1
WRITE(59,260)
READ(59,265) T2
IF(T2.LE.0.) GO TO 40
WRITE(59,270)
READ(59,275) DELTT
```

```
C C CALC. IDEAL GAS VOL.
```

```
T=T1
```

```
30 VIOL=82.05*T/P
```

```
C C CALC MODIFIED VAN DE WAALS VOL.
```

```
IFLAG1=0
```

```
IFLAG2=0
```

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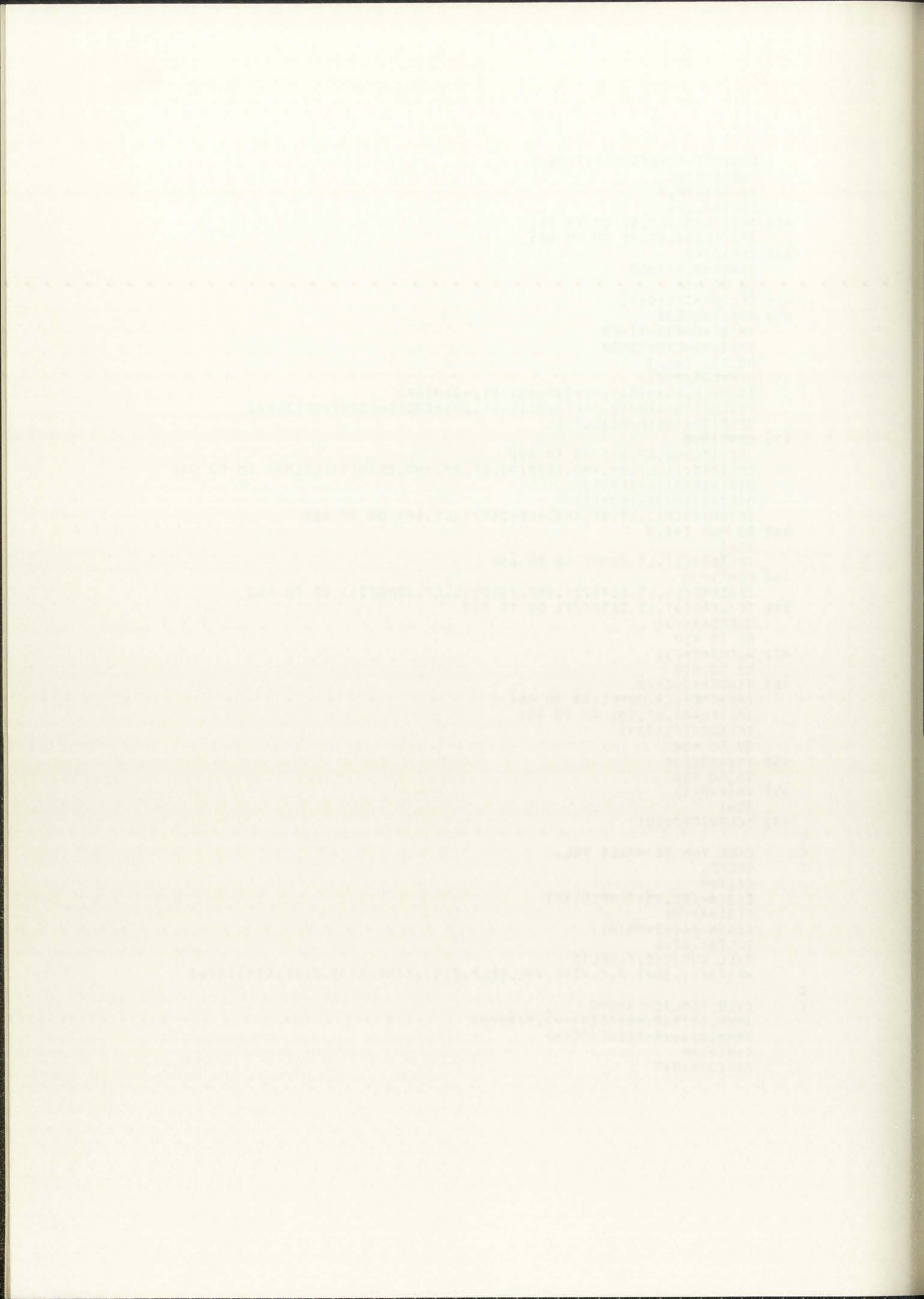
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```

CON=(PI*AV*SIG(N)**3)/6.0
GUESS=VIDL
VINCR=100.0
COMP=1.E-5
410 IF(IFLAG1.LT.5) GO TO 411
    IF(IFLAG2.GT.0) GO TO 411
420 IFLAG1=0
    VINCR=8.*VINCR
    GO TO 430
411 IFLAG1=IFLAG1+1
430 VM(1)=GUESS
    VM(2)=GUESS+VINCR
    VM(3)=GUESS+VINCR
    DO 431 I=1,3
    GAM=CON/VM(I)
    TGAM=(1.+GAM+GAM**2+GAM**3)/(1.+GAM)**3
    PCALC(I)=TGAM*82.05*T/VM(I)+41.293*EO(N)*VO(N)/VM(I)**2
    ZERO(I)=ABS(P-PCALC(I))
431 CONTINUE
    IF(IFLAG2.GT.27) GO TO 440
    IF(ZERO(1).LT.SM.AND.ZERO(2).LT.SM.AND.ZERO(3).LT.SM) GO TO 440
    DIF1=ZERO(1)-ZERO(2)
    DIF2=ZERO(2)-ZERO(3)
    IF(ABS(DIF1).LT.SM.AND.ABS(DIF2).LT.SM) GO TO 420
440 DO 460 I=1,3
    ID=I
    IF(ZERO(I).LT.COMP) GO TO 450
460 CONTINUE
    IF(ZERO(1).LT.ZERO(2).AND.ZERO(1).LT.ZERO(3)) GO TO 463
470 IF(ZERO(3).LT.ZERO(2)) GO TO 472
    GUESS=VM(2)
    GO TO 410
472 GUESS=VM(3)
    GO TO 410
463 VINCR=VINCR/2.
    IF(VINCR.LT.COMP) GO TO 451
    IF(IFLAG2.GT.50) GO TO 451
    IFLAG2=IFLAG2+1
    GO TO 430
450 VM1=VM(ID)
    GO TO 452
451 VM1=VM(1)
    ID=1
452 DELP=ZERO(ID)
C
C   CALC VAN DE WAALS VOL.
C   CDEFF.
C   C(1)=P
C   C(2)=- (82.05*T+AB(N)*P)
C   C(3)=AA(N)
C   C(4)=-AA(N)*AB(N)
C   DELT=1.0E-6
C   CALL CUBIC(C,E,DELT)
C   WRITE(11,300) P,T,VIDL,VM1,DELP,E(1),E(2),E(3),E(4),E(5),E(6)
C
C   CALC REDLICH KWONG
C   ARK=.4275*R**2+TC(N)**2.5/PC(N)
C   BRK=.3866*R*TC(N)/PC(N)
C   CRK(1)=P
C   CRK(2)=-R*T

```



```

CRK(3)=ARK/SQRT(T)-P*ARK**2-R*T*ARK
CRK(4)=-ARK*ARK/SQRT(T)
CALL CUBIC(CRK,ERK,DELT)
WRITE(11,305) P,T,ERK(1),ERK(2),ERK(3),ERK(4),ERK(5),ERK(6)
T=T+DELT
IF(T.LE.T2) GO TO 30
WRITE(11,280)
GO TO 20

```

C
C

```

OUTPUT CRIT VALUES
40 WRITE(11,200)
DO 50 I=1,NN
WRITE(11,320) ELEM(I),EO(I),VO(I),SIG(I),VC(I),PC(I),TC(I),
IZC(I),PCHK(I)
50 CONTINUE

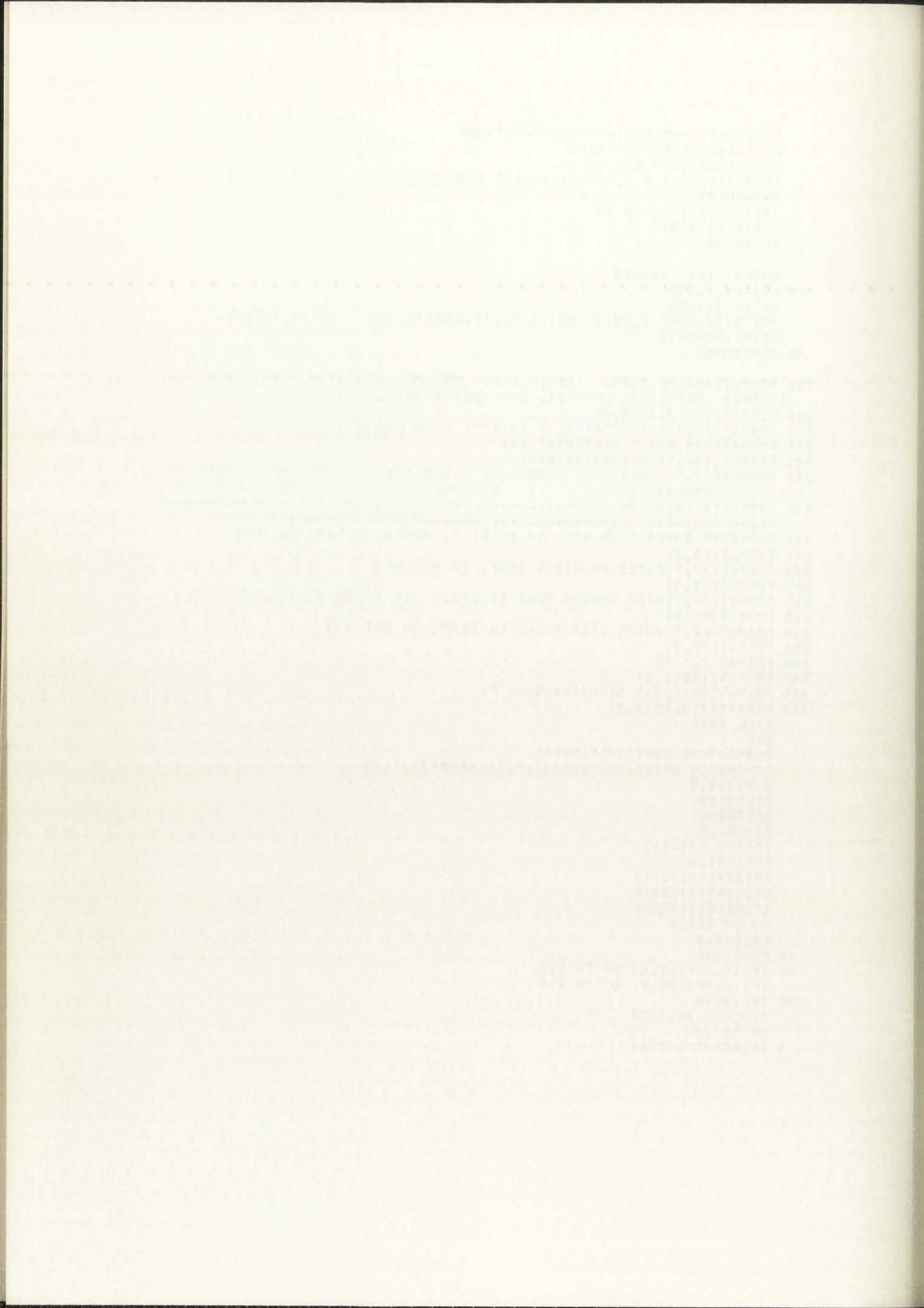
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C

```

200 FORMAT(///," ELEM. COH.F.(EO) MO.VOL. DIA. SIGMA CRIT. VOL CRIT
IT. PRES CRIT. TEM COMPRES. CHK PCRIT(VDWAALS)")
210 FORMAT(3X,A2,3E10,2)
215 FORMAT(//," V IN CMS**3, P IN ATM, T IN DEG.K")
220 FORMAT(///,40X," ELEMENT=",A2)
225 FORMAT(38X,"*****")
230 FORMAT(//," PRES. TEMP. ILO.VOL MOD VDW DELT PR.
1 VDW VOL.1 VDW VOL.2 VDW VOL.3")
235 FORMAT("-----")
1-----")
240 FORMAT(" ENTER P IN ATM IF ENTER 0. MOVES TO NEXT ELEM.")
245 FORMAT(F5.2)
250 FORMAT(//," ENTER STARTING TEMP. IN DEG.K")
255 FORMAT(F5.0)
260 FORMAT(//," ENTER ENDING TEMP IN DEG.K IF ENTER 0. WILL TERM.")
265 FORMAT(F5.0)
270 FORMAT(//," ENTER STEP INCR. IN TEMP. IN DEG.K")
275 FORMAT(F4.0)
280 FORMAT(/," ")
300 FORMAT(11E11.3)
305 FORMAT(8E11.3," REDLICH-KWONG ")
320 FORMAT(A10,8E10.2)
CALL EXIT
END
SUBROUTINE CUBIC(C,F,DELT)
DIMENSION CP(4),C(4),BN(3),P(3),ARSP(3),E(6)
GUESS=0.0
IFLAG1=0
IFLAG2=0
DINCR=.5
COMP=2.**(-16)
CP(1)=1.0
CP(2)=C(2)/C(1)
CP(3)=C(3)/C(1)
CP(4)=C(4)/C(1)
DO 50 I=1,6
E(I)=0.0
50 CONTINUE
100 IF(IFLAG1.LT.5) GO TO 110
IF(IFLAG2.GT.0) GO TO 110
200 IFLAG1=0
DINCR=.01*DINCR
GO TO 300
110 IFLAG1=IFLAG1+1

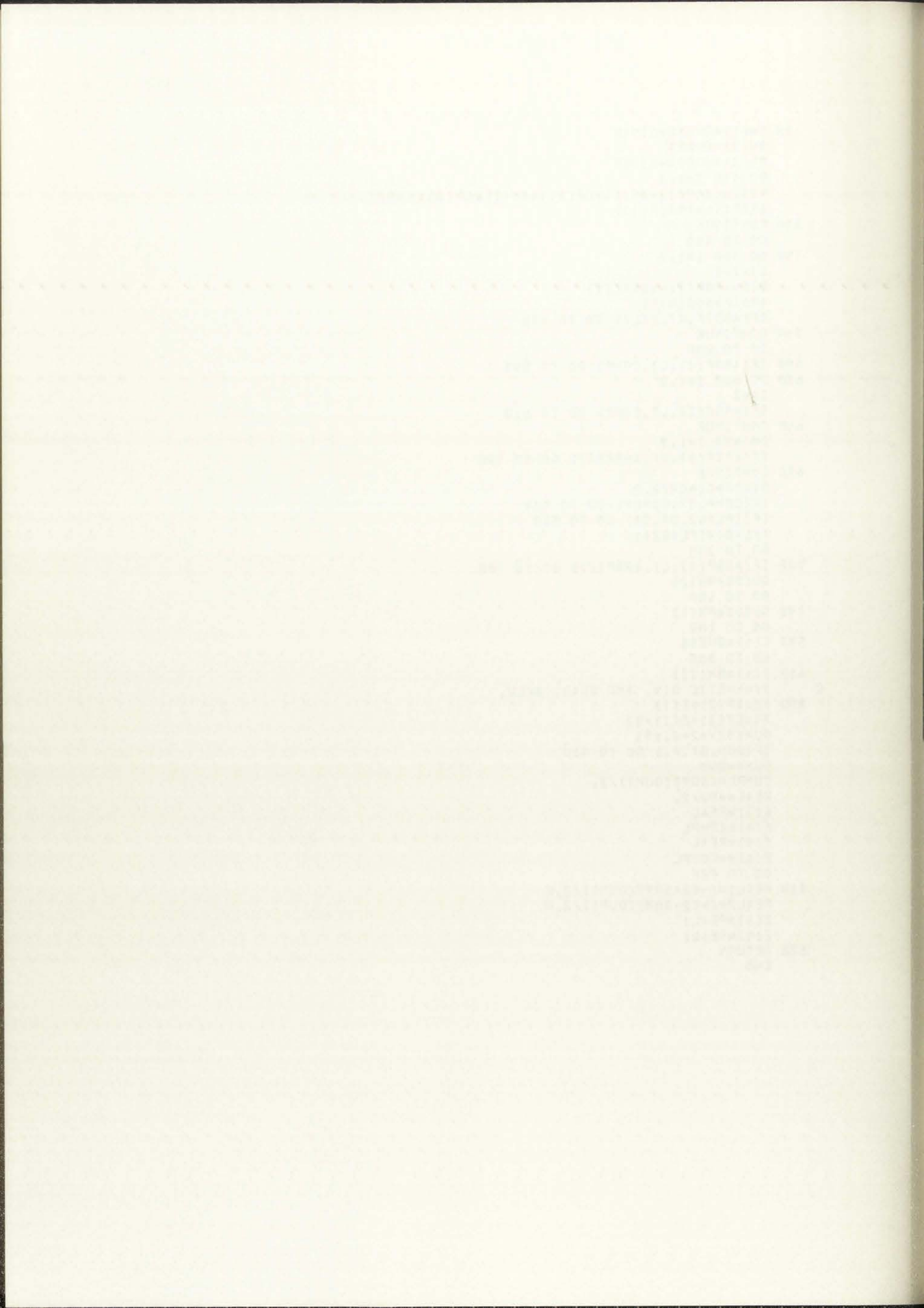
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```

300 RN(1)=GUESS+DINCR
   RN(3)=GUESS
   RN(2)=GUESS-DINCR
   DO 330 I=1,3
   P(I)=((CP(1)+RN(I)+CP(2))*RN(I)+CP(3))*RN(I)+CP(4)
   ABSP(I)=ABS(P(I))
330 CONTINUE
   GO TO 400
350 DO 360 I=1,2
   II=I+1
   DIF=ABSP(I)-ABSP(II)
   ABDIF=ABS(DIF)
   IF(ABDIF.GT.DELT) GO TO 400
360 CONTINUE
   GO TO 200
400 IF(ABSP(3).LT.COMP) GO TO 500
600 DO 660 I=1,2
   II=I
   IF(ABSP(I).LT.COMP) GO TO 610
660 CONTINUE
   DO 670 I=1,2
   IF(ABSP(3).GT.ABSP(I)) GO TO 700
670 CONTINUE
   DINCR=DINCR/2.0
   IF(OMP.GT.DINCR) GO TO 500
   IF(IFLAG2.GT.50) GO TO 500
   IFLAG2=IFLAG2+1
   GO TO 300
700 IF(ABSP(1).LT.ABSP(2)) GO TO 780
   GUESS=RN(2)
   GO TO 100
780 GUESS=RN(1)
   GO TO 100
500 E(1)=GUESS
   GO TO 800
610 E(1)=RN(II)
C SYNTHETIC DIV. AND QUAD. SOLU.
800 B2=CP(2)+E(1)
   B3=CP(3)+E(1)*B2
   DUM=B2**2-4.*B3
   IF(DUM.GT.0.) GO TO 810
   DUM=-DUM
   COMPL=(SQRT(DUM))/2.
   REAL=-B2/2.
   E(3)=REAL
   E(4)=COMPL
   E(5)=REAL
   E(6)=-COMPL
   GO TO 820
810 REAL1=(-B2+SQRT(DUM))/2.0
   REAL2=(-B2-SQRT(DUM))/2.0
   E(3)=REAL1
   E(5)=REAL2
820 RETURN
   END

```



APPENDIX G
DENSITY DETERMINATION OF CRBR TYPE FUEL

The theoretical density can be calculated via Eq. (G-1).

$$\rho_T = \frac{n M}{N_A v_0}, \quad (G-1)$$

where

- ρ_T = theoretical fuel density,
- n = number of molecules/unit cell,
- M = molecular weight,
- N_A = Avagadro's number = 6.023×10^{23} ,
- v_0 = volume of unit cell = a_0^3 ,
- a_0 = lattice parameter,

$$a_0 = 5.470 \times 10^{-8} (1.0 - .0133b) \left[1.0 + .0574 (2.0 - O/M) \right]^{\frac{1}{2}} \text{ cms} \quad (G-2)$$

where

- b = weight fraction of PuO_2 ,
- O/M = oxygen-to-metal ratio.

As a check to Eq. (G-2), if one assumes pure UO_2 , i.e., $b = 0$, and an $O/M = 2.00$, then $a_0 = 5.470$ as reported in GEAP-5583.²

To find M , molecular weight, let f_1 thru f_4 be the weight fraction of U^{234} thru U^{238} (normally only f_2 and f_4 will be

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significant). Let f_5 thru f_9 be Pu^{238} thru Pu^{242} .

$$\therefore \sum_{i=1}^4 f_i = 1, \quad \sum_{i=5}^9 f_i = 1, \quad (G-3)$$

$$M = (1 - b) \sum_{i=1}^4 f_i M_i + b \sum_{i=5}^9 f_i M_i + (O/M) M_{10},$$

where

M_i = molecular weight of each isotope,

M_{10} = molecular weight of oxygen.

Since UO_2 and PuO_2 are face-centered-cubic (FCC), then:

$$n = 4,$$

substituting Eq. (G-3) and (G-2) into (G-1):

$$\rho_T = \frac{4}{6.023 \times 10^{23}} \frac{(1 - b) \sum_{i=1}^4 f_i M_i + b \sum_{i=5}^9 f_i M_i + (O/M) M_{10}}{\left\{ 5.470 \times 10^{-8} (1.0 - .0133b) \left[1.0 + 0.574 \left(2.0 - \frac{O}{M} \right) \right] \right\}^3} \quad (G-4)$$

where

$$\begin{aligned} M_1 &= 234.0409 \text{ (U}^{234}\text{)}, & M_5 &= 238.0495 \text{ (Pu}^{238}\text{)}, \\ M_2 &= 235.0439 \text{ (U}^{235}\text{)}, & M_6 &= 239.0522 \text{ (Pu}^{239}\text{)}, \\ M_3 &= 236.0456 \text{ (U}^{236}\text{)}, & M_7 &= 240.054 \text{ (Pu}^{240}\text{)}, \\ M_4 &= 238.0508 \text{ (U}^{238}\text{)}, & M_8 &= 241.00 \text{ (Pu}^{241}\text{)}, \\ M_{10} &= 15.9994 \text{ (Oxygen)}, & M_9 &= 242.0587 \text{ (Pu}^{242}\text{)}. \end{aligned}$$

1. The first part of the problem is to find the value of the function $f(x)$ at $x = 1$.

$$f(x) = \frac{1}{x^2} + \frac{1}{x^3} + \frac{1}{x^4} + \dots$$

At $x = 1$,

$$f(1) = 1 + 1 + 1 + \dots$$

which is

divergent. Hence the function $f(x)$ is not defined at $x = 1$.

2. The second part of the problem is to find the value of the function $f(x)$ at $x = 2$.

At $x = 2$, the function $f(x)$ is defined and its value is $f(2) = \frac{1}{2^2} + \frac{1}{2^3} + \frac{1}{2^4} + \dots$

which is a convergent series. Hence the function $f(x)$ is defined at $x = 2$.

$$f(2) = \frac{1}{2^2} + \frac{1}{2^3} + \frac{1}{2^4} + \dots$$

$$= \frac{1}{2^2} \left(1 + \frac{1}{2} + \frac{1}{2^2} + \dots \right)$$

$$= \frac{1}{2^2} \left(\frac{1}{1 - \frac{1}{2}} \right)$$

$$= \frac{1}{2^2} \left(\frac{1}{\frac{1}{2}} \right)$$

$$= \frac{1}{2^2} \times 2$$

$$= \frac{1}{2}$$

$$= 0.5$$

$$= \frac{1}{2^2} \left(\frac{1}{1 - \frac{1}{2}} \right)$$

$$= \frac{1}{2^2} \left(\frac{1}{\frac{1}{2}} \right)$$

$$= \frac{1}{2^2} \times 2$$

$$= \frac{1}{2}$$

$$= 0.5$$

For CRBR

$$\frac{Pu}{Pu + U} = 22\% \text{ inner zone, } 32\% \text{ outer zone, }^3$$

volume average

$$\begin{aligned} \frac{\overline{Pu}}{\overline{Pu + U}} &= \frac{(.22) (V_{in} = 3.838 \times 10^5 \text{ cm}^3) + (.32) (V_{out} = 3.198 \times 10^5 \text{ cm}^3)}{V_{in} + V_{out}} \\ &= .265, \end{aligned}$$

thus

$$b \approx .265,$$

since CRBR O/M is unknown

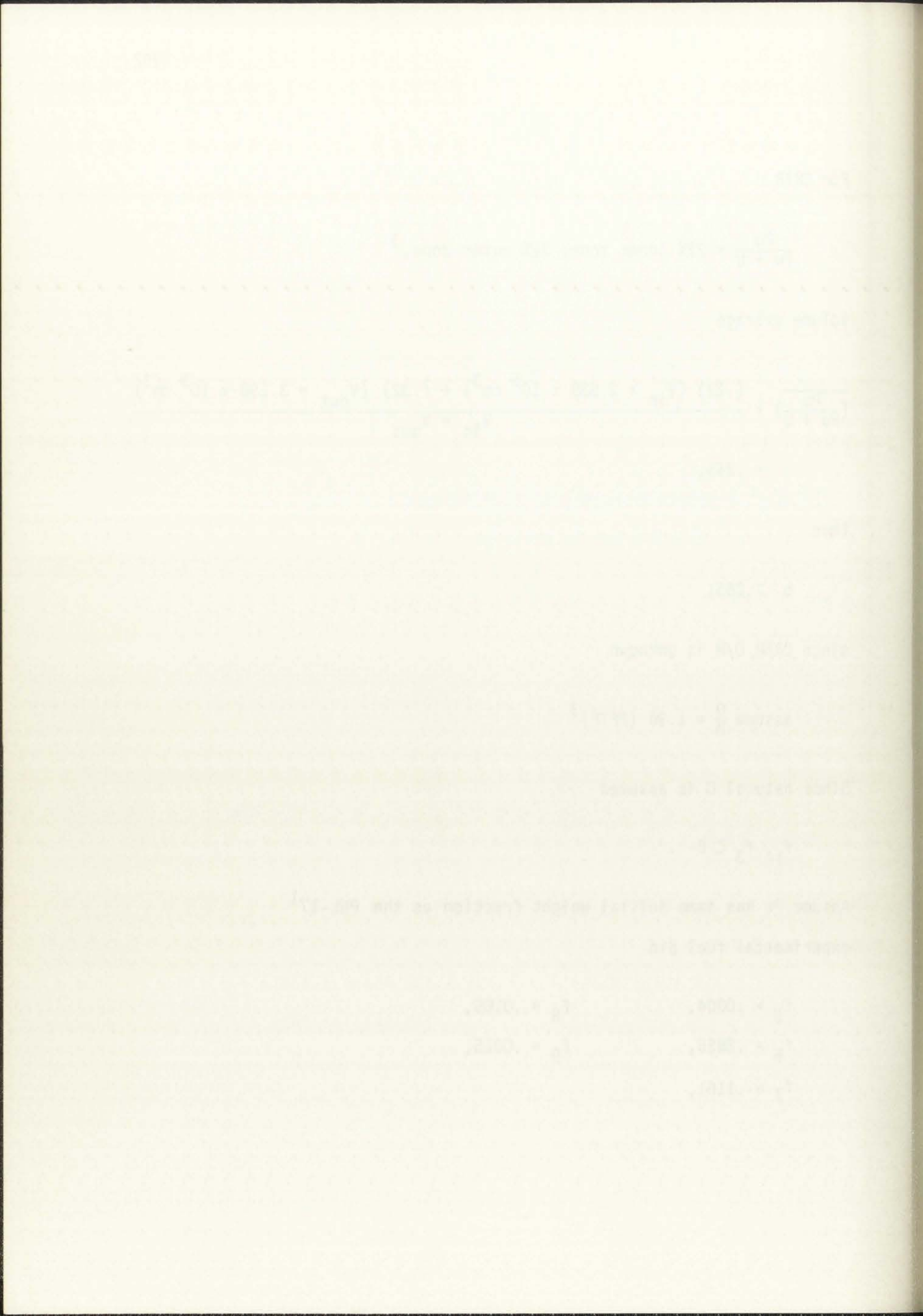
$$\text{assume } \frac{O}{M} = 1.96 (\text{FFTF})^3 .$$

Since natural U is assumed

$$f_1, f_3 \approx 0 .$$

Assume Pu has same initial weight fraction as the PNL-17¹
experimental fuel pin

$$\begin{aligned} f_5 &= .0004, & f_8 &= .0165, \\ f_6 &= .8655, & f_9 &= .0015, \\ f_7 &= .1161, \end{aligned}$$

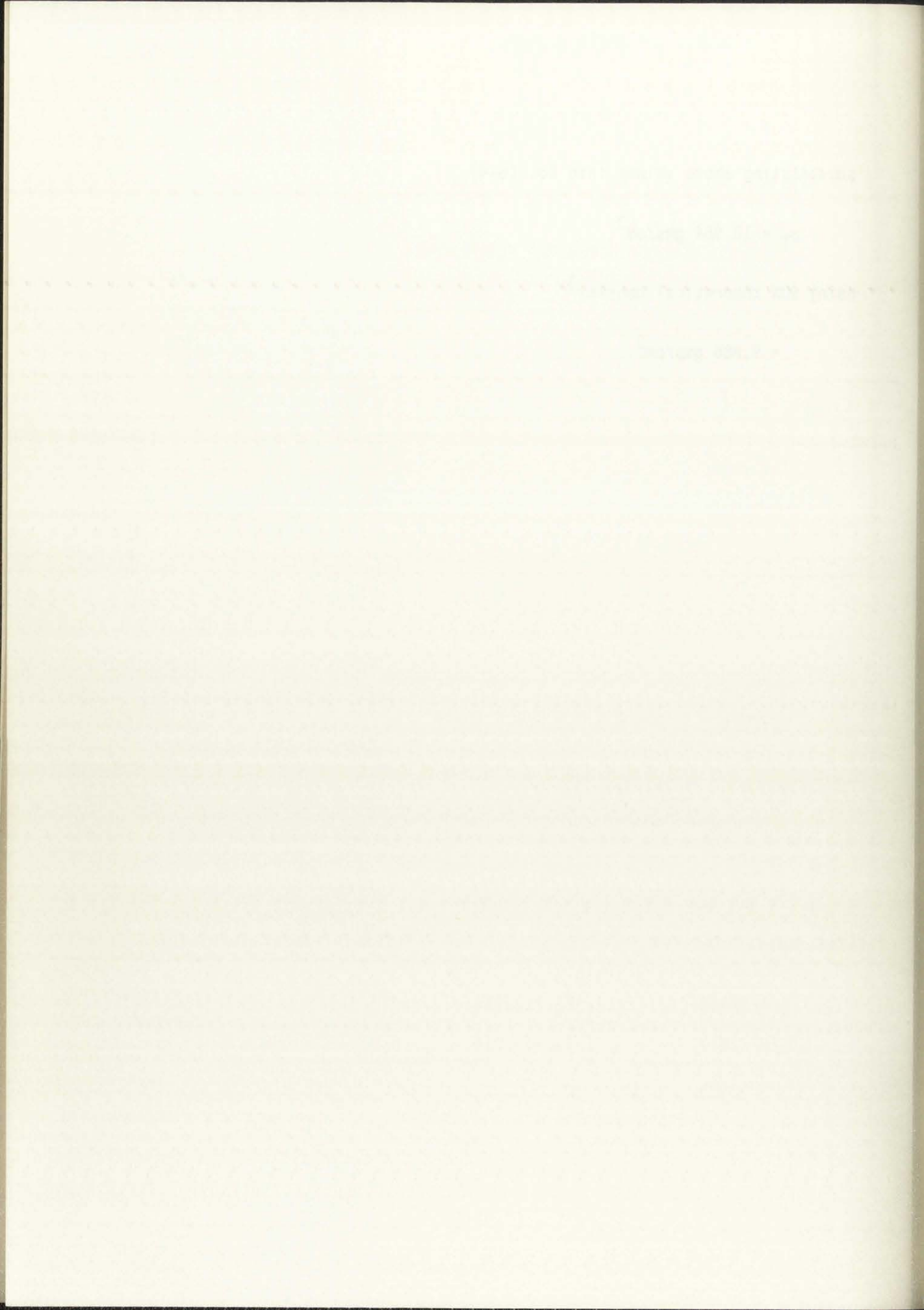


substituting above values into Eq. (G-4)

$$\rho_T = 10.984 \text{ gms/cm}^3,$$

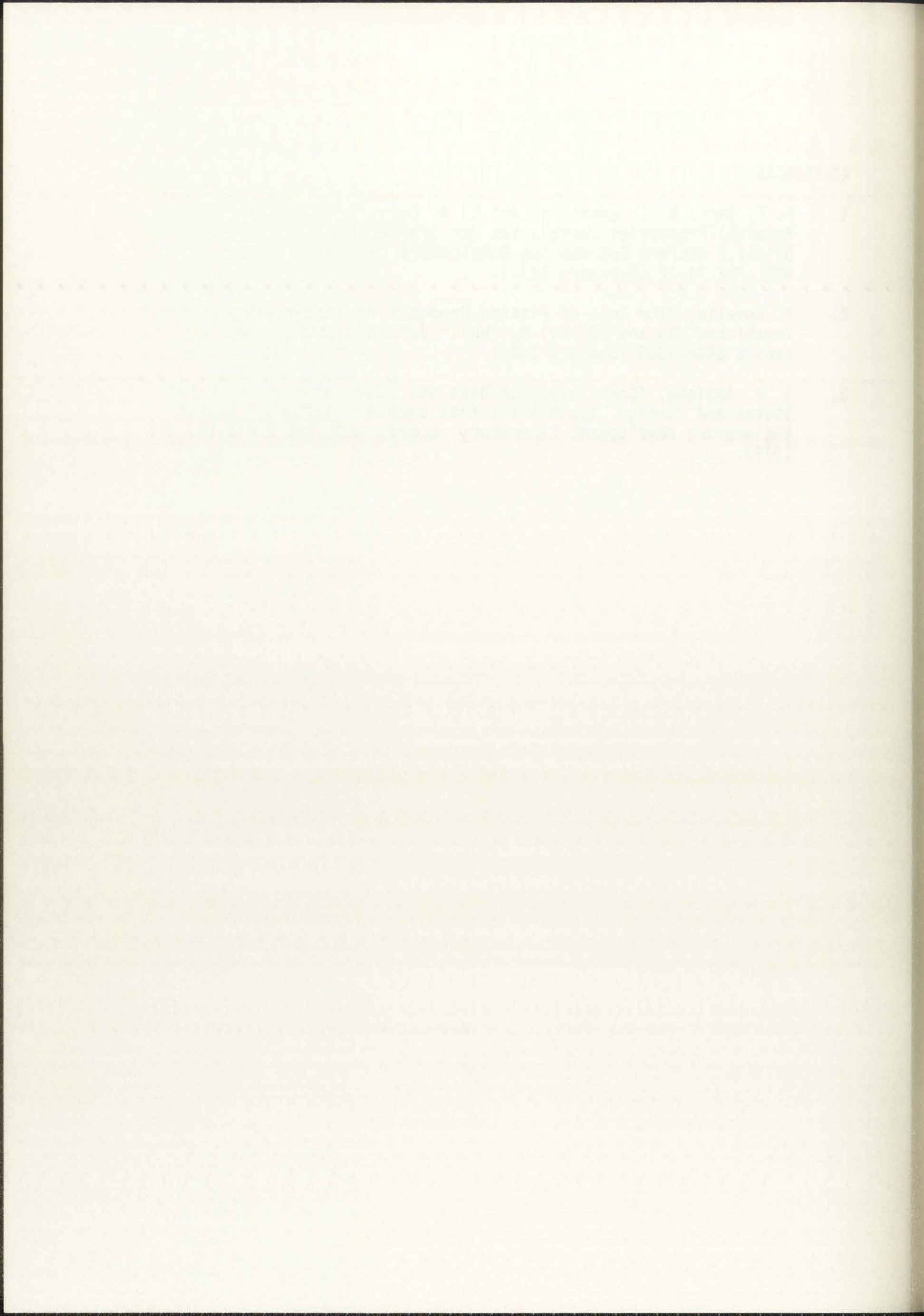
using 90% theoretical density³

$$= 9.886 \text{ gms/cm}^3.$$



REFERENCES

1. F. E. Bard, B. C. Gneiting, and C. M. Cox, "A Thermoelastic Material Properties Correlation for Uranium/Plutonium Mixed Oxides," Hanford Engineering Development Laboratory report HEDL-TME 74-12 (February 1974).
2. F. Anselin, "The Role of Fission Products in the Swelling of Irradiated UO_2 and (U, Pu) O_2 Fuel," General Electric Company report GEAP-5583 (January 1969).
3. E. A. Appleby, "Compilation of Data and Descriptions for United States and Foreign Liquid Metal Fast Breeder Reactors," Hanford Engineering Development Laboratory report, HEDL-TME 75-12 (August 1975).



APPENDIX H
CALCULATION OF FISSION PRODUCT CONCENTRATION
IN FUEL AT 3 ATOM % BURNUP

For unit cell of CRBR Fuel (U, Pu) O₂:

$$a_0 \approx 5.463 \times 10^{-8} \text{ cm}^3 \text{ }^{1,2},$$

$$v = a_0^3,$$

Assume 90% theoretical density,

$$(.90) \frac{(4 \text{ Fuel Atoms/Unit Cell})}{a_0^3} = 2.208 \times 10^{22} \text{ fuel atoms/cm}^3,$$

at 3 atom % Burnup (ignore transmutation):

$$\begin{aligned} (.03) (2.208 \times 10^{22} \text{ atoms/cm}^3) &= 6.624 \times 10^{20} \text{ fissions/cm}^3 \text{ fuel}, \\ &= 6.624 \times 10^{18} \text{ 100 fissions/cm}^3 \text{ fuel}. \end{aligned}$$

To obtain fission product volume:

$$\left(\frac{\text{fissions}}{\text{cm}^3 \text{ fuel}} \right) (\text{fission product yield}) (\text{atomic volume}) = \frac{\text{elemental volume}}{\text{cm}^3 \text{ fuel}}.$$

The fission product yield and atomic volume for appropriate fission products can be found in Table H.1.

CHAPTER 1

THE FUNDAMENTALS OF...

1.1. Introduction to the subject...

1.2. The basic principles of...

1.3. The role of the...

1.4. The importance of...

1.5. The scope of the...

1.6. The objectives of...

1.7. The structure of...

1.8. The significance of...

1.9. The contribution of...

1.10. The future of...

1.11. The conclusion...

1.12. The summary...

1.13. The final remarks...

1.14. The closing thoughts...

1.15. The end of the chapter...

TABLE H.1
YIELD DATA

Element	Yield		Pu ⁺⁺	m ⁺	Friedel Radii Å ^{***}		Atomic Volume Å ³	
	RIBD*	U**			Pure Element	Alloyed Element	Pure Element	Average Volume Alloyed Element
In	.07	.028		115. 115.	1.84	1.65	26.14	19.00
Sn	.73	.345	.089	120.2 121.2	1.86	1.66	26.88	19.20
Sb	.28	.228	.236	123.7 124.4	1.93	1.71	30.23	21.0
Ce	13.64	15.852	.406	141.5 141.7	2.95 ⁺⁺⁺	34.32 ⁺⁺⁺		
Te	3.05	2.375	13.403	129.3 129.2	2.94 ⁺⁺⁺		33.95 ⁺⁺⁺	
Ba	7.27	6.91	4.925	138.2 138.2	3.66 ⁺⁺⁺		65.16 ⁺⁺⁺	
Mo	19.93	21.344	6.304	97.3 93.2	1.56	1.55	15.51	15.49
Tc	4.34	6.01	18.265	99. 99.	1.50	1.50	14.21	14.21
Ru	22.96	16.091	5.721	102.17 103.17	1.48	1.48	13.57	13.57
			27.267					

TABLE H.1 (cont)

Element	Yield		Pu ^{††}	m [†]	Friedel Radii \AA^{***}		Atomic Volume \AA^3	
	RIBD*	U**			Pure Element	Alloyed Element	Pure Element	Average Volume Alloyed Element
Rh	4.39				1.49	1.49	13.77	13.77
		2.45		103.				
			4.033	103.				
Pd	14.35				1.52	1.52	14.79	14.65
		1.6		105.9				
			14.40	106.7				
Nb	.67				1.62	1.57	17.97	16.23
		1.473		95.0				
			1.148	95.0				
Ag	1.14				1.62	1.59	17.75	16.77
		.141		109.77				
			1.728	109.0				
Cd	1.33				1.73	1.63	21.58	18.30
		.204		113.7				
			.944	112.0				

*Calculation from RIBD code³ for 20% Pu, 80% depleted U, 3% B.U. (365-day irradiation) given in atoms/100 fissions. (Changes very little with B.U. past 1%.) Note this is effectively only Pu fission since depleted U converts to Pu with very little U fission.

TABLE H.1 (cont)

**Fission product spectrum for fast fission of U^{235} , irradiated 135 days, 0 days cooling, in atoms/100 atoms fissioned, ANL-5742.⁴

***Friedel radius² is the radius of the sphere occupying the equivalent volume of one atom in the lattice

$$R = \left(\frac{3}{4} v\right)^{1/3}$$

where for a face centered cubic (FCC) crystalline structure with 4 atoms/unit cell

$$v = \frac{a_0^3}{4}, \quad a_0 = \text{lattice parameter} .$$

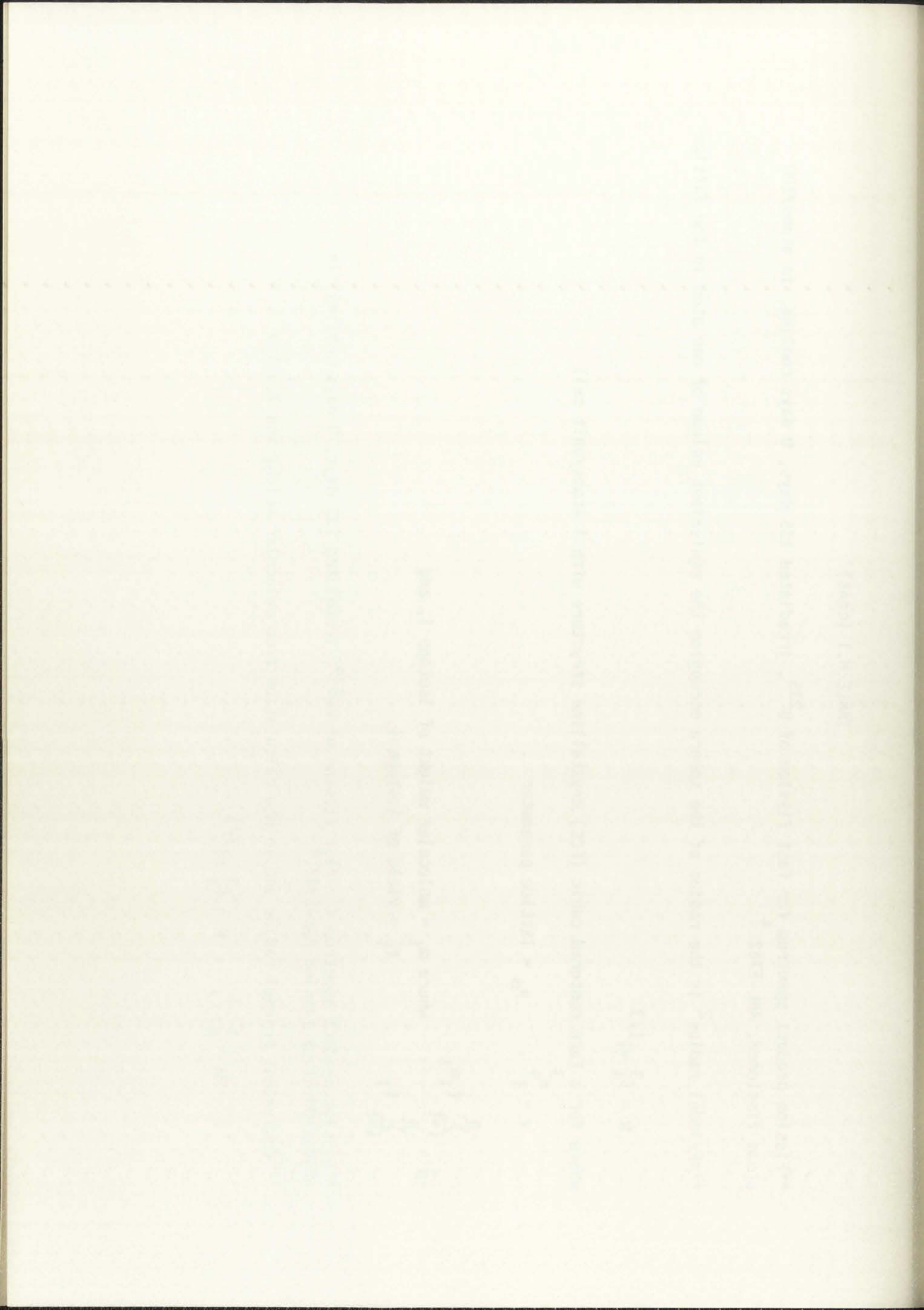
$$\bar{m} = \frac{\sum_{i=1}^n f_i m_i}{\sum_{i=1}^n f_i}$$

where m_i = molecular weight of isotope i , and
 f_i = yield of isotope i .

++Fission product spectrum for fast fission of Pu^{239} , irradiated 135 days, 0 days cooling, in atoms/100 atoms fission ANL-5742.⁴

+++Equivalent Friedel radius and volume calculation from molecular weight and density

$$v = MW \frac{1}{Na}, \quad R = \left(\frac{3}{4} v\right)^{1/3} .$$



The maximum (i.e. total segregation) individual fission product volume, molar, and mass concentration for 3 atom % burnup can be found in Table H.2 thru H.4.

If one assumes total segregation of the noble metal inclusion constituents, the following weight % shown in Table H.5 are found for the above yield data.

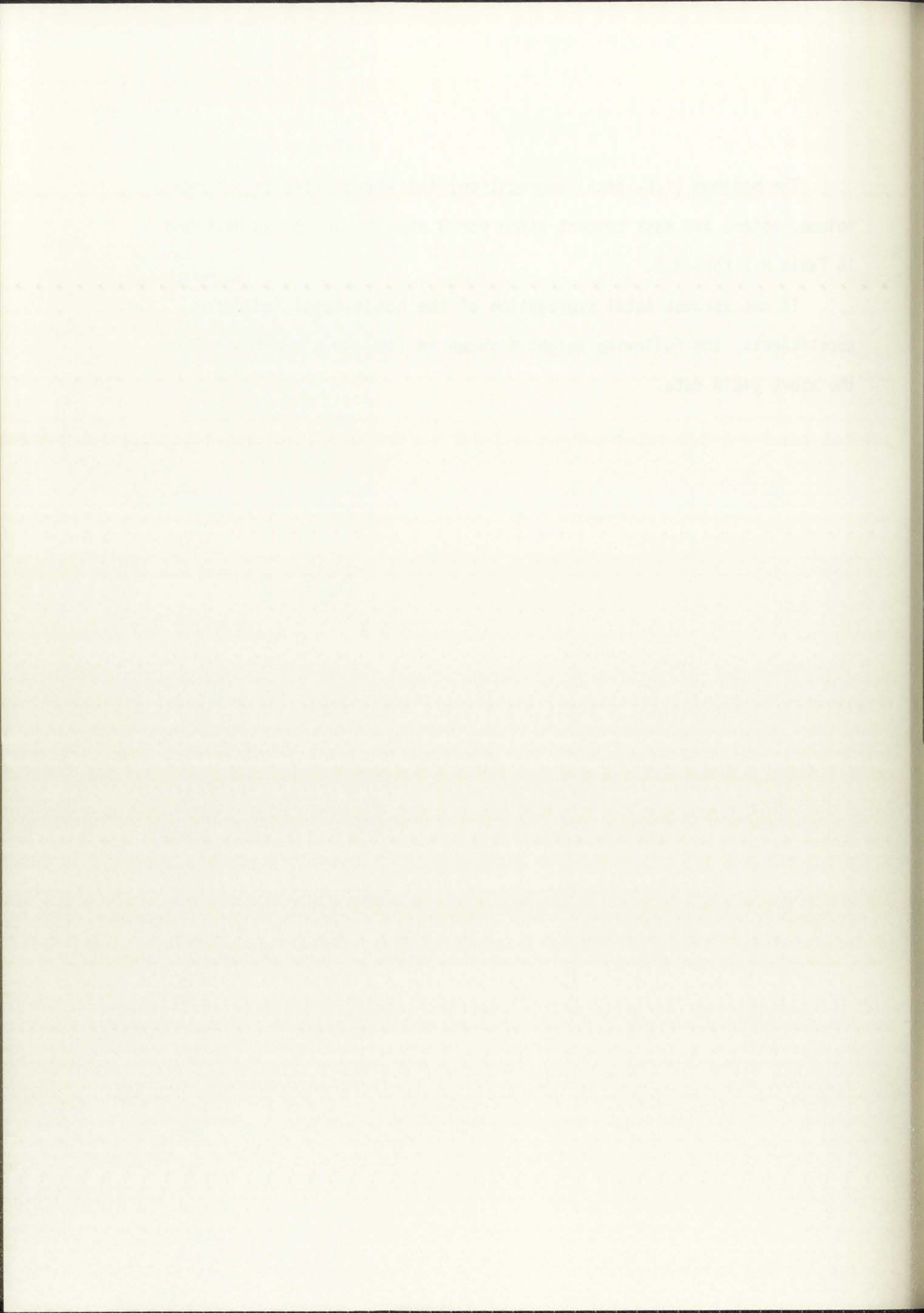


TABLE H.2
FISSION PRODUCT VOLUME CONCENTRATION FOR 3 ATOM % BURNUP

Element	Fission Product Volume/cm ³ Fuel					
	RIBD ³		Uranium ⁴		Plutonium ⁴	
	Pure Element	Alloyed	Pure Element	Alloyed	Pure Element	Alloyed
Mo	2.06×10^{-3}	2.04×10^{-3}	2.21×10^{-3}	2.20×10^{-3}	1.89×10^{-3}	1.87×10^{-3}
Tc	4.09×10^{-4}	4.09×10^{-4}	5.66×10^{-4}	5.66×10^{-4}	5.39×10^{-4}	5.39×10^{-4}
Ru	2.06×10^{-3}	2.06×10^{-3}	1.45×10^{-3}	1.45×10^{-3}	2.45×10^{-3}	2.45×10^{-3}
Rh	4.00×10^{-4}	4.00×10^{-4}	2.23×10^{-4}	2.23×10^{-4}	3.68×10^{-4}	3.68×10^{-4}
Pd	1.41×10^{-3}	1.39×10^{-3}	1.57×10^{-4}	1.55×10^{-4}	1.41×10^{-3}	1.40×10^{-3}
Te	6.36×10^{-4}		5.34×10^{-4}		1.11×10^{-3}	
Ba	3.14×10^{-3}		2.93×10^{-3}		2.72×10^{-3}	
Sb	5.61×10^{-5}	3.89×10^{-5}	4.57×10^{-5}	3.17×10^{-5}	8.13×10^{-5}	5.65×10^{-5}
Ce	3.10×10^{-3}		3.60×10^{-3}		3.05×10^{-3}	
Sn	1.30×10^{-4}	9.28×10^{-5}	6.14×10^{-5}	4.39×10^{-5}	4.20×10^{-5}	3.00×10^{-5}
In	1.21×10^{-5}	8.31×10^{-6}	4.35×10^{-6}	3.52×10^{-6}	1.54×10^{-5}	1.12×10^{-5}
Nb	7.98×10^{-5}	7.20×10^{-5}	1.75×10^{-4}	1.58×10^{-4}	1.37×10^{-4}	1.23×10^{-4}
Ag	1.34×10^{-4}	1.27×10^{-4}	1.66×10^{-5}	1.57×10^{-5}	2.03×10^{-4}	1.92×10^{-4}
Cd	1.90×10^{-4}	1.61×10^{-4}	2.92×10^{-5}	2.47×10^{-5}	1.35×10^{-4}	1.14×10^{-4}

Year	Area	Volume	Weight	Concentration
1960	100	100	100	100
1961	100	100	100	100
1962	100	100	100	100
1963	100	100	100	100
1964	100	100	100	100
1965	100	100	100	100
1966	100	100	100	100
1967	100	100	100	100
1968	100	100	100	100
1969	100	100	100	100
1970	100	100	100	100
1971	100	100	100	100
1972	100	100	100	100
1973	100	100	100	100
1974	100	100	100	100
1975	100	100	100	100
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2013	100	100	100	100
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2015	100	100	100	100
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2017	100	100	100	100
2018	100	100	100	100
2019	100	100	100	100
2020	100	100	100	100

LIST OF LITERATURE REFERENCES
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TABLE H.3
MOLAR CONCENTRATION FOR 3 ATOM % BURNUP

Element	RIBD	Moles/cm ³ Fuel ⁺	
		<u>U</u>	<u>Pu</u>
Mo	2.19 x 10 ⁻⁴	2.35 x 10 ⁻⁴	2.01 x 10 ⁻⁴
Tc	4.77 x 10 ⁻⁵	6.61 x 10 ⁻⁵	6.29 x 10 ⁻⁵
Ru	2.53 x 10 ⁻⁴	1.77 x 10 ⁻⁴	3.00 x 10 ⁻⁴
Rh	4.83 x 10 ⁻⁵	2.69 x 10 ⁻⁵	4.44 x 10 ⁻⁵
Pd	1.58 x 10 ⁻⁴	1.76 x 10 ⁻⁵	1.58 x 10 ⁻⁴
Te	3.35 x 10 ⁻⁵	2.61 x 10 ⁻⁵	5.42 x 10 ⁻⁵
Ba	8.00 x 10 ⁻⁵	7.60 x 10 ⁻⁵	6.93 x 10 ⁻⁵
Sb	3.08 x 10 ⁻⁶	2.51 x 10 ⁻⁶	4.47 x 10 ⁻⁶
Ce	1.50 x 10 ⁻⁴	1.74 x 10 ⁻⁴	1.47 x 10 ⁻⁴
Sn	8.03 x 10 ⁻⁶	3.79 x 10 ⁻⁶	2.60 x 10 ⁻⁶
In	7.70 x 10 ⁻⁷	3.08 x 10 ⁻⁷	9.79 x 10 ⁻⁷
Nb	7.37 x 10 ⁻⁶	1.62 x 10 ⁻⁵	1.26 x 10 ⁻⁵
Ag	1.25 x 10 ⁻⁵	1.55 x 10 ⁻⁶	1.90 x 10 ⁻⁵
Cd	1.46 x 10 ⁻⁵	2.24 x 10 ⁻⁶	1.04 x 10 ⁻⁵

$$^+ \text{Molar concentration} = \left(\frac{\text{fission}}{\text{cm}^3} \right) (\text{yield}) \frac{1}{NA}$$

TABLE 2. MEAN AND STANDARD DEVIATION OF THE

Logarithmic

Sample	Mean	Standard Deviation	Sample	Mean	Standard Deviation
1	1.00	0.00	11	1.00	0.00
2	1.00	0.00	12	1.00	0.00
3	1.00	0.00	13	1.00	0.00
4	1.00	0.00	14	1.00	0.00
5	1.00	0.00	15	1.00	0.00
6	1.00	0.00	16	1.00	0.00
7	1.00	0.00	17	1.00	0.00
8	1.00	0.00	18	1.00	0.00
9	1.00	0.00	19	1.00	0.00
10	1.00	0.00	20	1.00	0.00
21	1.00	0.00	22	1.00	0.00
23	1.00	0.00	24	1.00	0.00
25	1.00	0.00	26	1.00	0.00
27	1.00	0.00	28	1.00	0.00
29	1.00	0.00	30	1.00	0.00
31	1.00	0.00	32	1.00	0.00
33	1.00	0.00	34	1.00	0.00
35	1.00	0.00	36	1.00	0.00
37	1.00	0.00	38	1.00	0.00
39	1.00	0.00	40	1.00	0.00
41	1.00	0.00	42	1.00	0.00
43	1.00	0.00	44	1.00	0.00
45	1.00	0.00	46	1.00	0.00
47	1.00	0.00	48	1.00	0.00
49	1.00	0.00	50	1.00	0.00

NOTE: The values in parentheses are the standard deviations of the logarithmic data.

TABLE H.4
 MASS CONCENTRATION FOR 3 ATOM % BURNUP

<u>Element</u>	<u>RIBD*</u>	<u>gms/cm³ Fuel</u> <u>U**</u>	<u>Pu**</u>
Mo	2.10×10^{-2}	2.29×10^{-2}	1.97×10^{-2}
Tc	4.67×10^{-3}	6.54×10^{-3}	6.23×10^{-3}
Ru	2.56×10^{-2}	1.81×10^{-2}	3.10×10^{-2}
Rh	4.97×10^{-3}	2.77×10^{-3}	4.57×10^{-3}
Pd	1.68×10^{-2}	1.86×10^{-3}	1.69×10^{-2}
Te	4.27×10^{-3}	3.37×10^{-3}	7.00×10^{-3}
Ba	1.10×10^{-2}	1.05×10^{-2}	9.58×10^{-3}
Ce	2.10×10^{-2}	2.46×10^{-2}	2.08×10^{-2}
Sb	3.75×10^{-4}	3.10×10^{-4}	5.56×10^{-4}
Sn	9.53×10^{-4}	4.56×10^{-4}	3.15×10^{-4}
In	8.84×10^{-5}	3.54×10^{-5}	1.13×10^{-4}
Nb	6.85×10^{-4}	1.54×10^{-3}	1.20×10^{-3}
Ag	1.35×10^{-3}	1.70×10^{-4}	2.07×10^{-3}
Cd	1.64×10^{-3}	2.55×10^{-4}	1.16×10^{-3}

*Using molecular weight from Glasstone.⁵

**Using average molecular weight yield \bar{m} calculation earlier from Burris.⁴

TABLE 1. DATA FOR CALCULATING THE

Year	1951	1952	1953
1.00 x 10 ⁻¹	1.00 x 10 ⁻¹	1.00 x 10 ⁻¹	1.00 x 10 ⁻¹
2.00 x 10 ⁻¹	2.00 x 10 ⁻¹	2.00 x 10 ⁻¹	2.00 x 10 ⁻¹
3.00 x 10 ⁻¹	3.00 x 10 ⁻¹	3.00 x 10 ⁻¹	3.00 x 10 ⁻¹
4.00 x 10 ⁻¹	4.00 x 10 ⁻¹	4.00 x 10 ⁻¹	4.00 x 10 ⁻¹
5.00 x 10 ⁻¹	5.00 x 10 ⁻¹	5.00 x 10 ⁻¹	5.00 x 10 ⁻¹
6.00 x 10 ⁻¹	6.00 x 10 ⁻¹	6.00 x 10 ⁻¹	6.00 x 10 ⁻¹
7.00 x 10 ⁻¹	7.00 x 10 ⁻¹	7.00 x 10 ⁻¹	7.00 x 10 ⁻¹
8.00 x 10 ⁻¹	8.00 x 10 ⁻¹	8.00 x 10 ⁻¹	8.00 x 10 ⁻¹
9.00 x 10 ⁻¹	9.00 x 10 ⁻¹	9.00 x 10 ⁻¹	9.00 x 10 ⁻¹
1.00 x 10 ⁰	1.00 x 10 ⁰	1.00 x 10 ⁰	1.00 x 10 ⁰
1.10 x 10 ⁰	1.10 x 10 ⁰	1.10 x 10 ⁰	1.10 x 10 ⁰
1.20 x 10 ⁰	1.20 x 10 ⁰	1.20 x 10 ⁰	1.20 x 10 ⁰
1.30 x 10 ⁰	1.30 x 10 ⁰	1.30 x 10 ⁰	1.30 x 10 ⁰
1.40 x 10 ⁰	1.40 x 10 ⁰	1.40 x 10 ⁰	1.40 x 10 ⁰
1.50 x 10 ⁰	1.50 x 10 ⁰	1.50 x 10 ⁰	1.50 x 10 ⁰
1.60 x 10 ⁰	1.60 x 10 ⁰	1.60 x 10 ⁰	1.60 x 10 ⁰
1.70 x 10 ⁰	1.70 x 10 ⁰	1.70 x 10 ⁰	1.70 x 10 ⁰
1.80 x 10 ⁰	1.80 x 10 ⁰	1.80 x 10 ⁰	1.80 x 10 ⁰
1.90 x 10 ⁰	1.90 x 10 ⁰	1.90 x 10 ⁰	1.90 x 10 ⁰
2.00 x 10 ⁰	2.00 x 10 ⁰	2.00 x 10 ⁰	2.00 x 10 ⁰

Using average weights to calculate weight yield in calculation of the

TABLE H.5
TOTAL SEGREGATION

<u>Element</u>	<u>RIBD</u>	<u>Weight Fraction in %</u> <u>U</u>	<u>Pu</u>
Mo	28.75	43.89	25.13
Tc	6.39	12.54	7.95
Ru	35.05	34.69	39.54
Rh	6.80	5.31	5.83
Pd	23.0	3.57	21.56

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70	79	88
71	80	89
72	81	90
73	82	91
74	83	92
75	84	93
76	85	94
77	86	95
78	87	96
79	88	97
80	89	98
81	90	99
82	91	100

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4. L. Burris, Jr., and I. G. Dillon, "Estimation of Fission Product Spectra in Discharged Fuel from Fast Reactors," Argonne National Laboratory report ANL-5742 (July 1957).
5. S. Glasstone and A. Sesonske, Nuclear Reactor Engineering (Van Nostrand Reinhold Company, 1967).

1. The first part of the report is devoted to a description of the experimental apparatus and the method of measurement. The results of the measurements are given in the following tables.

2. The second part of the report is devoted to a discussion of the results of the measurements. It is shown that the results are in good agreement with the theoretical predictions.

3. The third part of the report is devoted to a discussion of the errors in the measurements. It is shown that the errors are small and that the results are reliable.

4. The fourth part of the report is devoted to a discussion of the conclusions of the report. It is shown that the results are in good agreement with the theoretical predictions.

APPENDIX I
 DERIVATION OF STEADY STATE TEMPERATURE PROFILES
 (SUBROUTINE SSTEMP)

A. Determination of heat transfer coefficient for the coolant

$$\text{Pec (Peclet number)} = \frac{D_e V \rho C_p}{K} , \quad (\text{I-1})$$

where

- D_e = equivalent diameter,
- V = coolant velocity,
- ρ = coolant density,
- C_p = coolant heat capacity,
- K = coolant thermal conductivity,

for assumed flow of liquid metals in annular channels

$$\text{Nu (Nusselt number)} = .8 \left(\frac{r_o}{r_i} \right)^{.3} \left(5.1 + .028 \text{ Pe}^{.8} \right)^{.1} , \quad (\text{I-2})$$

where

- r_i = outer clad radius (inner annulus radius),
- r_o = equivalent outer radius of coolant flow.

STABILITY
 ANALYSIS OF STEAM STATE TEMPERATURE PROFILES
 (CONTINUOUS STATE)

A. Introduction of the problem and definition of the system

$$(1) \quad \frac{d^2 T}{dx^2} + \frac{1}{x} \frac{dT}{dx} = -\frac{q}{k} \quad (1)$$

- 1. T = temperature
- 2. x = axial distance
- 3. q = constant heat source
- 4. k = constant thermal conductivity

The system is a solid cylinder of radius R in which a constant heat source q is present.

$$(2) \quad T(R) = T_0 \quad (2)$$

- where T_0 = surface temperature
- R = outer cylinder radius (inner cylinder radius)
- k = constant thermal conductivity

$$\text{Nu} = \frac{h D_e}{K} \Rightarrow h = \frac{k \text{Nu}}{D_e}, \quad (\text{I-3})$$

substituting Eqs. (I-1) and (I-2) into (I-3)

$$h \text{ (heat transfer coeff.)} = \frac{K}{D_e} \cdot 0.8 \left(\frac{r_o}{r_i} \right)^{.3} \cdot \left[5.1 + .028 \left(\frac{D_e V \rho C_p}{k} \right)^{.8} \right] \quad (\text{I-4})$$

B. Steady State Heat Transfer Equations

At steady state, heat stored term = 0.

1. Bulk Coolant Temperature.

$$\text{Axial heat in} = C_p \cdot V \cdot \rho \cdot \text{AEQ} \cdot T_{\text{Na},J-1}, \quad (\text{I-5})$$

$$\text{Axial heat out} = C_p \cdot V \cdot \rho \cdot \text{AEQ} \cdot T_{\text{Na},J}, \quad (\text{I-6})$$

$$\text{Radial heat in} = Q_{\text{Ave}} \cdot A_F \cdot \Delta Z, \quad (\text{I-7})$$

where

C_p = coolant heat capacity,

V = coolant velocity,

ρ = coolant density,

AEQ = cross-sectional coolant flow-area,

$T_{\text{Na},J}$ = axial node, J, coolant temperature,

A_F = cross-sectional area of fuel,

ΔZ = axial node length,

Q_{Ave} = average volumetric heat generation rate between axial nodes J, J-1, and

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10/10/10

$$f(x) = \frac{1}{2} \left(\frac{1}{x} + \frac{1}{x^2} \right)$$

1. Find the area under the curve

At $x=1$, $f(1) = \frac{1}{2} \left(\frac{1}{1} + \frac{1}{1^2} \right) = 1$

At $x=2$, $f(2) = \frac{1}{2} \left(\frac{1}{2} + \frac{1}{2^2} \right) = \frac{3}{8}$

At $x=3$, $f(3) = \frac{1}{2} \left(\frac{1}{3} + \frac{1}{3^2} \right) = \frac{4}{9}$

At $x=4$, $f(4) = \frac{1}{2} \left(\frac{1}{4} + \frac{1}{4^2} \right) = \frac{5}{16}$

At $x=5$, $f(5) = \frac{1}{2} \left(\frac{1}{5} + \frac{1}{5^2} \right) = \frac{6}{25}$

At $x=6$, $f(6) = \frac{1}{2} \left(\frac{1}{6} + \frac{1}{6^2} \right) = \frac{7}{36}$

At $x=7$, $f(7) = \frac{1}{2} \left(\frac{1}{7} + \frac{1}{7^2} \right) = \frac{8}{49}$

At $x=8$, $f(8) = \frac{1}{2} \left(\frac{1}{8} + \frac{1}{8^2} \right) = \frac{9}{64}$

At $x=9$, $f(9) = \frac{1}{2} \left(\frac{1}{9} + \frac{1}{9^2} \right) = \frac{10}{81}$

At $x=10$, $f(10) = \frac{1}{2} \left(\frac{1}{10} + \frac{1}{10^2} \right) = \frac{11}{100}$

At $x=11$, $f(11) = \frac{1}{2} \left(\frac{1}{11} + \frac{1}{11^2} \right) = \frac{12}{121}$

At $x=12$, $f(12) = \frac{1}{2} \left(\frac{1}{12} + \frac{1}{12^2} \right) = \frac{13}{144}$

At $x=13$, $f(13) = \frac{1}{2} \left(\frac{1}{13} + \frac{1}{13^2} \right) = \frac{14}{169}$

At $x=14$, $f(14) = \frac{1}{2} \left(\frac{1}{14} + \frac{1}{14^2} \right) = \frac{15}{196}$

$$= \frac{Q_J + Q_{J-1}}{2} ,$$

combining Eqs. (I-5), (I-6), and (I-7)

$$T_{Na,J} = T_{Na,J-1} + \frac{Q_{Ave} \cdot A_F \cdot \Delta Z}{C_p \cdot V \cdot \rho \cdot AEQ} , \quad (I-8)$$

where

T_0 = coolant inlet temperature.

2. Clad Outer Surface Temperature.

At axial node, J

$$\text{Radial heat in} = Q_J \cdot A_F \cdot \Delta Z , \quad (I-9)$$

$$\text{Radial heat out} = h \cdot 2 \pi R_{c1} \cdot \Delta Z (T_{c1,J} - T_{NA,J}) \quad (I-10)$$

Axial heat transfer = 0 (per assumptions) ,

where

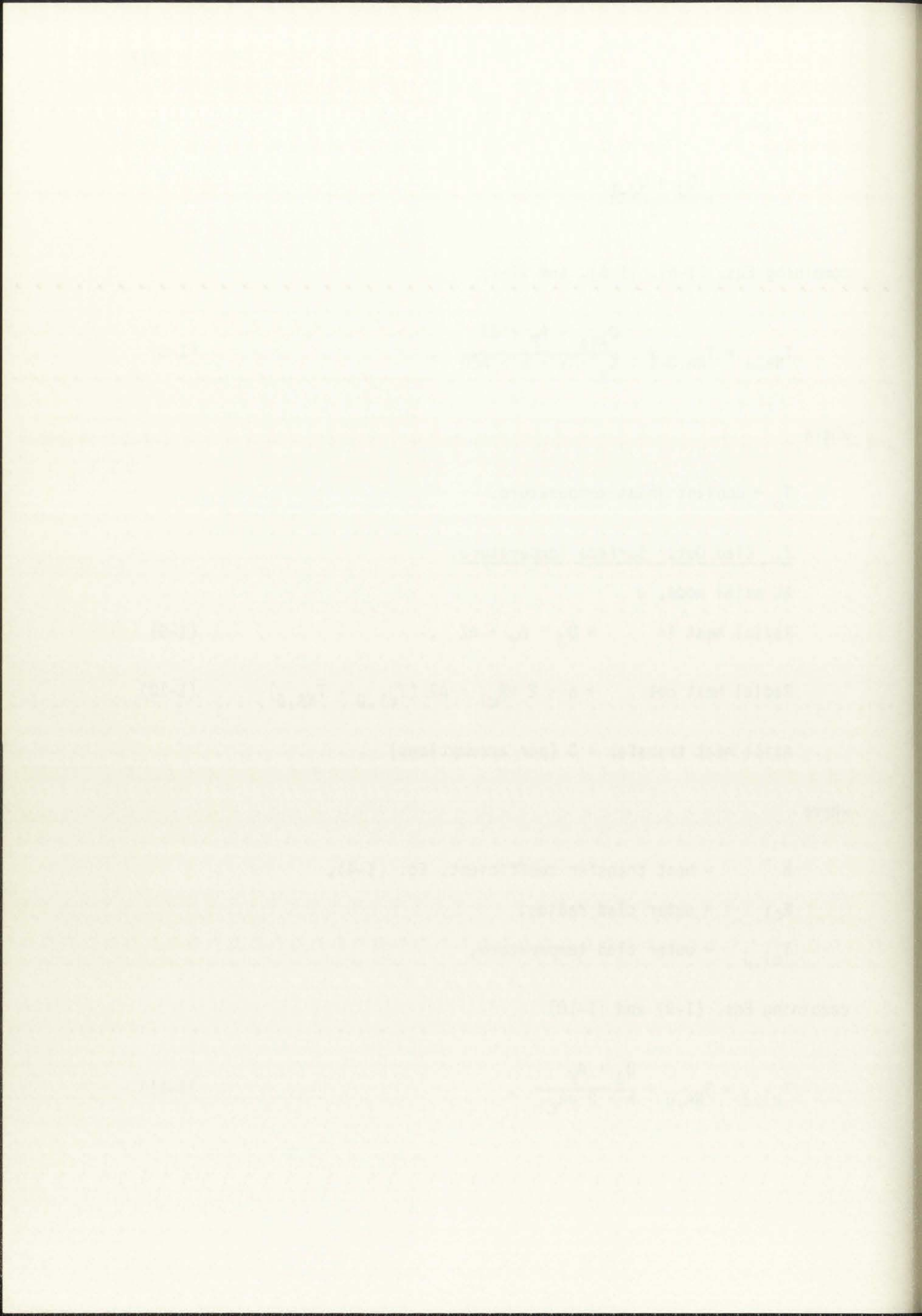
h = heat transfer coefficient, Eq. (I-4),

R_{c1} = outer clad radius,

$T_{c1,J}$ = outer clad temperature,

combining Eqs. (I-9) and (I-10)

$$T_{c1,J} = T_{NA,J} + \frac{Q_J \cdot A_F}{h \cdot 2 \pi R_{c1}} . \quad (I-11)$$



3. Clad-bond Interface Temperature.

at axial node, J

$$q = -k \cdot A \cdot \frac{dT}{dr} , \quad (I-12)$$

where

k = thermal conductivity of cladding,

A = radial heat transfer surface area = $2\pi r \Delta z$,

rearranging Eq. (I-12)

$$q \frac{dr}{r} = -k \cdot 2\pi \cdot \Delta z \cdot dT , \quad (I-13)$$

integrate Eq. (I-13) from clad inner to clad outer surface

$$q \ln \left[\frac{R_{in}}{R_{cl}} \right] = -k \cdot 2\pi \cdot \Delta z \left[T_{cl,J} - T_{in,J} \right] , \quad (I-14)$$

where

R_{in} = inner clad radius,

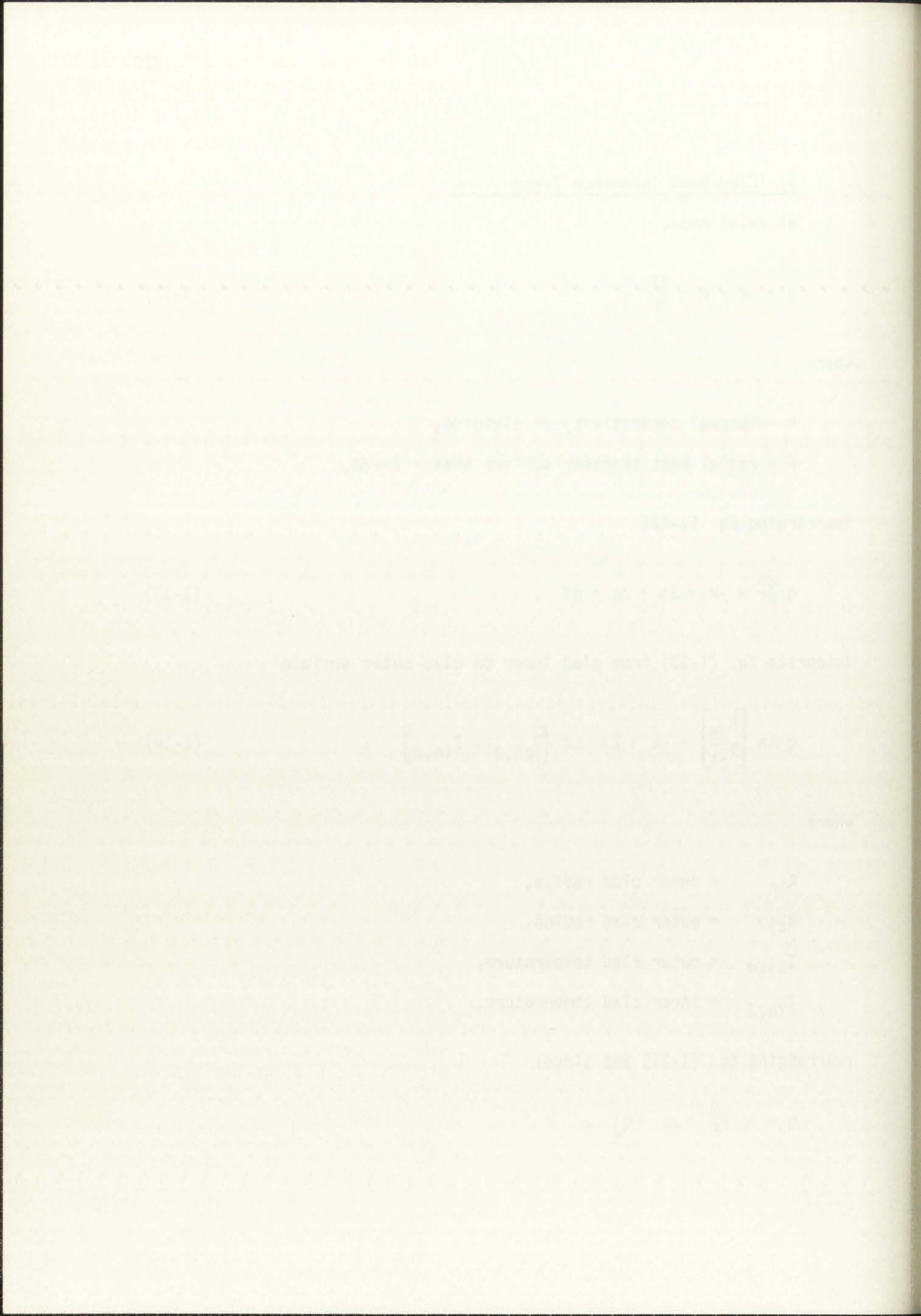
R_{cl} = outer clad radius,

$T_{cl,J}$ = outer clad temperature,

$T_{in,J}$ = inner clad temperature,

rearranging Eq. (I-14) and since:

$$q = \pi R_F^2 \cdot \Delta z \cdot Q_J ,$$



$$T_{in,J} = T_{cl,J} + \frac{Q_J \cdot R_F^2}{2k} \ln \left[\frac{R_{cl}}{R_{in}} \right] . \quad (I-15)$$

4. Fuel-bond interface

At axial node, J, assuming He bond,

$$\text{Radial heat in} = Q_J \cdot A_F \cdot \Delta z , \quad (I-16)$$

$$\text{Radial heat out} = h_{He} \cdot A_{He} \cdot (T_{F1,J} - T_{in,J}) , \quad (I-17)$$

$$\text{axial heat transfer} = 0 ,$$

where

h_{He} = helium heat transfer coefficient,

A_{He} = fuel heat transfer surface area = $2\pi \cdot R_F \cdot \Delta z$,

R_F = outer radius of fuel,

$T_{F1,J}$ = outer fuel temperature,

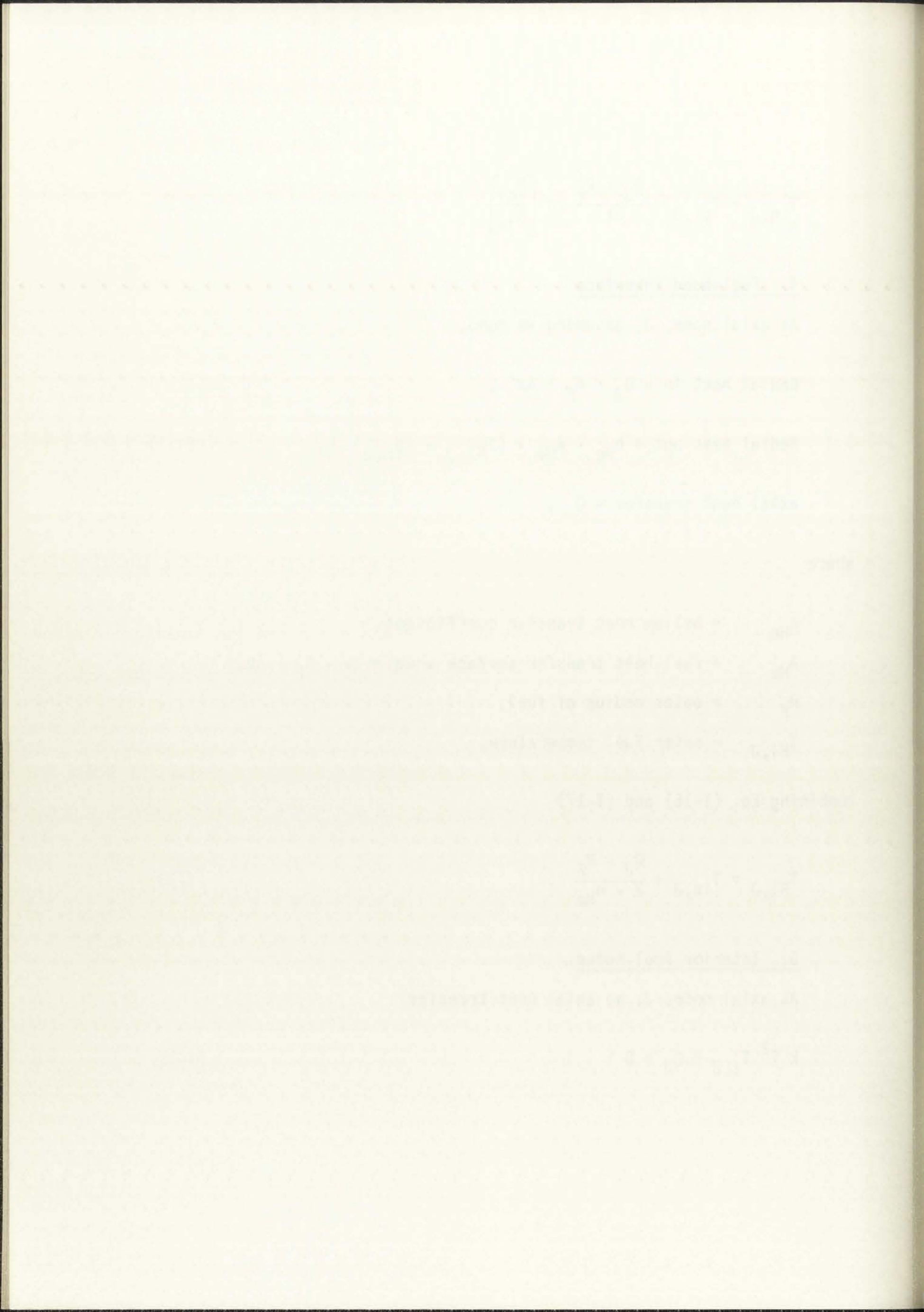
combining Eq. (I-16) and (I-17)

$$T_{F1,J} = T_{in,J} + \frac{Q_J \cdot R_F}{2 \cdot h_{He}} . \quad (I-18)$$

5. Interior fuel nodes.

At axial node, J, no axial heat transfer

$$k \nabla^2 T_{i,J} + Q_J = 0 \quad (I-19)$$



where

k = thermal conductivity of the fuel [assume $k \neq \text{func}(r)$],

$T_{i,J}$ = fuel temperature at radial node, i , axial node, J .

$$k \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right) T_{i,J} = -Q_J, \quad (\text{I-20})$$

$$Q_J r = -k \left(r \frac{\partial^2}{\partial r^2} + \frac{\partial}{\partial r} \right) T_{i,J}, \quad (\text{I-21})$$

$$\frac{-Q_J r}{k} = \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} T_{i,J} \right), \quad (\text{I-22})$$

integrate

$$r \frac{\partial T}{\partial r} = \frac{-Q_J r^2}{2k} + C_1, \quad (\text{I-23})$$

$$\frac{\partial T}{\partial r} = \frac{-Q_J r}{2k} + \frac{C_1}{r}. \quad (\text{I-24})$$

Boundary condition

$$\text{At } r = 0, \frac{\partial T}{\partial r} = 0 \quad C_1 = 0,$$

integrate Eq. (I-24)

$$T = \frac{-Q_J r^2}{4k} + C_2. \quad (\text{I-25})$$

$\int_{-\infty}^{\infty} \delta(x) dx = 1$
 $\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

(15-2) $\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

(15-3) $\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

(15-4) $\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

(15-5) $\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

(15-6) $\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

Integrate (15-6) with respect to x from $-\infty$ to ∞ .

(15-7) $\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

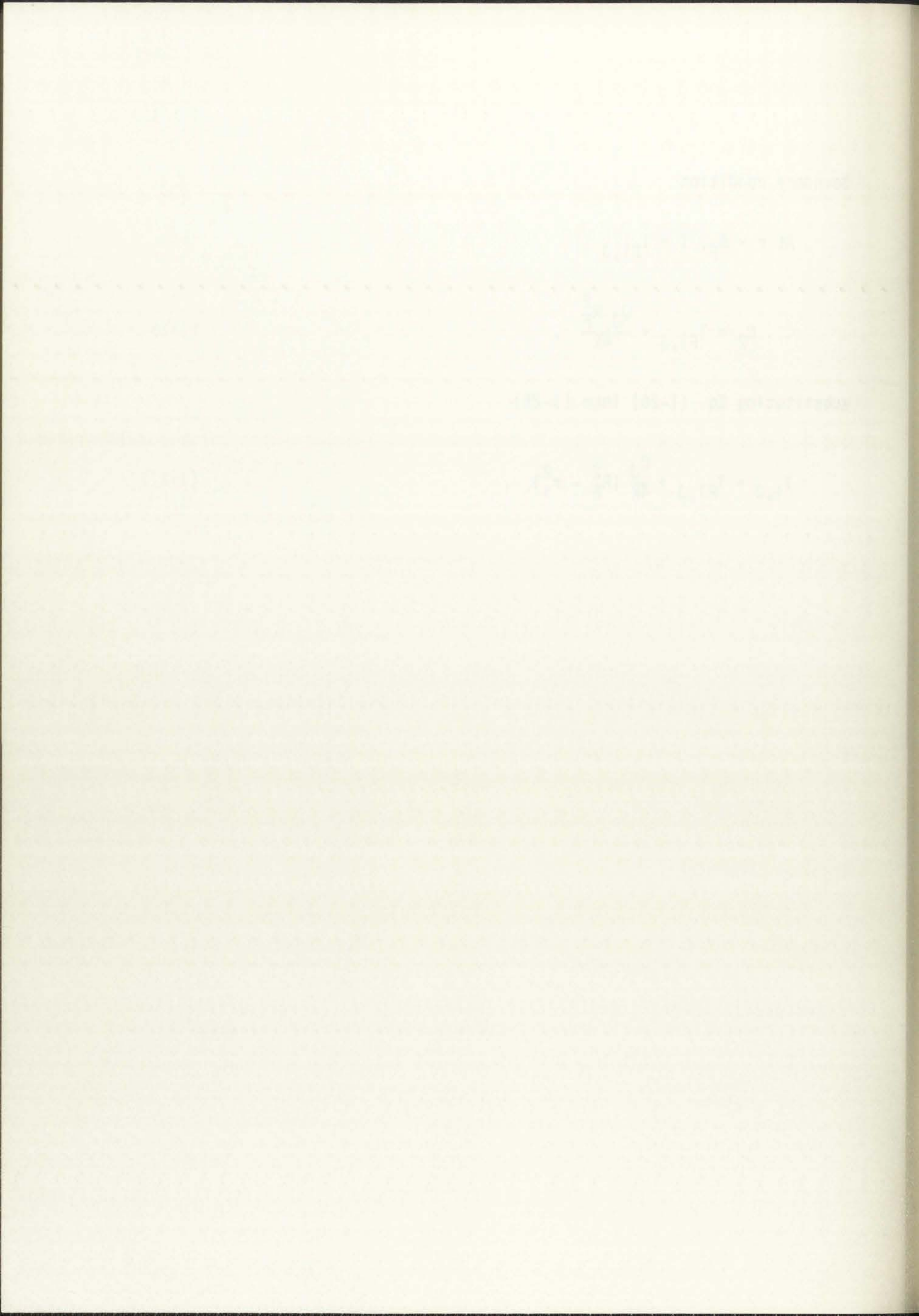
Boundary condition

$$\text{At } r = R_F, T = T_{F1,J}$$

$$\therefore C_2 = T_{F1,J} + \frac{Q_J R_F^2}{4k}, \quad (\text{I-26})$$

substituting Eq. (I-26) into (I-25)

$$T_{i,J} = T_{F1,J} + \frac{Q_J}{4k} (R_F^2 - r_i^2) . \quad (\text{I-27})$$



APPENDIX J
POINT KINETICS SOLUTION

Point kinetics is by definition spatially independent. One can put in finiteness by including the buckling terms. What will be assumed here is that the flux is defined as

$$\Phi(r,t) = S(r) P(t) \quad ,$$

where

$S(r)$ is a shape function (in this analysis taken as a chopped cosine).

$P(t)$ is the time dependent amplitude.

As stated in the text, the flux shape will be assumed constant in time during the transient. The flux amplitude equations can then be written as

$$\Lambda \frac{dP}{dt} = [\rho(t) - \beta] P(t) + \sum_{i=1}^n \lambda_i C_i(t) \quad , \quad (J-1)$$

$$\frac{d C_i(t)}{dt} = -\lambda_i C_i(t) + \beta_i P(t) \quad , \quad (J-2)$$

$$\beta = \sum_{i=1}^n \beta_i \quad , \quad (J-3)$$

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where

$\rho(t)$ = net reactivity feedback

$\Lambda = \frac{1}{v \sum_f} =$ prompt neutron generation time (for this analysis $\Lambda = 3.5 \times 10^{-7}$ sec),

β = total fraction of delayed neutrons (for this analysis $\beta = 3.01 \times 10^{-3}$),

λ_i = decay constant of the i th delayed neutron precursor group, sec^{-1} ,

C_i = reduced concentration of the i th delayed neutron precursors group,

β_i = fraction of neutrons from the i th delayed neutron precursor group,

t = independent variable, time, sec.

At steady state:

$$P(t) = 1,$$

$$\rho(t) = 0,$$

$$C_i = \frac{\beta_i}{\lambda_i},$$

$$\sum \lambda_i C_i = \sum \beta_i = \beta.$$

The integral solution of Kaganove² is used. His method is based on representing the amplitude function as a parabola. A simplifying modification made by Burns³ uses Lagrange interpolating polynomials to represent the amplitude function.

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$$P(t) = P_1 F_1(t) + P_2 F_2(t) + P_3 F_3(t) \quad , \quad (J-4)$$

where

P_1 = power amplitude at end of current time step, $t = t_1$

P_2 = power amplitude at beginning of current time step, $t = t_2$

P_3 = power amplitude at beginning of previous time step,
 $t = t_3$

and

$$F_1(t) = \frac{(t - t_2)(t - t_3)}{(t_1 - t_2)(t_1 - t_3)} \quad ,$$

$$F_2(t) = \frac{(t - t_1)(t - t_3)}{(t_2 - t_1)(t_2 - t_3)} \quad , \quad (J-5)$$

$$F_3(t) = \frac{(t - t_1)(t - t_2)}{(t_3 - t_1)(t_3 - t_2)} \quad .$$

Solving the ordinary nonhomogeneous Eq. (J-2)

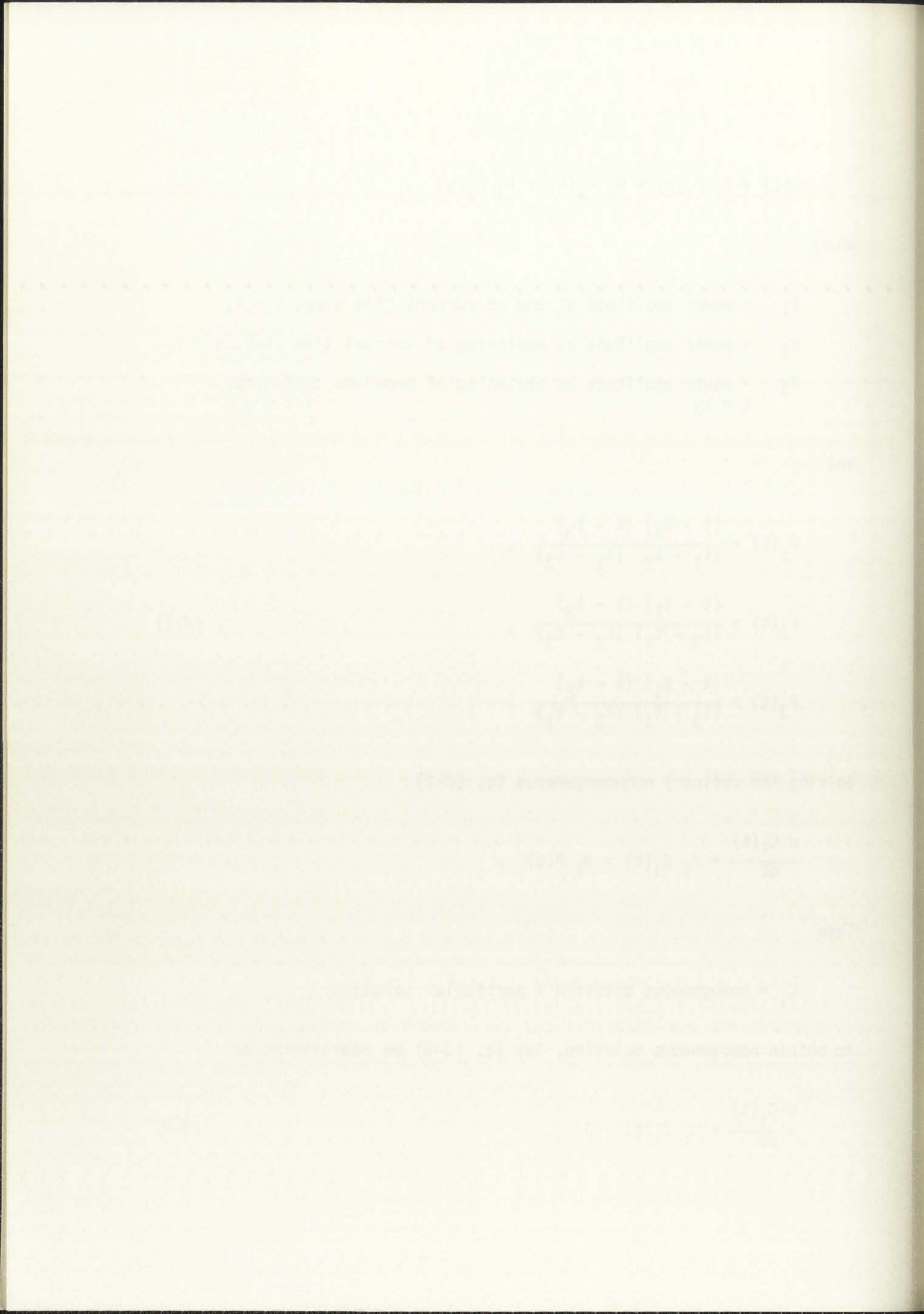
$$\frac{d C_i(t)}{dt} + \lambda_i C_i(t) = \beta_i P(t) \quad .$$

Then

C_i = homogeneous solution + particular solution

to obtain homogeneous solution, let Eq. (J-2) be represented as

$$\frac{d C_i(t)}{dt} + \lambda_i C_i(t) = 0 \quad , \quad (J-6)$$



and

$$C_i(t) \text{ homo} = Ke^{-\lambda_i t}, \quad (\text{J-7})$$

to obtain the particular solution use variation of parameters

$$C_i(t) \text{ part.} = e^{-\lambda t} \int_{t_2}^t e^{\lambda \tau} \beta_i P(\tau) d\tau, \quad (\text{J-8})$$

combining Eq. (J-7) and (J-8)

$$C_i(t) = Ke^{-\lambda_i t} + \beta_i \int_{t_2}^t e^{-\lambda(t-\tau)} P(\tau) d\tau, \quad (\text{J-9})$$

At $t = t_2$, $C_i(t) = C_i(t_2)$,

$$C_i(t_2) = Ke^{-\lambda_i t_2} + 0,$$

thus

$$K = C_i(t_2) e^{\lambda_i t_2}, \quad (\text{J-10})$$

and

$$C_i(t) = C_i(t_2) e^{-\lambda_i(t-t_2)} + \beta_i \int_{t_2}^t e^{-\lambda(t-\tau)} P(\tau) d\tau, \quad (\text{J-11})$$

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substituting Eq. (J-11) and (J-14) into Eq. (J-1)

$$\Lambda \left[P_1 \frac{dF_1(t)}{dt} + P_2 \frac{dF_2(t)}{dt} + P_3 \frac{dF_3(t)}{dt} \right] = [\rho(t) - \beta] [P_1 F_1(t) + P_2 F_2(t) + P_3 F_3(t)] + \sum_{i=1}^k \lambda_i \left[C_i(t_2) e^{-\lambda_i(t-t_2)} + \beta_i \int_{t_2}^t (P_1 F_1(\tau) + P_2 F_2(\tau) + P_3 F_3(\tau)) e^{-\lambda_i(t-\tau)} d\tau \right] \quad (J-12)$$

Let $t = t_1$, solve for P_1

$$P_1 = -\Lambda P_2 \frac{\frac{dF_2}{dt} \Big|_{t=t_1} - \Lambda P_3 \frac{dF_3}{dt} \Big|_{t=t_1} + \sum_{i=1}^k \left[\lambda_i C_i(t_2) e^{-\lambda_i(t_1-t_2)} + \lambda_i \beta_i (P_2 x_{i2} + P_3 x_{i3}) \right]}{\Lambda \frac{dF_1}{dt} \Big|_{t=t_1} - \rho(t_1) + \beta - \sum_{i=1}^k \beta_i \lambda_i x_{i1}}$$

where

$$x_{ij} = \int_{t_2}^{t_1} F_j(\tau) e^{-\lambda_i(t_1-\tau)} d\tau .$$

Thus P_1 can be solved directly, (t_1) is known since a ramp insertion of reactivity is used.

It should be noted that if one assumes a slow transient, i.e.,

$$\Lambda \frac{d\rho}{dt} \ll \sum_{i=1}^k \lambda_i C_i ,$$

Exercise 1.1.1. Let $f(x) = x^2 + 1$. Show that $f(x)$ is irreducible over \mathbb{Q} .

$$f(x) = x^2 + 1 = (x + i)(x - i)$$

$$= (x + \sqrt{-1})(x - \sqrt{-1})$$

$$= (x + \sqrt{-1})(x - \sqrt{-1})$$

Let $\alpha = i$, solve for β .

$$x^2 + 1 = (x + i)(x - i)$$

$$= (x + i)(x - i)$$

Since $i \notin \mathbb{Q}$, $f(x)$ is irreducible over \mathbb{Q} .

$$f(x) = x^2 + 1 = (x + i)(x - i)$$

Let $\alpha = i$, solve for β .

$$x^2 + 1 = (x + i)(x - i)$$

$$= (x + i)(x - i)$$

$$= (x + i)(x - i)$$

then Eq. (J-1) reduces to

$$P(t) \approx \frac{\sum_{i=1}^k \lambda_i C_i(t)}{\beta - \rho(t)} , \quad (J-14)$$

which is the same formula that Eq. (J-13) will reduce to for small time steps and small reactivity.

$$P_1 \approx \frac{\sum_{i=1}^k \lambda_i C_i(t_2)}{\beta - \rho_1} .$$

Convergence is determined by comparing the P_1 solution from Eq. (J-13) to solutions produced by taking smaller time steps, i.e., Eq (J-14). If the convergence criteria is not met, smaller time steps are used until the solution converges.

to be the case (see also [1, 2]) that the

$$\frac{1}{2} \frac{d}{dt} \left(\frac{1}{2} \frac{d}{dt} \right)$$

is proposed to be used to describe the

of the system. It is not clear, however, if

the system is stable or not. It is not clear

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1. S. Glasstone and A. Sesonske, Nuclear Reactor Engineering (Van Nostrand Reinhold Company, 1967).
2. J. J. Kaganove, "Numerical Solution of the One-Group, Space-Independent Reactor Kinetics Equations for Neutron Density Given the Excess Reactivity," Argonne National Laboratory report ANL-6132 (February 1960).
3. R. D. Burns, "A Parametric Approach to LMFBR Safety Evaluation," Purdue University report PNE-76-110 (August 1976).

THE UNIVERSITY OF CHICAGO

PHYSICS DEPARTMENT

PHYSICS 311

LECTURE 1

MECHANICS

1.1 Kinematics

1.2 Dynamics

1.3 Energy

1.4 Momentum

1.5 Angular Momentum

1.6 Relativity

1.7 Quantum Mechanics

1.8 Statistical Mechanics

1.9 Thermodynamics

1.10 Electrodynamics

1.11 Optics

1.12 Modern Physics

APPENDIX K
DERIVATION OF TRANSIENT TEMPERATURE PROFILES USING A FINITE
DIFFERENCING TECHNIQUE (SUBROUTINE TRANS)

In subroutine TRANS a node-by-node, finite differencing technique is utilized. Euler's method or forward differencing is used to approximate the time derivative of temperature.

$$\left. \frac{dT}{dt} \right|_{n,t} = \frac{T_n^{t+\Delta t} - T_n^t}{\Delta t} \quad (K-1)$$

The following finite-differences equations are generated using the general energy balance:

$$\text{heat in} - \text{heat out} + \text{heat generated} = \text{heat stored} \quad (K-2)$$

Again axial conduction heat transfer is assumed negligible. Axial convection heat transfer in the coolant channel is taken into account. Figure 4.1 shows the location of axial and radial nodes and node boundaries.

A. Fuel Centerline

$$\text{Radial heat in} = 0,$$

$$\text{Radial heat out} = k_f \cdot A \cdot \frac{dT}{dr} = k_f \cdot 2\pi \left(\frac{\Delta r}{2}\right) \Delta z \left(\frac{T_{1,j}^t - T_{2,j}^t}{\Delta r}\right), \quad (K-3)$$

$$\text{Heat generated} = Q_j \Delta V = Q_j \pi \left(\frac{\Delta r}{2}\right)^2 \Delta z, \quad (K-4)$$

APPENDIX I

EXPLANATION OF THE DATA IN THE TABLES

1. The data in the tables are the result of a series of experiments

conducted under the following conditions:

(a) The temperature was maintained at 25°C.

(b) The concentration of the reactants was 0.1 M.

(c) The reaction was allowed to proceed for a period of 10 minutes

before the measurements were taken.

(d) The reaction was carried out in a closed system.

(e) The reaction was carried out in the presence of a catalyst.

TABLE I

Reaction rate constants

Reaction rate constants for the reaction of A and B

at different temperatures and concentrations

Reaction rate constants for the reaction of A and B

$$\text{Heat stored} = \rho_F C_{pF} \Delta V \frac{dT}{dt} = \rho_F \cdot C_{pF} \cdot \pi \left(\frac{\Delta r}{2}\right)^2 \Delta z \frac{T_{1,J}^{t+\Delta t} - T_{1,J}^t}{\Delta t} \quad (\text{K-5})$$

note at axial nodes $J=1$ and $J=JMZ$ (top and bottom axial nodes) then Δz is replaced with $\frac{\Delta z}{2}$.

where

- k_f = thermal conductivity of the fuel,
- Δr = radial node distance in the fuel,
- Δz = axial node distance,
- Q_J = volumetric heat generation rate at axial node, J ,
- ρ_F = fuel density,
- C_{pF} = heat capacity of the fuel,
- Δt = time step,
- $T_{i,J}^t$ = temperature at node, i, J at time, t ,
- $T_{i,J}^{t+\Delta t}$ = temperature at node i, J at time, $t+\Delta t$ (end of time step),

combining Eqs. (K-3) thru (K-5) one obtains

$$T_{i,J}^{t+\Delta t} = T_{1,J}^t \left(1 - \frac{4\alpha}{\Delta r^2} \Delta t\right) + T_{2,J}^t \frac{4\alpha \Delta t}{\Delta r^2} + Q_J \frac{\Delta t}{\rho_F C_{pF}}, \quad (\text{K-6})$$

where

$$\alpha = \text{thermal diffusivity of the fuel} = \frac{k_F}{\rho_F C_{pF}}.$$

The first part of the paper is devoted to the study of the asymptotic behavior of the solutions of the system of equations (1) for large values of the parameter ϵ . It is shown that the solutions of this system are asymptotically equivalent to the solutions of the system of equations (2) for large values of ϵ .

In the second part of the paper, the asymptotic behavior of the solutions of the system of equations (1) is studied for small values of the parameter ϵ . It is shown that the solutions of this system are asymptotically equivalent to the solutions of the system of equations (3) for small values of ϵ .

In the third part of the paper, the asymptotic behavior of the solutions of the system of equations (1) is studied for intermediate values of the parameter ϵ . It is shown that the solutions of this system are asymptotically equivalent to the solutions of the system of equations (4) for intermediate values of ϵ .

In the fourth part of the paper, the asymptotic behavior of the solutions of the system of equations (1) is studied for large values of the parameter ϵ . It is shown that the solutions of this system are asymptotically equivalent to the solutions of the system of equations (5) for large values of ϵ .

It can be seen from Eq. (K-6) that for stability

$$\frac{\Delta r^2}{\alpha \Delta t} \gg 4 \quad \text{or} \quad \Delta t \ll \frac{\Delta r^2}{4\alpha} . \quad (\text{K-7})$$

B. Interior Fuel Nodes

$$\text{Radial heat in} = k_F A_{in} \frac{dT}{dr} = k_F \cdot 2\pi \Delta Z \left(r_i - \frac{\Delta r}{2} \right) \left(\frac{T_{i-1,J}^t - T_{i,J}^t}{\Delta r} \right) , \quad (\text{K-8})$$

$$\text{Radial heat out} = k_F A_{out} \frac{dT}{dr} = k_F \cdot 2\pi \Delta Z \left(r_i + \frac{\Delta r}{2} \right) \left(\frac{T_{i,J}^t - T_{i+1,J}^t}{\Delta r} \right) , \quad (\text{K-9})$$

$$\text{heat generated} = Q_J \Delta V = Q_J \cdot 2\pi \cdot r_i \cdot \Delta r \cdot \Delta Z \quad (\text{K-10})$$

$$\text{heat stored} = \rho_F C_{pF} \Delta V \frac{dT}{dt} = \rho_F C_{pF} 2\pi r_i \cdot \Delta r \cdot \Delta Z \left(\frac{T_{i,J}^{t+\Delta t} - T_{i,J}^t}{\Delta t} \right) , \quad (\text{K-11})$$

where

r_i = radius of i th radial node,

combining Eqs. (K-8) thru (K-11)

$$T_{i,J}^{t+\Delta t} = \frac{Q_J \cdot \Delta t}{\rho_F C_{pF}} + T_{i,J}^t \left(1 - \frac{2\cdot}{CM} \right) + \frac{T_{i-1,J}^t}{CM} \left(1 - \frac{\Delta r}{2r_i} \right) + \frac{T_{i+1,J}^t}{CM} \left(1 + \frac{\Delta r}{2r_i} \right) , \quad (\text{K-12})$$

It can be seen from equation (1) that the

$$\frac{d}{dt} \left(\frac{1}{r} \frac{dr}{dt} \right) = -\frac{1}{r^2} \left(\frac{dr}{dt} \right)^2 - \frac{1}{r} \frac{d^2 r}{dt^2}$$

Interior fuel nodes

$$\frac{d}{dt} \left(\frac{1}{r} \frac{dr}{dt} \right) = -\frac{1}{r^2} \left(\frac{dr}{dt} \right)^2 - \frac{1}{r} \frac{d^2 r}{dt^2}$$

$$\frac{d}{dt} \left(\frac{1}{r} \frac{dr}{dt} \right) = -\frac{1}{r^2} \left(\frac{dr}{dt} \right)^2 - \frac{1}{r} \frac{d^2 r}{dt^2}$$

$$\frac{d}{dt} \left(\frac{1}{r} \frac{dr}{dt} \right) = -\frac{1}{r^2} \left(\frac{dr}{dt} \right)^2 - \frac{1}{r} \frac{d^2 r}{dt^2}$$

$$\frac{d}{dt} \left(\frac{1}{r} \frac{dr}{dt} \right) = -\frac{1}{r^2} \left(\frac{dr}{dt} \right)^2 - \frac{1}{r} \frac{d^2 r}{dt^2}$$

radius of the radial node

comparing eqs (10) and (11)

$$\frac{d}{dt} \left(\frac{1}{r} \frac{dr}{dt} \right) = -\frac{1}{r^2} \left(\frac{dr}{dt} \right)^2 - \frac{1}{r} \frac{d^2 r}{dt^2}$$

where

$$CM = \frac{\Delta r^2}{\alpha \Delta t} \text{ (i.e., stability criteria Eq. K-7) .}$$

C. Fuel-Bond Interface

This node is located at the fuel surface and extends from $\frac{\Delta r}{2}$ into the fuel to half way between the fuel and clad, i.e. half the distance into the bond. The bond is assumed to be He with no heat generation occurring in the bond.

$$\text{radial heat in} = k_f A_{in} \frac{dT}{dr} = k_f \cdot 2\pi \left(r_f - \frac{\Delta r}{2} \right) \Delta z \left(\frac{T_{i-1,J}^t - T_{i,J}^t}{\Delta r} \right) , \quad (K-13)$$

heat generated = heat generated in fuel + heat generated in bond,

$$\text{heat generated} = Q_J \Delta z \cdot \pi \left[r_F^2 - \left(r_F - \frac{\Delta r}{2} \right)^2 \right] + 0 , \quad (K-14)$$

heat stored = heat stored in fuel + heat stored in bond,

$$\begin{aligned} \text{heat stored} = & \left[\frac{T_{i,J}^{t+\Delta t} - T_{i,J}^t}{\Delta t} \right] \pi \Delta z \left[\rho_b C_{pb} \left(r_F \cdot Thb + \frac{Thb^2}{4} \right) \right. \\ & \left. + \rho_F C_{pF} \left(r_F \Delta r - \frac{\Delta r^2}{4} \right) \right] , \quad (K-15) \end{aligned}$$

radial heat out = radial heat out of fuel surface - heat stored in nodal bond volume,

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$$\text{heat stored in nodal bond volume} = \rho_b C_{pb} \left(r_F \cdot Thb + \frac{Thb^2}{4} \right) \frac{dT}{dt} \pi \Delta z, \quad (K-16)$$

$$\text{radial heat out of fuel surface} = h_b \cdot 2\pi \cdot r_F \cdot \Delta z \left[T_{i,J}^t - T_{i+1,J}^t \right], \quad (K-17)$$

where

- r_F = fuel radius,
- ρ_b = bond density,
- C_{pb} = heat capacity of bond,
- Thb = bond thickness,
- h_b = bond heat transfer coefficient,

combining Eqs. (K-13) thru (K-17)

$$T_{i,J}^{t+\Delta t} = T_{i,J}^t + \frac{\Delta t}{\rho_F \cdot C_{pF} \left(r_F \Delta r - \frac{\Delta r^2}{4} \right)} \left[\frac{2 \cdot k_F}{\Delta r} \left(r_F - \frac{\Delta r}{2} \right) (T_{i-1,J}^t - T_{i,J}^t) - 2 \cdot h_b \cdot r_f (T_{i,J}^t - T_{i+1,J}^t) + Q_J \left(r_F \Delta r - \frac{\Delta r^2}{4} \right) \right]. \quad (K-18)$$

D. Bond-Clad Interface

This node is located at the clad inner surface and extends from halfway into the bond to halfway through the clad. It is assumed that heat generation does not occur either in the bond or clad. It should be noted that the heat out of a node is equal to the heat into the adjoining node.

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radial heat in = radial heat out of fuel surface - heat stored in nodal bond volume (see Eqs. (K-16), (K-17)),

$$\text{radial heat out} = k_c \cdot 2\pi \Delta z \left(r_c + \frac{\text{Thcl}}{2} \right) \cdot \left(\frac{T_{i,J}^t - T_{i+1,J}^t}{\text{Thcl}} \right), \quad (\text{K-19})$$

heat generated = 0,

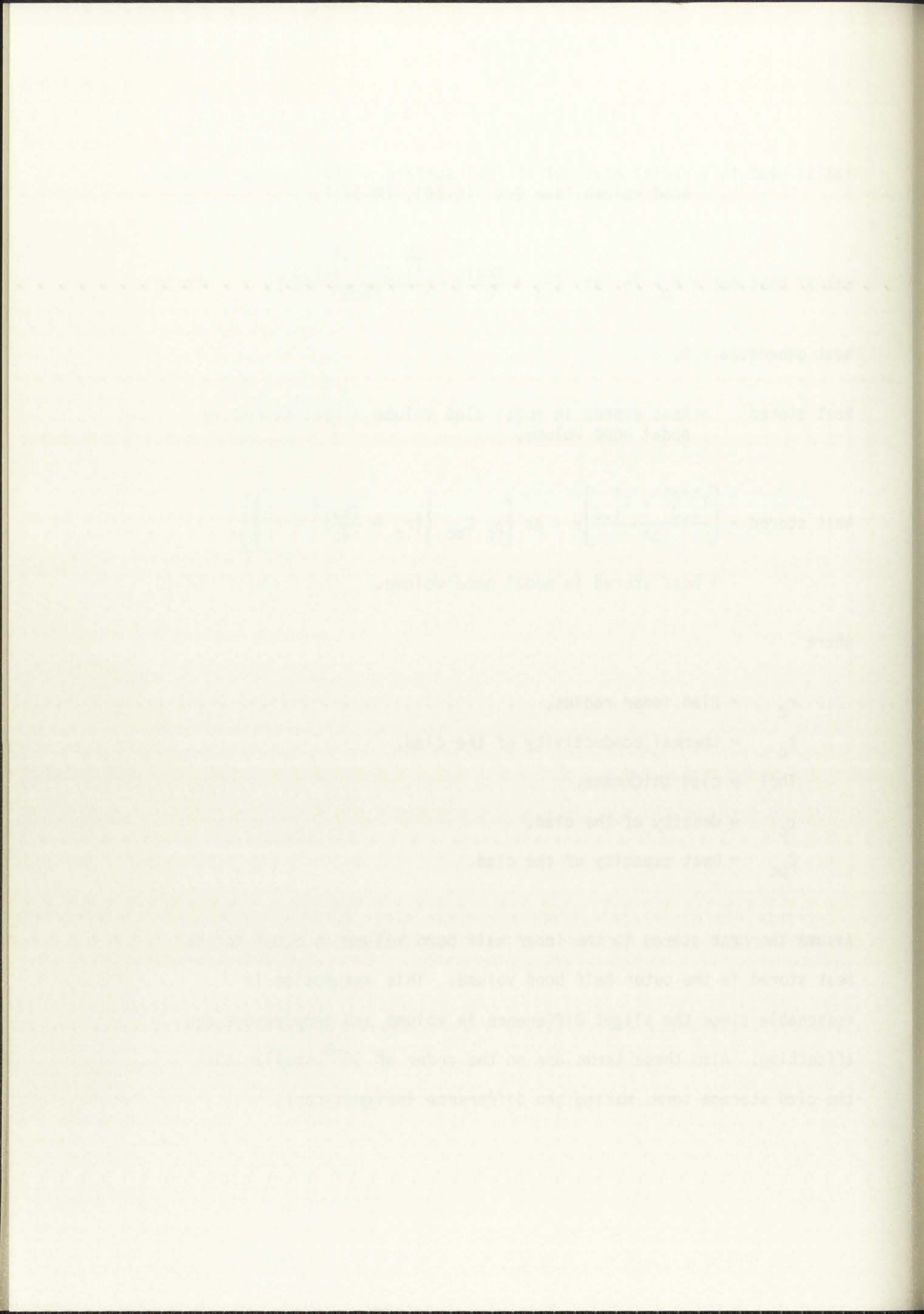
heat stored = heat stored in nodal clad volume + heat stored in nodal bond volume,

$$\begin{aligned} \text{heat stored} = & \left[\frac{T_{i,J}^{t+\Delta t} - T_{i,J}^t}{\Delta t} \right] \pi \cdot \Delta z \left[\rho_c C_{pc} \left\{ \left(r_c + \frac{\text{Thb}}{2} \right)^2 - r_c^2 \right\} \right] \\ & + \text{heat stored in nodal bond volume.} \end{aligned} \quad (\text{K-20})$$

where

- r_c = clad inner radius,
- k_c = thermal conductivity of the clad,
- Thcl = clad thickness,
- ρ_c = density of the clad,
- C_{pc} = heat capacity of the clad.

Assume the heat stored in the inner half bond volume is equal to the heat stored in the outer half bond volume. This assumption is reasonable since the slight difference in volume and temperature are offsetting. Also these terms are on the order of 10^{-3} smaller than the clad storage term, making the difference insignificant.



Combining Eqs. (K-16), (K-17), (K-19), and (K-20)

$$T_{i,J}^{t+\Delta t} = T_{i,J}^t + \frac{2 \Delta t}{\rho_c C_{pc} \left(r_c \cdot ThcL + \frac{ThcL^2}{4} \right)} \left[h_b \cdot r_F (T_{i-1,J}^t - T_{i,J}^t) - k_c \left(r_c + \frac{ThcL}{2} \right) \left(\frac{T_{i,J}^t - T_{i+1,J}^t}{ThcL} \right) \right] \quad (K-21)$$

E. Clad-Coolant Interface

This node is located at the clad outer surface and extends halfway through the clad. No coolant is included in this node since all the coolant is included in a bulk coolant node (see following section). Again it is assumed that heat generation only occurs in the fuel.

$$\text{radial heat in} = k_c \cdot 2\pi \cdot \Delta z \cdot \left(r_c + \frac{ThcL}{2} \right) \left(\frac{T_{i-1,J}^t - T_{i,J}^t}{ThcL} \right) \quad (K-22)$$

$$\text{radial heat out} = h_{NA} \cdot 2\pi \cdot r_o \cdot \Delta z \cdot (T_{i,J}^t - T_{i+1,J}^t) \quad (K-23)$$

heat generated = 0

$$\rho_c C_{pc} \pi \left[r_o^2 - \left(r_o - \frac{Thc}{2} \right)^2 \right] \Delta z \left(\frac{T_{i,J}^{t+\Delta t} - T_{i,J}^t}{\Delta t} \right) \quad (K-24)$$

where

h_{NA} = coolant heat transfer coefficient,

Continued on next page

1. The first part of the test is to determine the

total number of items in the test.

2. The second part of the test is to determine the

percentage of items that are correct.

3. The third part of the test is to determine the

percentage of items that are incorrect.

4. The fourth part of the test is to determine the

total

percentage of items that are correct.

5. The fifth part of the test is to determine the

total number of items

percentage of items that are correct.

6. The sixth part of the test is to determine the

percentage of items that are incorrect.

r_o = clad outer radius.

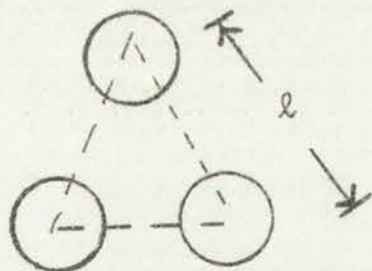
Combining Eqs. (K-22) thru (K-24)

$$T_{i,J}^{t+\Delta t} = T_{i,J}^t + \frac{2 \Delta t}{\rho_c C_{pc} (r_o \text{Thcl} - \frac{\text{Thcl}^2}{4})} \left[k_c (r_c + \frac{\text{Thcl}}{2}) \cdot \left(\frac{T_{i-1,J}^t - T_{i,J}^t}{\text{Thcl}} \right) - h_{NA} r_o (T_{i,J}^t - T_{i+1,J}^t) \right], \quad (\text{K-25})$$

F. Bulk Coolant

This node is located within the bulk coolant channel and includes all the coolant within an equivalent flow annulus. The expression for the equivalent area can be found below. Cross channel flow or heat conduction is not taken into account thus it is assumed an adiabatic surface is outside the coolant flow. The additional flow along the hex can walls is also ignored, thus the coolant/pin is lower than actual conditions.

1. Equivalent flow area for coolant flow,



area of equilateral triangle = $.43301 \ell^2$,

where

ℓ = pin pitch,

thus the area associated with $\frac{1}{2}$ fuel pins = $.43301 \ell^2 - \frac{1}{2} \pi r_o^2$

...
 ...

$$\left[\begin{matrix} \frac{1}{R_1} + \frac{1}{R_2} + \frac{1}{R_3} + \dots \\ \dots \\ \dots \end{matrix} \right] \left[\begin{matrix} \dots \\ \dots \\ \dots \end{matrix} \right]$$

Bolt Current

This node is located within the bolt current channel in the ...
 All the current within an equivalent flow channel ...
 The resistance will be found below. First, channel 1 is ...
 connected to the bolt head because it is adjacent to the ...
 surface is outside the bolt flow. The additional flow ...
 can walls is also shown, since the resistance to flow ...
 conditions ...
 1. Resistance flow was the bolt flow ...



...
 ...
 ...

where

r_o = clad outer radius,

thus for 1 pin

$$\text{AEQ (equivalent flow area)} = 2 \cdot (.43301 \ell^2 \approx \frac{1}{2} \pi r_o^2) \quad (\text{K-26}).$$

2. Bulk coolant temperature

at bottom axial node ($J=1$), $T_{i,J}^{t+\Delta t}$ = coolant inlet temperature

for $J > 1$

$$\text{Radial heat in} = h_{NA} \Delta Z 2\pi r_o [T_{i-1,J}^t - T_{i,J}^t] \quad (\text{K-27})$$

Radial heat out = 0,

$$\text{axial heat in} - \text{axial heat out} = \rho_{NA} C_{pNA} \cdot U \cdot \text{AEQ} \cdot [T_{i,J-1}^t - T_{i,J}^t] \quad (\text{K-28})$$

$$\text{heat stored} = \rho_{NA} C_{pNA} \Delta Z \cdot \text{AEQ} \left[\frac{T_{i,J}^{t+\Delta t} - T_{i,J}^t}{\Delta t} \right],$$

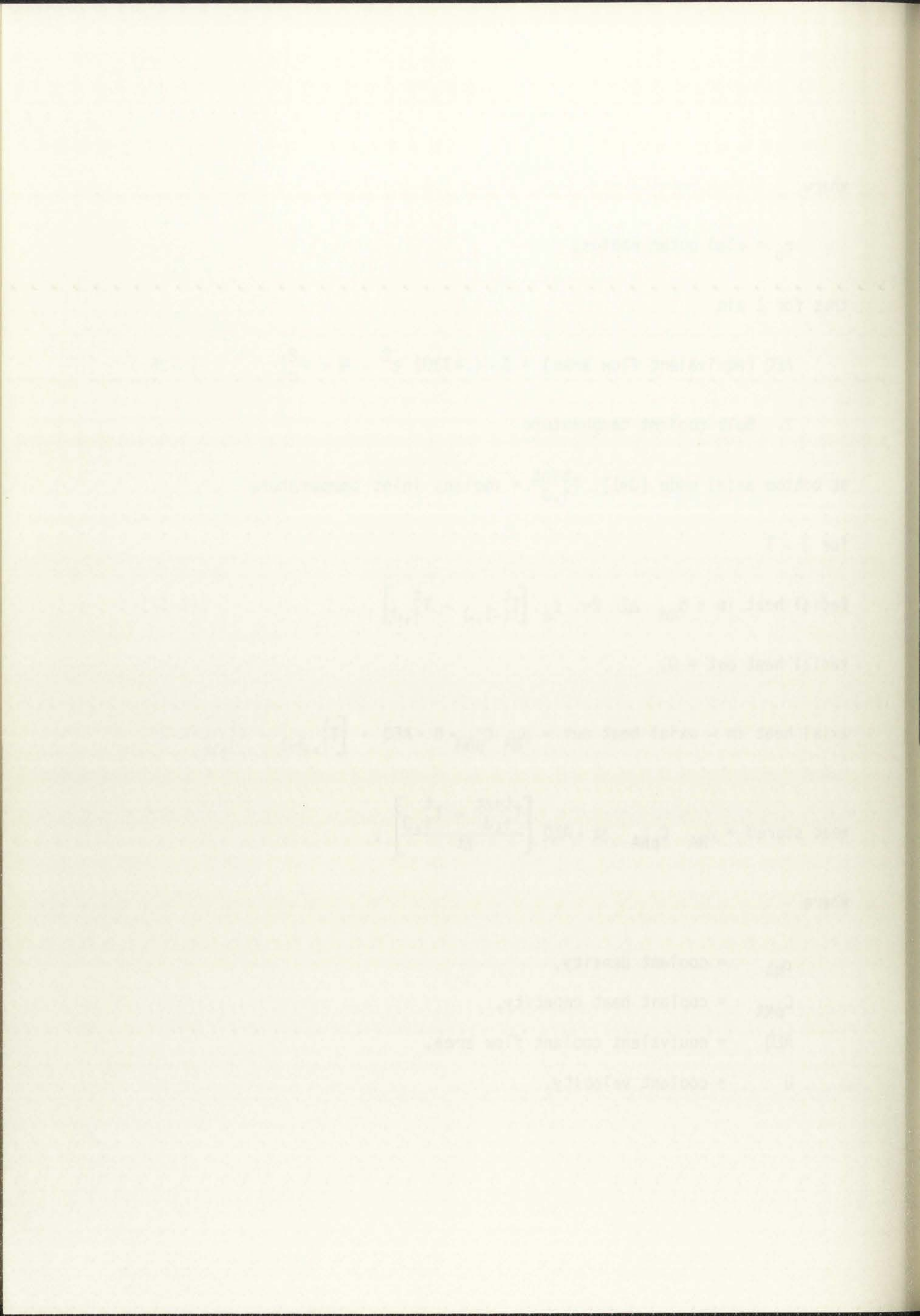
where

ρ_{NA} = coolant density,

C_{pNA} = coolant heat capacity,

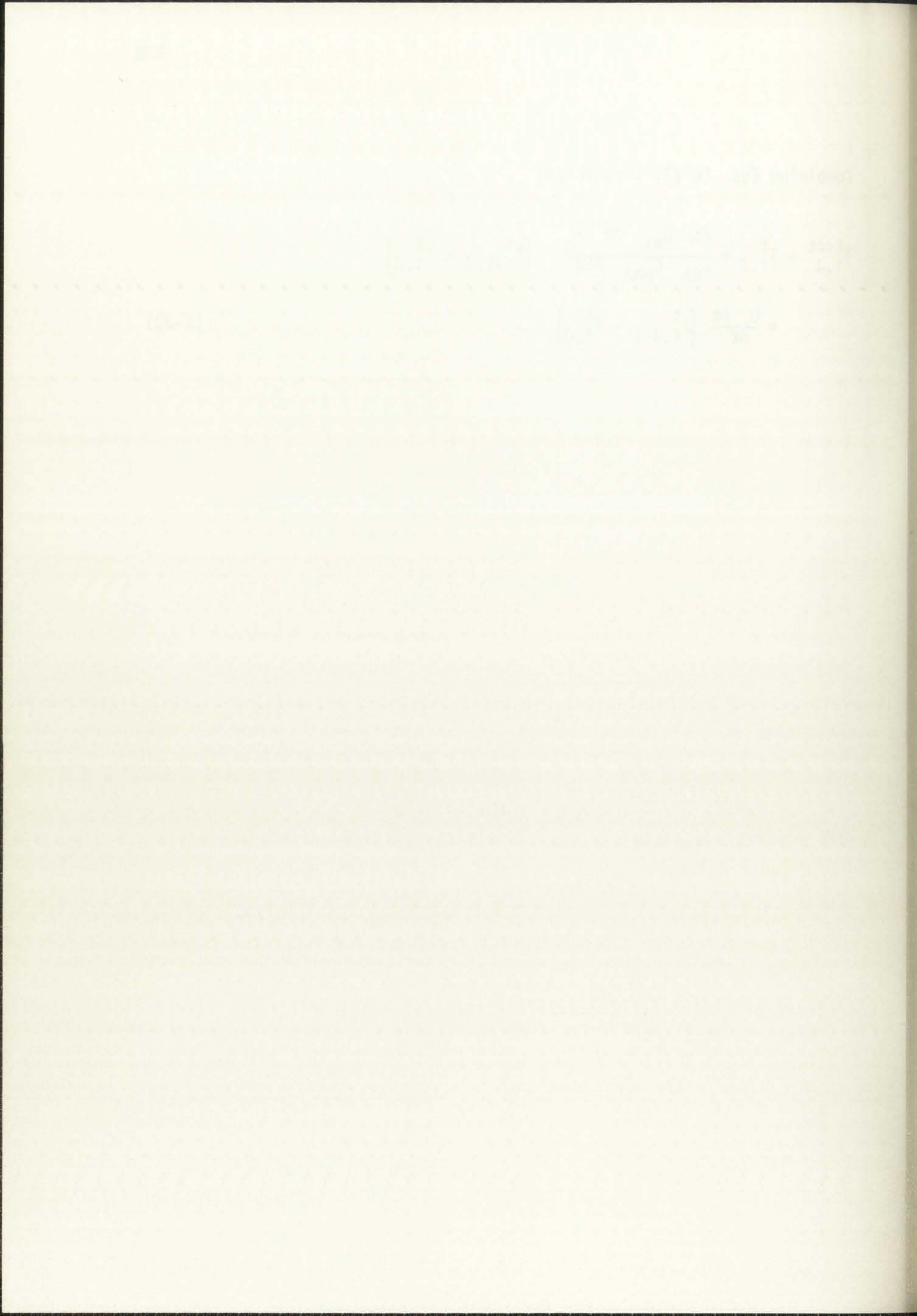
AEQ = equivalent coolant flow area,

U = coolant velocity.



Combining Eqs. (K-27) thru (K-29)

$$T_{i,J}^{t+\Delta t} = T_{i,J}^t + \frac{\Delta t}{\rho_{NA}} \frac{h_{NA}}{C_{pNA}} \frac{2\pi r_o}{AEQ} [T_{i-1,J}^t - T_{i,J}^t] \\ + \frac{U}{\Delta z} \Delta t [T_{i,J-1}^t - T_{i,J}^t] \quad (K-30)$$



APPENDIX L

VAPOR PRESSURE OF VOLATILE FISSION PRODUCTS OF INTEREST

A. Barium

The extrapolated vapor pressure of various investigators is plotted on Fig. L.1, and the tabular results are given in Tables L.1a-L.1c. Nesmeyanov's¹ curve is based on unverified experimental data in the temperature range 1333⁰ - 1419⁰ K. It should be noted that in this and all following partial pressure curves, theoretical or nonverified curves will be represented by dashed lines along with curves extrapolated beyond their valid or experimental limits.

Nesmeyanov's¹, Hultgren's², and the CRC's³ data all agree fairly well in the area below 2000 K. The difference between the linear extrapolation of Hornung⁴ and Hultgren, and the extrapolation containing phenomenological terms of Nesmayuanov can be seen in this Fig. L.1. The saturation curve of Hornung was determined over a larger experimental temperature range and will be used until more appropriate data can be found.

THE EFFECT OF TEMPERATURE ON THE RATE OF REACTION

Introduction

The rate of a chemical reaction is affected by many factors, one of which is temperature. In this experiment, the rate of reaction between hydrogen peroxide and potassium iodide was studied at different temperatures. The reaction is as follows:

$$2H_2O_2(aq) \rightarrow 2H_2O(l) + O_2(g)$$

The rate of reaction was measured by the volume of oxygen gas evolved over a fixed period of time. The results are shown in the table below.

Temperature (°C)	Volume of O_2 (cm ³)
10	10
20	20
30	40
40	80
50	160

From the table, it can be seen that the rate of reaction increases as the temperature increases. This is because the molecules have more kinetic energy and are therefore more likely to collide with sufficient energy to overcome the activation energy barrier.

Conclusion

The rate of reaction between hydrogen peroxide and potassium iodide increases as the temperature increases. This is due to the increase in the kinetic energy of the molecules, which allows them to overcome the activation energy barrier more easily.

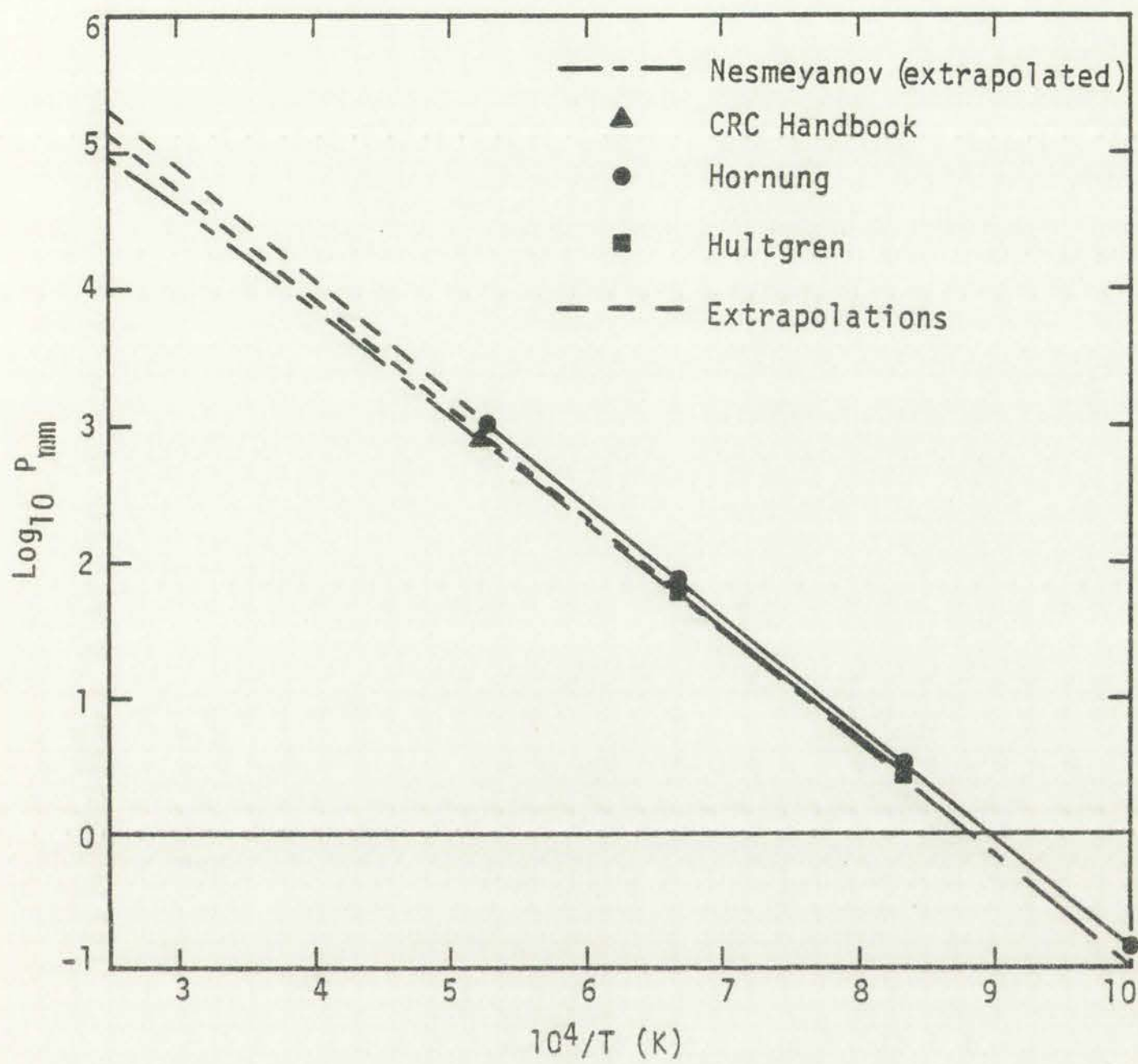


Figure L.1
Vapor pressure of barium.



Figure 1

Temperature vs. Time

Linear relationship between Temperature and Time

TABLE L.1a
NESMEYANOV BARIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
500	20.0	-9.382	4.15x10 ⁻¹⁰
1000	10.0	- .977	.106
1200	8.33	.394	2.48
1500	6.67	1.747	55.80
2000	5.0	3.069	1.17x10 ³
2500	4.0	3.838	6.88x10 ³
3000	3.33	4.334	2.16x10 ⁴

$$\text{Log } P_{\text{mm}} = 10.63717 - \frac{8703.64}{T} - .00001584 T - .96481 \text{ Log } T \text{ (K)}$$

(Based on nonverified data)

TABLE L.1b
HULTGREN BARIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{atm}	P _{atm}	Log P _{mm}
1000	10.0	-3.79	1.63x10 ⁻⁴	-.907
1200	8.33	-2.45	3.54x10 ⁻³	.430
1500	6.67	-1.12	7.68x10 ⁻²	1.77
2000	5.0	2.22x10 ⁻¹	1.667	3.10
2500	4.0	1.024	10.57	3.91

$$\text{Log } P_{\text{atm}} = \frac{-8020}{T} + 4.232 \text{ (1333 - 1419 K)}$$

TABLE 1.10
MUTUAL FUND DATA

Year	Assets	Assets	Assets
1970	1.0	1.0	1.0
1971	1.5	1.5	1.5
1972	2.0	2.0	2.0
1973	3.0	3.0	3.0
1974	4.0	4.0	4.0
1975	5.0	5.0	5.0
1976	6.0	6.0	6.0
1977	7.0	7.0	7.0
1978	8.0	8.0	8.0
1979	9.0	9.0	9.0
1980	10.0	10.0	10.0

TABLE 1.10
MUTUAL FUND DATA

Year	Assets	Assets	Assets
1970	1.0	1.0	1.0
1971	1.5	1.5	1.5
1972	2.0	2.0	2.0
1973	3.0	3.0	3.0
1974	4.0	4.0	4.0
1975	5.0	5.0	5.0
1976	6.0	6.0	6.0
1977	7.0	7.0	7.0
1978	8.0	8.0	8.0
1979	9.0	9.0	9.0
1980	10.0	10.0	10.0

TABLE L.1c
HORNING BARIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	$\ln P$	P_{atm}	Log P_{mm}
1000	10.0	-8.615	1.813×10^{-4}	- .86
1200	8.33	-5.477	4.18×10^{-3}	.502
1500	6.67	-2.34	.0964	1.865
2000	5.0	.799	2.224	3.23
2500	4.0	2.68	14.62	4.05
3000	3.33	3.94	51.3	4.59

$$\ln P_{\text{atm}} = 10.214 - 3.621 \frac{T_c}{T} \quad (983 - 1895 \text{ K})$$

where

$$T_c = 5200 \text{ K (critical temperature).}$$

From CRC handbook

$$\text{Boiling point} = 1913 \text{ K}$$

thus

$$\frac{10^4}{T} = 5.227 \text{ and } \log (760 \text{ mm}) = 2.88$$

B. Cerium

Tables L.2a thru c and Fig. L.2 contain the saturation vapor pressure information for cerium. Nesmeyanov's¹ curve is based on unreliable data determined in the temperature range of 1460 - 1720 K. Hultgren² based his curve on the results of Daane and Spedding,⁵

TABLE I

Year
1950
1951
1952
1953
1954
1955
1956
1957

(continued from previous page)

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and lies slightly above the curve determined by Ackermann, et al.⁶ Ackermann believed that the Daane and Spedding data, and thus Hultgren's curve, is slightly erroneous, not due to weighing or temperature errors but due to the vaporization of CeO(g). Ackermann, et al. did take experimental steps to eliminate oxygen from the liquid Ce, and their data will be used until better information can be found.

TABLE L.2a
NESMEYANOV CERIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
1460.	6.85	-4.447	3.57×10^{-5}
1720.	5.814	-2.025	9.45×10^{-3}
2000	5.0	- .12	.758
2500.	4.0	2.22	165.96
2690	3.717	2.88	760.0
3000	3.33	3.78	6.026×10^3
3500	2.857	4.89	7.84×10^4

$$\text{Log } P_{\text{mm}} = 11.58 - \frac{23400.}{T \text{ (K)}}$$

Unreliable data taken in temperature range 1470 - 1720 K.

1940

1941

1942

1943

1944

1945

1946

1947

1948

TABLE L.2b
HULTGREN CERIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	P_{atm}	Log P_{mm}
1600.	6.25	5.44×10^{-8}	-4.38
1800.	5.556	1.40×10^{-6}	-2.973
2000	5.0	1.88×10^{-5}	-1.85
2038	4.91	2.90×10^{-5}	-1.66
3000	3.33	4.54×10^{-2}	1.54
3500	2.86	4.21×10^{-1}	2.51
3742	2.67	1.0	2.88

$$\text{Log } P_{\text{atm}} = \frac{-20304.}{T} + 5.4254 \quad (1611 - 2038 \text{ K})$$

TABLE L.2c
ACKERMANN CERIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P_{atm}	P_{mm}	Log P_{mm}
1500.	6.667	-8.547	2.158×10^{-6}	-5.667
1750.	5.714	-6.54	2.19×10^{-4}	-3.66
2000.	5.0	-5.035	7.01×10^{-3}	-2.154
2250.	4.44	-3.86	.104	-.983

$$\text{Log } P_{\text{atm}} = 5.500 - \frac{21070.}{T} \quad (1525 - 2225 \text{ K})$$

TABLE 1

1950	100	100
1951	105	105
1952	110	110
1953	115	115
1954	120	120
1955	125	125
1956	130	130
1957	135	135
1958	140	140
1959	145	145
1960	150	150

Source: Bureau of Economic Analysis, Department of Commerce

TABLE 2

SELECTED ECONOMIC INDICATORS

1950	100	100
1951	105	105
1952	110	110
1953	115	115
1954	120	120
1955	125	125
1956	130	130
1957	135	135
1958	140	140
1959	145	145
1960	150	150

Source: Bureau of Economic Analysis, Department of Commerce

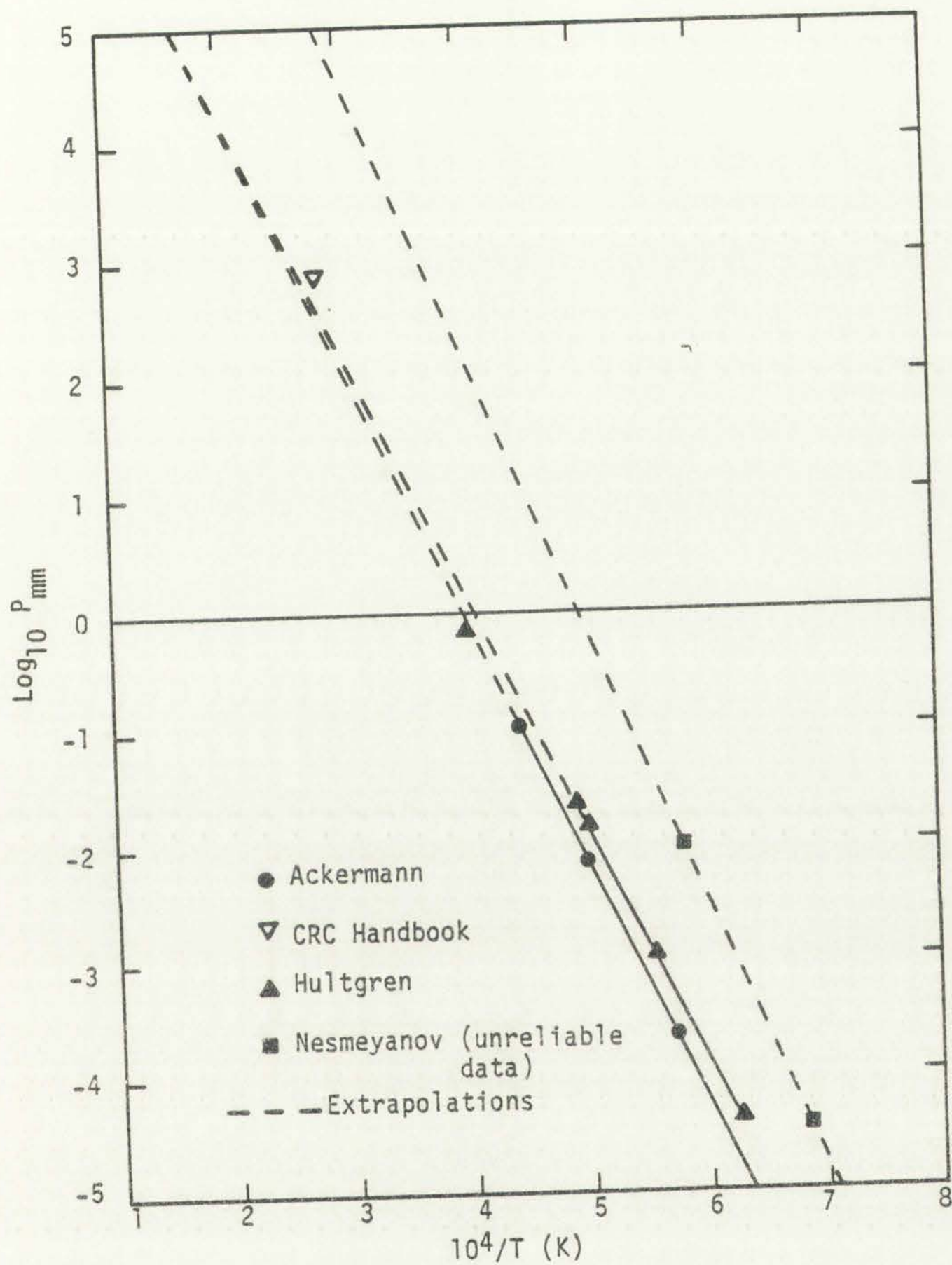


Figure L.2
Vapor pressure of cerium.



Faint text or labels, possibly a title or description, located below the diagram. The text is illegible due to fading.

From CRC³ handbook

Boiling Point = 3548 K

thus

$$\frac{10^4}{T} = 2.818 \quad , \quad \log (760 \text{ mm}) = 2.88$$

C. Palladium

Tables L.3a thru L.3c and Fig. L.3 contain the saturation vapor pressure data for palladium. Nesmeyanov's¹ curve is based on theoretical work only and gives a lower partial pressure than either Hultgren² or Wise.⁷ Wise in his book plots the saturation vapor pressure in the temperature range, 2000 - 3000 K. His plot, however, is based on the experiments of Dreger and Margrave,⁸ and Hampson and Walker⁹ both of which were done at temperature less than 1488 K. His curve should actually be regarded as an extrapolation. Thus Hultgren's curve will be assumed unless more suitable data is found.

$$10^6 \times 1.813 \quad \ln(1700 \text{ sec}) = 7.52$$

Discussion

Figure 1 is the plot of $\ln(t)$ versus $\ln(t)$ for the data obtained in the present study. The data points are shown in Figure 1 and the straight line is drawn through them. The slope of the line is 1.813×10^6 sec. This is in good agreement with the value of 1.813×10^6 sec obtained from the present study. The plot, however, is based on the experimental data of Deegan and Hargrave⁶ and Hargrave and Deegan⁷ both of which were done at temperatures less than 1400 K. The data actually reported as an extrapolation. This indicates that the data will be obtained under more reliable data if found.

TABLE L.3a
NESMEYANOV PALLADIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
1500	6.67	-4.249	5.64x10 ⁻⁵
2000	5.0	-1.053	.0886
2500	4.0	.868	7.376
3000	3.33	2.151	1.415x10 ²
3500	2.86	3.07	1.174x10 ³
4000	2.50	3.76	5.77x10 ³
4500	2.22	4.30	2.00x10 ⁴

$$\text{Log } P_{\text{mm}} = 8.76587 - \frac{19169.84}{T} + .00002347T - .08499 \text{ Log } T$$

(theoretical)

TABLE L.3b
HULTGREN PALLADIUM PARTIAL PRESSURE DATA

T(K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
1366	7.32	-4.12	1x10 ⁻⁷
1500	6.66	-2.95	1.48x10 ⁻⁶
1600	6.25	-2.2	8.21x10 ⁻⁶
2000	5.00	-.012	1.28x10 ⁻³
2600	3.85	1.95	.188
3200	3.125	3.22	2.18

$$\text{Log } P_{\text{mm}} = 8.6870 - \frac{17494}{T} \quad (1388 - 1675 \text{ K})$$

TABLE 1
 MEAN VALUES OF THE FACTORS

Factor	Mean	SD	CV
Factor 1	1.2	0.3	0.25
Factor 2	1.5	0.4	0.27
Factor 3	1.8	0.5	0.28
Factor 4	2.1	0.6	0.29
Factor 5	2.4	0.7	0.30
Factor 6	2.7	0.8	0.31
Factor 7	3.0	0.9	0.32
Factor 8	3.3	1.0	0.33
Factor 9	3.6	1.1	0.34
Factor 10	3.9	1.2	0.35

TABLE 2
 MEAN VALUES OF THE FACTORS

Factor	Mean	SD	CV
Factor 1	1.2	0.3	0.25
Factor 2	1.5	0.4	0.27
Factor 3	1.8	0.5	0.28
Factor 4	2.1	0.6	0.29
Factor 5	2.4	0.7	0.30
Factor 6	2.7	0.8	0.31
Factor 7	3.0	0.9	0.32
Factor 8	3.3	1.0	0.33
Factor 9	3.6	1.1	0.34
Factor 10	3.9	1.2	0.35

TABLE 3
 MEAN VALUES OF THE FACTORS

TABLE L.3c
WISE PALLADIUM PARTIAL PRESSURE DATA

T(K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
2000	5.0	- .638	.23
2273	4.40	.505	3.2
2500	4.0	1.312	20.5
2773	3.61	2.08	120.0
3077	3.25	2.792	620.0
3148	3.18	2.881	760.0

Based on experimental data.

From CRC³ Handbook

Boiling Point = 3413 K

thus

$$\frac{10^4}{T} = 2.93, \log (760 \text{ mm}) = 2.88.$$

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.....

100	100	100	100
200	200	200	200
300	300	300	300
400	400	400	400
500	500	500	500
600	600	600	600
700	700	700	700
800	800	800	800
900	900	900	900

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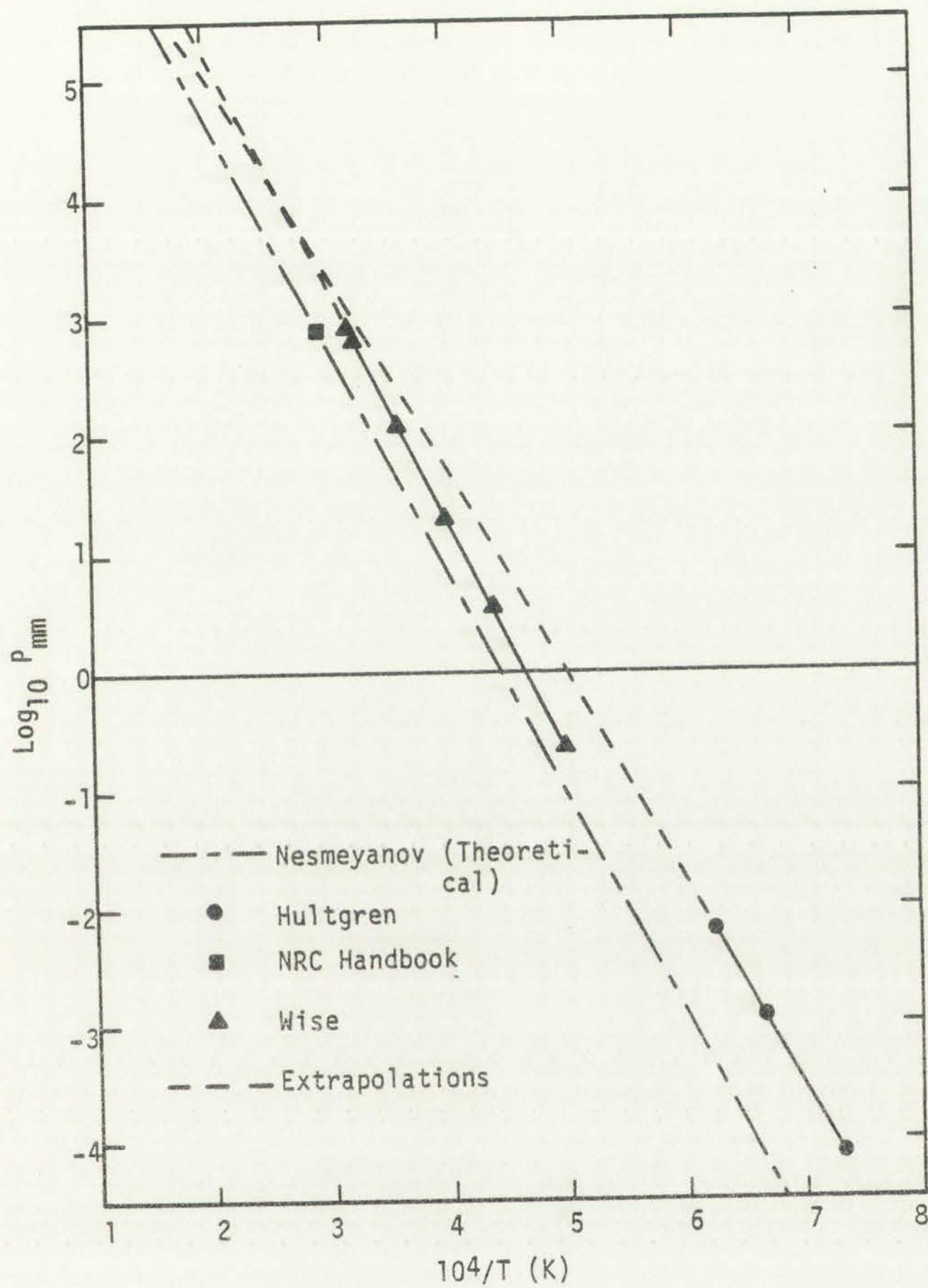


Figure L.3
Vapor pressure of Palladium.



(a) Class of

(b) Class of

(c) Class of

(d) Class of

(e) Class of

(f) Class of

(g) Class of

(h) Class of

(i) Class of

(j) Class of

D. Iron

The partial pressure data for iron is contained in Tables L.4a thru L.4c and Fig. L.4. Nesmeyanov's¹ curve is based on vapor pressures in the area of 10^{-4} - 10^{-5} mm Hg and is thus extrapolated well beyond its experimental limit. Hultgren's² curve is based principally on the experimental work of Morris, et al.¹⁰ (1810 - 1889 K). The vapor pressure curve of Hornung⁴ will be used due to its more appropriate experimental range (1809 - 3500 K).

TABLE L.4a
NESMEYANOV IRON PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
1453	6.882	-4.0	10^{-4}
1566	6.386	-3.0	10^{-3}
1698	5.889	-2.0	10^{-2}
1859	5.379	-1.0	10^{-1}
2063	4.847	0.0	1.0
2318	4.314	1.0	10.0
2649	3.775	2.0	100.0
3045	3.284	2.88	760.0

$$\text{Log } P_{\text{mm}} = -25.93396 - \frac{14124.5}{T} + .00113331T + 10.59505 \text{ Log } T$$

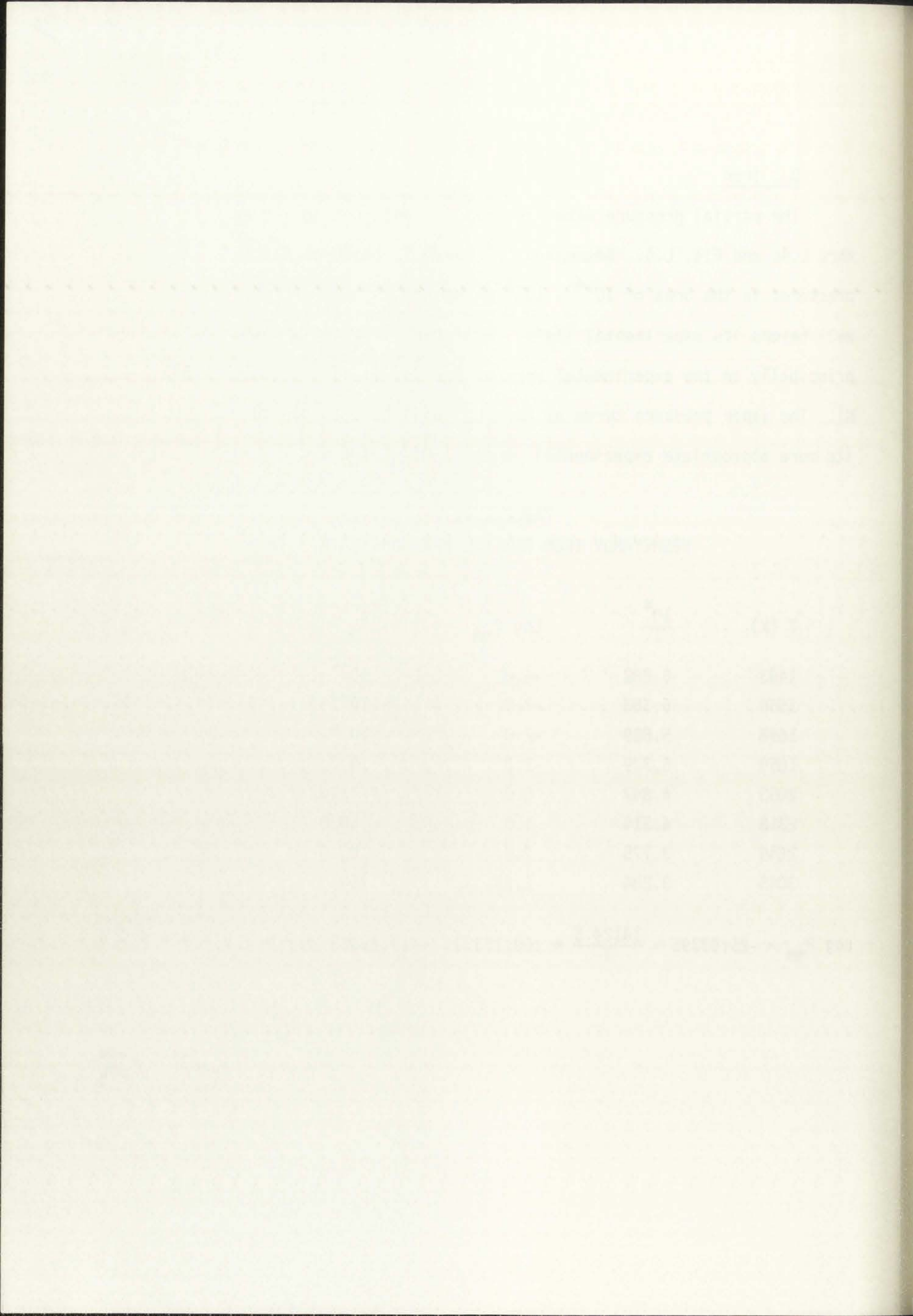


TABLE L.4b
HULTGREN IRON PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{mm}	P _{atm}
1387	7.21	-5.12	10 ⁻⁸
1485	6.73	-4.12	10 ⁻⁷
1599	6.25	-3.12	10 ⁻⁶
1732	5.77	-2.12	10 ⁻⁵
1895	5.28	-1.12	10 ⁻⁴

$$\text{Log } P_{\text{mm}} = 9.181 - \frac{19835}{T} \quad (1300 - 1889 \text{ K})$$

TABLE L.4c
HORNING IRON PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	$\ln P_{\text{atm}}$	P _{atm}	Log P _{mm}
1800	5.556	-10.42	2.98x10 ⁻⁵	-1.644
2000	5.0	-7.98	3.408x10 ⁻⁴	- .587
2500	4.0	-3.60	.0273	1.32
3000	3.33	- .679	.507	2.59
3500	2.86	1.408	4.09	3.49

$$\ln P_{\text{atm}} = 13.932 - \frac{4.693 T_c}{T} \quad (1809 - 3500 \text{ K})$$

where

$$T_c = 9340 \text{ K (critical temperature).}$$

TABLE 1

Year	1950	1951	1952
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...
...
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...
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TABLE 2

Year	1950	1951	1952
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Source: U.S. Bureau of Economic Analysis, *Survey of Current Business*, 1953, p. 10.

U.S. GOVERNMENT PRINTING OFFICE: 1953

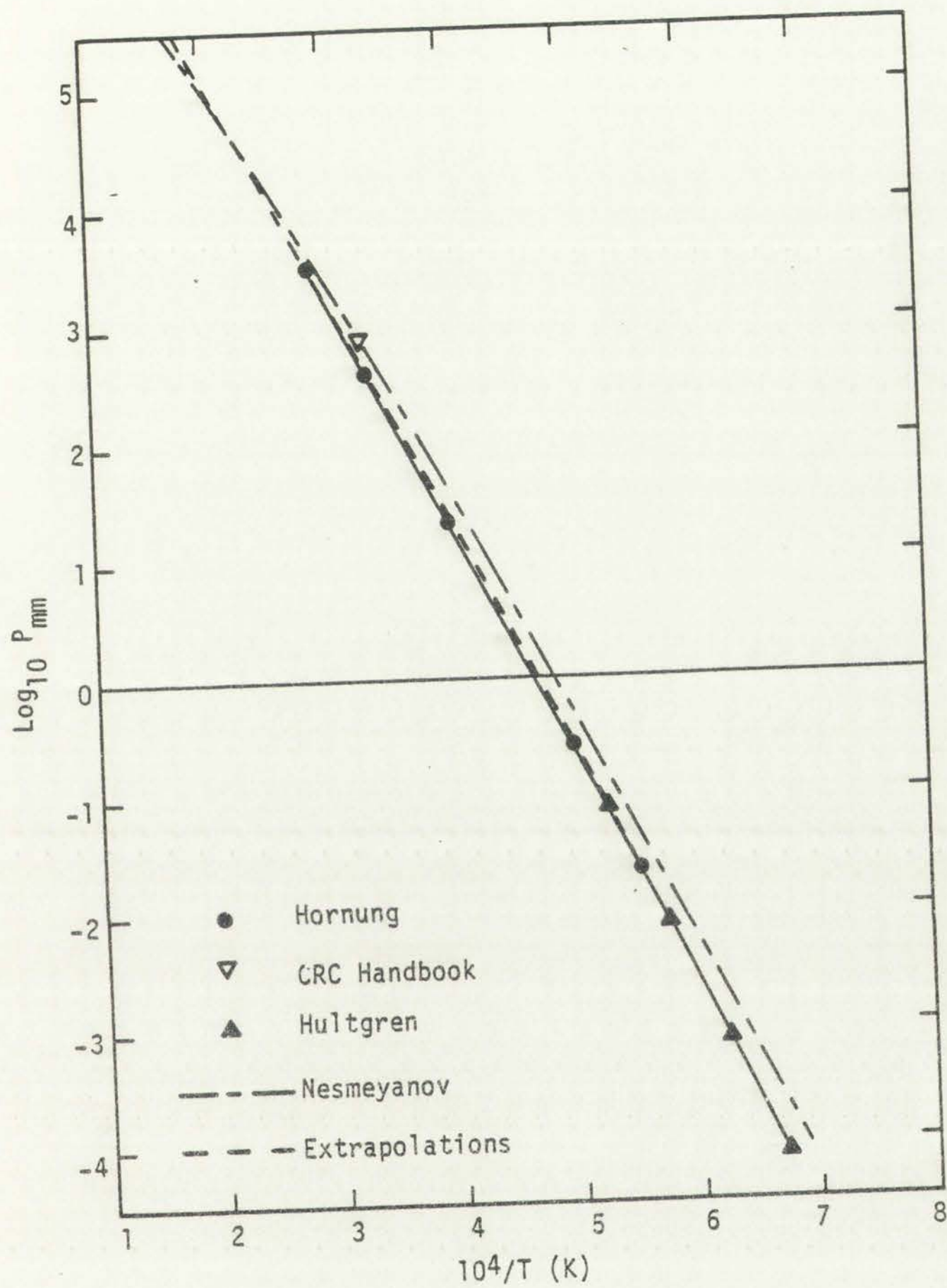


Figure L.4
Vapor pressure of iron.



(3) Fig. 1

Figure 1
 shows the relationship between
 temperature and resistance

From CRC³ Handbook

Boiling Point = 3033 K

thus

$$\frac{10^4}{T} = 3.297, \log (760 \text{ mm}) = 2.88.$$

E. Tellurium

Figure L.5 and Tables L.5a and L.5b contain the work of various investigators on the saturation pressure of tellurium. Nesmeyanov¹ considers his upper end of reliability to be 1100 K. Baker¹¹ however, experimentally determined the vapor pressure in the range 981-1680 K. It should be noted that tellurium, in the vapor phase, exists as predominantly $\text{Te}_2(\text{g})$ at least up until 1200 K. By observing the linear extrapolation of Baker's lower vapor pressure data, it appears that $\text{Te}_2(\text{g})$ is dominant into the 1800 K range, or at least the disassociation occurs linearly. Stull and Sinke¹² list thermodynamic properties of $\text{Te}_2(\text{g})$ to 3000 K. Baker's curve will be used unless more suitable data is found.

Section 1

Section 2

Section 3

Section 4

Section 5

Section 6

Section 7

Section 8

Section 9

Section 10

Section 11

Section 12

Section 13

Section 14

Section 15

Section 16

Section 17

Section 18

Section 19

Section 20

Section 21

Section 22

Section 23

Section 24

Section 25

TABLE L.5a
NESMEYANOV TELLURIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
1000	10.0	1.638	43.49
1250	8.0	2.7765	597.78
800	12.5	.1552	1.43

For Σ Te, i.e., Te(g) + Te₂(g)

$$\text{Log } P_{\text{mm}} = -32.44504 - \frac{4036.949}{T} - .00413735 T + 14.08592 \text{ Log } T$$

(500 - 1100 K)

STATE OF CALIFORNIA
COUNTY OF [illegible]

BEFORE ME, the undersigned authority, on this [illegible] day of [illegible], 20[illegible]

presented for my signature and attestation the foregoing instrument of writing, together with the authority to sign the same, and acknowledged to me that he executed the same for the purposes and consideration therein expressed.

Given under my hand and seal of office this [illegible] day of [illegible], 20[illegible].

Notary Public in and for the State of California

[illegible]

TABLE L.5b

BAKER TELLURIUM PARTIAL PRESSURE DATA

T(K)	$\frac{10^4}{T}$	P _{atm}	Log P _{mm}
981	10.19	.0434	1.518
1188	8.42	.494	2.574
1266	7.90	1.00	2.881
1323	7.56	1.58	3.079
1463	6.83	4.20	3.509
1580	6.33	8.16	3.792
1685	5.97	13.82	4.021
1780	5.62	21.00	4.203

$$\text{Log } P_{\text{atm}} = -\frac{6447}{T} - 1.0 \text{ Log } T + 8.1945 \quad (981 - 1780 \text{ K}).$$

From CRC³ handbook:

Boiling Point = 1263 K ,

thus

$$\frac{10^4}{T} = 7.92 \quad , \quad \log (760 \text{ mm}) = 2.88 \quad .$$

Year	1910	1920	1930	1940
1912	100	100	100	100
1915	100	100	100	100
1920	100	100	100	100
1925	100	100	100	100
1930	100	100	100	100
1935	100	100	100	100
1940	100	100	100	100
1945	100	100	100	100
1950	100	100	100	100
1955	100	100	100	100
1960	100	100	100	100
1965	100	100	100	100
1970	100	100	100	100
1975	100	100	100	100
1980	100	100	100	100
1985	100	100	100	100
1990	100	100	100	100
1995	100	100	100	100
2000	100	100	100	100
2005	100	100	100	100
2010	100	100	100	100
2015	100	100	100	100
2020	100	100	100	100

The following table shows the results of the survey conducted in the year 1910. The data is presented in a tabular format, with columns representing the years from 1910 to 2020. The values in the table represent the percentage of respondents who chose each option. The total percentage for each year is 100%.

The survey results indicate that the majority of respondents chose the first option in every year. The percentage of respondents who chose the first option ranged from 60% to 80%. The percentage of respondents who chose the second option ranged from 10% to 20%. The percentage of respondents who chose the third option ranged from 5% to 15%.

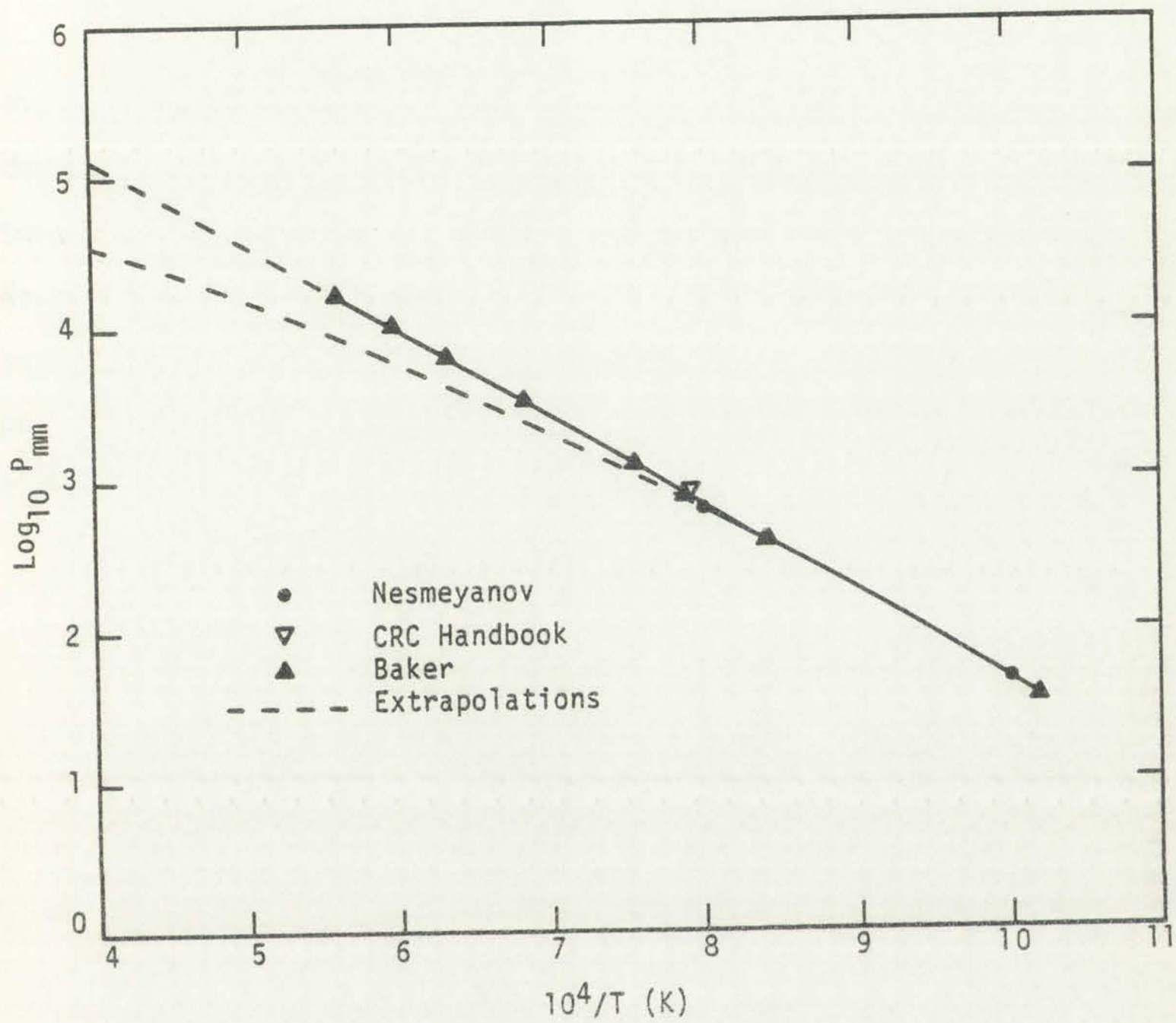


Figure L.5
Vapor pressure of tellurium.



Figure 1.3
 Vapor pressure of ethanol

F. Antimony

Gaseous Sb consists predominantly of polyatomic molecules, Sb_2 and Sb_4 . It appears from Fig. L.6 that a shift in the temperature dependence of the average molecular weight occurs at the melting temperature. Hultgren's² work is based partially on the data of Nesmeyanov¹ and thus the close correlation of two curves. Further saturation data for Sb should be found, since the disassociation of the polyatomic molecules could alter the high temperature portion of the curve.

TABLE L.6a
NESMEYANOV ANTIMONY PARTIAL PRESSURE DATA

T(K)	$\frac{10^4}{T}$	Log P_{mm}	P_{mm}
800	12.50	-2.117	7.64×10^{-3}
900	11.11	- .759	1.74×10^{-1}
1000	10.0	- .106	7.83×10^{-1}
1200	8.33	.816	6.54
1500	6.67	1.83	67.8
1800	5.56	2.63	427.0
1898	5.27	2.88	760.0

For Σ Sb, i.e., $Sb(g)$, $Sb_2(g)$ and $Sb_4(g)$.

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TABLE L.6b
HULTGREN ANTIMONY PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	P _{atm}	Log P _{mm}
693	14.43	10 ⁻⁷	-4.12
741	13.5	10 ⁻⁶	-3.12
803	12.45	10 ⁻⁵	-2.12
872	11.47	10 ⁻⁴	-1.12
1007	9.93	10 ⁻³	- .12
1225	8.16	10 ⁻²	.881
1520	6.58	10 ⁻¹	1.88
1908	5.24	1.0	2.88

For Σ Sb

From CRC³ handbook

Boiling Point = 2023 K

thus

$$\frac{10^4}{T} = 4.94, \log (760 \text{ mm}) = 2.88.$$

STATE OF TEXAS
COUNTY OF [illegible]

[illegible]	[illegible]	[illegible]	[illegible]
100	100	100	100
200	200	200	200
300	300	300	300
400	400	400	400
500	500	500	500
600	600	600	600
700	700	700	700
800	800	800	800
900	900	900	900
1000	1000	1000	1000

[illegible]

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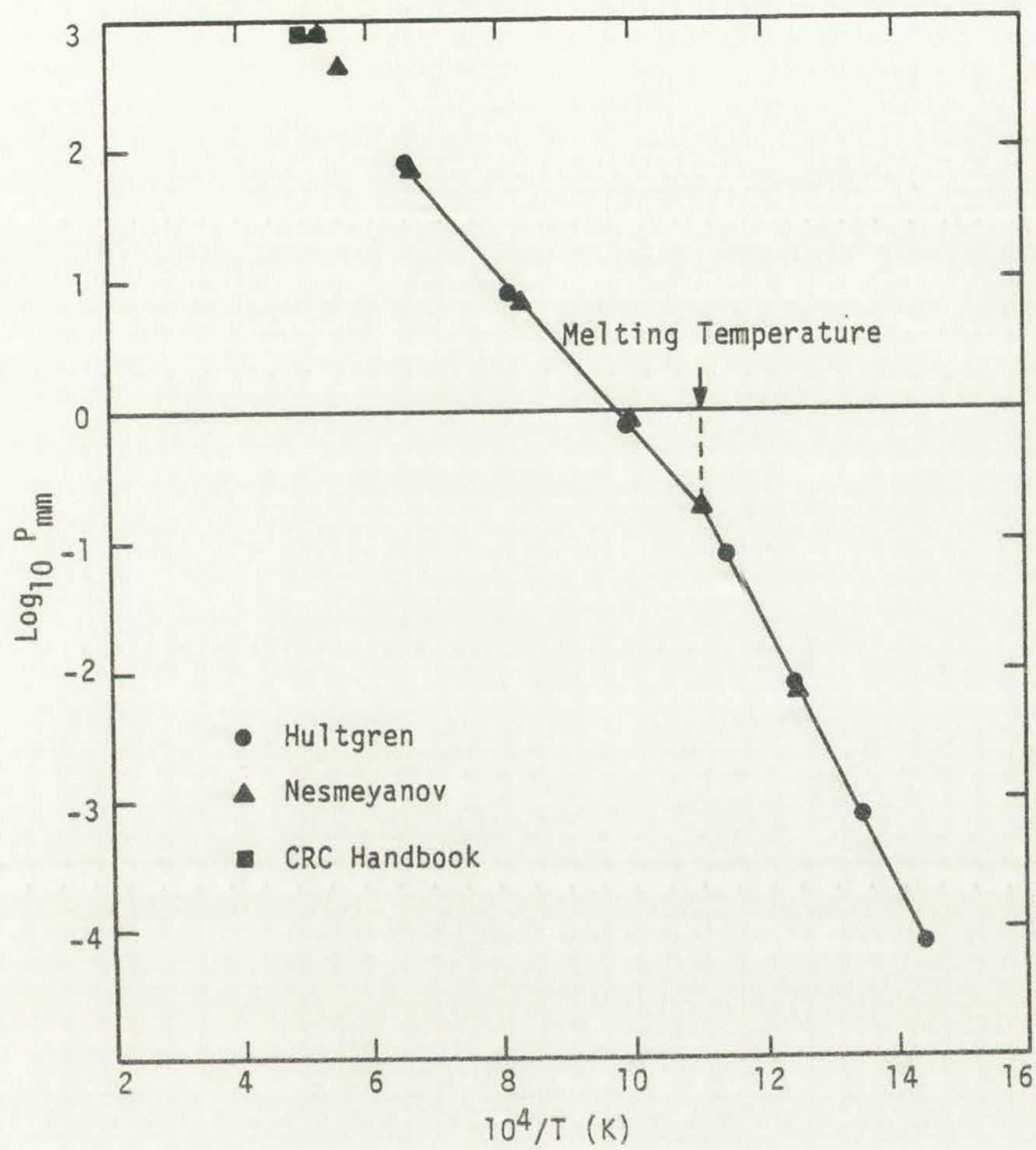


Figure L.6
Vapor pressure of Antimony.



Figure 1: A graph showing the relationship between X and Y. The X-axis represents the independent variable and the Y-axis represents the dependent variable. The data points are connected by a straight line, indicating a linear relationship.

The graph illustrates a positive linear relationship between the variables X and Y. The slope of the line is constant, and the data points are evenly spaced along the line. The dashed horizontal line represents a specific value on the Y-axis.

The following table represents the approximate data points from the graph:

X	Y
1	2
2	4
3	6
4	8
5	10
6	12
7	14
8	16
9	18
10	20

The dashed horizontal line is positioned at Y = 10. This line intersects the solid line at the point (5, 10).

The graph demonstrates that as the value of X increases, the value of Y also increases proportionally. The linear relationship is consistent across the entire range of the data shown.

The slope of the line is 2, and the y-intercept is 0. The equation of the line is $Y = 2X$.

The graph is a clear example of a linear function. The data points are perfectly aligned on a straight line, indicating a strong positive linear correlation between the two variables.

G. Cesium

Nesmeyanov's¹ curve is based on reliable data determined at pressures less than 10 mm Hg. Thus in Fig. L.7, his curve is extrapolated well beyond the upper experimental limit. Stone's¹³ curve is based on experimental points measured at higher temperatures than Hultgren² and will thus be assumed until better information is located. It should be noted in extrapolating the partial pressure Cs, that Cs(g) is made up of monatomic and diatomic molecules.

TABLE L.7a
NESMEYANOV CESIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	Log P _{mm}	P _{mm}
800	12.5	2.162	145.37
959	10.428	2.882	761.32
1000	10.0	3.025	1.0x10 ³
1250	8.0	3.656	4.532x10 ³
1600	6.25	4.126	1.336x10 ⁴
2000	5.00	4.367	2.326x10 ⁴

$$\text{Log } P_{\text{mm}} = 8.22127 - \frac{4006.048}{T} - .0060194 T - .19623 \text{ Log } T \text{ (Less 10 mm Hg)}$$

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Column 1	Column 2	Column 3	Column 4
100	100	100	100
200	200	200	200
300	300	300	300
400	400	400	400
500	500	500	500
600	600	600	600
700	700	700	700
800	800	800	800
900	900	900	900
1000	1000	1000	1000

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TABLE L.7b
HULTGREN CESIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	P _{atm}	Log P _{mm}
800	12.5	.172	2.116
900	11.11	.551	2.662
955	10.47	.932	2.850
963	10.38	1.0	2.881
1000	10.0	1.32	3.001

T < 1000 K

TABLE L.7c
STONE CESIUM PARTIAL PRESSURE DATA

T (K)	$\frac{10^4}{T}$	P _{atm}	Log P _{mm}
943.33	10.601	1.0169	2.89
1558.611	6.416	33.53	4.406
1526.611	6.55	30.071	4.359
1020.8	9.796	1.9968	3.181
1148.28	8.709	5.00	3.580
1267.833	7.887	9.998	3.881
1411.556	7.084	10.346	4.167
920.78	10.86	.811	2.790

$$\text{Log } P_{\text{atm}} = 5.87303 - \frac{7040.7}{T} - .5329 \text{ Log } T (^{\circ}\text{R}) \quad (920 - 1558 \text{ K})$$

TABLE 1
 STORE CUMULATIVE PRESSURE DATA

Time (min)	Pressure (mm Hg)	Temperature (°C)	Volume (ml)
0	100.0	25.0	100.0
10	101.5	25.5	101.5
20	103.0	26.0	103.0
30	104.5	26.5	104.5
40	106.0	27.0	106.0
50	107.5	27.5	107.5

TABLE 2
 STORE CUMULATIVE PRESSURE DATA

Time (min)	Pressure (mm Hg)	Temperature (°C)	Volume (ml)
0	100.0	25.0	100.0
10	101.5	25.5	101.5
20	103.0	26.0	103.0
30	104.5	26.5	104.5
40	106.0	27.0	106.0
50	107.5	27.5	107.5
60	109.0	28.0	109.0
70	110.5	28.5	110.5
80	112.0	29.0	112.0
90	113.5	29.5	113.5
100	115.0	30.0	115.0

TABLE 3
 STORE CUMULATIVE PRESSURE DATA

From CRC³ Handbook:

Boiling Point = 951.4 K

thus

$$\frac{10^4}{T} = 10.51, \log(760 \text{ mm}) = 2.88.$$

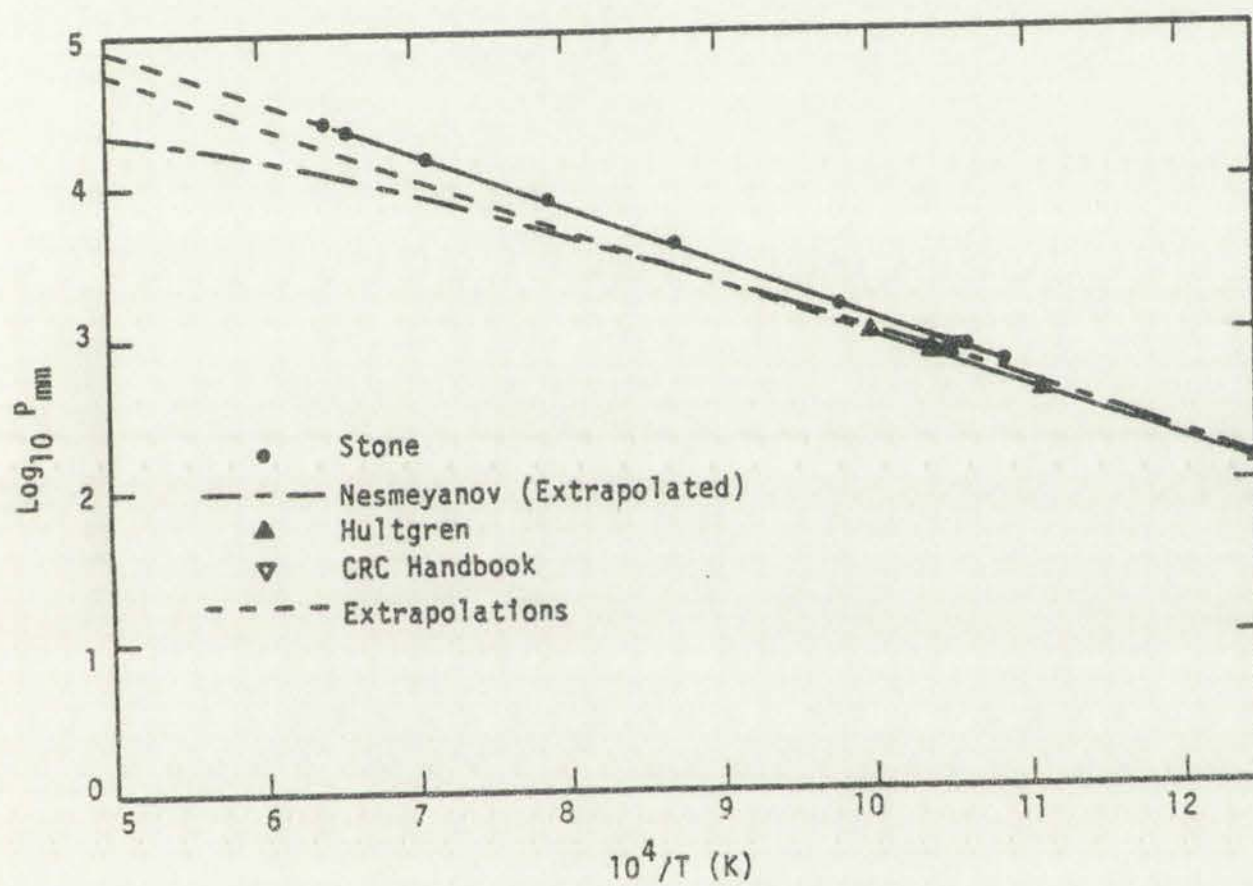


Figure L.7
Vapor pressure of Cesium.

1953

1954

1955



Figure 1
 Comparison of two series
 over the period 1953-1955

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APPENDIX M
DERIVATION OF VAPOR PRESSURE EQUATION
ASSUMING TEMPERATURE DEPENDENT LATENT HEAT
OF VAPORIZATION

For compressible substance

$$dU = TdS - PdV \quad (M-1)$$

where

U = internal energy,

T = temperature,

S = entropy,

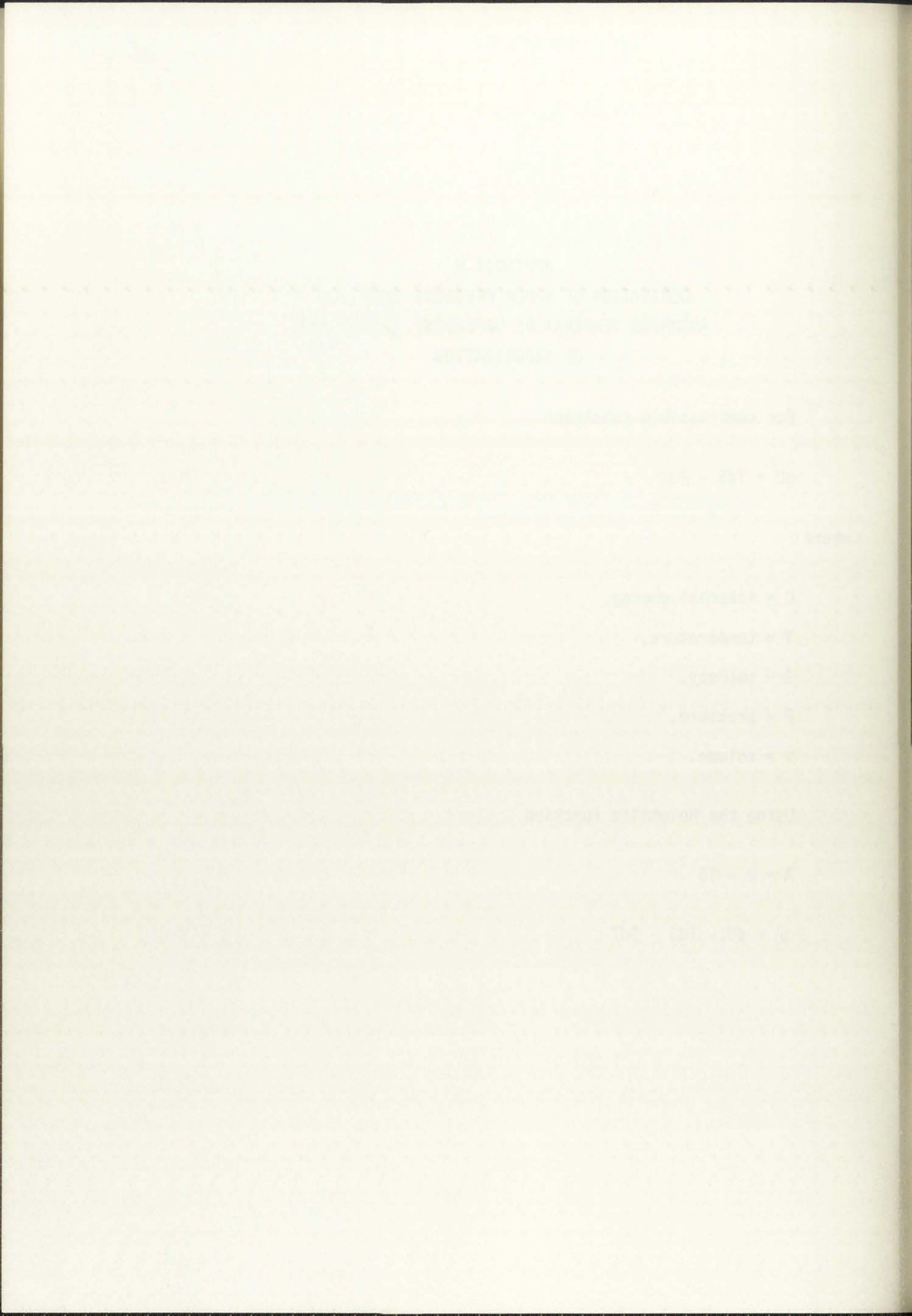
P = pressure,

V = volume.

Using the Helmholtz function

$$A = U - TS$$

$$dA = dU - TdS - SdT \quad (M-2)$$



Substitute Eq. (M-1) into Eq. (M-2)

$$dA = -PdV - SdT$$

$$-dA = PdV + SdT \quad (M-3)$$

For $z = f(x,y)$

$$dz = \left. \frac{\partial z}{\partial x} \right|_y dx + \left. \frac{\partial z}{\partial y} \right|_x dy = Mdx + Ndy \quad ,$$

then

$$\left. \frac{\partial M}{\partial y} \right|_x = \left. \frac{\partial N}{\partial x} \right|_y \quad ,$$

thus from Eq. (M-3)

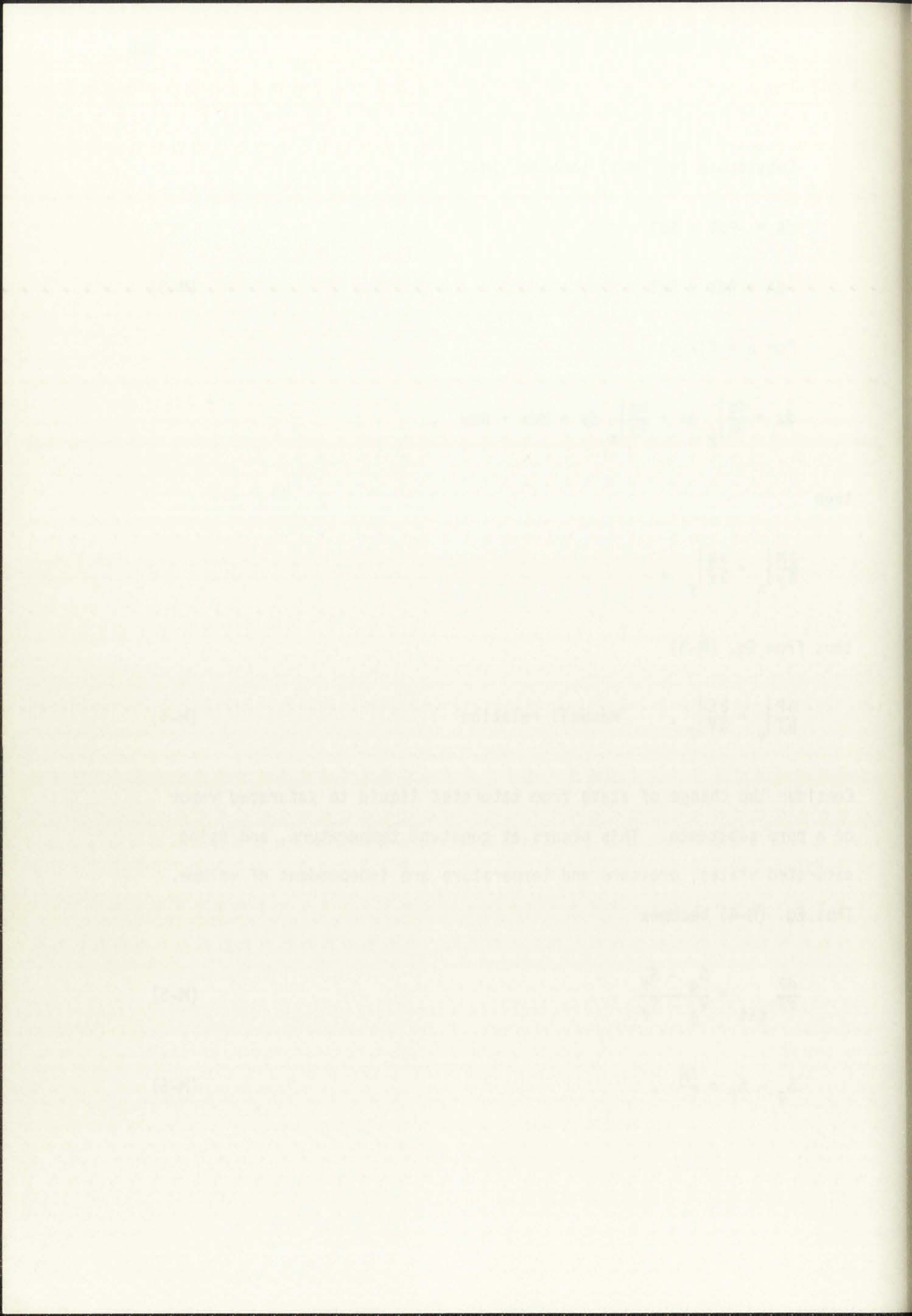
$$\left. \frac{\partial P}{\partial T} \right|_V = \left. \frac{\partial S}{\partial V} \right|_T \quad , \quad \text{Maxwell relation} \quad (M-4)$$

Consider the change of state from saturated liquid to saturated vapor of a pure substance. This occurs at constant temperature, and using saturated states, pressure and temperature are independent of volume.

Thus Eq. (M-4) becomes

$$\left. \frac{dP}{dT} \right|_{\text{sat}} = \frac{S_g - S_f}{V_g - V_f} \quad , \quad (M-5)$$

$$S_g - S_f = \frac{\Delta H}{T} \quad , \quad (M-6)$$



where ΔH is the latent heat of sublimation or vaporization thus Eq.

(M-5) becomes

$$\frac{dP}{dT} = \frac{\Delta H}{T\Delta V} \quad , \quad (M-7)$$

where

ΔV = change in volume during transition from condensed to vapor phase.

Assume the volume of the condensed phase is small compared to the vapor phase. Using the Ideal Gas law, Eq. (M-7) becomes

$$\frac{dP}{dT} = \frac{P\Delta H}{RT^2} \quad ,$$

or

$$\frac{d \ln P}{dT} = \frac{\Delta H}{RT^2} \quad . \quad (M-8)$$

Now if one assumes a constant ΔH

integrating Eq. (M-8)

$$\ln P = \frac{-\Delta H}{RT} + \text{constant} \quad ,$$

$$\text{Log } P = - \frac{\Delta H}{4.575T} + C = A + \frac{B}{T} \quad ,$$

which takes the straight line form.

Now assume ΔH is a function of temperature

$$\Delta H = \Delta H_0 + aT + bT^2 + cT^3 + \text{-----} \quad . \quad (M-9)$$

where ρ is the density of the liquid and ρ_v is the density of the vapor.

$$\rho = \rho_0 (1 - \beta \Delta T)$$

where ρ_0 is the density of the liquid at the normal boiling point and β is the coefficient of thermal expansion.

where

ΔT is the change in temperature during the process.

where ρ_0 is the density of the liquid at the normal boiling point and β is the coefficient of thermal expansion.

where ρ_0 is the density of the liquid at the normal boiling point and β is the coefficient of thermal expansion.

$$\rho = \rho_0 (1 - \beta \Delta T)$$

(2-3)

$$\rho = \rho_0 (1 - \beta \Delta T)$$

where ρ_0 is the density of the liquid at the normal boiling point and β is the coefficient of thermal expansion.

$$\rho = \rho_0 (1 - \beta \Delta T)$$

$$\rho = \rho_0 (1 - \beta \Delta T)$$

$$\rho = \rho_0 (1 - \beta \Delta T)$$

where ρ_0 is the density of the liquid at the normal boiling point and β is the coefficient of thermal expansion.

where ρ_0 is the density of the liquid at the normal boiling point and β is the coefficient of thermal expansion.

(2-4)

$$\rho = \rho_0 (1 - \beta \Delta T)$$

Substitute Eq. (M-9) into Eq. (M-8)

$$d \ln P = \frac{\Delta H_0}{RT^2} dT + \frac{a}{R} \frac{dT}{T} + \frac{b}{R} dT + \frac{c}{R} T dT + \text{-----} , \quad (\text{M-10})$$

integrate

$$\ln P = - \frac{\Delta H_0}{RT} + \frac{a}{R} \ln T + \frac{b}{R} T + \text{-----} + \text{constant} , \quad (\text{M-11})$$

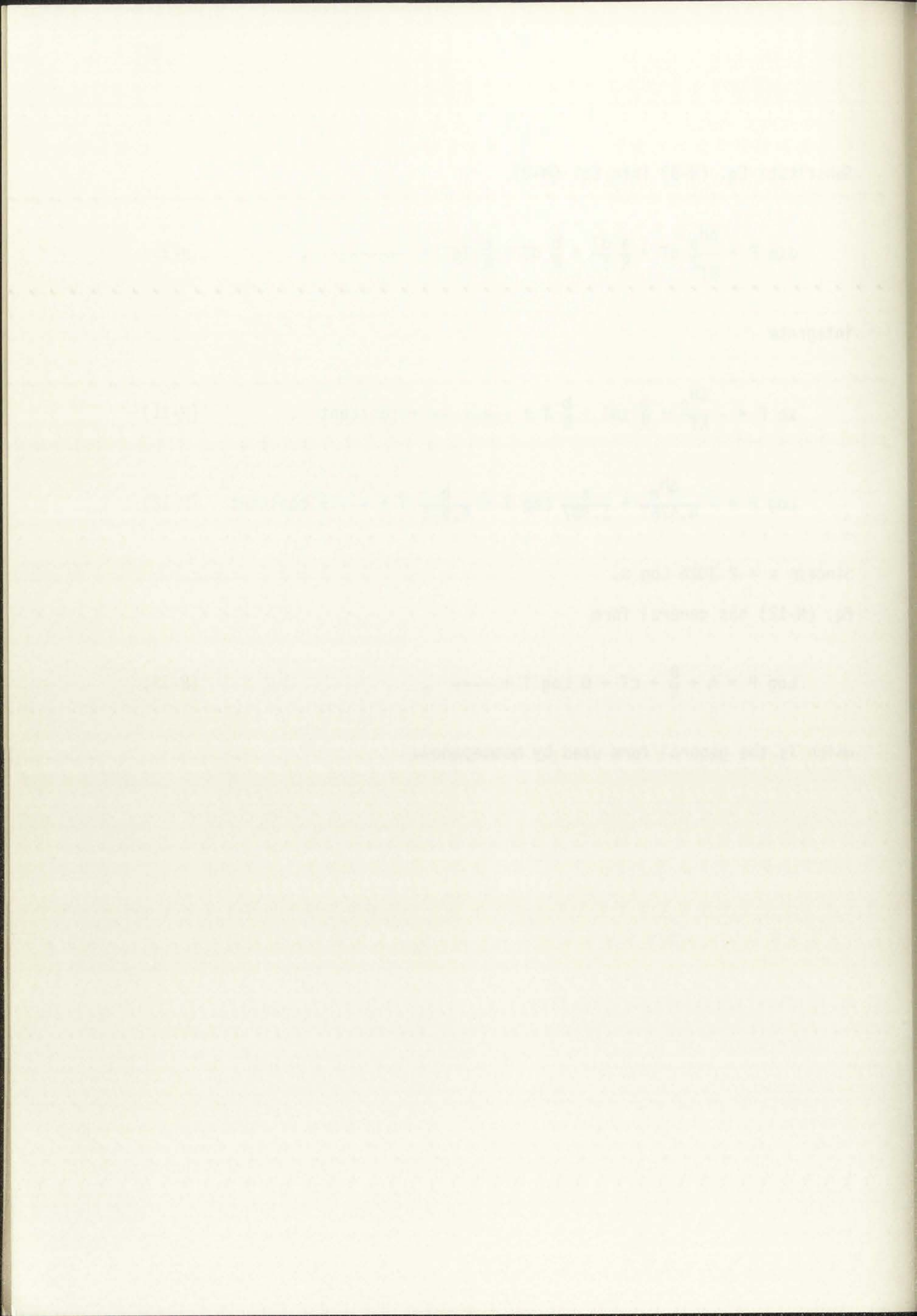
$$\text{Log } P = - \frac{\Delta H_0}{4.575T} + \frac{a}{1.987} \text{Log } T + \frac{b}{4.575} T + \text{---} + \text{constant} . \quad (\text{M-12})$$

Since $\ln x = 2.3026 \text{Log } x$,

Eq. (M-12) has general form

$$\text{Log } P = A + \frac{B}{T} + cT + D \text{Log } T + \text{----} , \quad (\text{M-13})$$

which is the general form used by Nesmeyanov.



APPENDIX N
PROGRAM LISTING

MEMORANDUM

DATE: 10/10/54

TO: SAC, NEW YORK

FROM: SAC, NEW YORK

SUBJECT: [Illegible]

RE: [Illegible]

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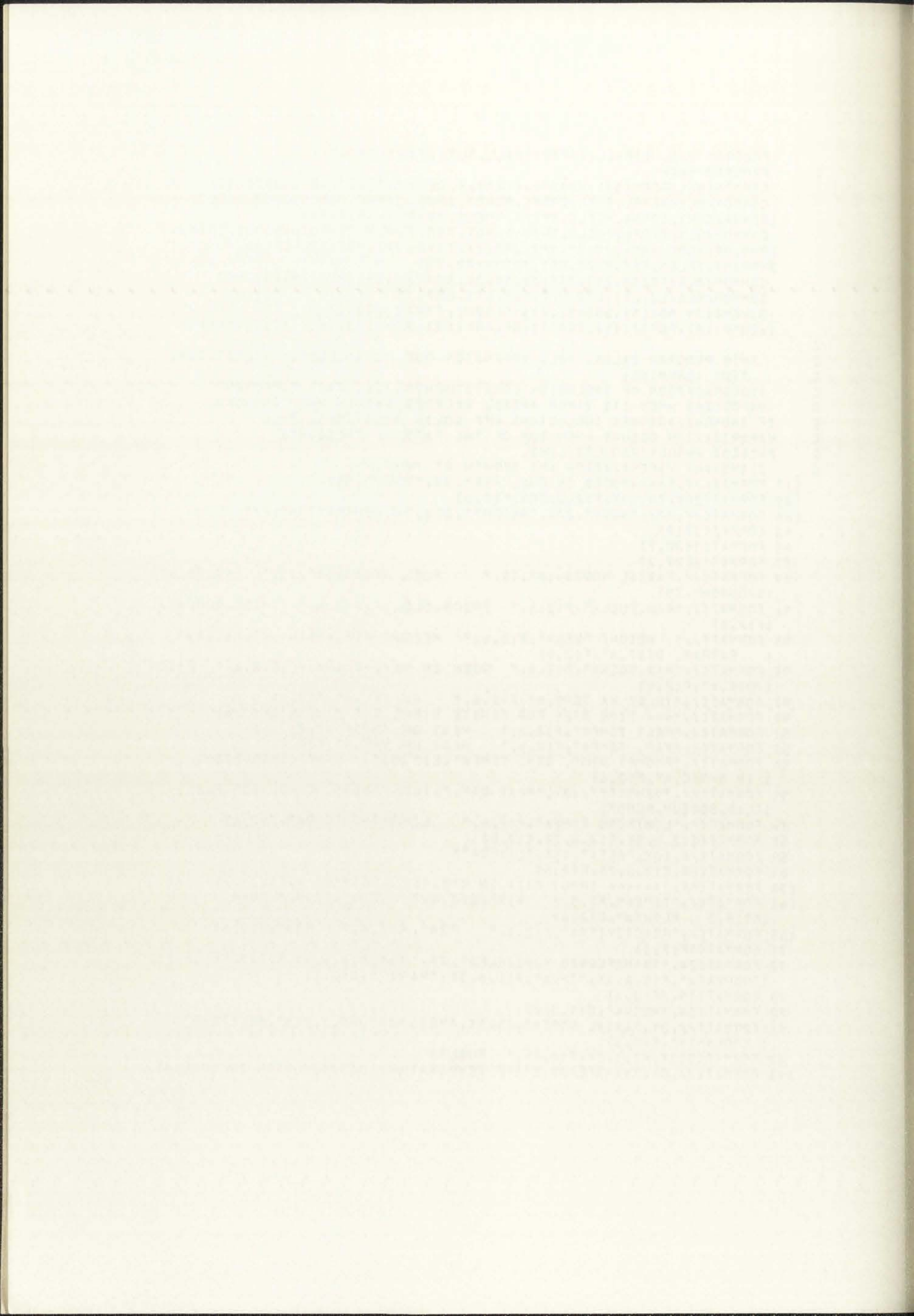
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PROGRAM VAIL (INALL,TAPE9=INALL,OUT1,TAPE10=OUT1)
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COMMON/BL2/DENFL,SHFL,CONF,DEBND,SHBD,CONBD,DENCD,SHCD,CONCD,
IDENNA,SHNA,CONNA,HCFLC,TMELT,HMELT,TVAP,HVAP,TEMAX
COMMON/BL3/RADFL,THCLD,THBND,HGT,DEC,THFLM,TEMPO,U,COOUT,COIN,
IDHG,DR,HCOV,ARFA,J4,IM,IMZ,JMZ,IA,TAVE,IPZ,HCFL0T,HCFL0B,
2NPRINT,TPLEN,TSTOR(20,25),TSTOV(20,25)
COMMON/BL5/TS(30,25),TSB(25,30,2),SGH(20,25),SVP(20,25),NCO
COMMON/BL6/LJ,LT1,LT2,VL1,VL2,LT3,LBP,JC
DIMENSION RS(15),DS(15),QYAYF(300),TTP2(300),E(15)
I,COMP(15),PCRT(15),TCRT(15),ARK(15),BRK(15),CHI(15),DRINC(15)

C THIS PROGRAM CALCS. VOL. EXPANSION DUE TO INCLUSION VOLITILIZA-
C TION ASSUMING:
C 1) SEGRAGATION OF INCLUSION CONSTITUENTS, I.E. EACH COMPONENT
C VAPORIZES WHEN ITS VAPOR PRESS. EXCEEDS P-BULK WHEN IHOMO=0.
C IF IHOMO=1, ASSUMES INCLUSIONS ARE SOLID SOLUTIONS, THUS
C VAPORIZATION OCCURS WHEN SUM OF THE PARTIAL PRESSURES
C EXCEEDS P-BULK (RAOULTS LAW).
C 2) INSTANT VAPORIZATION AND GROWTH AT TVAP.
117 FORMAT(/, "*****NODES IN FUEL ARE", I5, "THRU", I5)
129 FORMAT(20X, I4, 17X, F12.6, 20X, F12.6)
125 FORMAT(/, 20X, "NODE", 20X, "HEIGHT", 20X, "Q GENERATION", /)
83 FORMAT(3I10)
85 FORMAT(3E20, 7)
87 FORMAT(2E20, 7)
89 FORMAT(/, "AXIAL NODES=i=", I5, " FUEL NODES=i=", I5, " NO. DELAY
IGROUPS=", I5)
91 FORMAT(/, "RAD. FUEL=", F12.6, " THICK. CLD.=", F12.6, " THICK. BOND=",
IF12.6)
93 FORMAT(/, " HEIGHT FUEL=", F12.6, " HEIGHT REF.+BLANK.=", F12.6, "
1 EXTRAP. DIST.=", F12.6)
95 FORMAT(/, "MAX. QGEN=", F12.6, " QGEN IN REF.+BLANK.=", F12.6, " PITCH
1/DIA.=", F12.6)
97 FORMAT(/, "INLET NA TEMP.=", F12.6, " NA VEL.=", F12.6)
99 FORMAT(/, "*** TIME STEP FOR FINITE DIFF. AND PTKEN=", F12.6)
51 FORMAT(/, "MELT TEMP=", F12.6, " HEAT OF FUSION=", F12.6)
53 FORMAT(/, "VAP. TEMP=", F12.6, " HEAT OF VAP.", F12.6)
54 FORMAT(/, "PROMPT NEUT. GEN. TIME=", E12.6, " RAMP INSERTION
1 IN 1/SEC.=", F12.6)
55 FORMAT(/, "DENSITY", 10X, "HEAT CAP.", 10X, "THERM. COND. FOR FUEL.
ICLAD, SODIUM, BOND")
56 FORMAT(/, "LIMITING TIME=", F12.6, " LIMITING TEMP=", F12.6)
57 FORMAT(E12.6, 5X, F12.6, 7X, E12.6)
59 FORMAT(/, 10X, "BETA", 15X, "LAMBDA")
63 FORMAT(6X, E12.6, 7X, F12.6)
130 FORMAT(5X, "***** INPUT DATA IN CMS, SEC., DEGREES K, CAL.", /)
163 FORMAT(/, "TIME=", F7.5, " P1=", E12.6, " DT=", F7.5, " D=",
IF7.5, " P1. OUT=", E12.6)
165 FORMAT(/, "REACTIVITY=", E12.6, " P2=", E12.6, " P3=", E12.6)
71 FORMAT(2F10.3)
72 FORMAT(2X, "TRANSFERRED VARIABLES", 2X, "T=", F11.6, 4X, "DT=", F11.6, 4X,
1 "H0HEAT=", F15.8, 4X, "TMAX", F11.6, 3X, "RAVE ", E12.5)
78 FORMAT(15, 2F12.4)
80 FORMAT(3X, "HCOV=", E11.3, /)
81 FORMAT(/, 3X, "AXIAL NODES=", I3, 3X, "HEIGHT=", F9.3, "C4", 6X, "TEMP
1 COOLANT=", F10.3)
82 FORMAT(5(3X, F7.3, 2X, F10.3), " FUEL")
143 FORMAT(/, 8X, "***STEADY STATE TEMPERATURE DISTRIBUTION IN COOLANT

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1 AND FUEL PTN***",/)
147 FORMAT(2(3X,F7.3,2X,E10.3),," CLAD INNER AND OUTER TEMPS,")
202 FORMAT(3X,"DFLTT",F12.6,3X,"DT",F10.6,3X,"QZAV(CAL/CC SEC)",E12.5,
13X,"QZAW(WATTS/CC)",E12.5)
199 FORMAT(5(3X," R ",2X," TEMP "))
144 FORMAT(////,3X,"***** TRANSIENT CALCULATION *****",//)
21 FORMAT(I10)
22 FORMAT(/,"PLENPRESS=",F10.5," RAD. INCL=",E12.6," NO.
1 DENSITY OF INCL=",E12.6)
24 FORMAT(/,"MATERIAL=",10X," MOLES/INCL")
28 FORMAT(3X,IS,12X,E12.6)
37 FORMAT(/,"ELEMENT",10X,"PCRIT",10X,"TCRIT")
33 FORMAT(3X,IA,10X,E12.6,5X,E12.6)
49 FORMAT(/,"NODE",15X,"CHI")
301 FORMAT(/,10X,"***INCLUSION ASSUMED SEGREGATED***")
304 FORMAT(/,10X,"***INCLUSION ASSUMED HOMOGENEOUS***")

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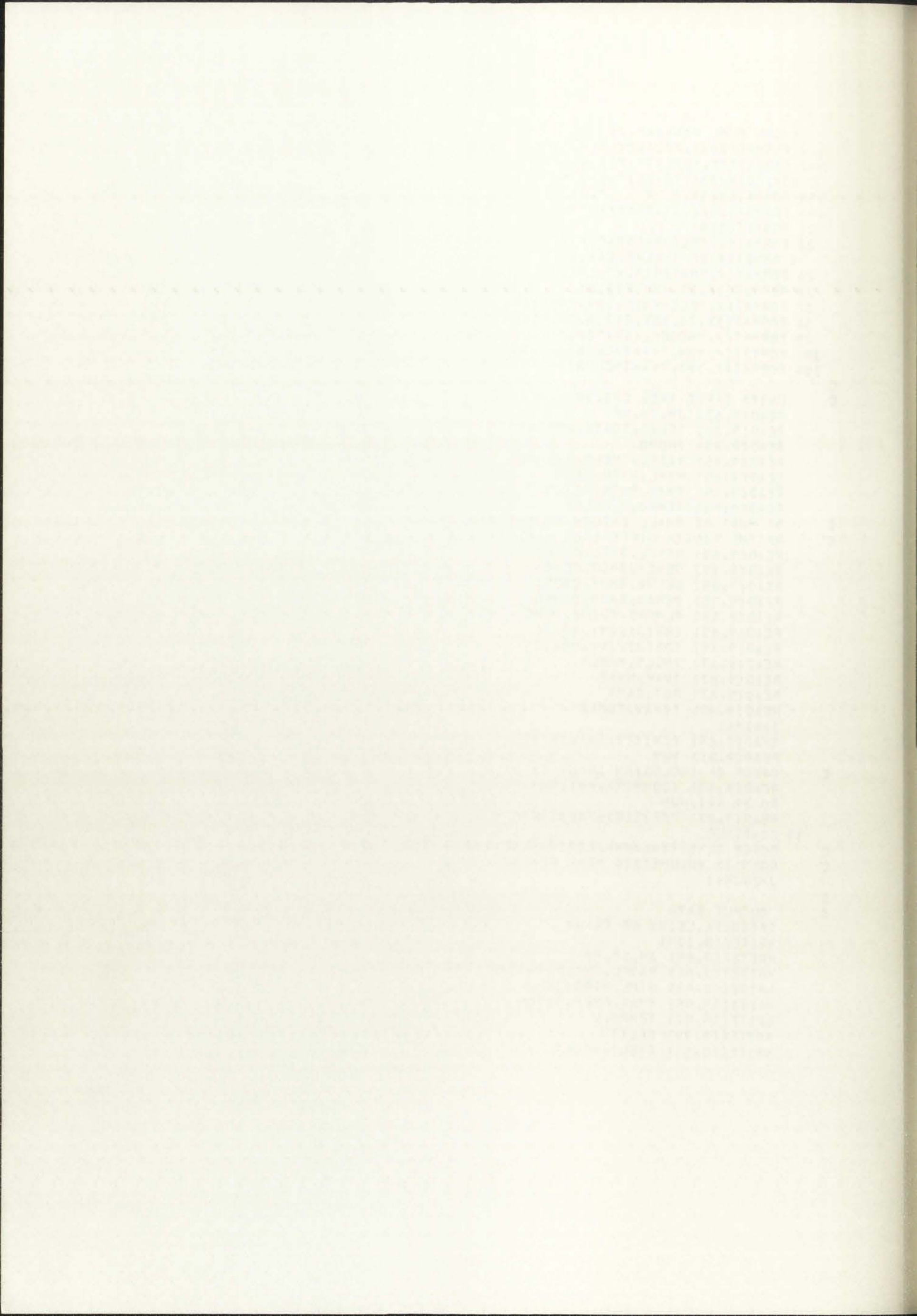
C
C UNITS INPUT ARE: CMS,SEC.,DEGREES K,CAL.
C READ(9,83) JM,IM,NP
C READ(9,83) IFLAG,ICATA,NPRINT.
C READ(9,83) IHOMO
C READ(9,85) RADFL,THCLD,THRONO
C READ(9,85) HTFL,HTRB,ZEXT
C READ(9,85) PMAX,PMIN,PITCH
C READ(9,85) TEMPO,U,DELTT
C DT MUST BE SMALL ENOUGH TO SATISFY THE CONVERGENCE CRITERION
C OF THE FINITE DIFFERENCE HEAT TRANSFER EQUATIONS
C READ(9,85) DENFL,SHFL,CONF1
C READ(9,85) DENC0,SHCD,CONCD
C READ(9,85) DENNA,SHNA,CONNA
C READ(9,85) DENRD,SHRD,CONRD
C READ(9,85) PLNPRS,ROINC,DINC
C READ(9,85) (BS(J),J=1,NP,1)
C READ(9,85) (DS(J),J=1,NP,1)
C READ(9,87) TMELT,HMELT
C READ(9,87) TVAP,HVAP
C READ(9,87) PGT,RAMP
C READ(9,87) TIMAX,TEMAX
C IA=IM+1
C READ(9,85) (CHI(I),I=1,IA,1)
C PEAD(9,21) NUM
C ORDER OF INCLUSION INPUT IS BA,CE,PD,FE,TE,SB,CS,MO,RU,RH,TC
C READ(9,85) (COMP(K),K=1,NUM,1)
C DO 39 K=1,NUM
C READ(9,87) PCRIT(K),TCRIT(K)
39 CONTINUE
C POWER DENSITY=6000KW/LITER=1400CAL/CM3.SEC
C QGEN IS VOLUMETRIC HEAT GENERATION
C J4Z=JM+1

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C
C OUTPUT DATA
C IF(ICATA,LE,0) GO TO 40
C WRITE(10,130)
C WRITE(10,89) JM,IM,NP
C WRITE(10,91) RADFL,THCLD,THRONO
C WRITE(10,93) HTFL,HTRB,ZEXT
C WRITE(10,95) PMAX,PMIN,PITCH
C WRITE(10,97) TEMPO,U
C WRITE(10,99) DFLTT
C WRITE(10,51) TMELT,HMELT

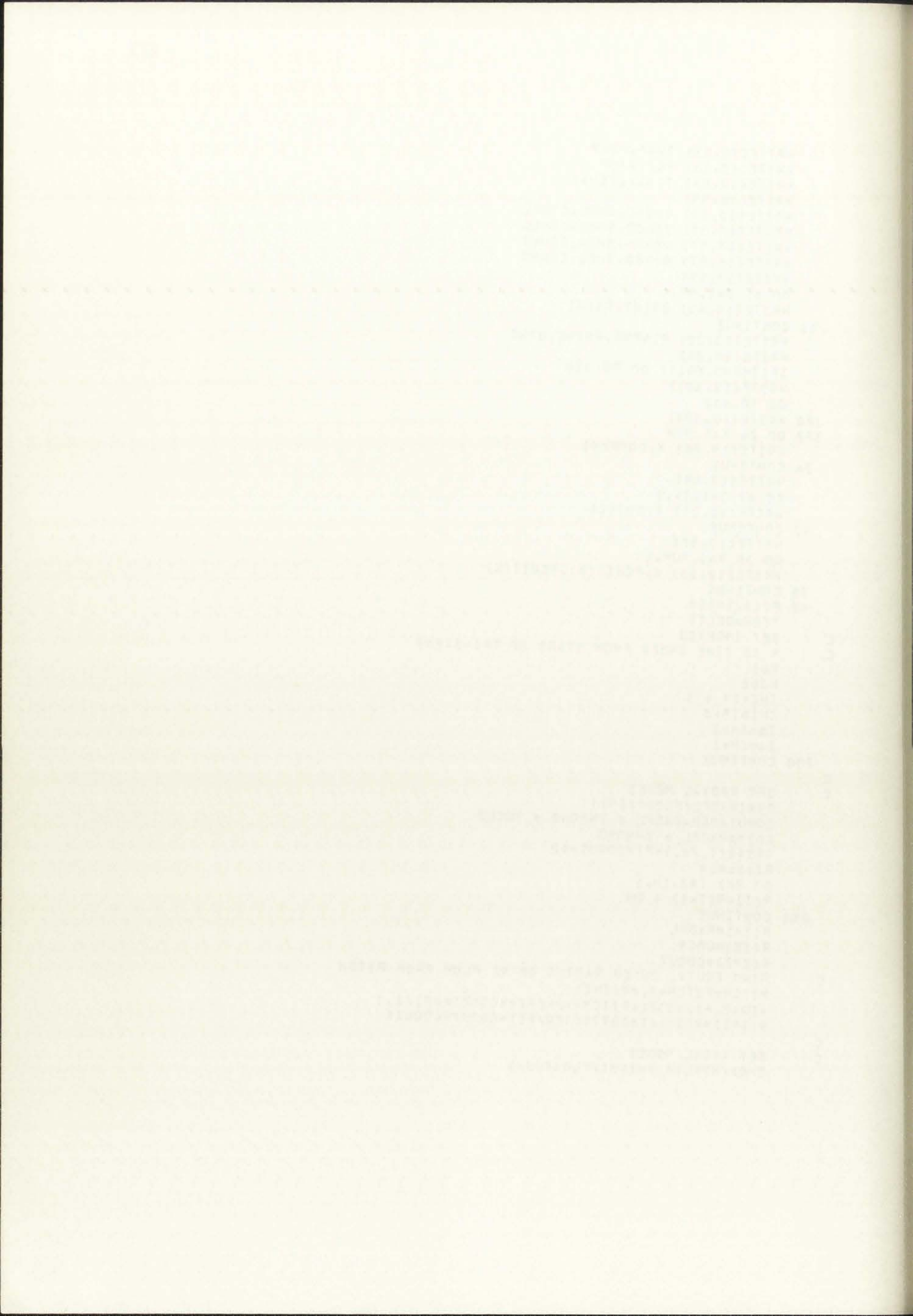
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WRITE(10,53) TVAP,HVAP
WRITE(10,54) PGT,RAMP
WRITE(10,56) TIMAX,TEMAX
WRITE(10,55)
WRITE(10,57) DENFL,SHFL,CONF
WRITE(10,57) DENCO,SHCO,CONCO
WRITE(10,57) DENNA,SHNA,CONNA
WRITE(10,57) DENBO,SHBO,CONBO
WRITE(10,59)
DO 61 J=1,NP,1
WRITE(10,63) BS(J),DS(J)
61 CONTINUE
WRITE(10,22) PLNPRS,ROINC,DINC
WRITE(10,24)
IF(IHOMO.EQ.1) GO TO 300
WRITE(10,301)
GO TO 302
300 WRITE(10,304)
302 DO 26 K=1,NUM
WRITE(10,28) K,COMP(K)
26 CONTINUE
WRITE(10,49)
DO 47 I=1,IA,1
WRITE(10,29) I,CHI(I)
47 CONTINUE
WRITE(10,37)
DO 35 K=1,NUM,1
WRITE(10,33) K,PCRT(K),TCRT(K)
35 CONTINUE
40 PI=3.14159
TTEM=DELTT
C
C SET INDEXES
C K IS TIME INDEX FROM START OF TRANSIENT
K=1
KJ=2
IMZ=IM+3
IPZ=IM+4
IB=IM+2
IA=IM+1
200 CONTINUE
C
C SET RADIAL NODES
DR=(RADFL/FLOAT(IM))
COOUT=DEQ=RADFL+THROND+THCLD
COIN=RADFL+THROND
AREA=(1./4.)*PI*COOUT**2
R(1)=0.0
DO 201 I=2,IM,1
R(I)=R(I-1)+DR
201 CONTINUE
R(IA)=RADFL
R(IB)=COIN
R(IMZ)=COOUT
C
C FIND EQUIV. OUTER RADIUS OF NA FLOW FROM PITCH
PITCM=PITCH*2.*R(IMZ)
AEQ=2.*(1.43301+PITCM**2-(PI*R(IMZ)**2)/2.)
R(IPZ)=R(IM+4)=SQRT((AEQ/PI)+COOUT*COOUT)
C
C SET AXIAL NODES
CHG=(HTFL+2.*HTRB)/FLOAT(JM)

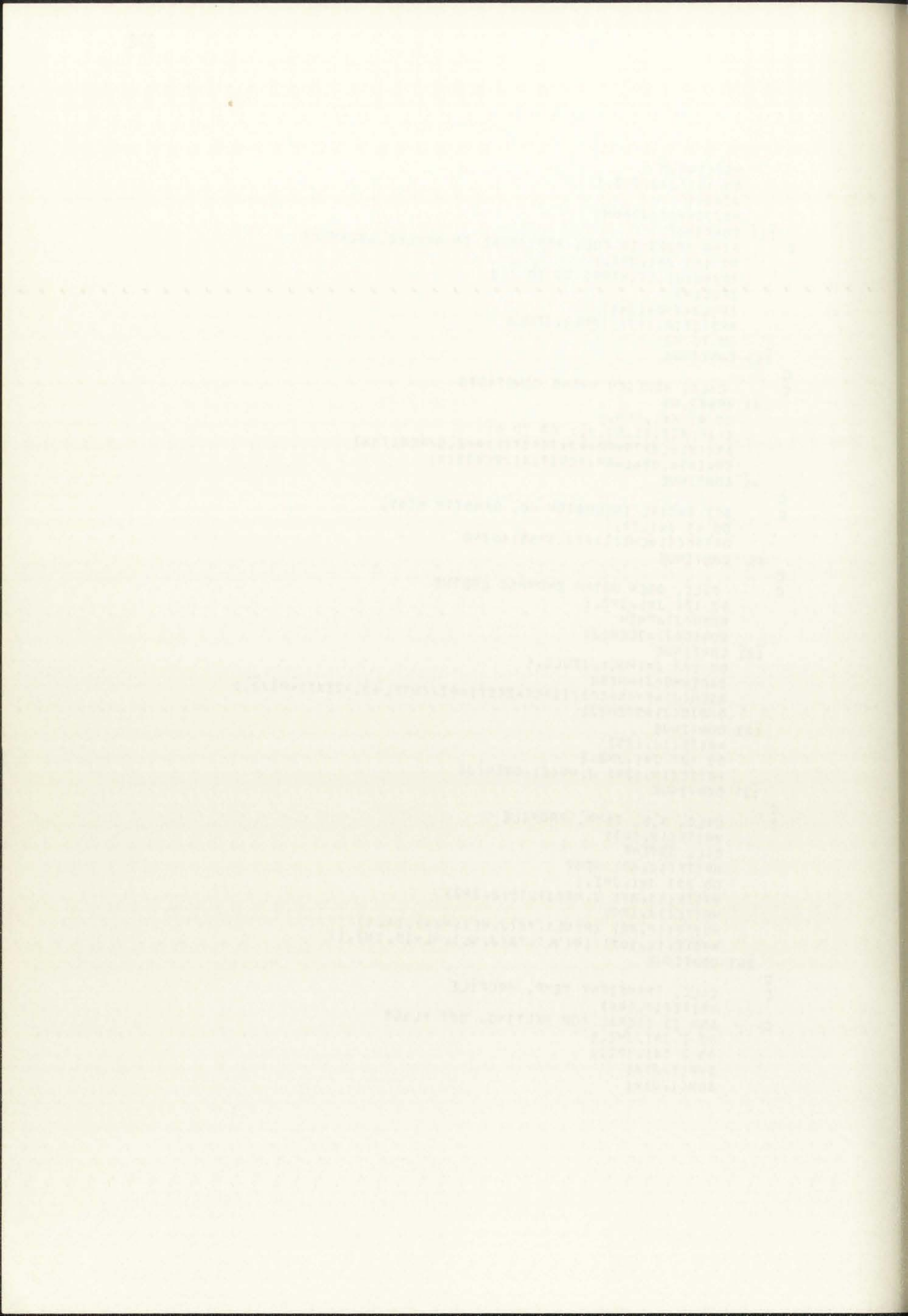
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HG(1)=0.0
DO 111 J=2, JMZ, 1
JJ=J-1
HG(J)=HG(JJ)+DHG
111 CONTINUE
C FIND NODES IN FUEL AND THOSE IN REFLEC.=BLANKET
DO 113 J=1, JMZ, 1
IF(HG(J).LT.HTRB) GO TO 113
IFUL1=J
IFUL2=JMZ-(J-1)
WRITE(10,117) IFUL1,IFUL2
GO TO 43
113 CONTINUE
C
C CALC. REDLICH KWONG CONSTANTS
43 RR=82.85
DO 41 K=1, NUM, 1
IF(PCRIT(K).EQ.0.) GO TO 41
ARK(K)=.4275*RR**2*TCRIT(K)**2.5/PCRIT(K)
BRK(K)=.2866*RR*TCRIT(K)/PCRIT(K)
41 CONTINUE
C
C SET RADIAL INCLUSION NO. DENSITY DIST.
DO 45 I=1, IA, 1
DRINC(I)=CHI(I)*(1.5955)*DINC
45 CONTINUE
C
C CALC. QGEN USING CHOPPED COSINE
DO 121 J=1, JMZ, 1
QGEN(J)=PMIN
QORIG(J)=QGEN(J)
121 CONTINUE
DO 123 J=IFUL1, IFUL2, 1
ZACT=HG(J)-HTRB
QGEN(J)=PMAX*COS((ZACT+ZEXT)*PI/(HTFL+2.*ZEXT)-PI/2.)
QORIG(J)=QGEN(J)
123 CONTINUE
WRITE(10,125)
DO 127 J=1, JMZ, 1
WRITE(10,129) J, HG(J), QGEN(J)
127 CONTINUE
C
C CALC. S.S. TEMP. PROFILE
WRITE(10,143)
CALL SSTEMP
WRITE(10,80) HCOV
DO 203 J=1, JMZ, 1
WRITE(10,81) J, HG(J), TS(J, IPZ)
WRITE(10,199)
WRITE(10,82) (R(NL), TS(J, NL), NL=1, IA, 1)
WRITE(10,147) (R(NL), TS(J, NL), NL=IB, IMZ, 1)
203 CONTINUE
C
C CALC. TRANSIENT TEMP. PROFILE
WRITE(10,144)
SGM IS SIGNAL FOR MELTING, SET FLAGS
DO 2 J=1, JMZ, 1
DO 2 I=1, IPZ, 1
SVP(I, J)=1
SGM(I, J)=1

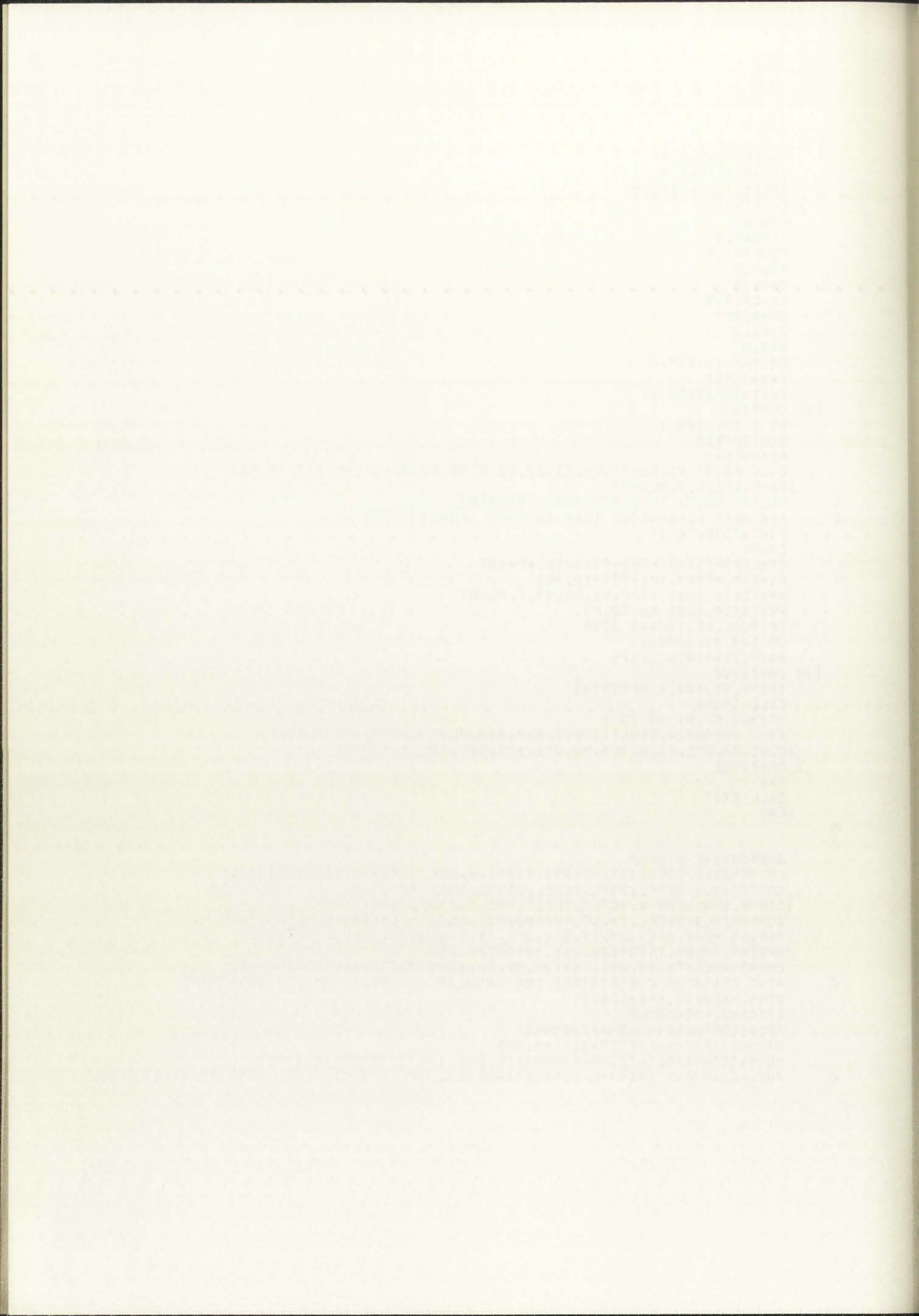
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TSTOR(I,J)=0.0
TSTOV(I,J)=0.0
TSR(I,J,1)=TS(J,I)
2 CONTINUE
NCO=0
TIME=0.0
P2=P3=1.0
R2=0.0
C0=1.0
C1=C2=0.0
DPM=.001
P1=1.0
B=0.0
DO 161 I=1, NP, 1
B=B+BS(I)
E(I)=BS(I)/DS(I)
161 CONTINUE
DO 3 I=1, 300, 1
DELTT=TTEM
NCO=NCO+1
CALL POINT(P1, DELTT, C0, C1, C2, R2, E, DS, BS, R, PGT, NP, DPM, P2, P3,
1 RAMP, IFLAG, D, PLOUT)
C DELTT= DELTA TIME FOR HEAT TRANSFER
C AVE HEAT GENERATION TERM IN WATT FOR COMPARE
C TIME=TIME+DELTT
C0=P1
C2=((P3-P1)-2.*(P2-P1))/(2.*D**2)
C1=(-4.*P2+3.*P1+P3)/(2.*D)
WRITE(10,163) TIME,P1,DELTT,D,PLOUT
WRITE(10,165) R2,P2,P3
IF(TIME.GE.TIMAX) STOP
DO 149 J=1, JMZ, 1
QGEN(J)=QORIG(J)*P1
149 CONTINUE
IF(P1.GT.100.) NPRINT=1
CALL TRANS
IF(NCO.GT.0) GO TO 3
CALL VAPOR(IA, IFUL1, IFUL2, SVP, SGM, PLNPRS, NUM, RDINC, COMP,
1 DINC, DR, DHG, PI, R, TSB, HG, JMZ, ARK, BRK, DRINC, IHOMO)
3 CONTINUE
K=1
CALL EXIT
END
C
C
SUBROUTINE SSTEMP
COMMON/BL1/QGEN(30), HG(30), R(20), K, DELTT, PI, IA, AEG, QORIG(30)
COMMON/BL2/DENFL, SHFL, CONFL, DENBD, SHBD, CONBD, DENCD, SHCD, CONCD,
1 DENNA, SHNA, CONNA, HCFLO, TMELT, HMELT, TVAP, HVAP, TMAX
COMMON/BL3/RAOFL, THCLD, THBND, HGT, DEQ, THFLM, TEMPO, U, CDOUT, CDIN,
1 DHG, DR, HCOV, AREA, JM, IM, IMZ, JMZ, IA, TAVE, IPZ, HCFLOT, HCFLOB,
2 NPRINT, TPLEN, TSTOR(20,25), TSTOV(20,25)
COMMON/BL5/TS(30,25), TSR(25,30,2), SGM(20,25), SVP(20,25), NCO
C HEAT TRANSFER COEFFICIENT FOR ANNULAR CHANNELS (PG 378, SENSORSKE)
DE=4.*AEG/(2.*PI*CDOUT)
CIRCD=2.*PI*CDOUT
PEC=((DE*U*DENNA*SHNA)/CONNA)
RANNU=((R(IM+4)/R(IM+3))**.30)
HCOV=(CONNA/DE)*(2.80*RANNU)*(5.1 + (0.226*(PEC**.80**R)))
C FUEL=CL40 GAP THERMAL CONDUCTANCE(CAL/SEC CM2 C) .45 USED BY MACFARLAND

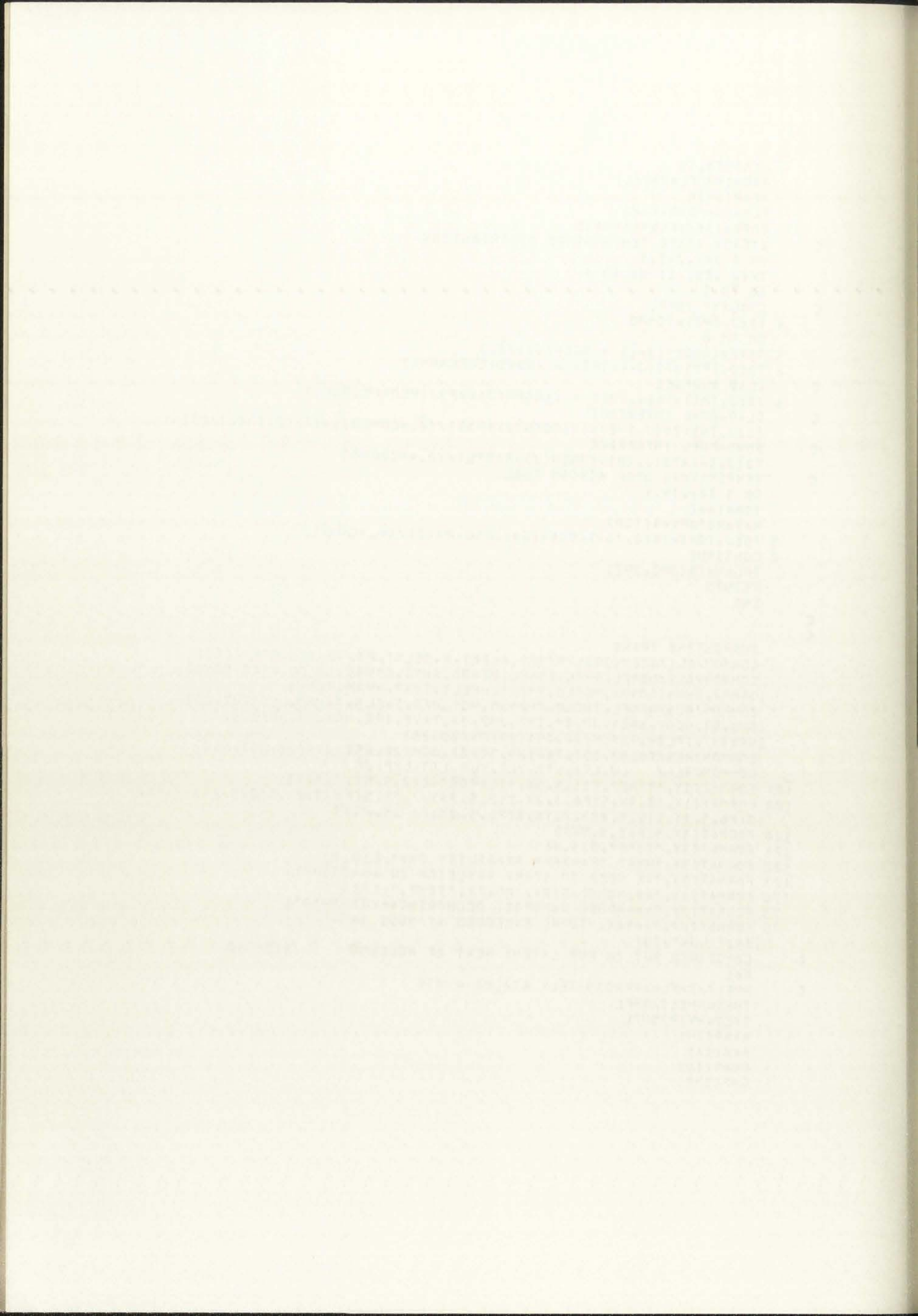
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HCBOND=.45
RSQ=(RADFL*ADFL)
AF=PI*RSQ
FLOW=U*DENNA*AEA
COFC=(AF/(FLOW*SHNA))
C
STADY STATE TEMPERATURE DISTRIBUTION
DO 2 J=1, JMZ, 1
IF(J.EQ. 1) GO TO 4
GO TO 5
C
COOLANT TEMP.
4 TS(J, IPZ)=TEMPO
GO TO 6
5 QAVE=((QGEN(J-1) + QGEN(J))/2.)
8 TS(J, IPZ)=TS(J-1, IPZ) + (QAVE*COFC*DHG)
C
CLAD SURFACE
6 TS(J, IMZ)=TS(J, IPZ) + ((QGEN(J)*AF)/(HCOV*CIROD))
C
CLAD-BOND INTERFACE
TS(J, IB)=TS(J, IMZ)+(((QGEN(J)*RSQ)/(2.*CONCD))*ALOG(COOUT/COIN))
C
BOND-FUEL INTERFACE
TS(J, IA)=TS(J, IB)+(QGEN(J)*RADFL)/(2.*HCBOND)
C
TEMPERATURE DROP ACROSS FUEL
DO 3 I=1, IM, 1
IQP=IA-I
RAT=R(IQP)*R(IQP)
3 TS(J, IQP)=TS(J, IA)+(QGEN(J)*(RSQ-RAT))/(4.*CONF)
2 CONTINUE
TLEN=TS(JMZ, IPZ)
RETURN
END
C
C
SUBROUTINE TRANS
COMMON/BL1/QGEN(30), HG(30), R(20), K, DELTT, PI, IR, AEO, CORRIG(30)
COMMON/BL2/DENFL, SHFL, CONF, DENBD, SHBD, CONBD, DENCD, SHCD, CONCD,
1 DENNA, SHNA, CONNA, HCFLC, TMELT, HMELT, TVAP, HVAP, TEMAX
COMMON/BL3/RADFL, THCLD, THBND, HGT, DEG, THFLM, TEMPO, U, COOUT, COIN,
1 CHG, DR, HCOV, AREA, JM, IM, IMZ, JMZ, IA, TAVE, IPZ, HCFLD, HCFLOB,
2 NPRINT, TLEN, TSTOR(20, 25), TSTOV(20, 25)
COMMON/BL5/TS(30, 25), TSB(25, 30, 2), SGM(20, 25), SVR(20, 25), NCO
COMMON/BL6/ LJ, LT1, LT2, VLT, VLR, LT3, LBP, JC
107 FORMAT(3X, "TIME", F11.5, 5X, "TLARGE", E12.5, 5X, "J", I3)
108 FORMAT(1X, I3, 3X, 5(F6.3, 2X, E12.5, 2X), /, 7X, 5(F6.3, 2X, E12.5, 2X), /, 7X,
15(F6.3, 2X, E12.5, 2X), /, 7X, 5(F6.3, 2X, E12.5, 2X))
120 FORMAT(3X, 5(F13.4, 5X))
121 FORMAT(3X, "TIME", E11.4)
122 FORMAT(3X, "HEAT TRANSFER STABILITY CM=", E10.4)
123 FORMAT(3X, "WE NEED TO START RAYLEIGH EQ ---STOP")
174 FORMAT(1X, "AX, NODE", 5(2X, "R", 7X, "TEMP.", 7X))
73 FORMAT(/, "****FUEL VAPORIZ. OCCURRING***STOPPED")
75 FORMAT(/, "****MAX. TEMP. EXCEEDED AT NODE I=",
1 I5, " J=", I5)
C
CONSTANTS PUT IN FOR LATENT HEAT OF MELTING STEP 50
K=1
C
HMELT/SHFL=APPROXIMATELY 67/.08 = 838
TMELT=HMELT/SHFL
TVEQ=HVAP/SHFL
AA=R(IM)
A=R(IA)
BB=R(IB)
C=R(IMZ)

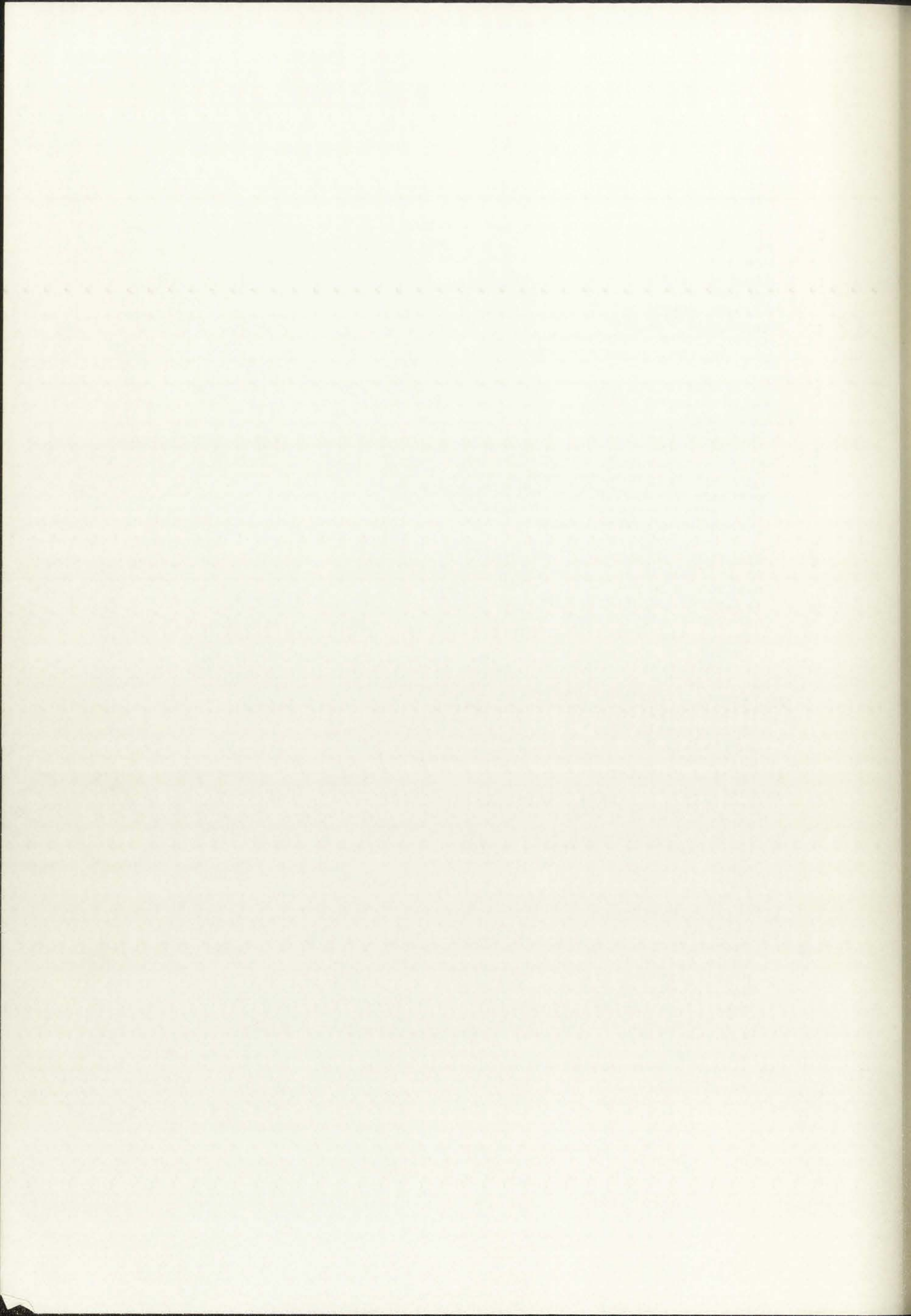
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DD=R(IPZ)
LA=10
NA=100
KA=1
C LOG MEAN DISTANCE BETWEEN CLAD SURFACE AND OUTSIDE EDGE OF COOLANT
RMN=((DD-C)/(ALOG(DD/C)))
HCSTG=(.8)*((R(IM+4)/R(IM+3))**.31*(5.1)*(CONNA/DEG)
C (PG 6=246, WASH=1106) 17608/HR F2 F = .239CAL/CM2 SEC C
HCROND=.45
DQ2=(DEG*DEG)
C CONSTANTS FOR FUEL
ALPHFL=(CONFL/(DENFL*SHFL))
CM=((OR*DR)/(ALPHFL*DELTT))
C
C CM IS STABILITY CRITERIA OF TRANSIENT HEAT TRANSFER EQS. CM>0
WRITE(10,122) CM
16 CONTINUE
TIE=TIE + DELTT
C
C CALC. COEF. NEEDED FOR TRANS. SOLUTION
COEF1=DENFL*SHFL*(PADFL+DR-DR*DR/4.)
COEF2=DENCD*SHCD*(CDIN+THCLD+THCLD*THCLD/4.)/2.
COEF3=DENCD*SHCD*(CDOUT+THCLD+THCLD*THCLD/4.)/2.
COEF4=DHG*DENNA*SHNA*AEG
C
C SOLUTION FOR OVERPOWER TRANSIENT, GGEN VARIABLE
DO 60 J=1, JMZ, 1
QAVE=GGEN(J)
C TRANSIENT SOLUTION AT R=0
GGP=((QAVE*DELTT)/(SHFL*DENFL))
TSB(1, J, K+1)=(TSB(1, J, K)*(1.-(4./CM))) + (TSB(2, J, K)*(4./CM))
+ QGP
1 IF(TSB(1, J, K+1) .GE. TMELT .AND. SGM(1, J) .LE. 2.) GO TO 22
GO TO 24
22 TSTOR(1, J)=TSTOR(1, J)+TSB(1, J, K+1)-TMELT
IF(TSTOR(1, J).LT.TMEQ) GO TO 80
TSB(1, J, K+1)=TMELT+TSTOR(1, J)-TMEQ
SGM(1, J)=3.0
GO TO 24
80 TSB(1, J, K+1)=TMELT
24 CONTINUE
IF(TSB(1, J, K+1) .GE. TVAP .AND. SVP(1, J) .LE. 2.) GO TO 68
GO TO 64
68 TSTOV(1, J)=TSTOV(1, J)+TSB(1, J, K+1)-TVAP
IF(TSTOV(1, J).LT.TVEQ) GO TO 81
TSB(1, J, K+1)=TVAP+TSTOV(1, J)-TVEQ
SVP(1, J)=3.0
GO TO 64
81 TSB(1, J, K+1)=TVAP
64 CONTINUE
C TRANSIENT SOLUTION ACROSS THE FUEL PIN
DO 29 I=2, IM, 1
PMP=(1./CM)*(1.0+(DR/(2.*R(I))))
PMM=(1./CM)*(1.0-(DR/(2.*R(I))))
TSB(I, J, K+1)=(TSB(I-1, J, K)*PMM) + (TSB(1, J, K)*(1.-(2./CM)))
+ (TSB(I+1, J, K)*PMP) + QGP
1 IF(TSB(I, J, K+1) .GE. TMELT .AND. SGM(I, J) .LE. 2.) GO TO 28
GO TO 27
28 TSTOR(I, J)=TSTOR(I, J)+TSB(I, J, K+1)-TMELT
IF(TSTOR(I, J).LT.TMEQ) GO TO 82

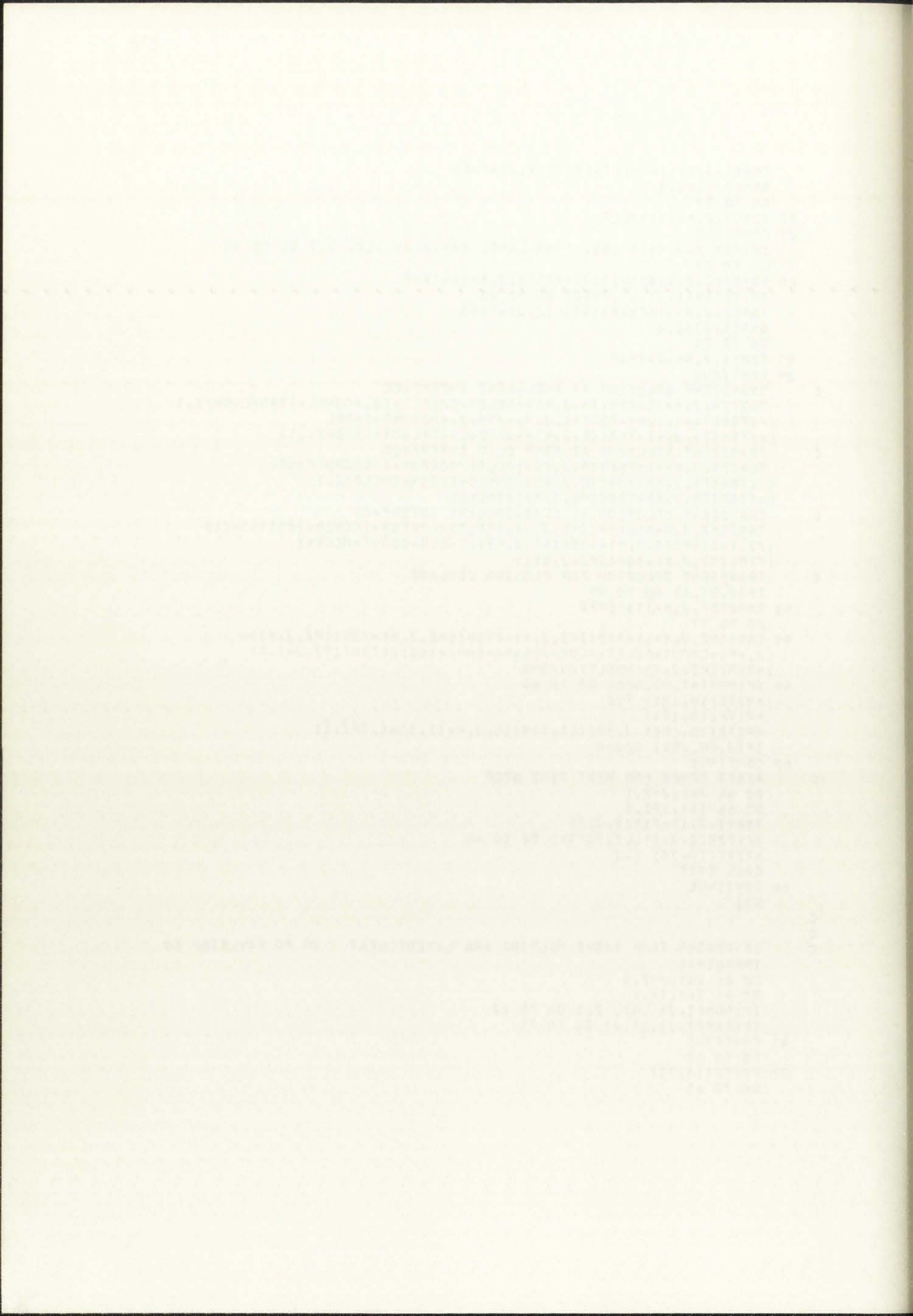
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      TSB(I,J,K+1)=TMELT+TSTOR(I,J)-TMEQ
      SGM(I,J)=3.0
      GO TO 27
82  TSB(I,J,K+1)=TMELT
27  CONTINUE
      IF(TSB(I,J,K+1) .GE. TVAP .AND. SVP(I,J) .LE. 2.) GO TO 45
      GO TO 29
45  TSTOV(I,J)=TSTOV(I,J)+TSB(I,J,K+1)-TVAP
      IF(TSTOV(I,J).LT.TVEQ) GO TO 83
      TSB(I,J,K+1)=TVAP+TSTOV(I,J)-TVEQ
      SVP(I,J)=3.0
      GO TO 29
83  TSB(I,J,K+1)=TVAP
29  CONTINUE
C   TRANSIENT SOLUTION AT FUEL-BOND INTERFACE
      TSB(IA,J,K+1)=TSB(IA,J,K)+(DELTT/COEF1)*(2.*CONFL*(RADFL-DR/2.)
1*(TSB(IA-1,J,K)-TSB(IA,J,K))/DR-2.*HCBOND*RADFL
1*(TSB(IA,J,K)-TSB(IB,J,K))+QAVE*(RADFL*DR-DR*DR/4.))
C   TRANSIENT SOLUTION AT BOND CLAD INTERFACE
      TSB(IB,J,K+1)=TSB(IB,J,K)+(DELTT/COEF2)*(HCBOND*RADFL
1*(TSB(IA,J,K)-TSB(IB,J,K))-CONCD*(CDIN+THCLD/2.)
1*(TSB(IB,J,K)-TSB(IMZ,J,K))/THCLD)
C   TRANSIENT SOLUTION AT CLAD-COOLANT INTERFACE
      TSB(IMZ,J,K+1)=TSB(IMZ,J,K)+(DELTT/COEF3)*(CONCD*(CDIN+THCLD
1/2.)*(TSB(IB,J,K)-TSB(IMZ,J,K))/THCLD-CDOUT*HCOV*(
1TSB(IMZ,J,K)-TSB(IPZ,J,K)))
C   TRANSIENT SOLUTION FOR FLOWING COOLANT
      IF(J.GT.1) GO TO 99
90  TSB(IPZ,J,K+1)=TEMPO
      GO TO 97
99  TSB(IPZ,J,K+1)=TSB(IPZ,J,K)+(TSB(IMZ,J,K)-TSB(IPZ,J,K))*
12.*PI*CDOUT*DELTT*HCOV/(DENNA*SHNA*AEQ)+(TSB(IPZ,J-1,K)
1-TSB(IPZ,J,K))*DELTT*U/DHG
97  IF(NPRINT.GT.NCO) GO TO 60
      WRITE(10,121) TIE
      WRITE(10,174)
      WRITE(10,108) J,(R(IC),TSB(IC,J,K+1),IC=i,IPZ,i)
      IF(J.EQ.JMZ) NCO=0
60  CONTINUE
C   RESET TEMPS FOR NEXT TIME STEP
      DO 66 J=1,JMZ,1
      DO 66 I=1,IPZ,1
      TSB(I,J,1)=TSB(I,J,2)
      IF(TSB(I,J,1).LT.TEMAX) GO TO 66
      WRITE(10,75) I,J
      CALL EXIT
66  CONTINUE
      K=1
C
C
C   IF REGION TEMP ABOVE MELTING AND LATENT HEAT GO TO RAYLEIGH EQ
      IPPA=IM+1
      DO 61 J=1,JMZ,1
      DO 61 I=1,IA,1
      IF(SGM(I,J) .GT. 2.) GO TO 62
      IF(SVP(I,J) .GT. 2) GO TO 71
61  CONTINUE
      GO TO 63
71  WRITE(10,73)
      GO TO 63

```



```

62 WRITE(10,123)
63 RETURN
END

```

C
C

```

SUBROUTINE POINT(P1,DT,C0,C1,C2,R2,E,DS,BS,B,PGT,NP,DPM,P2,P3
1,RAMP,IFLAG,D,PLOUT)
DIMENSION E(6),EL(6),DS(6),BS(6),AI(3,6),CI(6),BI(6)
P1=1.0
IF(DPM.EQ.0.0) RETURN
DTEX=100.0
IF(C2.NE.0.0) DTEX=-C1/2./C2
IF(DTEX.GT.0.0) DT=AMINI(DT,DTEX/3.)
12 SD=0.0
R1=R2+RAMP*DT*B
DO 9 J=1,NP
EL(J)=E(J)
SD=SD+DS(J)*E(J)
9 CONTINUE
PL=P1+SD/(B+R1)
PLOUT=PL
IF(PL.LE.0.0) PL=P2**2/P3
N=1
1 D=DT/FLOAT(N)
DO 3 J=1,NP
X=DS(J)*D
TERM=PGT/(2.*D)
BI(J)=EXP(-X)
CI(J)=1.-BI(J)
IF(X.GT.0.1) GO TO 2
AJ2=(1.-((1.-((1.-((1.-X/8.)*X/7.)*X/6.)*X/5.)*X/4.))/3.
AJ1=(1.-X+AJ2)/2.
AJ0=1.-X*AJ1
GO TO 8
2 AJ2=CI(J)/X
AJ1=(1.-AJ0)/X
AJ2=(1.-2.*AJ1)/X
8 F(J)=EL(J)
AI(1,J)=D*(AJ2+AJ1)/2.
AI(2,J)=D*(-AJ2+AJ0)
AI(3,J)=D*(AJ2-AJ1)/2.
3 CONTINUE
P2=C0
P3=C0+(C1+C2+(-D))*(-D)
10 DO 6 M=1,N
R1=R2+RAMP*D*B
SUM1=SUM2=0.0
DO 4 J=1,NP
SUM1=SUM1+DS(J)*(BS(J)+(P2+AI(2,J)+P3*AI(3,J))+E(J)*BI(J))
SUM2=SUM2+DS(J)*BS(J)+AI(1,J)
4 CONTINUE
P1=(TERM+(4.*P2+P3)+SUM1)/(3.*TERM+B+R1+SUM2)
IF(P1.LE.0.0) GO TO 7
DO 5 J=1,NP
E(J)=E(J)*BI(J)+(AI(1,J)*P1+AI(2,J)*P2+AI(3,J)*P3)+BS(J)
5 CONTINUE
T=T+D
P4=P3
P3=P2
P2=P1

```

THE UNIVERSITY OF CHICAGO

PHILOSOPHY DEPARTMENT

PHILOSOPHY 101

LECTURE 1

THE PHENOMENON OF CONSCIOUSNESS

1. THE PROBLEM OF CONSCIOUSNESS

2. THE HARD PROBLEM OF CONSCIOUSNESS

3. THE EASY PROBLEM OF CONSCIOUSNESS

4. THE MEASUREMENT OF CONSCIOUSNESS

5. THE NEURAL CORRELATES OF CONSCIOUSNESS

6. THE EVOLUTION OF CONSCIOUSNESS

7. THE FUNCTION OF CONSCIOUSNESS

8. THE CONSCIOUSNESS OF OTHERS

9. THE CONSCIOUSNESS OF THE FUTURE

10. THE CONSCIOUSNESS OF THE PAST

11. THE CONSCIOUSNESS OF THE PRESENT

12. THE CONSCIOUSNESS OF THE SELF

13. THE CONSCIOUSNESS OF THE WORLD

14. THE CONSCIOUSNESS OF GOD

15. THE CONSCIOUSNESS OF THE UNIVERSE

```

6 CONTINUE
  IF(ABS((PL-P1)/(PL+P1)).LT.DPH) GO TO 30
  GO TO 7
30 P2=P3
   P3=P4
   R2=R1
   RETURN
7 PL=P1
  WRITE(10,14)
  IF(IFLAG.LE.0) GO TO 24
  WRITE(10,22) P1,P3,P4
24 N=N+5
  IF(N.LT.125) GO TO 1
  WRITE(10,20) N
  WRITE(10,15)
  DT=DT/2.
  IF(DT.GT.1.E-6) GO TO 12
  WRITE(10,16)
14 FORMAT(/,13X,"***NOTE D: TIME STEP, HAS CHANGED***")
16 FORMAT(/,13X,"*** SEVERE PROB. IN POINT, NO CONVERG.***")
15 FORMAT(/,13X,"*** NOTE DT CHANGED FOR CONVERG.***")
20 FORMAT(" ***NOTE N,GE.125 BUT P1.GT.0,***",14)
22 FORMAT("TEST CONVERG. P1,P2,P3=",3E14.6)
  CALL EXIT
  END

```

C
C

```

SUBROUTINE VAPOR(IA,IFUL1,IFUL2,SVP,SGM,PLNPRS,NUM,ROINC,COMP,
  IDINC,DR,DHG,PI,R,TSB,HG,JMZ,ARK,BRK,DRINC,IHQHO)
  DIMENSION PINC(20,25,15),SVP(20,25),SGM(20,25),COMP(15),R(20),
  TSB(25,30,2),PP(20,25,15),VOL(15),IGRW(20,25),RADR(20,25)
  I,HG(30),CONT(15),CRK(5),VIC(15),ARK(15),BRK(15),ERK(8),X(8),
  DRINC(15)

```

C

```

  CONV=1.E-6
  PTOT=0.0
  TVOL=0.0
  TMOLE=0.0
  GAS CONST. IN CM**3 ATM/K MOLE
  RR=82.05
  DO 125 K=1,NUM
  TMOLF=TMOLE+COMP(K)
  VOL(K)=0.0
125 CONTINUE
  DO 123 I=1,IA
  DO 123 J=IFUL1,IFUL2
  IGRW(I,J)=1
  RADR(I,J)=ROINC
123 CONTINUE
  ASSUME SURFACE AREA PROP. TO MOLAR X
  DO 101 J=IFUL1,IFUL2
  DO 101 I=1,IA
  IF(I.GT.1) GO TO 115
  DVOL=PI*DHG*DR*DR/4.
  GO TO 117
115 IF(I.LT.1A) GO TO 116
  DVOL=PI*DHG*(R(I)*DR*DR*DR/4.)
  GO TO 117
116 DVOL=PI*DHG*2.*DR*R(I)
117 IF(SVP(I,J).GT.1) GO TO 127
  PINC(I,J,1)=EXP(10.214-3.621*5200./TSB(I,J,1))

```

THE UNIVERSITY OF CHICAGO

PHYSICS DEPARTMENT

5720 S. UNIVERSITY AVENUE

CHICAGO, ILLINOIS 60637

TEL: 773-936-3700

FAX: 773-936-3700

WWW: WWW.PHYSICS.UCHICAGO.EDU

WWW: WWW.PHYSICS.EDU

WWW: WWW.PHYSICS.ORG

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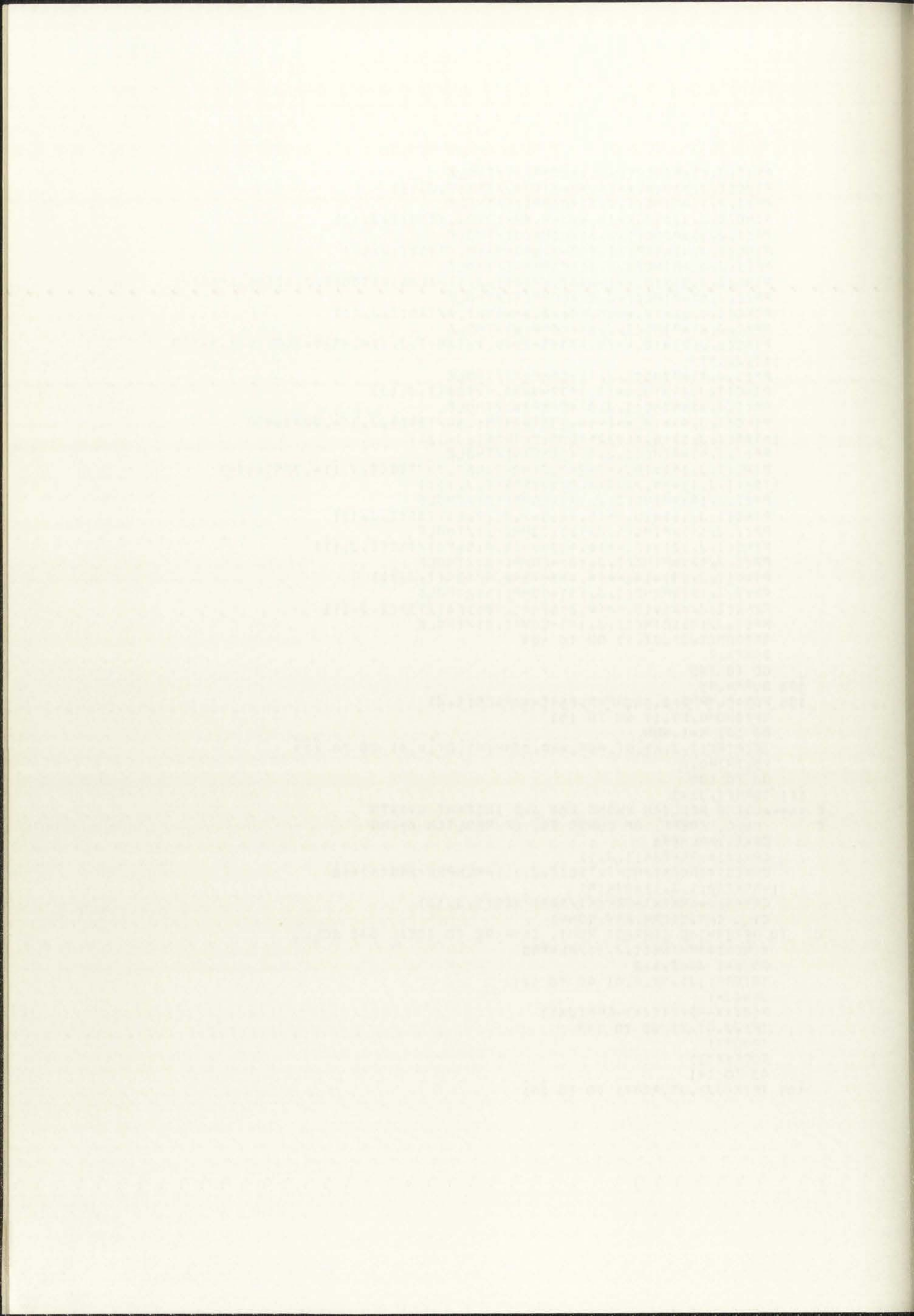
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```

PP(I,J,1)=PINC(I,J,1)*COMP(1)/TMOLE
PINC(I,J,2)=10.**((5.58-21070./TSB(I,J,1)))
PP(I,J,2)=PINC(I,J,2)*COMP(2)/TMOLE
PINC(I,J,3)=10.**((8.687-2.88-17494./TSB(I,J,1)))
PP(I,J,3)=PINC(I,J,3)*COMP(3)/TMOLE
PINC(I,J,4)=EXP(13.932-4.693+9340./TSB(I,J,1))
PP(I,J,4)=PINC(I,J,4)*COMP(4)/TMOLE
PINC(I,J,5)=10.**((-6447./TSB(I,J,1)-ALOG10(TSB(I,J,1))+8.1945))
PP(I,J,5)=PINC(I,J,5)*COMP(5)/TMOLE
PINC(I,J,6)=10.**((5.896-2.88-5967.4/TSB(I,J,1)))
PP(I,J,6)=PINC(I,J,6)*COMP(6)/TMOLE
PINC(I,J,7)=10.**((5.87303-7040.7/TSB(I,J,1)-.5329*ALOG10(1.8*TSB
1(I,J,1)))
PP(I,J,7)=PINC(I,J,7)*COMP(7)/TMOLE
PINC(I,J,8)=10.**((7.1872-4280./TSB(I,J,1)))
PP(I,J,8)=PINC(I,J,8)*COMP(8)/TMOLE
PINC(I,J,9)=10.**((-14.3373-29751.34/TSB(I,J,1)-.00054932
1*TSB(I,J,1)+6.41032*ALOG10(TSB(I,J,1)))
PP(I,J,9)=PINC(I,J,9)*COMP(9)/TMOLE
PINC(I,J,10)=10.**((-267.2102+22487.72/TSB(I,J,1)-.00596694*
1TSB(I,J,1)+79.2243*ALOG10(TSB(I,J,1)))
PP(I,J,10)=PINC(I,J,10)*COMP(10)/TMOLE
PINC(I,J,11)=10.**((5.8265-2.91176E4/TSB(I,J,1)))
PP(I,J,11)=PINC(I,J,11)*COMP(11)/TMOLE
PINC(I,J,12)=10.**((6.43266-(3.0156E4)/TSB(I,J,1)))
PP(I,J,12)=PINC(I,J,12)*COMP(12)/TMOLE
PINC(I,J,13)=10.**((4.488-7396.5/TSB(I,J,1)))
PP(I,J,13)=PINC(I,J,13)*COMP(13)/TMOLE
PINC(I,J,14)=10.**((4.2162-(1.4061E4)/TSB(I,J,1)))
PP(I,J,14)=PINC(I,J,14)*COMP(14)/TMOLE
IF(SGM(I,J).GT.1) GO TO 103
SURF=.7
GO TO 105
103 SURF=.45
105 PGR=PLNPRS+2.*SURF*0.869E-6/RADR(I,J)
IF(IHOMO.EQ.1) GO TO 151
DO 121 K=1,NUM
IF(PINC(I,J,K).GT.PGR.AND.COMP(K).GT.0.0) GO TO 111
VOL(K)=0.0
GO TO 109
111 IGRW(I,J)=3
C *****USING REDLICH KWONG EOS AND INSTANT GROWTH
C CALC. COEFF. OF CUBIC EQ. OF REDLICH KWONG
CRK(1)=PLNPRS
CRK(2)=-RR+TSB(I,J,1)
CRK(3)=ARK(K)/SQRT(TSB(I,J,1))-PLNPRS*BRK(K)**2
1-RR*TSB(I,J,1)*BRK(K)
CRK(4)=-ARK(K)*BRK(K)/SQRT(TSB(I,J,1))
CALL CURIC(CRK,ERK,CONV)
C TO DETERMINE CORRECT ROOT, COMPARE TO IDEAL GAS SOLU.
VIG(K)=RR*TSB(I,J,1)/PLNPRS
DO 141 JJ=2,6,2
IF(ERK(JJ).NE.0.0) GO TO 141
JK=JJ-1
X(JJ)=ABS(VIG(K)-ERK(JK))
IF(JJ.GT.2) GO TO 143
1ROOT=1
ROOT=X(2)
GO TO 141
143 IF(X(JJ).GT.ROOT) GO TO 141

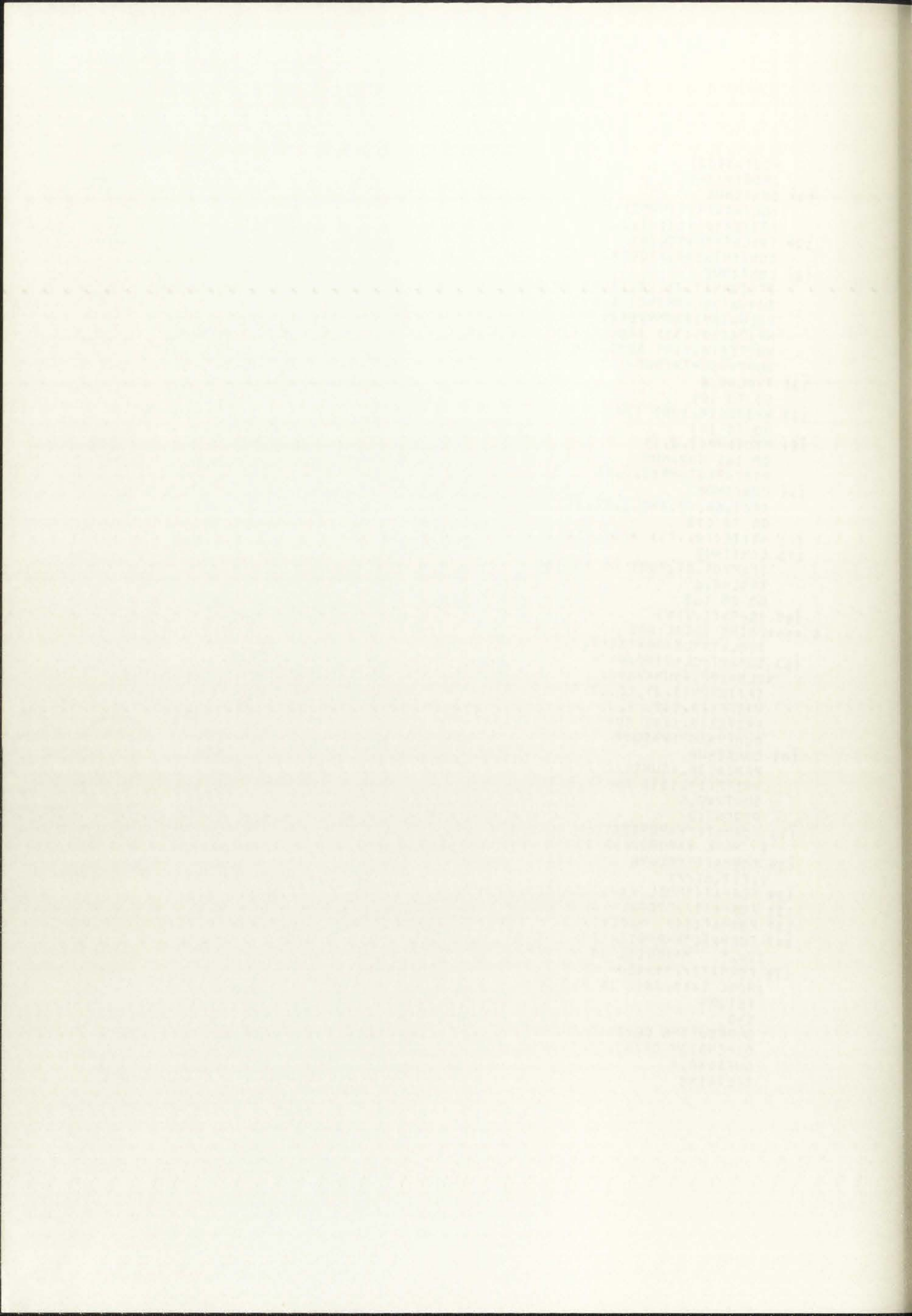
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      ROOT=X(JJ)
      IROOT=JJ+1
141  CONTINUE
      VOL(K)=ERK(IROOT)*COMP(K)
      WRITE(10,113) I,J,K
109  TVOL=TVOL+VOL(K)
      CONT(K)=100.*VOL(K)*DRINC(I)
121  CONTINUE
      IF(IGRW(I,J).LE.1) GO TO 131
      SUMV=TVOL*DRINC(I)*DVOL
      VOLN=100.*SUMV/DVOL
      WRITE(10,137) (KK,CONT(KK),KK=1,NUM,I)
      WRITE(10,119) SUMV,TSB(I,J,1),VOLN
      SUMTV=SUMTV+SUMV
131  TVOL=0.0
      GO TO 101
127  WRITE(10,129) I,J
      GO TO 101
151  PTOT=PP(I,J,1)
      DO 161 K=2,NUM
      PTOT=PTOT+PP(I,J,K)
161  CONTINUE
      IF(I.EQ.10.AND.J.EQ.11) GO TO 171
      GO TO 173
171  WRITE(10,175) PTOT,TSB(I,J,1)
173  CONTINUE
      IF(PTOT.GT.PGR) GO TO 165
      TVOL=0.0
      GO TO 163
165  IGRW(I,J)=3
C ****USING IDEAL GAS AND INSTANT GROWTH
      TVOL=TMOLE*RR*TSB(I,J,1)/PLNPRS
163  SUMV=TVOL*DRINC*DVOL
      VOLN=100.*SUMV/DVOL
      IF(IGRW(I,J).LE.1) GO TO 101
      WRITE(10,147) I,J
      WRITE(10,119) SUMV,TSB(I,J,1),VOLN
      SUMTV=SUMTV+SUMV
101  CONTINUE
      PERC=100.*SUMTV/(PI*R(TA)*R(TA)*HG(JMZ))
      WRITE(10,133) SUMTV,PERC
      SUMTV=0.0
      PERC=0.0
113  FORMAT("VAPORIZATION OCCURRING AT NODE I=",I4," J=",I4,"
1 MATL VAPORIZING IS K=",I4)
119  FORMAT("VOLUME INCREASE=",F12.6," TEMP=",E12.6," VOL% IN NODE="
1,E12.6,/)
129  FORMAT("FUEL VAPORIZATION OCCURRING AT NODE I=",I5," J=",I5)
133  FORMAT(", TOTAL VOL FROM INCL=",E12.6," VOL%=",E12.6)
137  FORMAT(3(" MATL=",I2," VOL% CONTR.=",E12.6))
147  FORMAT("VAPORIZATION OCCURRING AT NODE I=",I4," J=",
1I4," MATERIAL IS HOMOGEN. MIXTURE")
175  FORMAT(", ***SUM OF P,P.=",E12.6," ATM. TEMP. IN
1 NODE I=10,J=11 IS ",E12.6)
      RETURN
      END
      SUBROUTINE CUBIC(C,E,DELT)
      DIMENSION CP(4),C(4),BN(3),P(3),ARSP(3),E(6)
      GUESS=0.0
      IFLAG=0

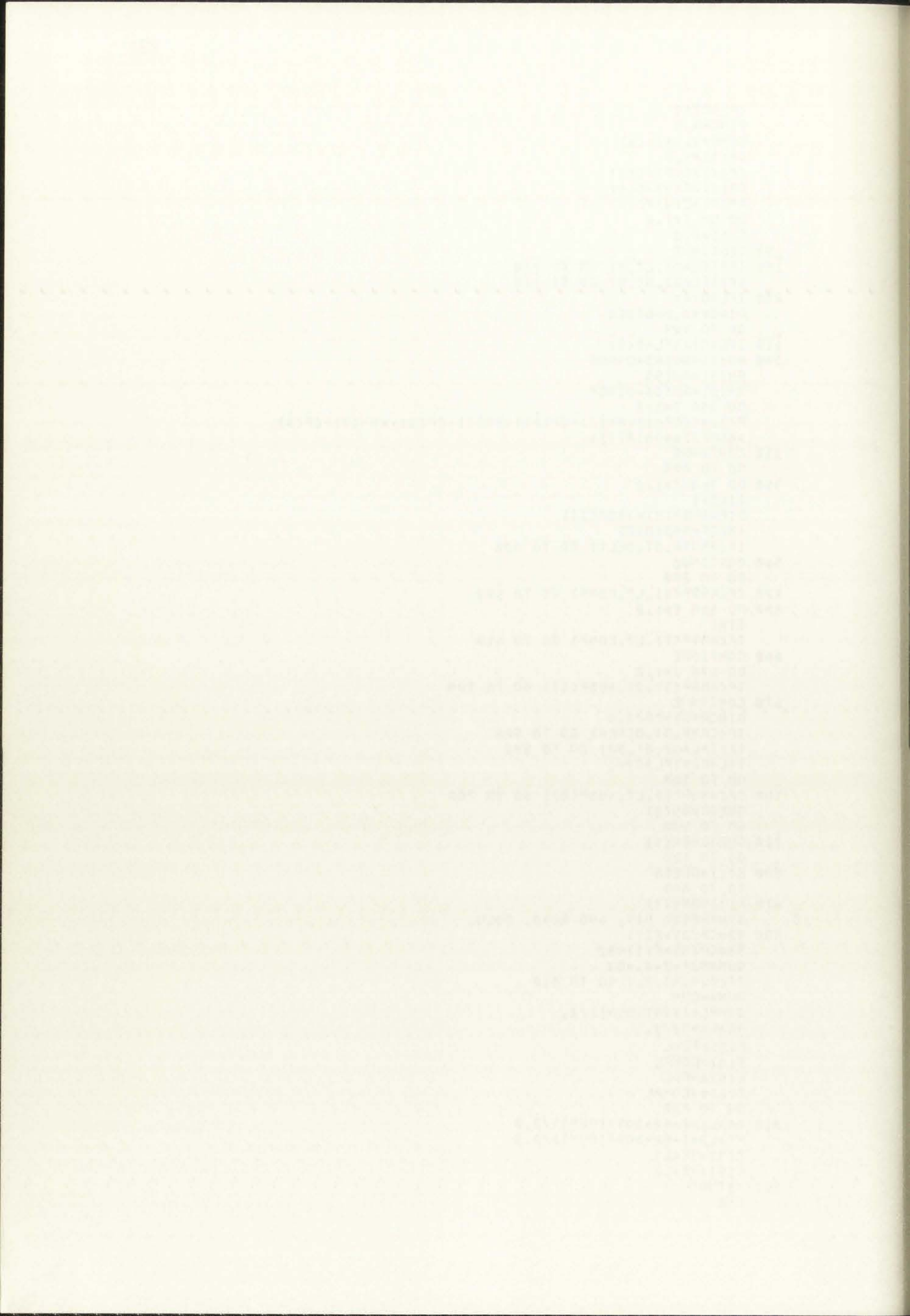
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IFLAG2=0
DINCR=.5
COMP=2.**(-16)
CP(1)=1.0
CP(2)=C(2)/C(1)
CP(3)=C(3)/C(1)
CP(4)=C(4)/C(1)
DO 50 I=1,6
F(I)=0.0
50 CONTINUE
100 IF(IFLAG1.LT.5) GO TO 110
IF(IFLAG2.GT.0) GO TO 110
200 IFLAG1=0
DINCR=.001*DINCR
GO TO 300
110 IFLAG1=IFLAG1+1
300 BN(1)=GUESS+DINCR
BN(3)=GUESS
BN(2)=GUESS-DINCR
DO 330 I=1,3
P(I)=(CP(1)*BN(I)+CP(2))*BN(I)+CP(3))*BN(I)+CP(4)
ABSP(I)=ABS(P(I))
330 CONTINUE
GO TO 400
350 DO 360 I=1,2
II=I+1
DIF=ABSP(I)-ABSP(II)
ABDIF=ABS(DIF)
IF(ABDIF.GT.DELT) GO TO 400
360 CONTINUE
GO TO 200
400 IF(ABSP(3).LT.COMP) GO TO 500
600 DO 660 I=1,2
II=I
IF(ABSP(I).LT.COMP) GO TO 610
660 CONTINUE
DO 670 I=1,2
IF(ABSP(3).GT.ABSP(I)) GO TO 700
670 CONTINUE
DINCR=DINCR/2.0
IF(COMP.GT.DINCR) GO TO 500
IF(IFLAG2.GT.50) GO TO 500
IFLAG2=IFLAG2+1
GO TO 300
700 IF(ABSP(1).LT.ABSP(2)) GO TO 780
GUESS=BN(2)
GO TO 100
780 GUESS=BN(1)
GO TO 100
500 E(1)=GUESS
GO TO 800
610 F(1)=BN(II)
C SYNTHETIC DIV. AND QUAD. SOLU.
800 B2=CP(2)+E(1)
B3=CP(3)+E(1)*B2
DUM=B2**2-4.*B3
IF(DUM.GT.0.) GO TO 810
DUM=-DUM
COMPL=(SQRT(DUM))/2.
REAL=-B2/2.
F(3)=REAL
F(4)=COMPL
E(5)=REAL
E(6)=-COMPL
GO TO 820
810 REAL1=(-B2+SQRT(DUM))/2.0
REAL2=(-B2-SQRT(DUM))/2.0
F(3)=REAL1
E(5)=REAL2
820 RETURN
END

```



APPENDIX O
DETERMINATION OF SURFACE TENSION

From Overbury:¹

$$A = fN^{1/3} \left(\frac{M}{\rho}\right)^{2/3} \quad (0-1)$$

where

A = area occupied by Avogadro's Number of atoms,

N = Avogadro's number,

M = atomic weight,

ρ = density,

f = structure factor, f = 1 simple cubic structure,

f = 1.09 for face centered cubic (fcc),

f = 1.12 for body centered cubic (bcc),

f = 1.14 for orthorhombic structure,

and

$$\sigma_{LM} (T) = A \sigma_L (T) \quad , \quad (0-2)$$

where

σ_{LM} = molar surface Free Energy,

$$\sigma_{LM} = .15 \Delta H_{\text{vap}} \quad (0-3)$$

DETERMINATION OF SURFACE TENSION

(10-1)

10-10-10

A = area enclosed by liquid's surface of glass

ρ = liquid's density

h = static height

g = gravity

The pressure, P , of a static liquid structure,

$P = \rho gh$ for a static liquid (10-1)

$P = \rho gh$ for a static liquid (10-1)

$P = \rho gh$ for a static liquid (10-1)

(10-1) $P = \rho gh$ for a static liquid (10-1)

10-1

A = area enclosed by liquid's surface of glass

(10-1)

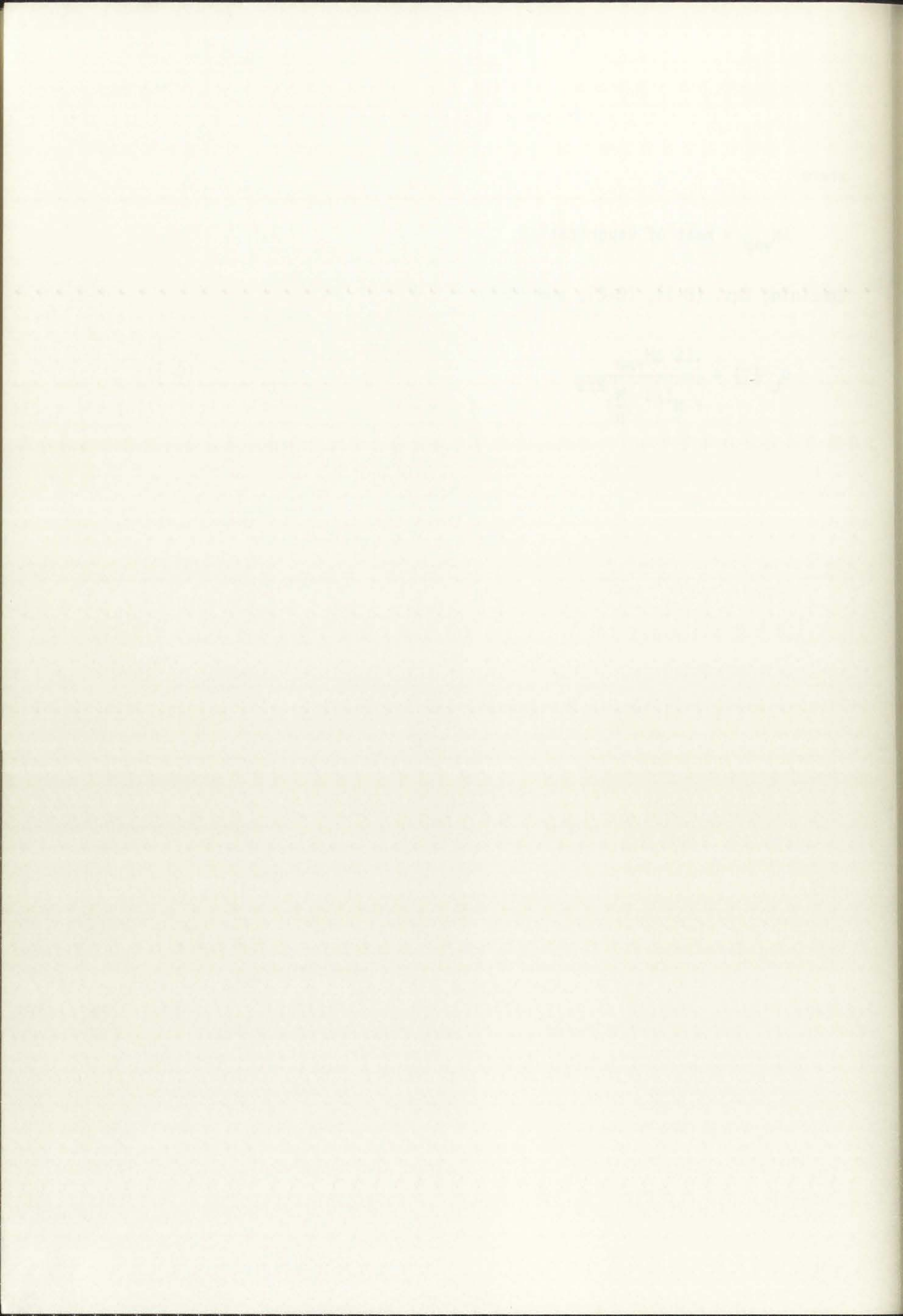
10-10-10

where

ΔH_{vap} = heat of vaporization.

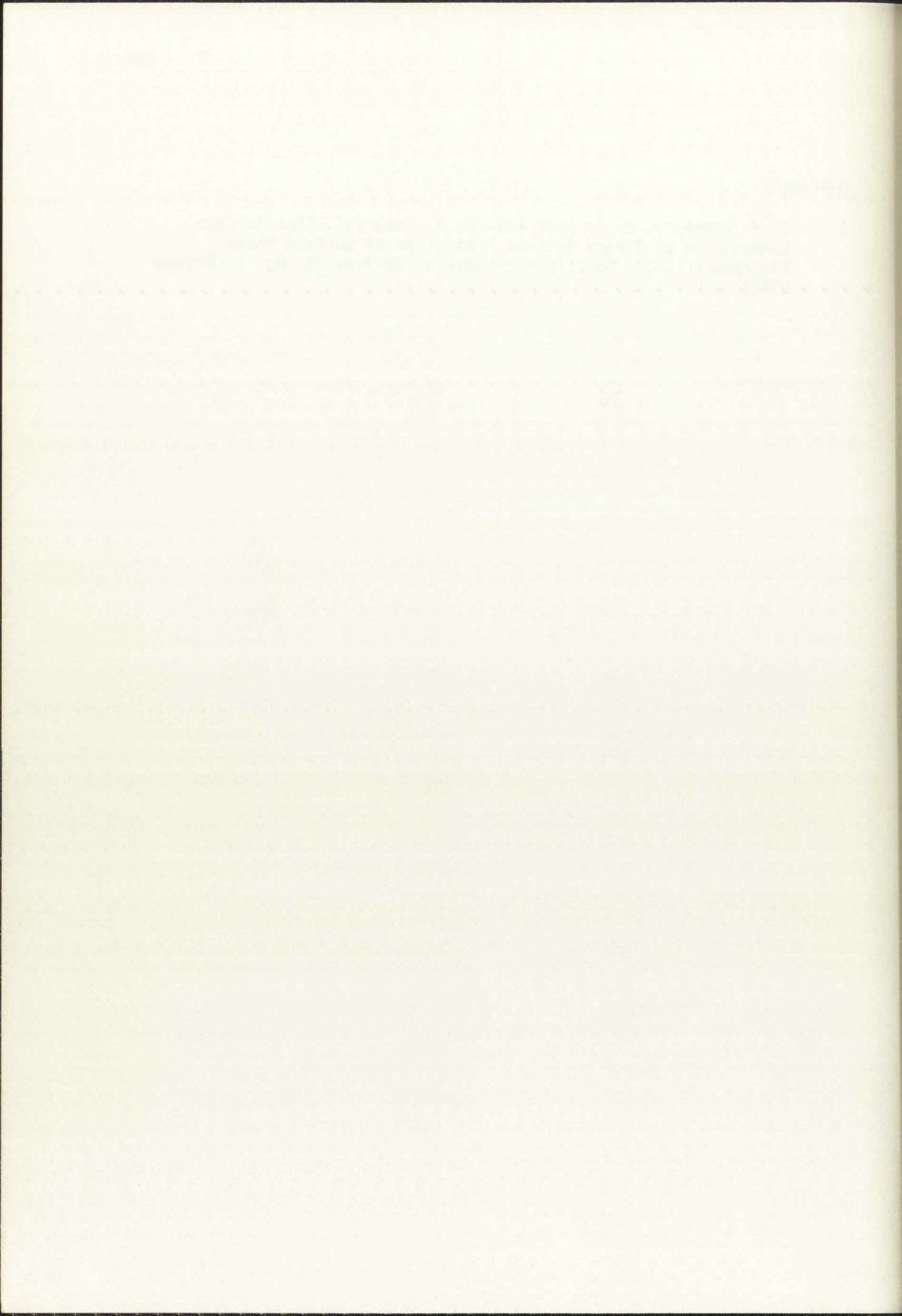
Combining Eqs. (0-1), (0-2), and (0-3)

$$\sigma_L (T) = \frac{.15 \Delta H_{\text{vap}}}{f N^{1/3} \left(\frac{M}{\rho}\right)^{2/3}} \cdot \quad (0-4)$$



REFERENCE

1. S. H. Overbury, P. A. Bertrand, G. A. Somorjai, "The Surface Composition of Binary Systems Prediction of Surface Phase Diagrams of Solid Solutions," *Chemical Reviews* 75, No. 5 (October 1975).



VITA

Paul Sasa was born on November 27, 1945, in Brighton, Colorado. Upon graduating from Brighton High School in 1963, he went to the University of Colorado where he received his B.S. in Engineering Physics in 1968. After graduation, he worked one year for the Naval Missile Systems Engineering Station in Port Hueneme, California and then four years for the Bendix Corporation in Kansas City, Missouri. In 1973 he entered graduate school at the University of New Mexico and received his M.S. in Nuclear Engineering in 1974. In the summer of 1975, he was associated with Argonne National Laboratory in its Reactor Analysis and Safety Division. His Ph.D. research was conducted in the Fast Reactor Safety Division of the Los Alamos Scientific Laboratory in Los Alamos, New Mexico, and after graduation, he will join Rockwell International in Golden, Colorado. He has a wife, Janet.

