HYDRODYNAMIC ANALYSIS OF ELECTRON-BEAM HEATED UO₂ VAPORIZATION EXPERIMENTS

by

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1979
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APPROVAL BY THESIS DIRECTOR

This thesis has been approved on the date shown below:

B. D. Ganapol
Assistant Professor of Nuclear Engineering

Date
To my Mother, my Father, and my Wife
ACKNOWLEDGMENTS

I would like to express my sincere gratitude to Dr. Barry Ganapol for his assistance and guidance over the duration of this study.
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ABSTRACT

A hydrodynamic analysis of electron-beam heated, UO$_2$ vaporization experiments is performed. The analysis uses the SIMMER-II fast reactor safety code. The SIMMER-II analysis indicates that complicated hydrodynamic effects prevent simple analyses from providing meaningful data. It is doubtful that a UO$_2$ equation of state should be based upon the e-beam experiments.
CHAPTER 1

INTRODUCTION

The liquid metal fast breeder reactor (LMFBR) has the potential for providing large quantities of electrical energy in a world of increasing energy shortage. Utilization of the LMFBR will require a proven level of safety. LMFBR safety analysis is concerned with core disruptive accidents (CDAs). The analysis of CDAs includes three general modeling areas: neutronics, hydrodynamics, and thermodynamics. Thermodynamic models provide temperatures and pressures of the disrupted core. The thermodynamic pressure-temperature relationship, or equation of state, is an important part of the thermodynamic model. This work is concerned with the equation of state (EOS) of uranium dioxide.

In order to obtain vapor pressure data in the 3000°K to 6000°K temperature range, Sandia Laboratories performed a series of UO$_2$ experiments. The results of these experiments have established an algebraic equation of state for UO$_2$. The Benson EOS is named for the author of the report analyzing the experiments.

Previous equations of state have been based upon extrapolation of low temperature data. The extrapolation process introduces error into the resulting EOS. The choice of the appropriate physical extrapolation model also introduces uncertainty into the EOS.

The Benson EOS yields larger vapor pressures than the previously reported values. Questions have arisen concerning the analysis of the...
Sandia results as well as the applicability of the experiment itself. This work is concerned with answering some of the questions which have arisen concerning the analysis. Hopefully, this new analysis will add to the knowledge of the UO$_2$ EOS.

This research will be based on numerical hydrodynamic and thermodynamic simulation of the e-beam experiments. For this purpose, the SIMMER-II$^2$ code was chosen. SIMMER-II is a fast reactor safety code with neutronic, hydrodynamic, and thermodynamic models. The results of the analysis were not completely satisfactory; however, some conclusions can be drawn. In particular, some phenomena may be identified as playing no significant role in experimental analysis.
CHAPTER 2

SANDIA E-BEAM EXPERIMENTS

The electron-beam heating experiments are described by Benson\textsuperscript{1,3-5}. In this chapter, the geometry, energy deposition, and results of the experiment are described. The description is limited to points of interest in this analysis. Detailed information is available in References 3-6.

2.1 Geometry

The experimental geometry is shown schematically in Fig. 1. Note that Fig. 1 is not to scale. The UO\textsubscript{2} sample is confined on all sides by graphite. Two graphite disks form the side surfaces of the powdered UO\textsubscript{2} sample disk. The motion of the pistons is later used to infer the UO\textsubscript{2} vapor pressure. The powder grains average 2 microns in diameter. Benson\textsuperscript{1} expresses the sample thickness as a mass per unit area, or area density. The macroscopic smeared UO\textsubscript{2} density was later reported by Benson\textsuperscript{6} to be \(2.0 \times 10^3\) kg/m\(^3\) with an estimated error of 50 to 80%. The piston and sample diameter was \(\frac{1}{8}\)" (6.35\times10\(^{-3}\) meters). The sample area densities and ranges of thicknesses based on the density error estimate are presented in Table 1.

Following the energy deposition, described later in this chapter, the graphite pistons move under the influence of all forces acting upon them. The forces include, but are not limited to, the vapor pressure of
Fig. 1. Experiment Schematic (Dimensions in mm).
Table 1. Sample Thicknesses.

<table>
<thead>
<tr>
<th>E (J/g)</th>
<th>Area Density (kg/m²)</th>
<th>Sample Thickness (micron)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1860</td>
<td>0.12</td>
<td>6 - 60</td>
</tr>
<tr>
<td>1990</td>
<td>0.12</td>
<td>6 - 60</td>
</tr>
<tr>
<td>2030</td>
<td>0.12</td>
<td>6 - 60</td>
</tr>
<tr>
<td>2490</td>
<td>0.25</td>
<td>12 - 120</td>
</tr>
<tr>
<td>3030</td>
<td>0.25</td>
<td>12 - 120</td>
</tr>
</tbody>
</table>

$^{235}$UO$_2$ and dissolved impurities, and any sample material which might impact the pistons. The piston motion is recorded with a streak camera and flash lamp. The displacement recorded on film may be differentiated to obtain the piston velocity and acceleration. The acceleration may then be used to calculate the forces acting on the pistons. The experiment was proposed with the idea that the force on the piston could be related to the sample vapor pressure. The vapor pressure was assumed constant throughout the sample.

2.2 Energy Deposition

The source of energy for the experiments was Sandia's Relativistic Electron Beam Accelerator (REBA). REBA supplies an electron beam with 1.2 Mev average electron energy. The accelerator operates in a pulsed mode. Each pulse is approximately Gaussian in time with a 0.6 microsecond full width at half-maximum (FWHM). The beam cross section may be altered to vary the total energy deposition in the sample.
The variation of the energy deposition spatially is one dimensional. The calculated variation is shown in Fig. 2. Figure 2 is the result of an electron transport calculation performed at Sandia. The axial variation of the energy deposition is important only in the sample region. The large graphite heat capacity keeps the graphite temperature below 2000°C. Since the graphite temperature remains below its melting temperature, energy deposition in the graphite need not be modeled.

During each experiment the energy deposition is measured using a fast infrared pyrometer. The pyrometer views a calorimeter plate behind the sample, see Fig. 1. The energy deposition in the sample is calculated from the data used to generate Fig. 2. The calorimeter plate is destroyed in each experiment by the moving graphite piston. The pyrometer measurement must take place after the energy deposition and prior to the destruction of the calorimeter plate.

2.3 Sandia's Experimental Results

The primary data of the experiments are obtained from streak camera photographs and energy deposition measurements. The data are most easily presented as a plot of velocity versus time for several energy depositions, shown in Fig. 3. Benson's analysis begins by splitting the velocity data into two time intervals. The first interval is characterized by large acceleration of the piston. All of the remaining data points are fit to a straight line. The fit lines are also shown in Fig. 3.
Fig. 2. Spatial Variation of the Energy Deposition.
Fig. 3. Piston Velocity.
In Benson's analysis, the slope of the fit line is used to calculate the piston acceleration. The experimental acceleration is assumed to arise completely from the vapor pressure of the UO\textsubscript{2} sample\textsuperscript{1}. The piston area density (mass per unit area) is used to calculate the pressure from the assumed constant acceleration. The source of the initially large acceleration is assumed to come from the thermal expansion of the sample\textsuperscript{4}. The forces acting on the piston will be examined in greater detail in Chapter 5.

The data from Sandia's experiments (after conversion to S.I. units) is presented in Table 2.

Table 2. Benson's Pressure Data Points.

<table>
<thead>
<tr>
<th>Energy Deposition (J/g)</th>
<th>Pressure (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1860</td>
<td>4.3</td>
</tr>
<tr>
<td>1990</td>
<td>6.6</td>
</tr>
<tr>
<td>2030</td>
<td>9.6</td>
</tr>
<tr>
<td>2490</td>
<td>32.2</td>
</tr>
<tr>
<td>3030</td>
<td>150.0</td>
</tr>
</tbody>
</table>

These results are in the pressure-internal energy format. Benson has suggested that this is a logical format for EOS tabulations. Conventionally, the EOS has been tabulated and fit to a pressure-temperature format. The EOS is considered in greater detail in Chapter 3.
CHAPTER 3

STATUS OF THE UO$_2$ EQUATION OF STATE

Most UO$_2$ EOS models are based upon extrapolation of low temperature measurements. The number of vapor pressure measurements in the 3100°K to 6000°K temperature range is small. Correlations in use are based upon extrapolation of lower temperature data or methods with limited applicability in the high temperature range. Errors in extrapolation and uncertainty in the correct model to use for extrapolation lead to uncertainties in the UO$_2$ EOS. An excellent review of UO$_2$ equations of state is given by Ostensen$^7$.

Conventionally the EOS has been expressed in a pressure-temperature format. More recently, Benson$^1$ has proposed a pressure-internal energy format. In order to compare the temperature and internal energy formats, a heat capacity model is required. The heat capacity model becomes a part of the EOS in a pressure-energy format. This chapter examines models for the heat capacity and vapor pressure relations in both formats.

3.1 Heat Capacity

The heat capacity is required to interpret Sandia's data points in a pressure-temperature format. Experimental evaluations of the UO$_2$ heat capacity have been reviewed by Fink et al$^8$. The recommended

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constant liquid heat capacity is 504 J/kg°K. The solid heat capacity displays a decided variation with temperature.

The solid heat capacity exhibits a significant increase as the temperature approaches melting. The solid heat capacity data has been fit assuming that it is made up of three components. The phonon and thermodynamic contributions are well accepted. The third model component is oxygen Frenkel defect formation. The controversy surrounding the solid UO₂ heat capacity concerns the third anomalous contribution. The three components and the total fit heat capacity are shown in Fig. 4.

Bergeron has analyzed Frenkel defect formation in UO₂. The analysis indicates that times on the order of milliseconds are necessary for defect formation. Benson argued that since the e-beam experiments are completed after 20 microseconds, the defect formation would not contribute to the experimentally observed heat capacity. Recent solid-state analysis by Young indicates that Frenkel defect formation could not produce the UO₂ heat capacity anomaly. Young argues further that the increase is electronic in nature. MacInnes has also put forth the thesis that the anomaly is electronic. In general, the time scale for the electronic contribution is much shorter than 20 microseconds; and, therefore, if the anomaly were electronic, it would be observed on the time scale of the e-beam experiments. At this point in time some question exists concerning the correct solid heat capacity to be used in the e-beam experimental analysis.

In order to avoid this controversy, two average solid heat capacities were calculated. The averages are based on the assumption
Fig. 4. Solid UO\textsubscript{2} Heat Capacity.
that the three component fit is accurate. This assumption is valid as long as the anomalous contribution is qualitatively fit by the Frenkel defect model. Average heat capacities are calculated with and without the defect contribution. The temperature range for the averaging is 300°K to melting. The average solid heat capacities are 330.7 J/kg-°K without the anomalous contribution, and 399.5 J/kg-°K with the anomalous contribution. The anomaly contributes an additional 20.8% to the average heat capacity. The two solid heat capacities are used in computer simulations to provide estimates of the effects of the different solid heat capacity models.

3.2 Vapor Pressure versus Temperature

The vapor pressure of UO$_2$ is conventionally tabulated as a function of the UO$_2$ liquid temperature. Despite new experimental data, there is a great deal of uncertainty in the correct vapor pressure relation. Figure 5 illustrates that the range of vapor pressures at 6000°K spans almost two orders of magnitude.

In Fig. 5, Benson's data was placed in this format using the two-component heat capacity described in the previous section. In the two-component model, the anomalous contribution to the solid heat capacity was neglected. If the three component heat capacity is used, Benson's data is shifted higher. The Menzies EOS is the most widely accepted equation of state. The standard EOS in SIMMER-II$^2$ is so close to Menzies as to be indistinguishable from it in Fig. 5. The Ackermann EOS is generally accepted as the upper bound on the UO$_2$ vapor pressure.
Fig. 5. UO$_2$ Equations of State.
Computer codes usually require an algebraic formulation of the vapor pressure relation. Table look-up is not normally used. A typical form is shown in Eq. (3.1)

\[ P = e^{A-B/T} \]  

(3.1)

Ostensen has published fits of various equations of state to the form of Eq. (3.1). The coefficients of the most often used relations are given in Table 3. The coefficients in Table 3 yield pressures in Pascals.

Table 3. Equation of State Parameters.

<table>
<thead>
<tr>
<th>EOS Name</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
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<tr>
<td>Menzies</td>
<td>25.859</td>
<td>53137</td>
</tr>
<tr>
<td>Ackermann</td>
<td>35.327</td>
<td>82880</td>
</tr>
<tr>
<td>Benson</td>
<td>26.142</td>
<td>49729</td>
</tr>
<tr>
<td>SIMMER-II</td>
<td>25.693</td>
<td>51708</td>
</tr>
</tbody>
</table>

3.3 Vapor Pressure versus Internal Energy

Figure 6 indicates how fit lines may be shifted depending upon the heat capacity model used. Benson's data points are also shown. Benson argues that energy is a better dependent variable for EOS tabulations. Given the current uncertainty in the heat capacity, and the widespread use of the P-T format, the pressure-temperature format seems the more logical choice. For comparison purposes, the pressure-temperature format will be used throughout the remainder of this work.
Fig. 6. Energy Format for EOS.
CHAPTER 4

EXPERIMENTAL ANALYSIS

This work is primarily concerned with computer simulation and analysis of Sandia's electron-beam experiments. The SIMMER-II code was chosen for the analysis. SIMMER-II was chosen for its extensive phase transition and two-phase inhomogeneous flow models. Concurrent with this analysis, studies using other codes and models took place. It was hoped that the combination of models would identify all hydrodynamic and thermodynamic processes of importance in the experiments. The results of this analysis and the other studies in Reference 12 will be published in a Nuclear Regulatory Commission NUREG report. In this chapter, SIMMER-II is briefly described. Modifications and additions to SIMMER-II are also explained.

4.1 SIMMER-II Description

SIMMER-II is a fast reactor accident analysis code under continuing development at the Los Alamos Scientific Laboratory (LASL). In its most complete form, SIMMER-II includes a transport or diffusion neutronics calculation. The neutronics package was not used in this analysis. SIMMER-II solves the Eulerian hydrodynamics equations in an r-z geometry. The solution algorithm contains both implicit and explicit methods. The combined method is usually described as "semi-implicit". SIMMER-II allows for solid, liquid and gaseous phases in
each mesh cell. The solution algorithm solves the hydrodynamics equations for three fields: structure, liquid, and vapor. Solid particles may be included in the liquid field. The distinction is necessary because the structure field remains motionless. Liquid and vapor field velocities are calculated. Relative motion is allowed. A single vapor temperature is calculated. A liquid temperature is calculated for each liquid field component present in a cell. The temperature solutions allow non-equilibrium thermodynamic situations to be modeled.

The three fields may contain several components. Depending upon the particular field, up to six components may be selected: fissile fuel, fertile fuel, steel, sodium, control material, and fission gas. The two fuel components share the same equation of state. In this analysis, fissile fuel, fertile fuel, steel, and fission gas components are used. The UO$_2$ sample is initially modeled as solid fissile fuel particles in the liquid field. The steel equation of state is modified to match graphite properties.

Heat transfer is important in this SIMMER-II analysis. All phase transition models in SIMMER-II are heat transfer limited. Detailed explanation of the models may be found in Reference 2. The models within a given cell include convection and conduction between all fields and components. Radiation heat transfer is not considered. No heat transfer is modeled between mesh cells.

Figure 1 shows that the piston geometry is not symmetric. Asymmetry effects would cause displacement of the center of mass of the sample. Benson$^1$ has reported that streak camera photographs indicate
that there was no sample motion of that kind. Therefore, the sample can be considered as two separate halves. Half of the problem geometry is simulated in SIMMER-II. Sample properties are assumed symmetric about the sample center-line. The sample occupied 10 mesh cells. Graphite was placed in all remaining mesh cells. Graphite motion is simulated by moving the graphite-\( \text{UO}_2 \) interface.

4.2 Graphite Motion Model

The graphite motion model was incorporated into SIMMER-II to allow limited motion of the structure field. The graphite-\( \text{UO}_2 \) interface is assumed to move under the influence of forces at the boundary. Forces on the graphite are assumed to arise from two sources. The pressure difference across the graphite plug yields a net body force. The sample pressures involved in these experiments are two to three orders of magnitude greater than the pressure outside the plug. The pressure outside the pistons was not reported. The external pressure was assumed to be 0.8 atmospheres. This assumption is one of convenience and has little bearing on the results.

The second source of acceleration is impulse due to liquid or vapor field components impacting the graphite. This source is important in modeling the effects of liquid and vapor motion in the system.

The pressure force, \( F_p \), is defined as

\[
F_p = (P_u - P_0) \cdot A
\]

where, \( P_u \) is the \( \text{UO}_2 \) pressure at the graphite surface, \( P_0 \) is the pressure outside the graphite, and \( A \) is the sample area. The convective
force is defined as

\[ F_c = \frac{\Delta (mv)}{\Delta t} \]  

(4.2)

where, \( \Delta (mv) \) is the fluid momentum change due to impact on the graphite which occurs during the time interval \( \Delta t \). The mass \( (m) \) is constant during the impact. The velocity \( (v) \) is the fluid velocity relative to the graphite plug. Equation (4.2) may be re-written.

\[ F_c = \frac{m \cdot \Delta v}{\Delta t} \]  

(4.3)

Calculation of \( \Delta v \) is dependent upon an assumption concerning fluid impact. Such impacts may be idealized as elastic or completely inelastic. The real case is at some situation between the two ideal cases. The elastic collision will result in the liquid traveling at its previous velocity in the opposite direction after the collision. An inelastic collision will result in zero relative velocity after collision. A parameter \( e \) may be introduced as follows:

\[ \Delta v = e \cdot v \]  

(4.4)

Recall that \( v \) is relative to the graphite piston. The parameter \( e \) may take on a range of values from 1.0 (completely inelastic collision) to 2.0 (elastic collision). The convective force may be written as

\[ F_c = \frac{emv}{\Delta t} \]  

(4.5)

The two forces are summed to calculate the acceleration of the graphite. Benson\(^1\) reports the mass per unit area, \( \xi \), of the piston.
The piston mass is $\xi \cdot A$. The acceleration, $a$, is defined as

$$a = \frac{P - P_0}{\xi} + \frac{\epsilon \cdot m \cdot v}{\xi \cdot A \cdot \Delta t} \quad (4.6)$$

The acceleration is calculated at the beginning of each time step. The new acceleration and the acceleration at the prior time step are linearly extrapolated to estimate the average acceleration during the advanced time step. The average acceleration, $\bar{a}$, is assumed constant during the advanced time step. The average acceleration is used to calculate the velocity, $v$, and the displacement, $x$, of the piston during the advanced time step.

$$v = v_0 + \bar{a} \cdot \Delta t \quad (4.7)$$

$$x = x_0 + v_0 \cdot \Delta t + \frac{\bar{a} \Delta t^2}{2} \quad (4.8)$$

The zero subscript indicates a value at the beginning of time step $\Delta t$.

Equation (4.8) is used to calculate the displacement during a time step. Graphite motion is simulated by decreasing the graphite density in the cell containing the $\text{UO}_2$-graphite interface. An additional time step limit was included in SIMMER-II for this analysis. The time step limit is based upon a maximum fraction of the original graphite density which may be displaced during a single time step. Typically the code was run so that no more than 10% of the interface cell volume may be depleted during a given time step. Numerical results using a 1% limit were essentially the same as those using a 10% limit. The model simulates the motion of the graphite plug inner surface only. All non-sample volume in the simulation is filled with
graphite. The parameter $\xi$ is input; it is not calculated from the graphite present in the simulation. The graphite motion is based on the input parameter $\xi$.

4.3 Global Momentum Model

The results of simulations using the graphite motion model are described in Chapter 5. It is sufficient to note here that the results using that model were not completely satisfactory. The piston velocities were much less than the velocity data reported by Sandia. To account for the discrepancy, an alternate motion model, the Global Momentum Model (GMM), was developed. The model presumably yields an upper bound on the acceleration of the graphite piston. An upper bound was required after the results using the graphite motion model became known.

The GMM assumes that all of the increase in the sample momentum during a time interval is instantaneously imparted to the graphite piston. STIMMER-II calculates the total sample momentum at each time step. The piston average acceleration, $\bar{a}$, is given by Eq. (4.9).

$$\bar{a} = \frac{M^n - M^{n-1}}{\Delta t^{n-1}} + \frac{P_u - P_0}{\xi} \quad (4.9)$$

where, $M^n$ is the sample momentum at time step $n$, and $\Delta t^{n-1}$ is the time interval between time step $n$ and time step $n-1$. The acceleration calculated by Eq. (4.9) is also used in Eqs. (4.7) and (4.8) to calculate piston velocity and displacement.
4.4 Energy Deposition

The temporal variation of the energy deposition has a Gaussian shape. For this analysis, the distribution was neglected beyond $3\sigma$ of the distribution maximum. The duration of the approximated pulse is $6\sigma$. The SIMMER-II calculation begins after $1\%$ of the sample has melted. This condition was required because initially there must be liquid in every SIMMER-II cell. In order to correctly calculate the system energy deposition, the Gaussian was integrated to solve for the time necessary to reach the $1\%$ melt condition, $t_{1\%}$. This is illustrated in Fig. 7. Values of the Gaussian at times later than $t_{1\%}$ are tabulated and input into SIMMER-II. The spatial energy variation (see Fig. 2) is also input into SIMMER-II in a tabular format.
Fig. 7. Normalized Power Variations in Time.
CHAPTER 5

RESULTS

This chapter presents the results of the SIMMER-II analysis of Sandia's electron-beam experiments. The SIMMER-II results of the 2030 J/g run along with the experimental data points are shown in Fig. 8. The agreement between data and simulations is not good. The SIMMER-II simulation is believed to be correct insofar as its models allow it to be. Other codes\textsuperscript{12} modeling even fewer phenomena yield similar results. Further, the relative insensitivity of the result to changes in model parameters provides further confidence in the result. It is possible that some phenomena which are not modeled in SIMMER-II are causing the discrepancy. Reasons for the discrepancy will be discussed.

The experimental results naturally separate into three distinct time scales. The three time scales are shown in Fig. 8 for the 2030 J/g case. The initial time scale is characterized by large increases in graphite piston velocity. The initial time scale spans the interval from the beginning of the experiment to a maximum of 2.0 microseconds. The actual duration varies with the total energy deposition.

The second time interval begins immediately after the first. It is characterized by smaller increases in piston velocity. The duration of the second time scale varies from experiment to experiment, and
Fig. 8. SIMMER-II Velocity Results.
it may not be present at all. The third time scale is characterized by a return to large increases in the graphite acceleration.

Benson's experimental data points and fit lines are shown in Fig. 3. Data points are given only for two extreme cases. Some features of Fig. 3 demand attention in the analysis of the experiments. In both cases where data points are shown, the data exhibits a systematic deviation from the fit line. Understanding the systematic deviation is a goal of the analysis along with the determination of the nature of the initial acceleration. Also, it should be noted that the velocities for the 2030 J/g case are less than those for the 1860 J/g and 1990 J/g cases. The reasons for this variation need to be identified.

5.1 Initial Acceleration

Previous analysis has asserted that the initial sharp increases in piston velocity are due to sample thermal expansion. The basis of the statement is Sandia's electron-beam heated gold experiments. The gold experiment involved the e-beam heating of two samples. One of the samples was gold powder, the other was a gold metal foil. These results are shown in Fig. 9. Thermal expansion effects are enhanced in the foil experiment. Some of the expansion in the powder sample is into the volume between particles.

Thermal expansion effects are separated into three individual effects. Thermal expansion of solid particles and liquid UO\textsubscript{2} is calculable using thermal expansion coefficients given in Reference 8. The third effect is an 11% expansion of the UO\textsubscript{2} upon melting.
Fig. 9. Gold Experiment Results.
The following analysis indicates that thermal expansion cannot produce the velocities observed. Each of the expansion rates may be calculated as a function of the peak power in the sample. Velocities can then be estimated for each of the experiments.

An incremental piston displacement, $dz$, can be related to the temperature increase, $dT$, by Eq. (5.1).

$$dz = \frac{\alpha l}{2} dT$$

(5.1)

The variable $l$ is the sample thickness and $\alpha$ is the thermal expansion coefficient. The factor $1/2$ is due to the fact that expansion will be relieved on both sides of the sample. The incremental temperature change, $dT$, may be related to an incremental time change, $dt$, by Eq. (5.2).

$$dT = \frac{P}{C_p} dt$$

(5.2)

The variable $P$ is the peak specific power in the sample (J/kg-sec), and $C_p$ is the sample heat capacity.

Substitution of (5.2) into (5.1) yields Eq. (5.3) for the velocity, $dz/dt$.

$$v = \frac{\alpha l P}{2C_p}$$

(5.3)

The above analysis applies equally to the liquid expansion. Equation (5.4) will allow calculation of the expansion through melting.

$$v = \frac{\beta l P}{2h}$$

(5.4)
The variable $\beta$ is the fractional expansion through melting, and $h$ is the heat of fusion. Values for the expansion parameters are given in Reference 8.

The above analysis will yield a maximum for the velocity due to expansion. The model overestimates since it does not allow for expansion into the volume between particles. Evaluation of Eq. (5.3), for solid and liquid, and Eq. (5.4) yields the maximum velocities shown in Table 4. These velocities are clearly less than 10% of the observed velocities.

Table 4. Velocities from Thermal Expansion.

<table>
<thead>
<tr>
<th>Energy Deposition (J/g)</th>
<th>Velocity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1860</td>
<td>9.6</td>
</tr>
<tr>
<td>1990</td>
<td>10.3</td>
</tr>
<tr>
<td>2030</td>
<td>10.4</td>
</tr>
<tr>
<td>2490</td>
<td>26.0</td>
</tr>
<tr>
<td>3030</td>
<td>33.0</td>
</tr>
</tbody>
</table>

Analysis of the experiments using SIMMER-II indicates an additional source of piston acceleration. A pressure gradient within the sample causes the liquid to impact the graphite piston. Representative sample liquid densities and velocities are shown in Figs. 10 and 11. The SIMMER-II analysis does not predict the large graphite velocities that are observed. The SIMMER-II analysis predicts a rather slow
Fig. 10. Sample Liquid Velocities (2030 J/g case).
Fig. 11. Sample Liquid Densities (2030 J/g case).
movement of the sample toward the piston. The observed piston velocity would be produced in the SIMMER-II analysis if the sample motion was faster. The GMM was used to immediately transfer all sample momentum to the piston. The use of the GMM should have provided an upper bound on the piston velocity. The velocity predicted by SIMMER-II, using each of the motion models, was much less than experimentally observed. The results of some of the SIMMER-II simulations are shown in Fig. 12. Though many other model parameters were modified, the velocities were consistently less than observed, as shown in Figs. 8 and 12.

The discrepancy in the SIMMER-II analysis is that the liquid velocity never becomes large enough to produce the observed accelerations. Estimation of the velocity required to produce the acceleration will become important later in this chapter. Figure 10 shows the velocity of the liquid. In order to produce the observed velocities, the SIMMER-II simulation velocity would have to be increased by a factor of 24. The resulting liquid velocity would be approximately 200 meters per second, or approximately 56% of the vapor speed of sound.

The duration of the initial time scale varies with the energy deposition. Since data is available only for the extreme cases, only these two time scales may be defined. The 2030 J/g run initial acceleration period ends at about 2.5 microseconds. The end is less clear for the 3030 J/g run, but it appears to be at approximately 1.0 microsecond.

5.2 Medium Time Scale

In Benson's analysis this time scale covers the remainder of the experiment. In this time frame, Benson assumed that the
Fig. 12. SIMMER-II Piston Velocities.
acceleration of the piston was due only to the vapor pressure of the UO$_2$ sample. The SIMMER-II analysis indicates that other effects may influence the piston acceleration during the remainder of the experiment. Liquid "sloshing" is one possibility which will be discussed in the next section. The SIMMER-II analysis also indicates that although the motion is due to vapor pressure, it is not a single pressure which can be easily correlated with the energy deposition. The pressure effects are considered below.

The SIMMER-II analysis indicates that during the motion of the piston significant changes in pressure occur. The changes are large enough at the piston surface to affect the piston motion. There are three important effects which are noted in the sample: a spatial pressure gradient, a temporal variation of that gradient, and a temporal dependence of the gross sample pressure. Figure 13 shows the three effects in the 2030 J/g case.

The initial pressure gradient is caused by the spatial variation of the energy deposition; see Fig. 2. The plot at 4 microseconds in Fig. 13 shows a decrease in the gradient. This equalization of pressure occurs because the piston velocities remain small. At 6 microseconds the piston has moved and pressure gradients are re-established. Pressure equalization then occurs by 15 microseconds. The temporal variation of the gross sample pressure is also notable in Fig. 13. The depressurization occurs as the sample volume increases.

Figure 13 shows that the acceleration of the graphite piston is not characteristic of a single pressure during the middle time interval.
Fig. 13. Spatial Variation of the Sample Pressure (2030 J/g case).
The lack of a single pressure brings into question the simple analysis previously presented. Meaningful analysis of the experiments will require an even more extensive hydrodynamic examination.

5.3 Long Time Results

The beginning of the long time frame is defined by the return to larger increases in piston velocity. In the 2030 J/g case, the acceleration begins at about 15 microseconds. This acceleration has not been calculated by SIMMER-II. The acceleration is apparent in the Sandia data. Benson has attributed the deviation of data points about the fit line to random measurement error. The deviation, however, appears to be systematic. Figure 3 illustrates the deviations. The 2030 J/g and 3030 J/g data points as well as the gold experimental data, exhibit the same oscillatory deviation from the line. The following analysis indicates the possibility that the second upward deviation is due to liquid impact on the graphite piston.

Earlier in this chapter, the liquid velocity necessary for the initial acceleration of the 2030 J/g case was estimated. Following initial fluid impact, at approximately 1 microsecond, the liquid will reflect off of the piston. If it is assumed that the collision is elastic, the liquid speed will remain the same. Traveling at that constant velocity, the liquid would impact the opposite piston at 13 microseconds. The impact location is based on the piston displacement data from Reference 1. For the 3030 J/g case, the same analysis indicates liquid impact at 2.5 microseconds. These times seem to correspond with
observed upward trends in the data points. The times are one to two microseconds earlier than the recorded acceleration times. The analysis is approximate. Deviation from an elastic collision will reduce the velocity and delay the impact. It is doubtful that waves travel through the medium at constant velocity.

The second liquid impact has not been predicted by the SIMMER-II code. The prediction would not be expected unless SIMMER-II could produce realistic initial liquid velocities prior to the first liquid sample-piston impact. Whatever the reason for the upward trend in the data, it is present. Fitting a line which includes the upward trend will result in an overestimation of the $\text{UO}_2$ vapor pressure. Since the acceleration is not due to vapor pressure it should not be included in the fitting procedure. Possible wave propagation further complicates the problem of finding a single characteristic pressure for a given experiment.

5.4 Motion Models

Details of the piston motion models are described in Chapter 4. The graphite motion model is a "best estimate" model. The GMM is a "maximum possible" model. Results from the two models are shown in Fig. 12. Both models predict velocities which are low compared to the data. These results indicate that the velocities from SIMMER-II analysis may be too small.
5.5 Velocity Variation with Energy Deposition

The piston velocities shown in Fig. 3 exhibit an unusual variation with the total energy deposition. Specifically, the 2030 J/g velocities are less than the 1860 J/g and 1990 J/g velocities. This behavior has not been addressed in prior analyses. In order to shed light on the phenomena, SIMMER-II was applied to the problem.

Benson has estimated relative errors in the initial UO₂ sample densities to be 50 to 80%. SIMMER-II was run with sample densities modified to the limits of these error bounds. Although all of the SIMMER-II piston velocities are less than the data, they may be compared with other SIMMER-II simulations. The results of the runs are shown in Table 5.

Table 5. Piston Velocities.

<table>
<thead>
<tr>
<th>Case (J/g)</th>
<th>Velocity at 20 μsec (m/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1860</td>
<td>19.0</td>
</tr>
<tr>
<td>1990</td>
<td>29.0</td>
</tr>
<tr>
<td>2030</td>
<td>33.1</td>
</tr>
<tr>
<td>2030 (low density sample)</td>
<td>28.6</td>
</tr>
<tr>
<td>2030 (high density sample)</td>
<td>26.9</td>
</tr>
</tbody>
</table>
Table 5 shows that the velocities depend upon the initial density of the sample. Since the sample area density is known, density variations between runs cause the sample thickness to change (see Table 1). The magnitude and timing of the acceleration from the liquid slosh will depend upon the sample density and thickness. The 2030 J/g case can give smaller piston velocities than the 1990 J/g nominal density case. The thickness of the sample also has an effect on piston velocity. The piston velocity is a complicated function of the sample density and thickness. This dependence is illustrated in Table 5 by the decrease in the 2030 J/g velocity on either side of the nominal density and thickness.

5.6 Non-Equilibrium Effects

The SIMMER-II code was chosen because it allowed simulation of non-equilibrium situations. The deviation from equilibrium could be caused by superheating of the vapor. Phase transition limits could also cause a deviation from thermal equilibrium. Heat transfer to the graphite might also cause non-equilibrium situations to persist.

Thermal equilibrium was established by approximately 1.4 microseconds for all cases. This is due to the decrease in the energy deposition near that time, see Fig. 7. After piston motion begins, the liquid UO₂ becomes superheated as the sample depressurizes. The SIMMER-II results indicate that the superheat remains less than 5⁰K. The low superheat indicates that the system is very close to equilibrium during the depressurization.
Heat transfer to the graphite was modeled at the piston only. Heat transfer increased piston velocities by approximately 15%. This occurs because the heat transfer increases the pressure gradient in the sample. The larger pressure gradient increases the sample velocities.

5.7 Benson EOS Results

The Benson EOS does not agree with the well accepted Menzies EOS. In order to evaluate the sensitivity of the simulations to changes in the EOS, simulations were run using the Benson EOS. The piston velocity was found to increase from the Menzies EOS case as expected. The velocity increase was 55% for the 2030 J/g case and 19% for the 3030 J/g case. The velocities exhibited the same time variation as shown in Fig. 12.

The use of the anomalous solid heat capacity model yielded lower sample pressures and piston velocities, as expected. The difference in velocities is inadequate to judge the actual heat capacity observed.
CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

The Sandia electron-beam heated UO$_2$ experiments have been analyzed using the SIMMER-II code. The analysis has identified important phenomena present in the experiments and parameters which have little effect on the final results have been identified.

1) The experimental data shows large increases in velocity during the first one to two microseconds of the experiment. Thermal expansion of the solid and liquid UO$_2$ is not large enough to produce the observed piston velocities. The motion of the sample material into the piston is responsible for the large accelerations. The SIMMER-II code severely underpredicts the observed piston velocities. This is due to an underprediction of the sample velocities as they impact the piston.

2) The prior analysis of these experiments has fit all velocity data following the initial acceleration to a straight line. This procedure has been shown to be oversimplified. During the experiment, the sample pressure is a complicated function in space and time. Therefore, the piston acceleration is not the result of a single pressure characteristic of the total energy deposition.
3) Later time results are dominated by what is believed to be a reflected liquid wave impacting the piston. The sample "slosh" has not been directly simulated. Simple analysis indicates that the slosh is possible. The data certainly indicates that some phenomenon causes an increase in the piston velocity.

4) The piston velocity was found to depend on the initial macroscopic sample density. The sample thickness is also an important parameter. Density variations are thought to be the reason for unusual trends in the velocity data as a function of energy deposition.

5) The prior analyses of these experiments have neglected hydrodynamic phenomena. The hydrodynamics dominates the experimental analysis. The lack of detailed geometric and accurate density data have made hydrodynamic analysis difficult at best. The analysis has shown that the hydrodynamics has a profound effect on the experimental results.

6.2 Recommendations

There are features of the experiments which could be changed to provide better data. The most important change would be a better definition of initial sample dimensions. The initial smeared sample density would also be necessary. The information would be required for a more detailed hydrodynamic analysis. Lighter graphite pistons would also assist in the analysis. The lighter piston motion would be more sensitive to accelerations. Lighter pistons would also reduce the effects of any "sloshing" which might occur.
One area seems to be open to further analysis. The area for further development seems to be the explosive dispersal of the individual \( \text{UO}_2 \) particles. This behavior may occur during the heating, and may provide some of the initial acceleration.

Future experiments should include extensive pre-analysis of the hydrodynamics involved. The initial conditions of the experiments should be known well enough to perform the necessary analysis.

6.3 Summary

In summary, the e-beam experiments have been analyzed hydrodynamically. There are complex hydrodynamic effects which make analysis of the experiments difficult. Inferring an EOS from the experiments is exceedingly difficult, and may be impossible with current computational tools. The benefit of further analysis of the experimental data is questionable.
REFERENCES


