FINAL PROJECT REPORT
ON

The Development of a Chemical Kinetic Measurement Apparatus and the Determination of the Reaction Rate Constants For Lithium-Lead/Steam Interaction

Prepared by:
Dr. Paul Orlean Biney
Department of Mechanical Engineering

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COLLEGE OF ENGINEERING AND ARCHITECTURE

Mechanical Engineering Department

Prairie View A&M University

Prairie View, Texas 77446

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Prepared by:
Dr. Paul Orlean Biney
Department of Mechanical Engineering
P.O. Box 397
Prairie View, TX. 77446
Telephone: 409-857-4023
Fax: 409-857-2222

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PRINCIPAL INVESTIGATOR

Paul Orleans Biney, Ph. D.
Assoc. Professor and Head
Mechanical Engineering Dept.

MASTER

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Abstract

The objective of this research is to experimentally determine the hydrogen generation rate during the beginning and subsequent stages of liquid metal ($Li_{17}Pb_{83}$) and water reaction. The experimental set-up has been built. It includes a metal sample preparation apparatus, a reaction system, a measurement system and a PC based data acquisition and control system. The most important feature of the reaction system is a pneumatic actuated quick opening and closing high temperature, all stainless steel valve used in the system for reaction time control. The PC system provides remote process sequencing, acquisition and control of all the systems except the metal preparation apparatus. Due to the reactivity of the lithium, all the metal sampling, preparation and loading procedures are executed in a glove box under argon protection. The metal temperature was varied between 350°C-650°C and water temperature fixed at 60°C during the experiments. A set of experimental procedures and two analyses methods: (1) thermodynamics method and (2) heat transfer method are discussed. All the measurements and data collections are executed under the PC system control. A data analysis program is used to calculate both the partial pressure of hydrogen and the hydrogen generation rate. The experiment results indicate that the amount of hydrogen generated is relate to the initial liquid metal temperature when the reaction surface is fixed. The mass of hydrogen generated as a function of initial liquid metal temperature and time of reaction is presented. The hydrogen generation over a time period of 240 seconds and the calculated errors are summarized in Table 1.1

Table 1.1 Summary of Hydrogen Generation

Liquid Metal Temperature T (°C)	Hydrogen Generation $\overline{N}_{H_2Max}(g-mole)$	Total Error $\varepsilon_{H_2tot}(g-mole)$	Percentage of Error $\frac{\varepsilon_{H_2tot}}{\overline{N}_{H_2Max}} \times 100\%$
350	0.0067	0.00147	22.6%
400	0.0072	0.00053	8.95%
600	0.0102	0.00158	15.9%

The maximum amount of hydrogen generation ranged from 0.0064 g-mole at 350°C to 0.0102 g-mole at 600°C over a time period of 240 seconds. The maximum hydrogen generation rate range was from 0.0025 g-mole/sec (350°C) to 0.0045 g-mole/sec (600°C) at the beginning of the reaction phase. The average hydrogen generation flux ranged from 0.0551 g-mole/m^2 sec (350°C) to 0.0838 g-mole/m^2 sec (600°C) over a time period of 240 seconds.

The Arrhenius reaction rate constants in the equation $\frac{dN_{H_2}(t)}{dt} = B*\exp(-\frac{\Delta E}{RT})$ are determined from the experimental rate curves. The constant B as a function of time was determined to be, $B = A*\alpha*\beta*(t^{\beta-1})*\exp[-\alpha(t^{\beta})]$, where A=0.052025 (g-mole), α=0.28 (sec^{-1}), β=0.68 and ΔE=1.0336×10^5(J/g-mole).

Nomenclature

Cp	Heat capacity (kJ/kg K)
LGP	Gas pressure in the lower chamber (bar)
LGT	Gas temperature in the lower chamber (°C)
LMT	Liquid metal temperature (°C)
LWT	Water temperature in the lower chamber (°C)
M	Mass (gm)
m.w	Molecule weight (gm/mole)
N	Moles (g-mole)
P_{ardn}	Argon pressure in lower chamber during countdown phase (bar)
P_{arup}	Argon pressure in upper chamber during countdown phase (bar)
PC-DAS	PC-Data Acquisition and Control System
P_{H_2}	Partial pressure of hydrogen (bar)
P_{H_2O}	Water vapor pressure (bar)
P_{sat}	Saturated pressure (bar)
$P_{sys}(t)$	System pressure was measured as function of time (bar)
P_{sysdn}	System pressure in lower chamber during countdown phase (bar)
P_{sysup}	System pressure in upper chamber during countdown phase (bar)
R	Molar gas constant (83.14395 bar cm^3/g-mole K)
$T_{gas}(t)$	Gas temperature was measured as function of time (°C)
T_{gasdn}	Gas temperature in lower chamber during countdown phase (°C)
T_{gasup}	Gas temperature in upper chamber during countdown phase (°C)

$T_{wat}(t)$	Water temperature was measured as function of time (°C)
UGP	Gas pressure in the upper chamber (°C)
UGT	Gas temperature in the upper chamber (°C)
UWT	Water temperature in the upper chamber (°C)
V_{gas}	Gas volume (cm^3)
V_{gasdn}	Gas volume in lower chamber during countdown phase (cm^3)
V_{gasup}	Gas volume in upper chamber during countdown phase (cm^3)
V_{wat}	Water volume (cm^3)
α	Constant in reaction equation (67) in page 85
β	Constant in reaction equation (67) in page 85
ρ	Density (gm/cm^3)

I. Introduction

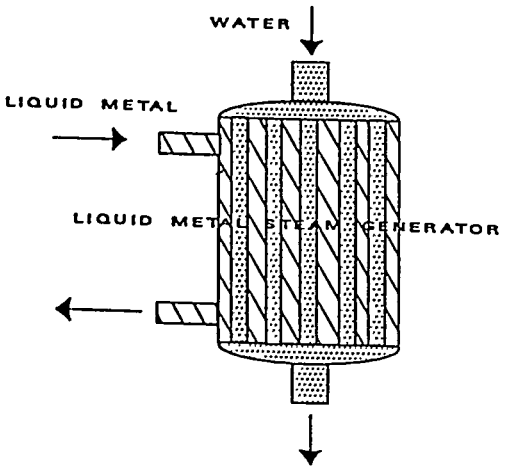
The main purpose of this research is to determine the chemical kinetics of the lithium-lead/water interaction by conducting a series of small scale experiments and to develop the theoretical groundwork to analyze the result of the experiments.

A. Background

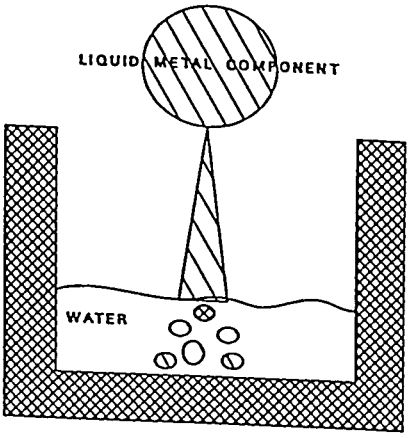
In its general design, fusion power reactors use tritium as their principal fuel. The tritium is bred by capturing neutrons from the fusion reaction in a blanket containing lithium in some form which include liquid lithium metal, lithium-lead alloy $Li_{17}Pb_{83}$, lithium-lead compound (Li_7Pb_2), lithium oxide (Li_2O), and lithium based ceramics [1] [2]. Along with their breeding capabilities, the blanket represents the primary fusion energy heat sink and heat transfer medium. Lithium-lead is being considered as the breeder and coolant, since it has a high tritium breeding ratio, good neutron multiplication and acceptable corrosion rates. Water could be present as an auxiliary cooling fluid or as the working fluid for the power cycle. It is necessary to consider accidental contact of these liquid metals and water in their fusion application. For various accident sequences between the molten metal breeder and the water, four contact modes (coolant injection mode, metal pouring mode, spray mode and water pouring mode) are possible, and described below.

(i) Coolant Injection Contact Mode

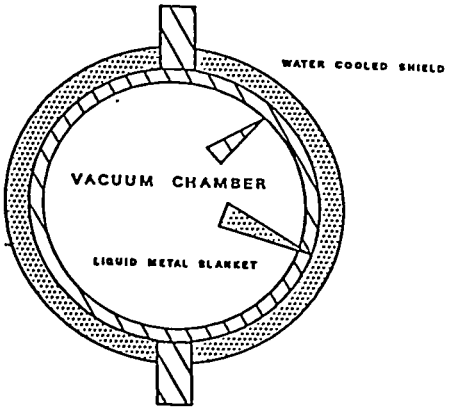
The coolant injection contact mode occurs after a tube rupture in a liquid metal steam generator due to the high pressure injection of the steam/water into the low pressure liquid metal as shown in Figure 1.1a. This contact mode is characterized by rapid mixing, due to the initially enormous pressure difference between the two species.



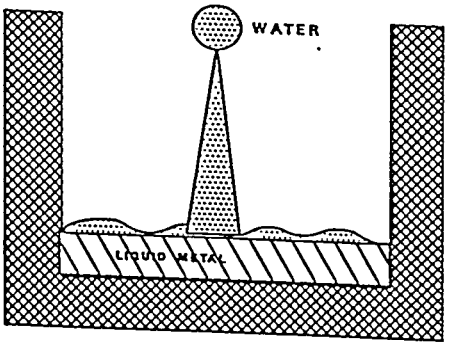
a.Coolant Injection Contact Mode



b. Metal Pouring Contact Mode



c. Spray Contact Mode



d. Water Pouring Contact Mode

Figure 1.1 Four Possible Contact Mode

(ii) Metal Pouring Contact Mode

The metal pouring contact mode occurs in a fusion reactor, after a severe accident in which molten metal is poured from a ruptured component into a stagnant pool of water in the containment vessel as shown in Figure 1.1b. This contact mode would be characterized by less rapid mixing than the coolant injection contact mode, because the two species are initially at the same pressure.

(iii) Spray Contact Mode

The spray contact mode occurs after the rupture of water and breeder-blanket tubes in the vacuum vessel (i.e. central cell), resulting in a spray of these reactants into a common volume as shown in Figure 1.1c. This contact mode is of special concern in a fusion reactor because the major radioactive inventory resides within the vacuum vessel. One may consider this contact mode to be a subset of the previous two, because it is due to the simultaneous injection of the liquid metal breeder and water into a common volume.

(iv) Water Pouring Contact Mode

The water pouring contact mode occurs when the liquid metal and the water come into contact such that the reaction limited their interfacial area of contact is constant. In this research we only consider the last contact mode with its hydrogen production from the interaction with water as shown in Figure 1.1d.

B. Literature Review

In an European research program, based at the European Communities Joint Research Center, ISPRA Italy, a series of small scale liquid lithium-lead alloy/water tests were performed to investigate hydrogen generation during the liquid metal/water interaction. These included the two experiments described below.

(i) Small Scale Experiments

1. The liquid metal drop experiments

In a preliminary test, a 100 gm sample of liquid lithium-lead was poured into excess water; but there appeared to be no difference between this test and a test in which pure lead was poured into water [3]. In two other tests, a stream of lithium-lead was poured into a large beaker, open to air, and partially filled with water [4]. In the first test, the temperature of the lithium-lead stream was 350° C, and the water temperature was 20° C. The second test consisted of pouring a 500° C stream of lithium-lead into 90° C water. In these experiments, the lithium-lead and water interacted in an indiscernible manner. In both experiments, bubbles formed as the stream of liquid metal flowed to the bottom of the container. These bubbles consisted mostly of steam and entrained air. Any hydrogen formed in this phase of the interaction did not reach a sufficient concentration for it to be ignited above the water surface with a fine burner flame. At a later stage, the lithium-lead lying on the bottom of the beaker, became coated with a thin bubble film which later became detached as larger bubbles. These bubbles could be ignited with a flame. Repeating these two tests, but in a closed vessel, the rise in pressure measured after 12 hours, was interpreted to mean that only 16% of the lithium in the alloy had reacted during this period [4]. In these experiment, the contact mode is pouring liquid metal into water, the reaction surface area varied with time during experiments and the hydrogen generation also varied with time. The hydrogen generation rate cannot be determined accurately using experiments based on this contact mode. This contact mode is different with ours experiment but we can use this result to estimate the amount of hydrogen generated in our experiment. We patterned our work on the last contact mode (pouring water onto liquid metal surface) using a reaction chamber with fixed reaction surface area to determine hydrogen generation rate.

2. The liquid metal/steam interaction.

The experiments were designed to facilitate the measurement of the average rate of reaction of various breeder materials with steam [5]. The reaction was initiated by passing steam through a heated test chamber containing the breeder samples. Tests have been performed with three different breeder materials: liquid $Li_{17}Pb_{83}$, with initial temperatures from 310° C to 450° C; solid and liquid Li_7Pb_2, with initial temperatures from 550° C to

850° C; and liquid Li, with initial temperatures from 700° C to 900° C. After the steam passed over the exposed surface of a breeder sample, the resulting steam and hydrogen mixture was passed through a condenser, which separated the unreacted water from the gas mixture. The free hydrogen was then collected. By measuring the amount of hydrogen collected, the average rate of reaction could be inferred. The results of these experiments are summarized in Figure 1.3 [5]. This figure shows that the rate of reaction of steam with $Li_{17}Pb_{83}$ is a function of the initial breeder temperatures and shows an approximate range of hydrogen generation that can help us to estimate the matrix of our experiment. The hydrogen generation rate is a function of time during the reaction. However, in this experiment, the hydrogen generation cannot be measured in a short time interval. We cannot use this method to determine the hydrogen generation rate. A wide range of small scale lithium lead alloy/water experiments performed in Europe lead to the conclusions that the extent of the hydrogen generation is a function of initial liquid metal temperature and contact area.

(ii). Large Scale Experiments

A series of large scale lithium-lead and lithium/material compatibility experiments were performed at the Hanford Engineering Development Laboratory (HEDL) in Richland, Washington [6]. The experimental program consisted of three liquid metal/material groups; liquid metal/atmosphere (air, nitrogen, and carbon dioxide atmospheres), liquid metal/steam, and liquid metal/concrete. The experimental conditions were chosen to reflect the conditions of postulated accident scenarios. Accident scenarios considered included rupture of breeder material lines or modules allowing breeder material spillage to containment cells, and rupture of coolant lines to allow coolant breeder material contact. The lithium-lead/steam reaction test consisted of injecting 335° C superheated steam at about 7 gm/sec into a 200 kg pool of 500° C lithium-lead for 325 seconds. A schematic of the experimental apparatus used in the test is given in Figure 1.2 [6]. The open reaction chamber was placed in a containment vessel containing an argon atmosphere. The reaction chamber was covered with three inches of insulation to minimize heat loss. The reaction chamber was vented by a line that passed through a condenser.

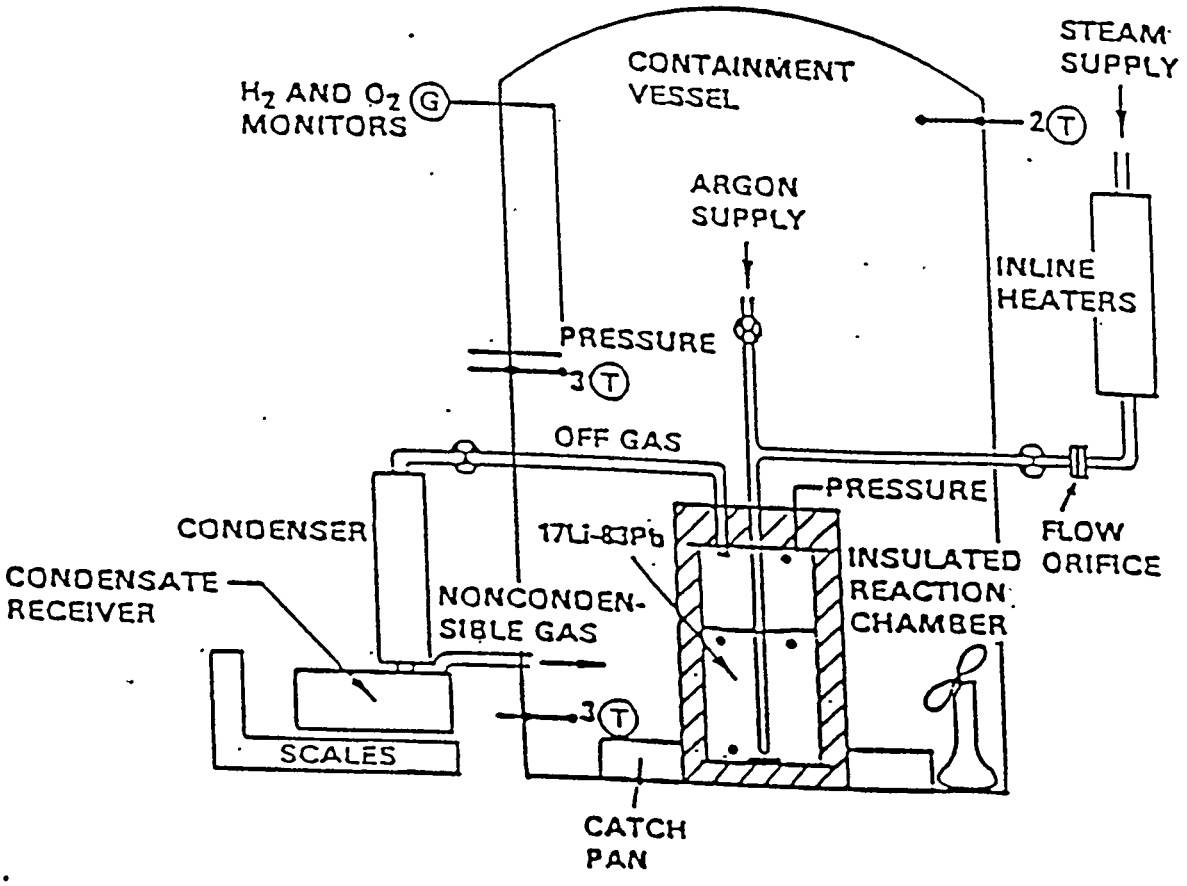


Figure 1.2 Large Scale Lithium-lead/steam Reaction Test Chamber [6]

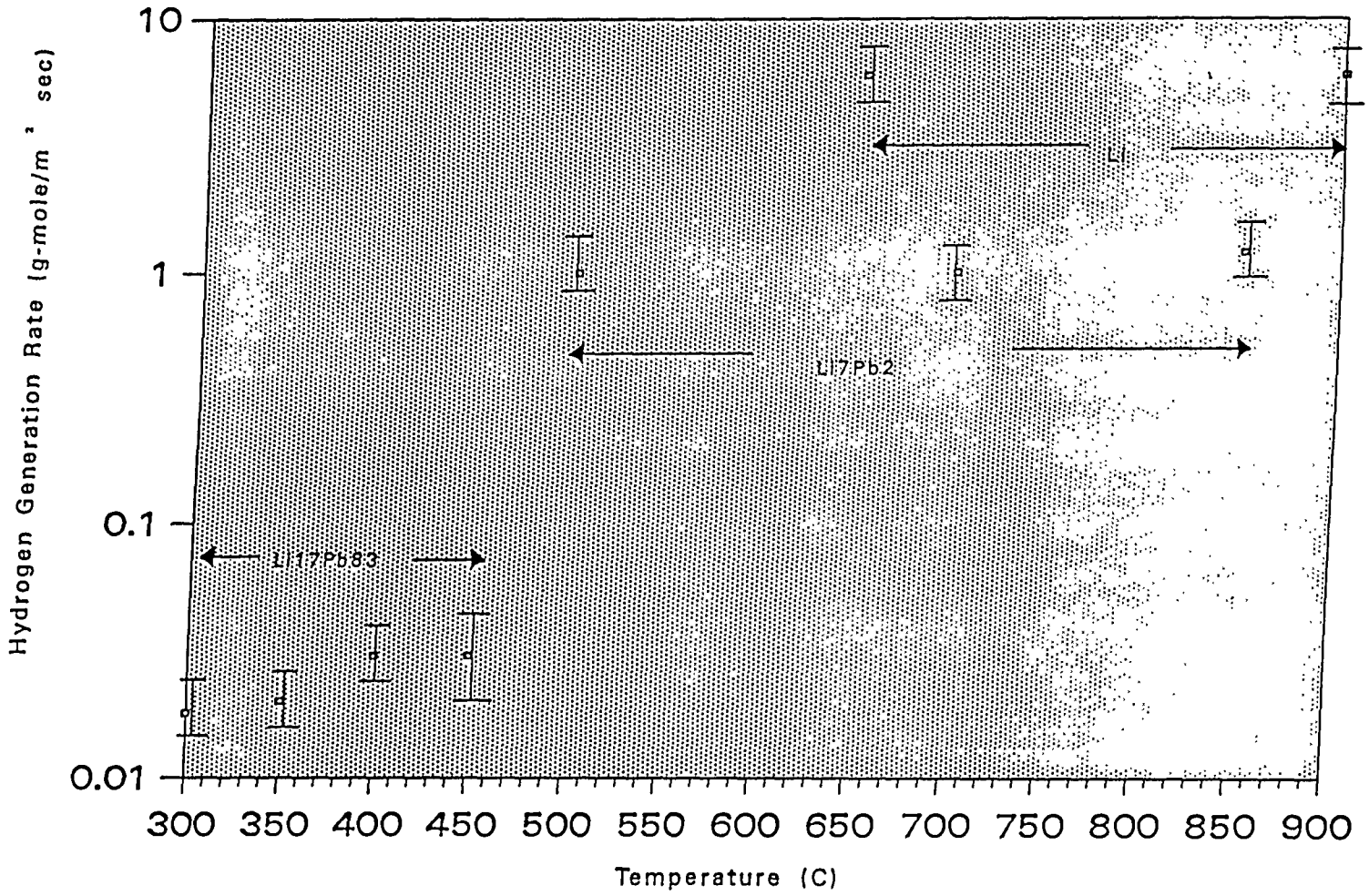


Figure 1.3 Rates of Hydrogen Generation for LiPb and Li Reacted with Water Steam [5]

The condenser was attached to the vent line to condense any exiting steam, allowing the hydrogen to pass on through to the containment vessel atmosphere. The hydrogen release was measured by a hydrogen monitor. The lithium-lead pool temperature response was measured by five thermocouples placed throughout the alloy pool. After the test, the reaction chamber contents were chemically analyzed to determine the extent of the reaction. The lithium-lead pool reached a maximum temperature of 870° C, 240 seconds after the system injection began. The pool temperature remained near the maximum temperature for the remainder of the experiment. Roughly all of the steam injected into the lithium-lead reacted. This conclusion is supported by the fact that only very little steam condensate was collected in the condensers during the experiment. Most of the hydrogen release occurred during the first 240 seconds of the experiment. This result can help us to determine the reaction time in our experiment. In this experiment, the system is an open system. The amount of steam coming into the system is a function of time and some of hydrogen will dissolve into water. As a result, the accuracy of measurement will be limited.

They used a closed system and account the dissolved hydrogen in the total amount of hydrogen generation. The lithium and water react to form LiOH by:

$$Li + H_2O \rightarrow LiOH + \frac{1}{2}H_2 + 2.0*10^5 \text{ J/Mole Li} \qquad (1)$$

Chemical analysis of the reaction products showed that only 0.37% of the lithium content of the pool remained unreacted at the end of the experiment. Hydrogen released amounted to about 0.56 mole H_2 / mole of reacted lithium. The fact that essentially all of the lithium was depleted from the alloy was supported by a measurement of the melting point of the final metal, which was 327° C (the melting point of pure lead) [6]. The chemical analysis also showed that no oxide or hydroxide compounds of lead were formed during the experiment. There was no reaction during the lead/water interaction.

$$Lead + H_2O \rightarrow Lead + H_2O \qquad (2)$$

The reaction equations (1) and (2) are two of the basic equations to be used in our analysis.

Other small scale experiments were performed by J. P. Herzog [7] to determine the amount of hydrogen generation under different initial liquid metal and water temperatures. This experiment was performed with a closed low pressure (<2.0 bar) system and fixed reaction surface area. In the experiments, the extent of reaction was found to vary over the range of initial liquid metal temperatures between 350°C and 600°C. For the 600°C initial liquid metal temperature tests, the average mass of hydrogen at 200 s was 13.4 +/- 0.61 mole/m^2. For the 500° C initial liquid metal temperature tests, the average mass of hydrogen at 200 s was 3.77 +/- 1.01 mole/m^2. For the 400° C initial liquid metal temperature tests, the average mass of hydrogen at 200 s was 10.7 +/- 1.05 mole/m^2, and for the 350° C initial liquid metal temperature tests, the average mass of hydrogen at 200 s was 1.80 +/- 1.16 mole/m^2. In these experiments, the large error was due to measurement system error. The low pressure range (<2 bar) limited the accuracy of pressure measurement. The pressure transducer resolution is limited. If we reduce the gas volume in the system, that will increase the accuracy of pressure measurement. Therefore, our system is designed to operate around 7 bar which is the full range of the transducer used. This will increase the accuracy as much as possible.

(iii) Liquid Metal Transport Reaction Model

A liquid metal transport reaction model was modified by P. O. Biney [8] to estimate the reaction coefficient (ΔE) in the Arrhenius equation $D_{lm} = D_o * \exp(-\frac{\Delta E}{RT})$. This model is based on the premise that the rate of reaction during LiPb/water interaction is controlled by the rate of diffusion of lithium atoms and products Li_2O or LiOH in the liquid metal. Thus the rate of the reaction at the interaction surface will be far greater than the rate of diffusion of lithium to the interaction surface.

The liquid metal transport reaction model is based on the following assumptions: (1) the reaction occurs only at the surface, (2) the system is assumed to be one dimensional, (3) the concentration of lead is assumed to be constant throughout the interaction since there

are 83 atoms of lead to 17 atoms of lithium in the alloy and lead is chemically inactive during the interaction, (4) the liquid metal is incompressible, (5) the gases produced during the reaction are ideal, (6) once reaction begins, the concentration of lithium at the interaction surface is zero, and (7) there is no bulk mixing within the liquid metal pool. Figure 1.4 shows the reference coordinate system used for the model. In the figure, the interaction surface is shown located a distance (s) from the bottom of the liquid metal pool. Hypothetical concentrations of the products and recants are also indicated on the figure. A vapor film of thickness (δ) is shown above the interaction surface and a pool of subcooled water above the vapor film.

Using this reference coordinate and modified model, the value of reaction constant (ΔE) in the Arrhenius equation $D_{lm} = D_o * \exp(-\frac{\Delta E}{RT})$ was estimated. ΔE is 1.09×10^5 J/mole for lithium-lead/water interaction and it is independent of initial liquid metal temperature.

C. Objectives and Scope

The objectives of this research are:

1. To make design improvements in an existing experimental setup and to develop a set of experimental procedure for studying liquid metal/water reactions.
2. To develop mathematical models for predicting the hydrogen generation rate during $LI_{17}Pb_{83}$/water reaction.
3. To determine the hydrogen generation rate and the empirical chemical kinetics reaction rate constants from the hydrogen generation curve during lithium lead/water reaction.

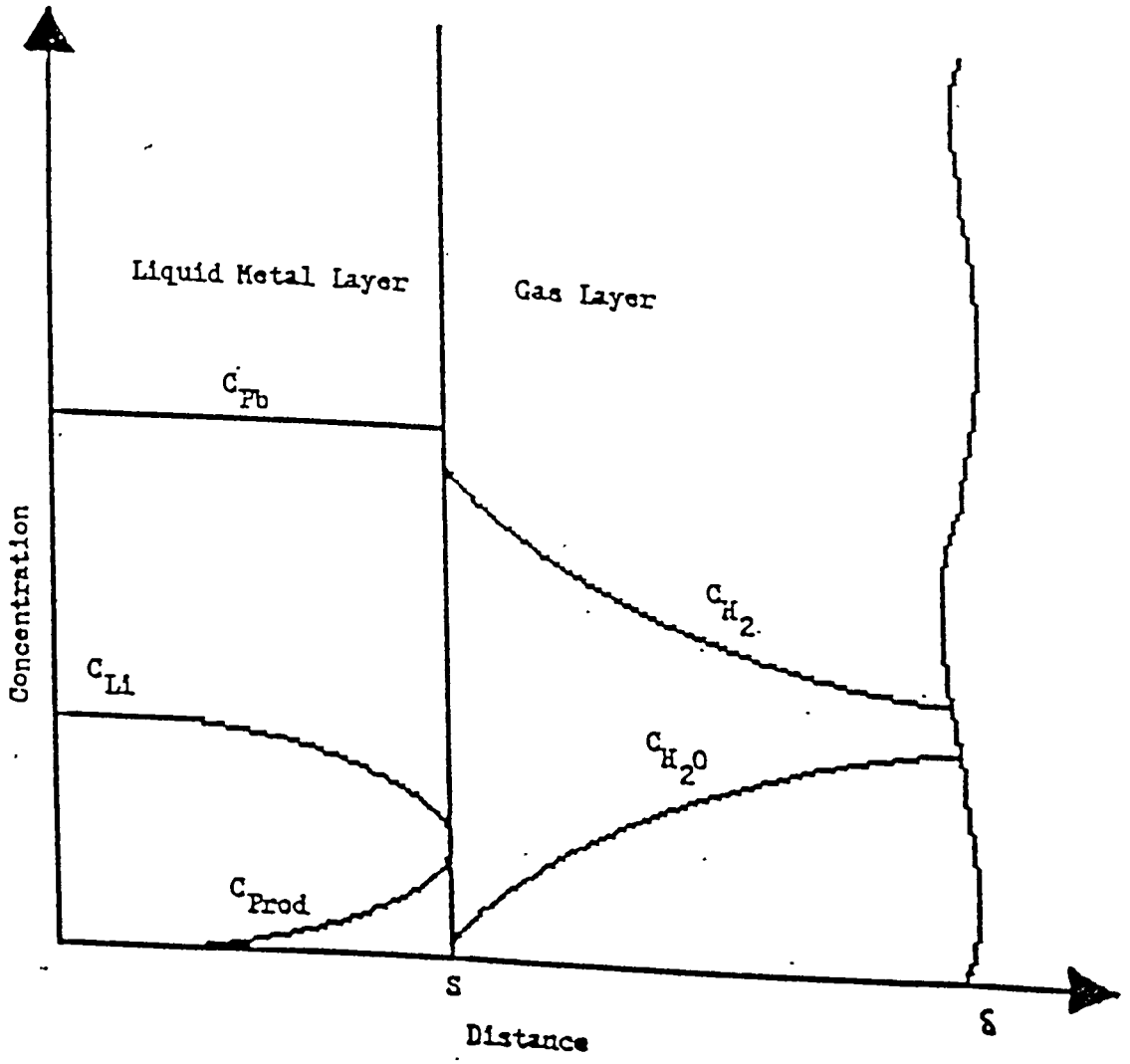


Figure 1.4 The coordinate of Liquid Metal Transport Reaction Model

II. PRELIMINARY DESIGN OF EXPERIMENTAL SYSTEM

In this chapter, the details of an initial experimental setup will be presented. Additional changes made in the setup for the final experiments will also be discussed.

A. Experimental Test Matrix

To enable us to determine the operating condition of the system to be designed, a detailed experimental matrix was initially developed. The matrix has been modified to enable only the most important parameters to be varied. The primary experimental variables are:

1. Initial Liquid Metal Temperature
2. Initial Water Temperature T_{iuw}
3. Initial System Pressure P_{iug}
4. Total reaction time t_r and
5. Initial Mass of liquid Metal M_{lm} (de-emphasized)

To ensure that the surface area for reaction is constant throughout an experiment, the area was selected to be the maximum that prevents Taylor instability. These instability waves can grow if the characteristic length of the liquid metal surface is greater the Taylor wavelength (λ) [10]. This wavelength (λ) is calculated using.

$$\lambda = 2\pi\sqrt{\left(\frac{3\sigma}{g^{*}\Delta\rho}\right)}$$

where

σ is water surface tension $58.9*10^{-3}$ N/m (at water temperature 100°C),

g is gravity acceleration 9.807 m/s^2,

$\Delta\rho$ is density difference 960.6 kg/m^3 between water and water vapor at (100°C).

Since, for our experiment, the Taylor wavelength equals 2.721 cm, we used a tube of 2.54 cm inside diameteras the liquid metal chamber. Thus the liquid metal surface is impervious to Taylor instabilities, which implies that the contact area will remain relatively constant throughout the experiment.

The Secondary variables measured included

1. Reaction product gas temperature T_{ug}.
2. Reaction product gas pressure P_{ug}.
3. Liquid Metal Temperature T_{lm} (t) (350°C-650°C).
4. Lower gas chamber volume V_{lg}.
5. Low gas chamber pressure P_{lg}.
6. Lower gas chamber temperature T_{lm}.
7. Initial Upper Gas Chamber Volume V_{iug}.

The final experimental test matrix for lithium lead/water reaction is shown in Table 2.1.

Table 2.1 Final Experimental Test Matrix for Lithium-lead/Water Reaction with Fixed Reaction Area (5.06 cm^2)

Liquid Metal Temperature °C	Initial Water Temperature °C	Reaction Time s	Liquid Metal Mass gm
350	90	5,10,20,200	60
350	70	5,10,20,200	60
400	60	5,10,20,200	60
400	90	5,10,20,200	60
400	90	5,10,20,200	30
500	90	5,10,20,200	60
500	70	5,10,20,200	60
500	90	5,10,20,200	30
600	90	5,10,20,200	60
600	70	5,10,20,200	60
650	90	5,10,20,200	60
650	70	5,10,20,200	60

B. Preliminary Determination of Hydrogen Gas Pressure in the Gas Region of the Upper Chamber

In order to provide estimates of gas pressures and concentration of hydrogen gas in the gas region, a preliminary analysis was made to obtain the range of hydrogen gas concentration and partial pressures that may be encountered in the course of the experiment. The analysis was based on the following:

1. The mass of liquid metal initially in the lower reaction vessel shown in Figure 2.1 was known.
2. The percent of metal reacted was varied from 5% to 100% (a typical range for such nonmixing reactions).
3. The upper chamber gas region volume shown in Figure 2.1 was varied by varying the water level in the upper chamber (of diameter 3.81 cm) to produce gas volume heights of from 5 cm to 25 cm.
4. Saturated liquid is assumed to be in the upper chamber, and the gas temperature was assumed to be 100 °C.

The above information were used in conjunction with the chemical reaction equation for lithium-lead ($Li_{17}Pb_{83}$)/water reaction to determine the theoretical partial pressure of hydrogen generation during the reaction. The details of the calculation are given in Appendix F. Table 2.2 gives sample calculation results for ($Li_{17}Pb_{83}$)/water reaction. From Table 2.2, it is evident that in addition to serving as a reactant and condensing medium for any water vapor generated as a result of the reaction, the water in the upper chamber shown in Figure 2.1 also can be used to control the partial pressure of the hydrogen produced in the upper gas region by varying its column height. In doing so, we can also have control over the partial pressure of the hydrogen and therefore its concentration. These calculation results also provided us with the upper bounds of pressures to be expected in the system, and this information was used in designing for the minimum thickness of both the upper and lower vessels.

Table 2.2 Theoretical Pressure of Hydrogen Generated form $Li_{17}Pb_{83}$/Water Reaction

Percent Reaction	5%	10%	20%	100%
Gas Accumulation Height in Upper Chamber (cm)	Gas Pressure (kPa)	Gas Pressure (kPa)	Gas Pressure (kPa)	Gas Pressure (kPa)
5	195.5	391.1	782.1	3910.6
10	97	195.5	391.1	1955.3
15	65.2	130.4	260.7	1303.5
20	48.9	97.8	195.5	977.7
25	39.1	78.3	156.4	782.1

C. Intermediate Experimental System Design

Several changes were made in the conceptual design shown in Figure 2.1, the most important of which is the cooling method for the ball valve section. As a result of the high temperatures encountered by the lower reaction chamber and subsequently conducted to the ball valve, it is extremely important that the section close to the valve seat be effectively cooled. Provision was made for cooling the valve by incorporating an internal cooling channel in the lower flange connecting the ball valve to the lower chamber. The details of this design is shown in Figure 2.2. The detail design of the various components of the system is described below.

(i) Details of Lower Reaction Vessel

Figure 2.3 shows the details of the lower reaction vessel which was designed to contain the liquid lithium lead. The flange at the top was welded to the lower part of this section. The flange has an internal cooling channel just beneath the butterfly valve seat. Chilled water from a bath is circulated through this channel to maintain satisfactory temperatures at the valve section. This section is constructed of 316 stainless steel. At the lower section, a 4 inch long NANMAC eroding tip fast response thermocouple is permanently inserted - the tip of this thermocouple is just 1.5 mm below the liquid metal pool and thus closely

measures the liquid metal temperature. All basic dimensions of the lower reaction chamber are provided in Figure 2.3.

(ii) The Furnace

Figure 2.4 shows the details of the design of the furnace into which the lower section described in Figure 3 containing the lithium-lead is inserted, and heated to required liquid metal temperature. Parts A and B constitute a Watlow semi cylindrical high watt density ceramic fiber heater (750 Watts). Two such heaters are used in the furnace providing a total heating power of 1500 watts. Parts C and D are cylindrical ceramic fiber insulation modules used to insulate the lower section of the furnace. Part E is made of ceramic fiber blanket insulation. The outer shell of the furnace is made of stainless steel metal sheet.

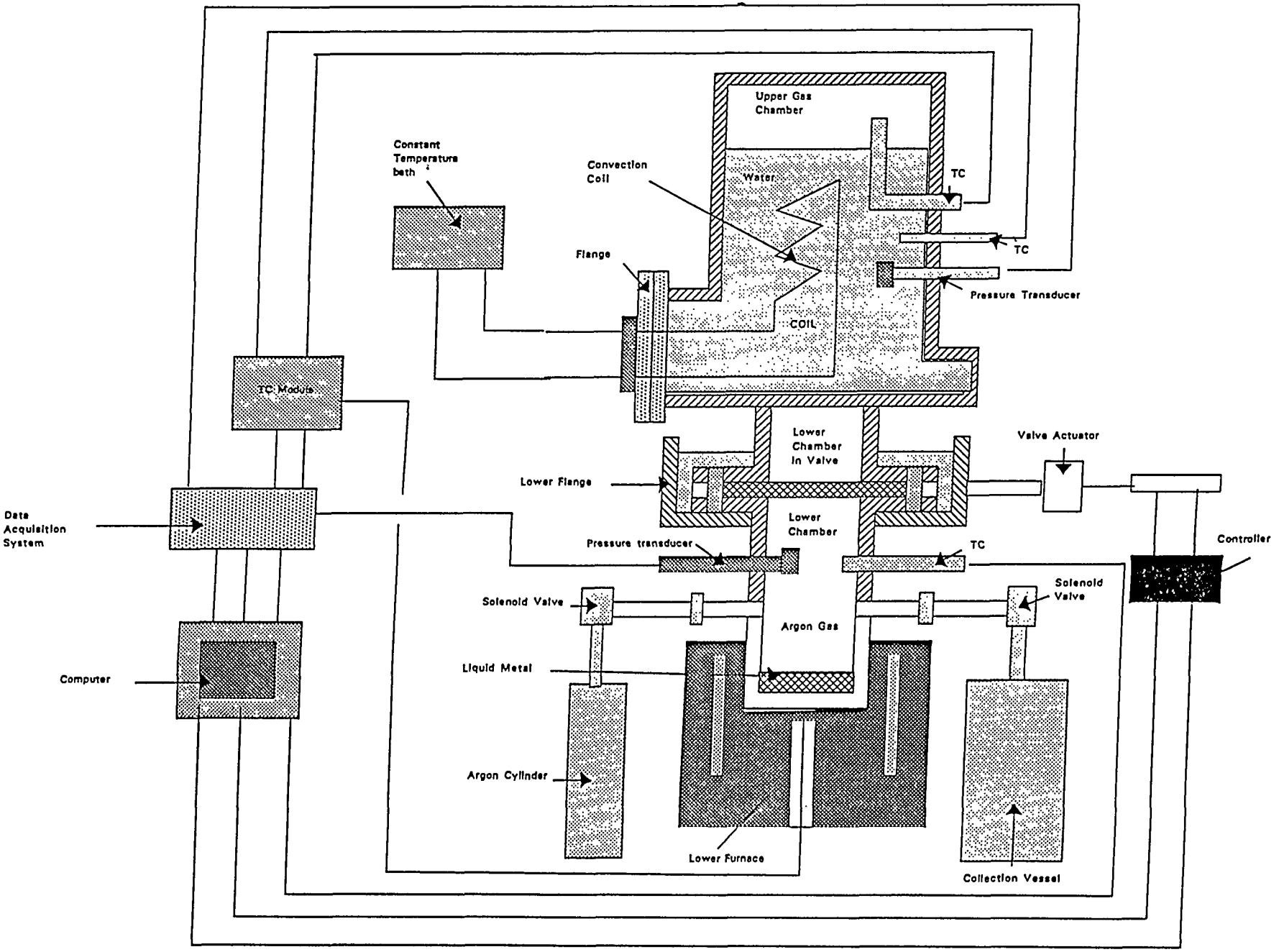


Figure 2.1 Conceptual System Design

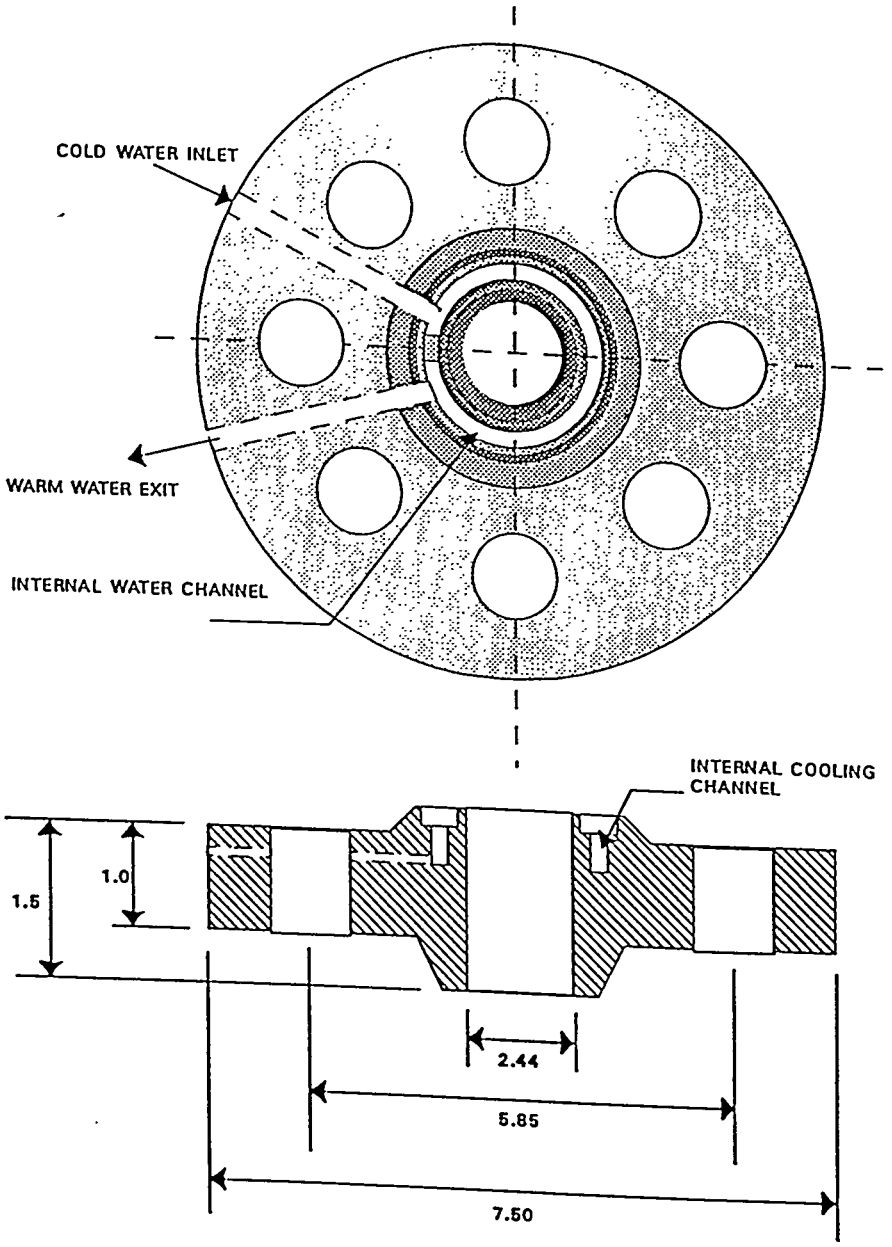


Figure 2.2 Details of Internal Cooling Channel in Lower Flange.

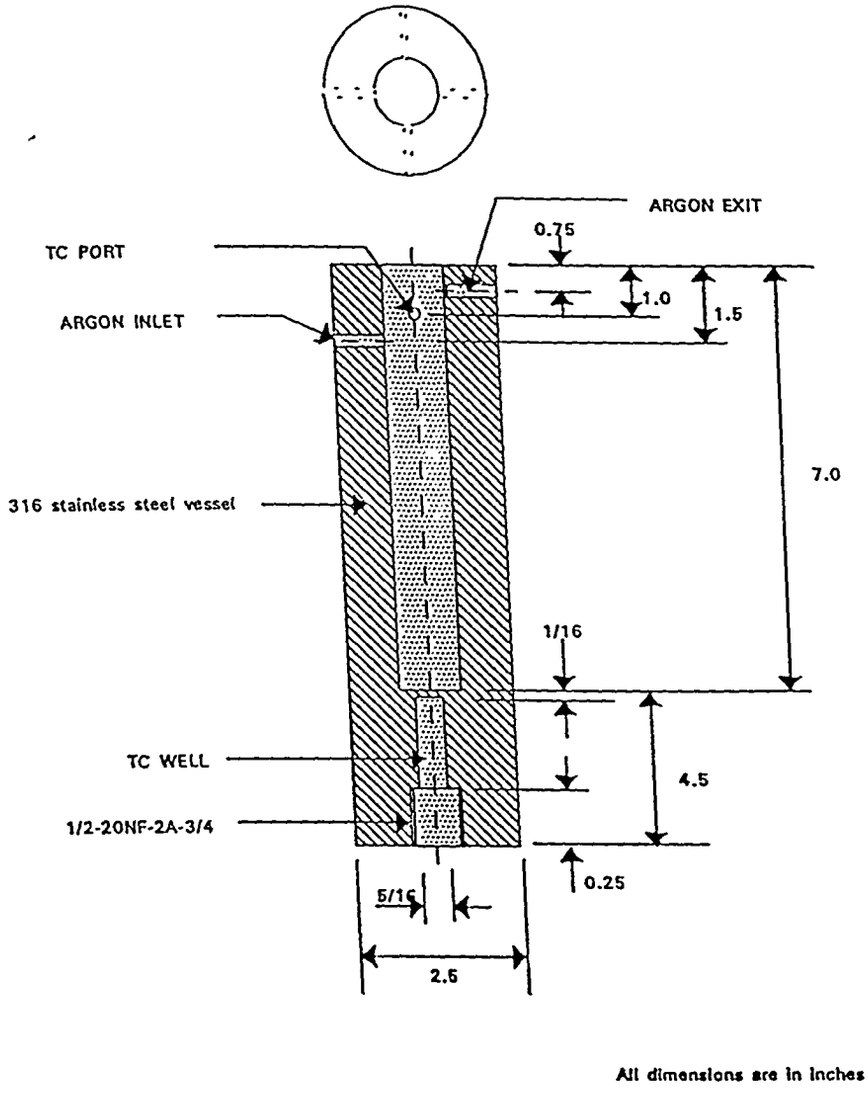


Figure 2.3 Details of Lower Reaction Vessel

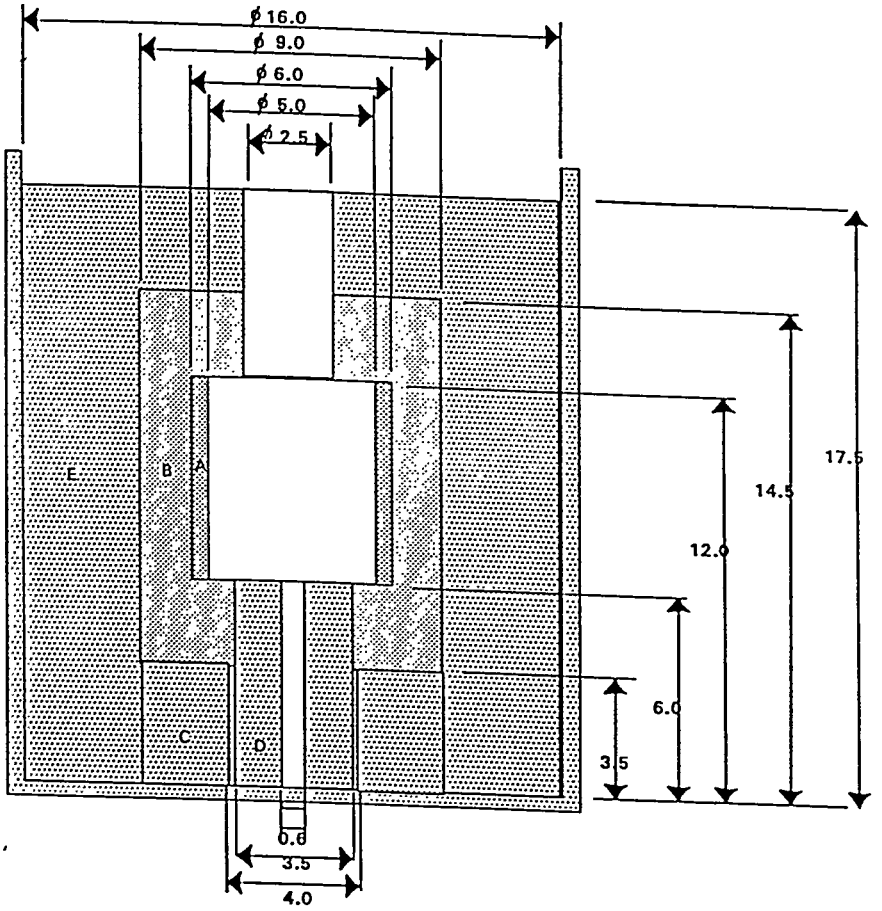
A---Heater Coil

B---Insulation

A and B---Heater Assembly

C and D---Cylindrical Ceramic Fiber Insulation

E---Ceramic Fiber Blanket Insulation



All dimensions are in inches

Figure 2.4 Details of Lower Furnace Design

(iii) Upper Vessel Details

The upper vessel, constructed with 316 stainless steel is shown in figure 2.5. Initially, space V contains saturated water vapor, whose temperature is measured using a adjustable probe NANMAC right angle thermocouple (not shown) connected to port A, which also eventually measures the upper gas temperature once reaction is initiated. A second thermocouple connected to port C measures the temperature of the water in the upper chamber. A convection coil is connected to ports E and F, and hooked to a constant temperature bath and is used to control the initial temperature of the water. The upper chamber is bolted to the butterfly valve through a flange F.

(iv) Mid-Section Butterfly Valve

A pneumatic controlled 2-1/2 inch size 316 stainless steel butterfly valve, shown in Figure 2.6, separated the lower reaction chamber from the upper collection chamber. The valve is an ANSI class 300 high temperature valve, the valve was chosen due to its negligible leakage characteristic, sealing capacity and cycle time (250 ms). The upper and lower sections of the apparatus are connected to the butterfly valve through a flange with graf oil gaskets used to prevent leakage. The flange connection also facilitates easy disconnection of the lower portion of the apparatus for the purpose of loading and unloading the liquid-metal into and out of the vessel in a glove box. To ensure that the butterfly valve and its actuator are operated within their specified temperature range, the valve section is water-cooled internally as described earlier.

(v) Design of Convection Coil

The experimental determination of the rate of hydrogen production during Lithium-Lead/Water reaction involves two distinct stages, the heating stage and the reaction stage. During the heating stage, the lower portion of the apparatus is electrically heated to melt the lithium-lead and to bring it to the required initial temperature, T_{LM}. The reaction stage begins when the butterfly valve is opened and water from the upper chamber makes contact with the liquid metal in the lower section. This stage ends when the butterfly valve is closed at the end of a pre-determined reaction time, t_R.

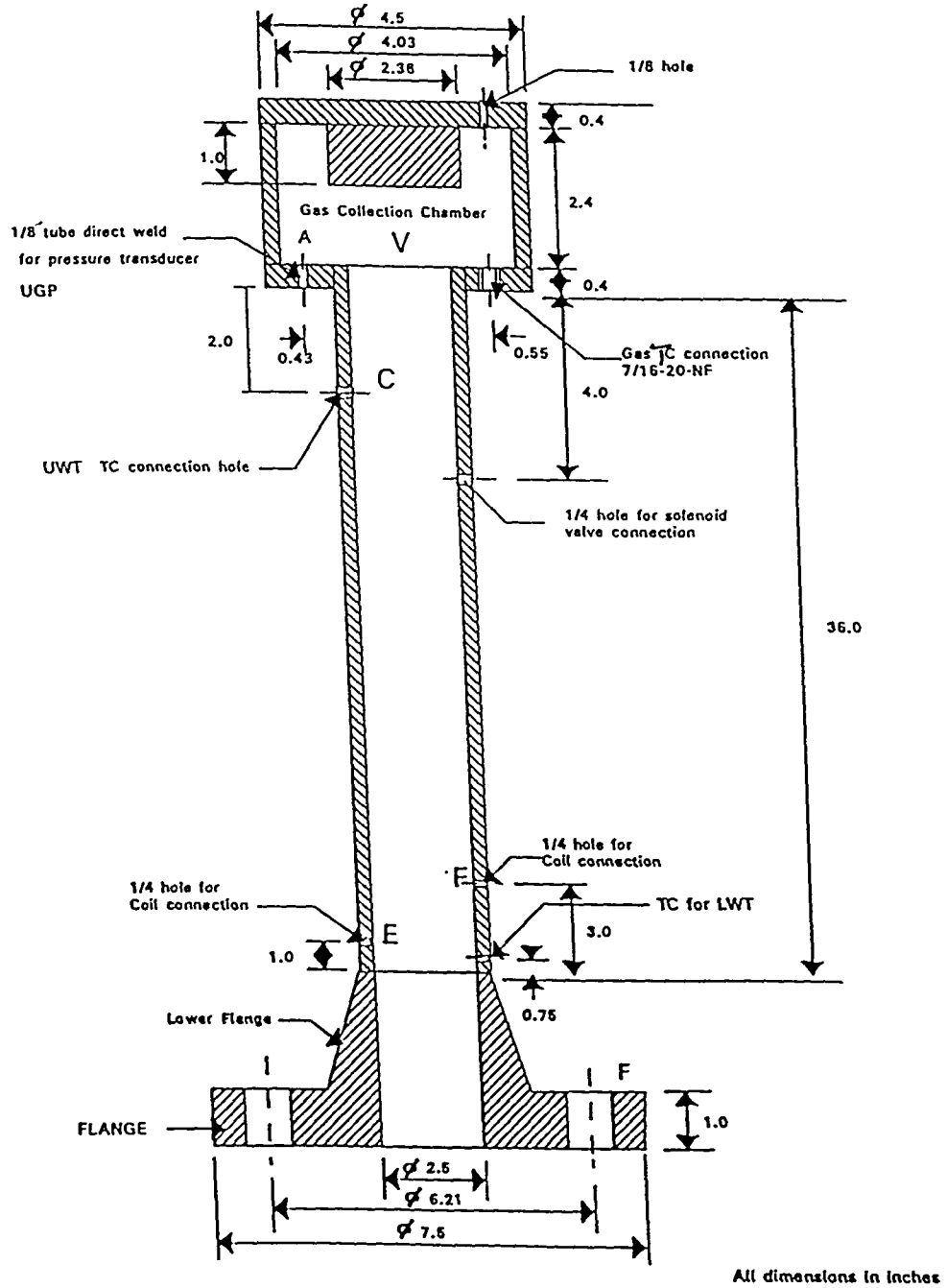


Figure 2.5 Details of Upper Vessel

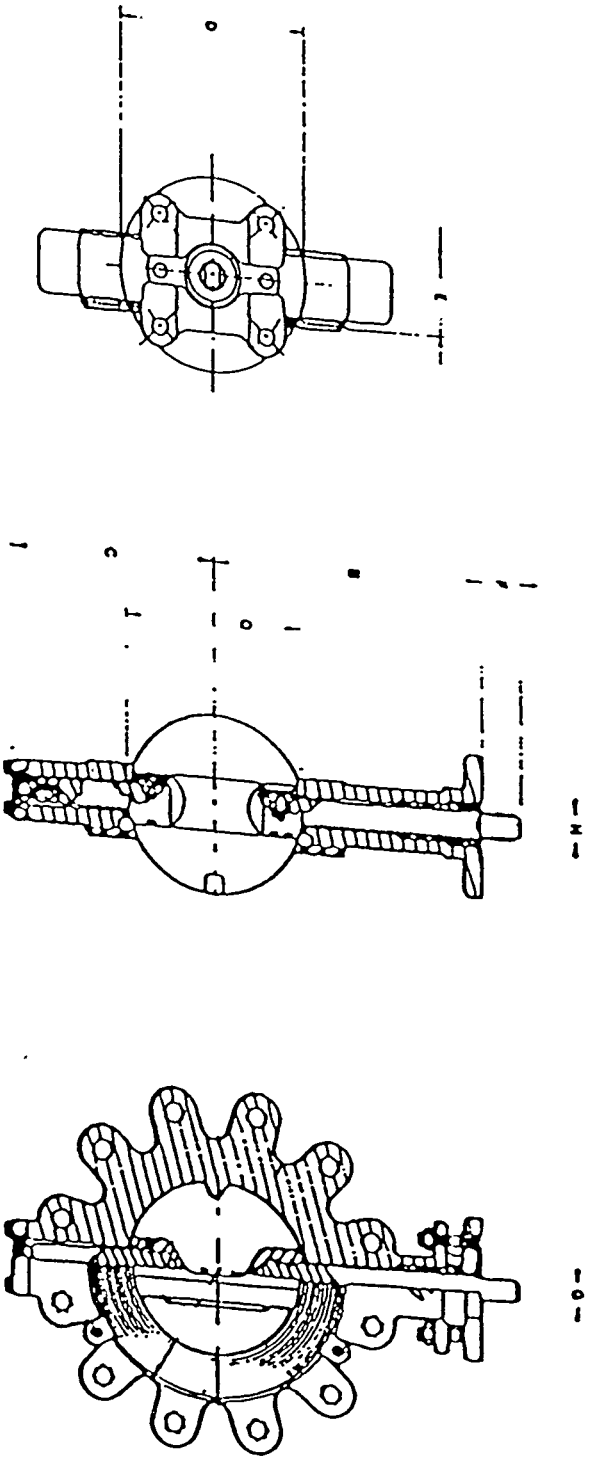


Figure 2.6 Pneumatic Controlled Butterfly Valve

During the heating stage, it is important to ensure that both the butterfly valve and the electrical resistance heating elements are maintained within their stated operating temperature range. It is also important to ensure that right size heaters and adequate insulation is provided to obtain a reasonable heating time (30-45 minutes). These require that a heat transfer analysis be done at the early design stages of the system to ensure that the system under design will satisfy the required constraints. A two-dimensional finite element analysis was used to analyze the heat transfer characteristics of the lower portion of the apparatus during the heating stage. During the heating stage of the experiment, heat is transferred from the lower chamber to the upper chamber, and subsequently by convection to the water in that chamber. This heat has to be removed to maintain a constant water temperature in the upper chamber. The description below gives summary of analysis performed to ensure that the convection coil selected has adequate heat transfer area to remove this heat. Finite element analysis described earlier indicated a total of 375 Watts of heat will have to be removed. Based on this a number of constant temperature baths were reviewed to provide the cooling capacity and flow. Also the pump characteristics of the baths were noted. From the experimental test matrix given earlier in Table 1, the temperature of the pool of water outside the coil ranges from 60°C to 90°C. The above information, together with an assumed bulk inlet temperature of 5°C at the inlet of the coil were used to estimate the heat transfer area, the length of tube required, the head loss in the cooling coil circuit and the flow rate for the given system characteristics. The results of the coil design calculator are summarized in Table 2.3.

Figure 2.7 shows a partial assembly of the furnace, the lower reaction chamber, the mid-section pneumatic controlled butterfly valve, the cooling coil and the upper collection chamber.

D. Initial Testing of Intermediate Experimental System

The assembly of the experimental setup shown in Figure 2.7 was completed. The first test performed was the system pressure tests, and during this test, it was found that the system could not hold pressure. Systematic pressure test performed on the individual component indicated a welding imperfection on the cooling coil.

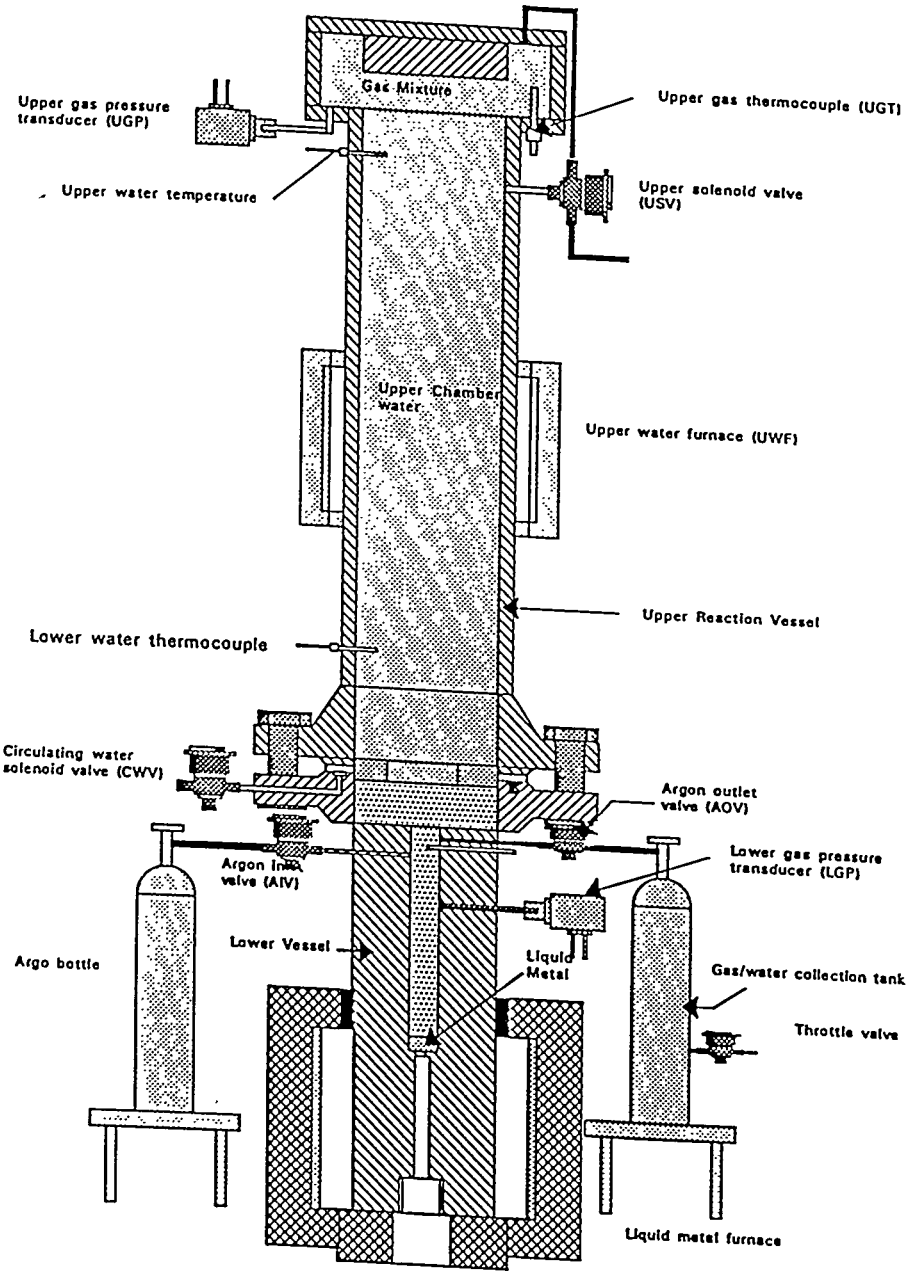


Figure 2.7 Partial Assembly of Preliminary System

Table 2.3 Design Specifications for Cooling Coil

Parameter	Design Selection/Value
Tube Material	316 Stainless Steel
Tube Inside Diameter	3/16 Inch
Tube Outside Diameter	1/4 Inch
Minimum Tube Length Required	28 Inches
Design Tube Length	40 Inches
Mean Coil Diameter	1 3/8 Inches
Bulk Fluid Inlet Temperature	5°C
Flow Rate Through Tube	5 Liters/min

It was also found that the butterfly valve had a higher leakage rate than specified. The failure of the butterfly valve to perform to specification was a big blow to the progress of research. A representative of the valve manufacturer was brought on sight and upon inspection, found the valve to be defective. The manufacturer recommended the use of a zero-leak all stainless steel Vitron ball valve. It was also necessary to change the valve size from 2 1/2" to 1" due to the high cost of 2 1/2" Vitron ball valve. This valve was ordered to be manufactured in August 1992. The new valve was not received until December, 1992. Upon inspection, it was found that a wrong valve stem length was attached. It was returned to the manufacturer. The final valve with the right specification was received in January 15, 1993. As a result of a change in valve size from 2 1/2 inches to 1 inch, several modifications had to be made in both the lower and upper vessels.

E. Final Experimental System Design

A new upper vessel was designed and fabricated to match the new valve between January and March 1993. Several modifications were made in the lower vessel to fit the new valve. Figure 2.8 shows the details of the modified lower vessel. Due to the reduction in size of the valve and its flanges the details of the internal cooling were modified as shown in the Figure 2.8.

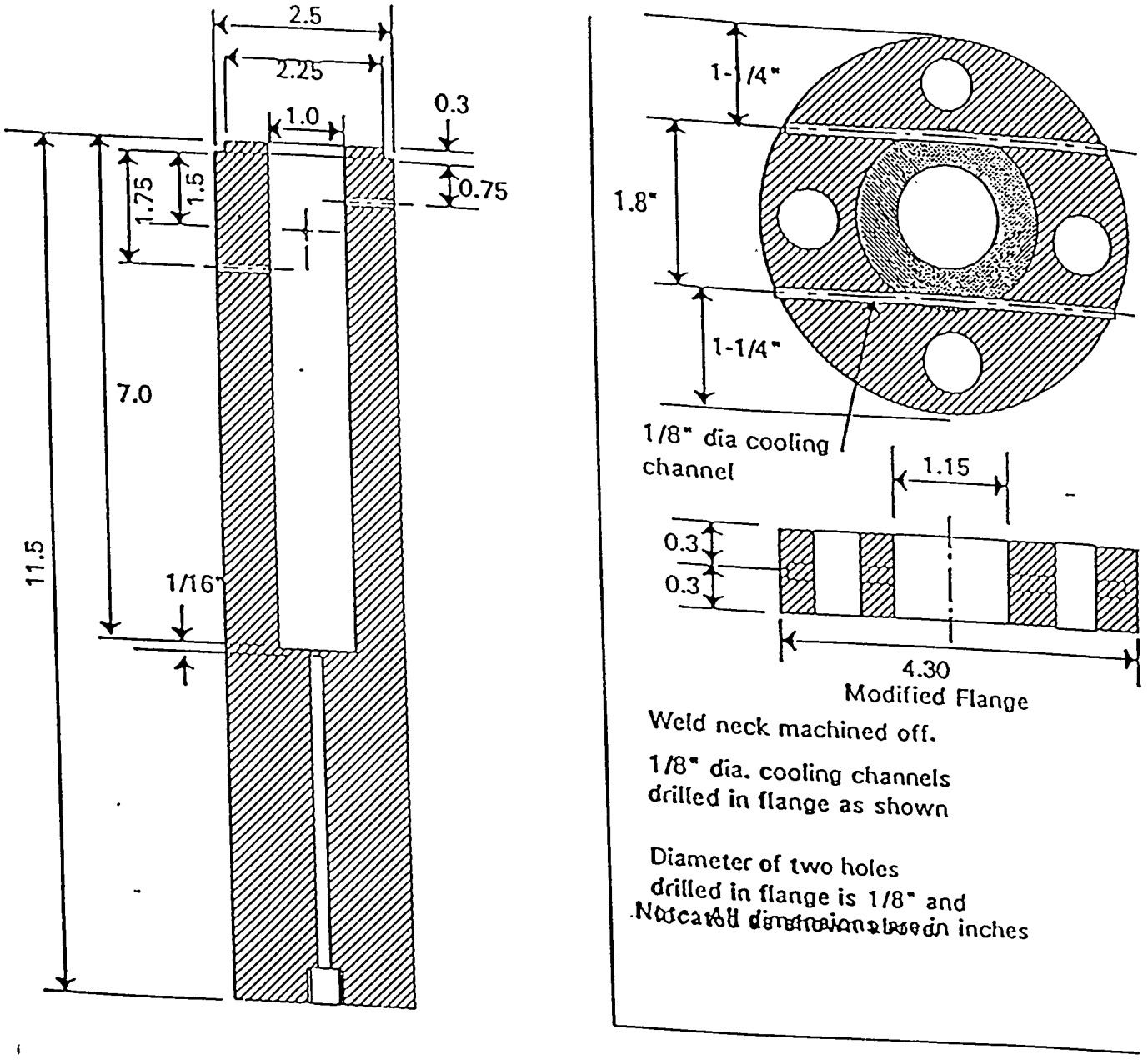


Figure 2.8 Final Design Details of Lower Vessel

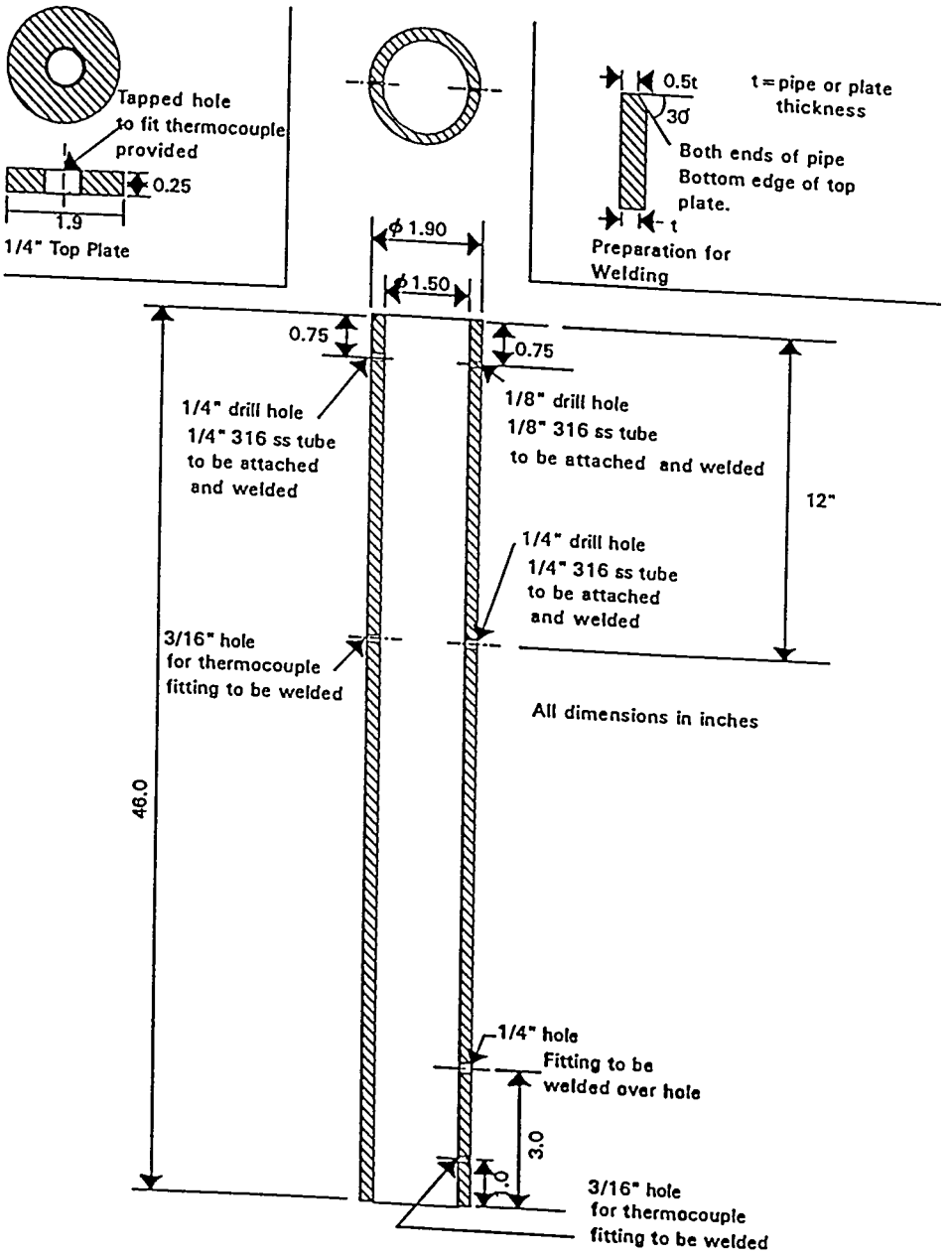


Figure 2.9 Final Design Details of Upper Vessel

Figure 2.9 shows the details of the final upper chamber design. The enlarged section previously on top of this chamber was eliminated to reduce fabrication cost and for simplicity.

All the good leakage prevention features in the preliminary design were retained in this final design. The new experimental design was assembled and all instrumentation attached. Figure 2.10 shows a schematic assembly of the final experimental system. The control panel and the data acquisition and control systems when they were being assembled.

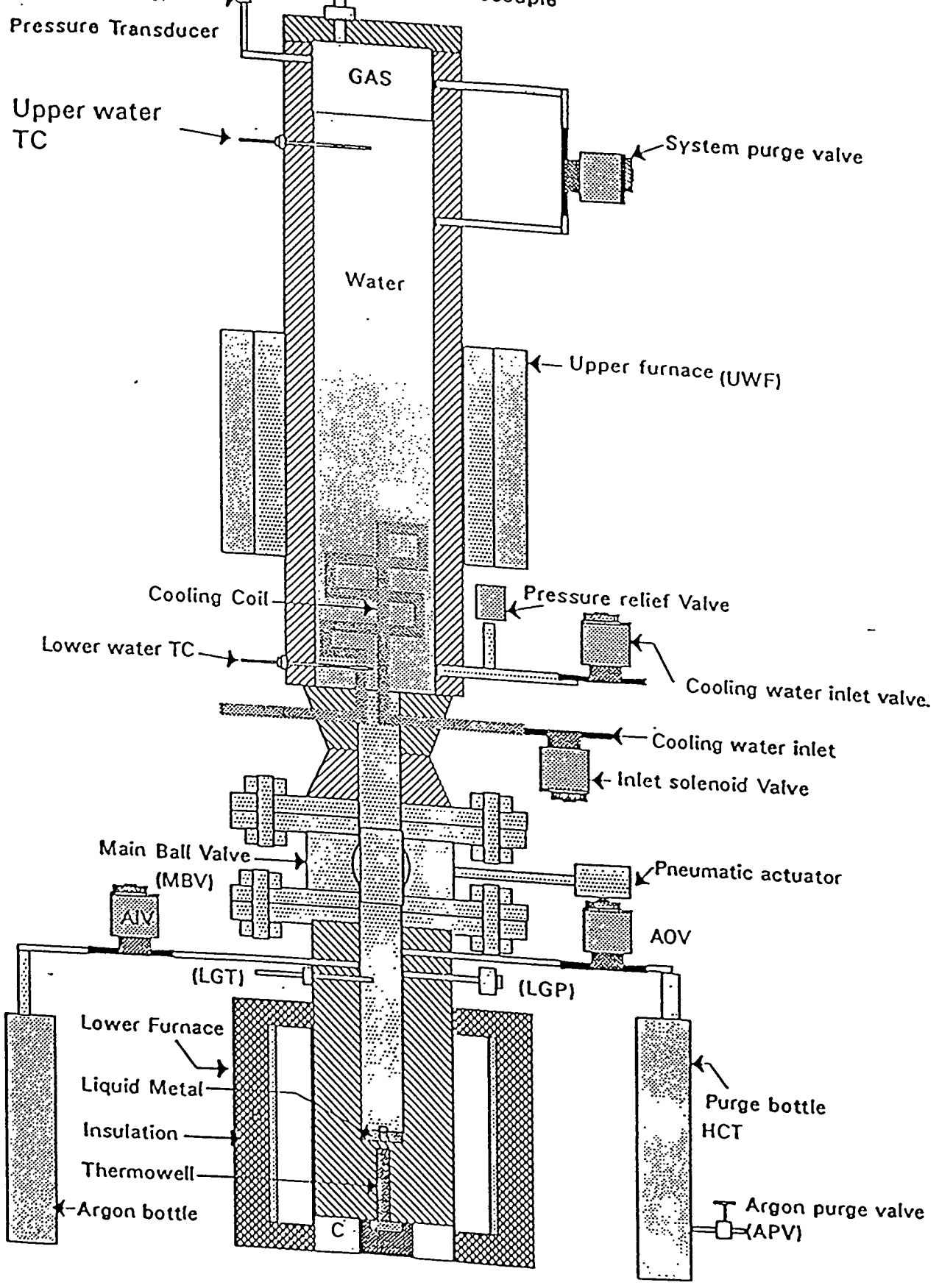


Figure 2.10 Assembly of Final Experimental System

III. DATA ACQUISITION AND CONTROL HARDWARE

In this chapter, the details of an initial experimental will be presented. Additional changes made in the setup for the final experiments will also be discussed.

At the heart of the data acquisition and control system is a Keithly Model 575-2 Measurement and Control unit. A summary of the analog input/output and digital input/output features of the unit are given in Tables 3.1 and 3.2 respectively.

Table 3.1 Analog Input/Output Features of Data Acquisition and Control System

Feature	Description/Range
Speed	50,000 Readings/s
Resolution	16 Bits
Full Scale Ranges	+100 mV, +200 mV, +500 mV +1 V, +2 V, +5 V, +10 V
Channels	8 Differential 16 Single Ended Plus 8 Additional Single Ended
Analog Output Channels	2, Single Ended
Output Ranges	+10 V, +5 V, +2 V, +1 V
Resolution	13 Bits

Table 3.2 Digital Input/Output and Power Control Features of Data Acquisition and Control System

Feature	Description/Range
Channels	32 Non-Isolated, programmable for Input or Output in Groups of 8 Channels. 16 Channels can Drive Power Control Rack for On/Off Control of Power Devices
Trigger Functions Channels	1, Differential Input
Trigger Source	External Input, Any Input Channel, or Software Storable
Ranges	0 to -10 V, 0 to -1 V, 0 to +1 V, 0 to +10 V
Resolution	8 Bit
Input Coupling	AC or DC

Sixteen of the 32 digital input/output channels are dedicated for power control of on/off devices including all solenoid valves and the ball valve through the use of a power control module and relay board. The power control module (PCM-3) is a general purpose remote relay card for the control of power AC and DC devices. It permits direct interface of relays, heaters, meters, actuators, and other AC and DC devices over the full range of voltages from 10 to 280 V. A 16-channel thermocouple module capable of handling J,K,S,T,B,E and R single or mixed thermocouples and having an iso-thermal block is used for all temperature measurements. Figure 3.1 shows the simplified schematic control diagram. The solid state relays SSR-0 through SSR-6 are operated through software, (the Data Acquisition and control program (DACP) developed for this work) and serve as the main on-off switches for all equipment.

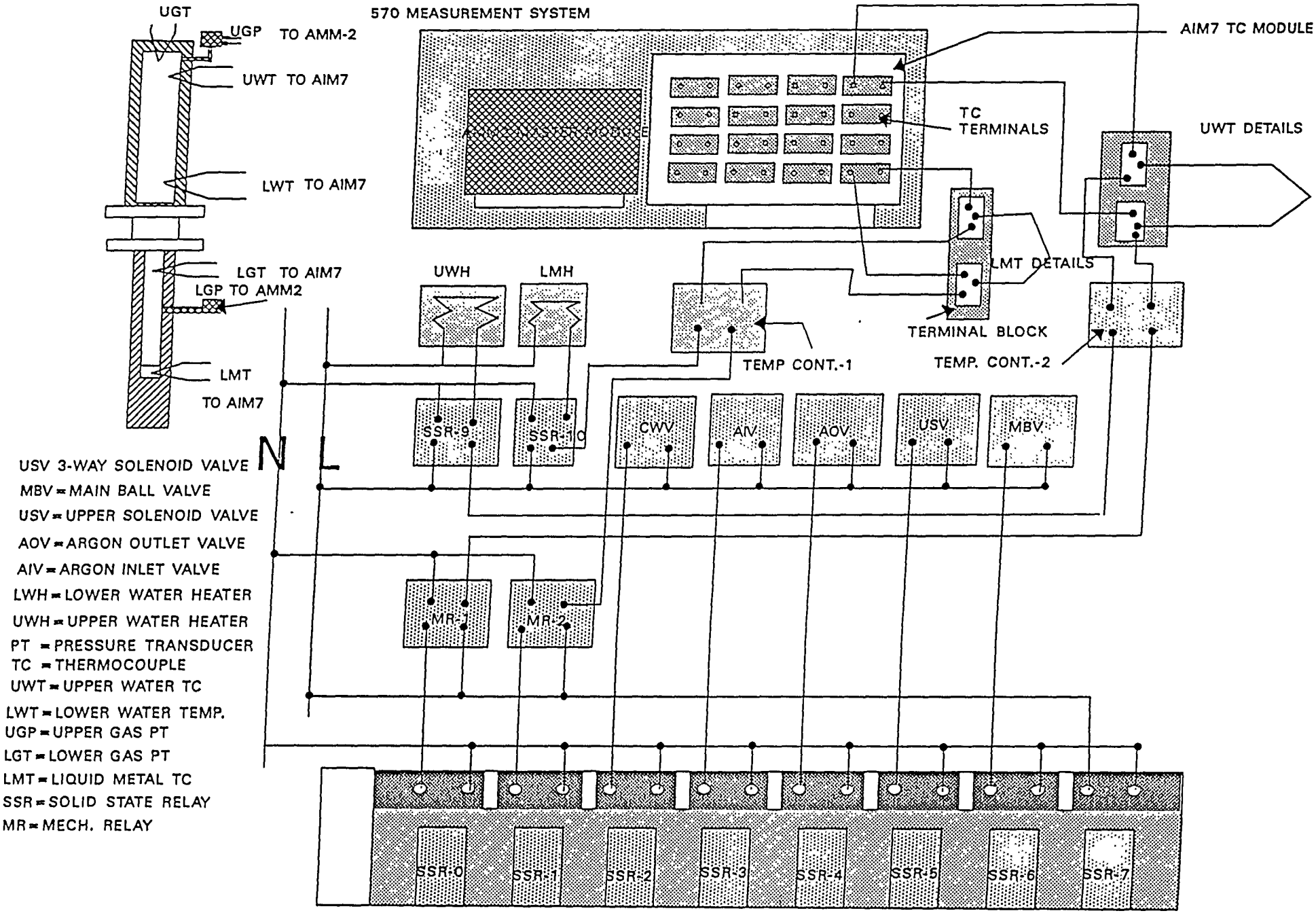


Figure 3.1 *Simplified Schematic Control Diagram*

A. Control of Solenoid Valves

Relays SSR-2 though SSR-6 control the on-off states of the cooling coil/flange circulating water (CWV), the argon inlet valve (AIV), the argon outlet valve (OAV), the upper-purge valve (UPV), and the main ball valve (MBV) respectively. The sequencing timing and duration of operation of these valves are done through DACP.

B. Control of Liquid Metal Temperature

Liquid metal thermocouple (LMT) reads the liquid metal temperature. LMT terminates on a terminal strip from where two sets of thermocouple extension wires take off, one set to a temperature controller (Temp. Cont.-1) and the other set to the temperature measurement module in the 575-2 DAC System. The preset liquid metal temperature is programmed into Temp. Cont.-1, and this controller uses the temperature output of the LMT to control the liquid metal heater LMH, and thus the liquid metal temperature. LMH could not be directly connected to SSR-1 due to the high current pulled by the heater. High line current solid state relay (SSR-10) was initially connected between SSR-1 and the heater, thereby enabling SSR-1 to energize SSR-10 to turn the LMH on. That arrangement did not work due to the leakage current of the two solid states relays SSR-1 and SSR-10. It became necessary to install a mechanical relay MR-2 between SSR-1 and SSR-10. The signal to energize SSR-1 is obtained from the temperature reading on the lower furnace thermocouple (LFT) which reads the heater surface temperature that has been preset to protect the heater element from overheating. As long as the experiment has been initiated and LFT is below the set point, the DAP energizes SSR-1 which in turn energizes MR-2 and MR-2 energizes SSR-10. The dynamic control of liquid metal temp through on/off power regulation of LMT is done by the programmable temperature controller Temp. Cont.-1.

C. Control of upper water temperature

The control of the upper water temperature is identical to the control of the liquid metal temperature. The solid state relays involved are SSR-0, MR-1, SSR-9 and temperature

controller T-C2. The thermocouples involved are the upper water thermocouple (UWT) and the upper furnace thermocouple (UFT).

D. Pressure Transducers

Two pressure transducers are used to measure the major pressures of the system as shown in Figure 2.10.

(i) Upper Chamber Pressure

The upper chamber system pressure is the pressure of the gas mixture above the water level in the upper chamber and it is measured by a high accuracy Setra absolute pressure transducer (UGP). The 0-5 VDC linear output of the transducer is connected to the 575-2 DAC system and converted to kilopascals by DACP. This transducer requires 15-24 Volts DC Supply for excitation.

(ii) Lower Gas Pressure

The lower gas pressure is the pressure of the argon gas in the space between the main ball valve and the liquid metal as shown in Figure 2.10. This pressure is used in conjunction with the temperature of the gas in that chamber and the total volume of the chamber to calculate the amount of argon gas initially in the system. This pressure is measured by a Setra absolute pressure transducer (LGP). The 0-5 VDC linear output is also converted to kilopascals by the DACP through the 575-2 DAC system.

E. Data Acquisition and Control Program

A brief description of the important features of a basic program for acquisition and control of the experiment is described in this section. The important equipment to be controlled is connected to relays on a Keithley PCM3 Relay Board. Table 3.3 gives the description of the relay connections.

Table 3.3 summary of Controlled Equipment and Relays

Relay Number	Input/Output Name	Description of Equipment Attached
0	UWH	Upper Water Heater
1	LMH	Liquid Metal Heater
2	CWV	Circulating Water Valve
3	AIV	Argon Inlet Valve
4	AOV	Argon Outlet Valve
5	USV	Upper Solenoid Valve
6	MBV	Main Ball Valve
7	VAC	Vacuum Valve
9	WIV	Water Inlet Valve

Seven thermocouples (TC) are installed in the system and directly connected to the thermocouple module (AIM7). Two extension wires carry signals from the liquid metal TC temperature and the upper water temperature TC to two temperature controllers. Table 3.4 gives a summary of thermocouples and channel connections.

Table 3.4 Summary of Thermocouples and Channel Connections

Description	Input/Output Names	Channel Number	Thermocouple Type
Upper Gas Temp.	UGT	1	E
Upper Water Temp.	UWT	2	K
Upper Water Temp.-C	Controller-2		K
Lower Water Temp.	LWT	3	E
Lower Gas Temp.	LGT	4	K
Liquid Metal Temp.	LMT	5	K
Liquid Metal Temp.-C	Controller-1		K
Upper Furnace Temp.	UFT	6	K
Lower Furnace Temp.	LFT	7	K

The two setra pressure transducers are directly connected to the AMM2 master module. Each experiment is divided into six phases, and Table 3.5 gives the summary of the important features of these phases.

Phase 1

During this phase, the upper water, the liquid metal heater and the circulating bath are turned on to heat the water in the upper chamber to a pre-determined temperature at which time a vacuum pump is used to control the pressure to obtain a saturated liquid in the upper chamber.

Phase 2

This phase involves activation of the liquid metal heater and the liquid metal heated to a pre-determined temperature.

Table 3.5 Description of the Six Phases of Each Lithium-lead/Water Reaction Experiment

Phase #	Phase Description	Time Interval Between Readings (sec)	No. of Data acquired (Maximum)	Data Saved for Analysis	Data Not Saved
1	Upper Water Heating	20	100		x
2	Liquid Metal Heating	20	150		x
3	Water & Metal Temp. Control	20	90		x
4	Countdown to Reaction	1	60	x	
5	Chemical Reaction	.2	100	x	
6	Equilibrium Period	20	100	x	

Phase 3

This phase involves controlling the upper water and the liquid metal temperatures until they are within a given tolerance of their preset values. This step was found necessary for repeatability of the experiments to ensure an accurate generation of the reaction rate curves from different experiments with identical values of the liquid metal & upper water temperatures. When these two temperatures are within their proper range, phase 4 is activated automatically by the DACP.

Phase 4

This is the count down phase. There is a 60 seconds countdown, during which all pressures and temperatures are read every 1 second and stored later. The average value of each set of reading is used to establish the initial conditions in the system. Particularly, the temperature and the pressure of the argon gas in the lower chamber, which is completely closed at this time, is used to determine the amount of argon in the system. At the end of the 60 seconds countdown, the fifth phase is initiated.

Phase 5

This phase, the reaction phase, begins with the automatic opening of the main ball valve, to initiate the reaction. The valve remains open for a preset reaction time period after which the valve closes, indicating end of reaction. All temperature and pressure readings are recorded and saved during the reaction phase.

Phase 6

Phase 6 involves recording of pressure and all temperatures in the upper chamber for a period of 10 to 20 minutes or until the temperature in the chamber is uniform. The data at this phase is used to obtain the average value of the total amount of hydrogen generated during the reaction time period. Figure 3.2 gives a simplified flow chart of the Data Acquisition and Control Program. The complete program is given in Appendix B.

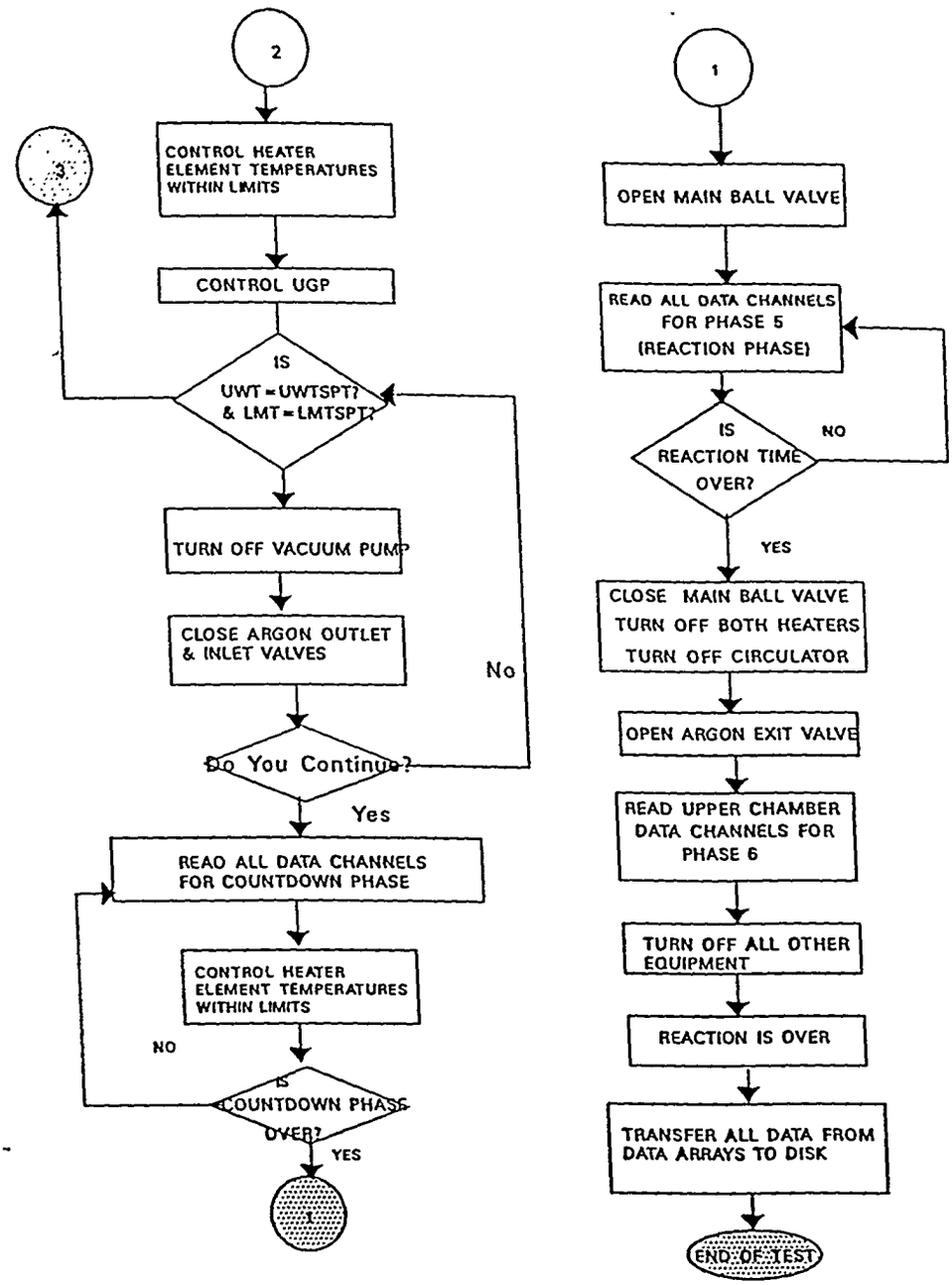


Figure 3.2 Simplified Flow Chart of Data Acquisition and Control Program

IV. CALIBRATION AND TESTING OF EXPERIMENTAL HARDWARE

In this chapter, the details of an initial calibration of the experimental setup will be presented.

A. Initial System Test

The initial system tests performed included a check of continuity of all electrical connections, testing of all instruments with and without the use of data acquisition and control system, calibration of upper and lower vessel volumes.

B. Calibration of Upper Gas Volume

In order to obtain an accurate measurement of the gas space above the water in the upper chamber, it was necessary to accurately calibrate of calculate the volume and to determine the mean and standard deviation of the measurement for statistical analysis of the final experimental data. Figure 4.1 shows the experimental set up for calibration of the upper gas volume. With the upper solenoid valve (USV) closed, upper pressure transducer (UGP) and upper gas thermocouple (UGT) removed, the upper chamber is filled (through valves A and B) with water until the system is completely filled. The chamber is slowly drained through valves A and B into a finely graduated cylinder. The volumes and mass of water collected at different water levels on finely graduated indicator on the upper chamber are recorded. The measured results are then compared to the calculated results obtain from dimensions of the vessel and tubes. Table 4.1 summarizes the results of the upper chamber calibration tests. The experimental values of the volumes agree well with those calculated using vessel and tube dimensions. In the useful water level range of 0-9 inches, the maximum standard deviation is 0.5 cc. Thus all upper gas volumes will be repeated as xxx.xx + 0.50 cc. The total volume of the space in upper chamber was measured to be 1384 cc. The calculated value obtained from system dimensions is 1386 cc. The volume used in all calculations is the average of the two, 1385.0 cc $\pm$ 1 cc.

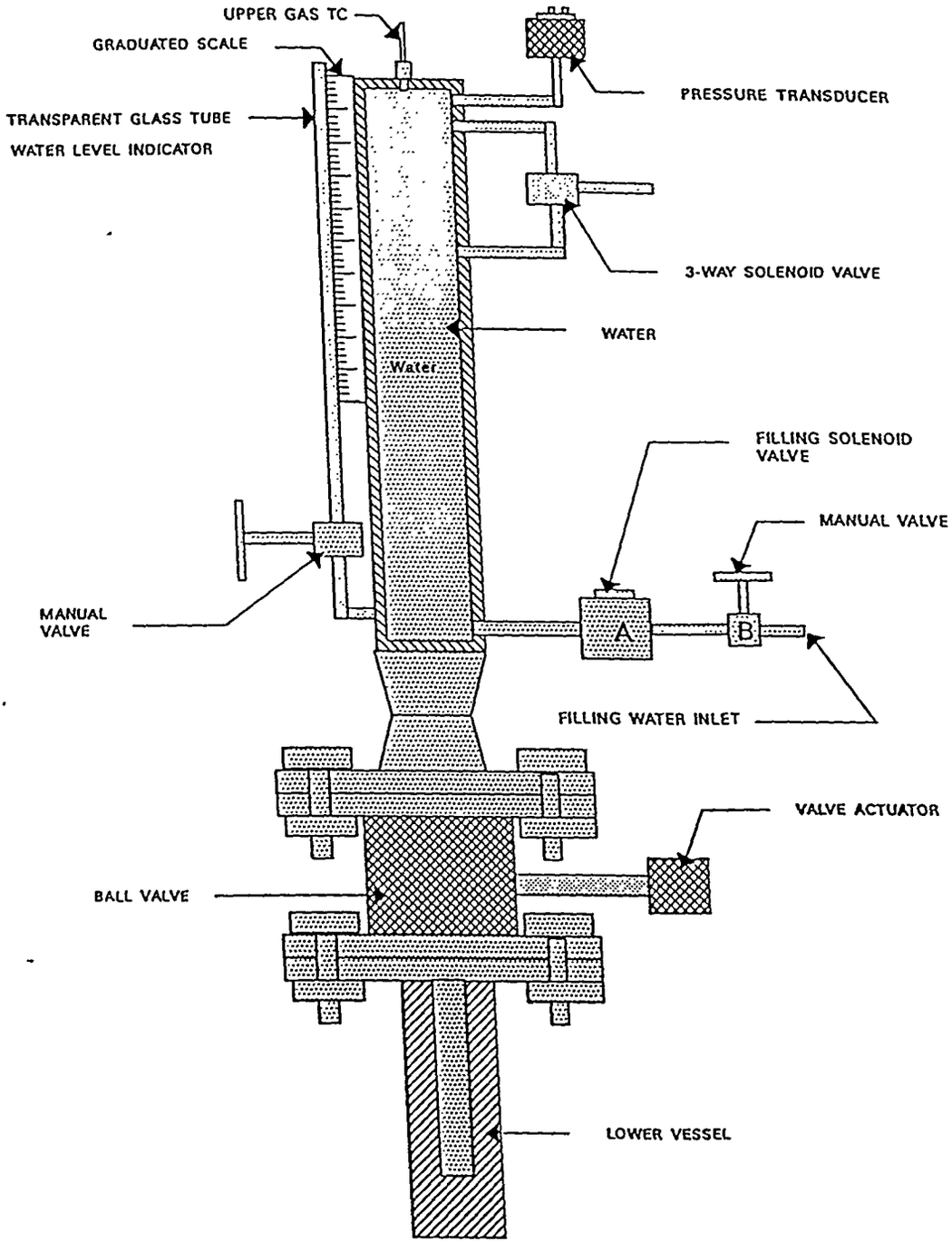


Figure 4.1 Setup for Calibrating Upper Gas Volume

Table 4.1 Summary of Upper Chamber Calibration results

Water Level Mark Inches	Expt. #1 Volume cc	Expt. #2 Volume cc	Expt. #3 Volume cc	Calculated Volume cc	Mean	Standard Deviation
1	29.0	28.5	28.5	27.93	28.48	0.14
2	57.5	58.0		56.88	57.26	0.25
3	86.0	86.5	86.5	85.85	86.21	0.09
4	114.5	115.5	115.1	114.80	115.0	0.14
5	144.0	144.0	143.1	143.76	143.8	0.03
6	172.5	173.0	172.5	172.72	172.7	0.04
7	201.5	202.0	201.5	201.68	201.7	0.04
8	230.0	230.5	230.0	230.64	230.3	0.08
9	259.5	260.5	258.5	259.60	259.5	0.50
10	285.0	286.0	286.3	288.55	286.5	1.68
11	315.5	316.5	315.5	317.51	316.3	0.69
12	346.0	346.0	344.0	346.47	345.6	0.91
13	375.5	375.5	373.0	375.43	374.9	1.15

The total volume of space in the lower chamber below the main ball valve (when in closed position) was to be 114.2 cc and the calculated valve is 114.3 cc. This volume is represented as 114.25. The total volume of space in the lower chamber with the ball valve opened (volume in ball included) is 138.0 $\pm$ 1 cc.

C. Upper Chamber Pressure Test

Two pressure tests were performed on the upper chamber to check for leakage and the ability of the vessel to hold pressure. In the first test, with the ball valve closed the upper vessel was pressurized to 650 KPa. The pressure was monitored for three hours. The total pressure drop during this period was 5.5 Kpa.

In the second test, the upper chamber was filled with water to a level just below the purge line and the system pressurized to 650 KPa. After three hours, the pressure drop was 0.52 KPa, well within the tolerance of the pressure transducer accuracy. From the pressure test, we were satisfied with the ability of the experimental set-up hold pressure over expended period of time.

V. Modifications of Experimental Set-Up and Procedures

In this chapter, all the final modifications made on the experimental set-up are discussed. The modifications described were to simplify the experimental procedure and also to increase the accuracy and repeatability of the measurements.

A Modifications of the Experimental Matrix

From the literature review, the main experimental variables are liquid metal temperature and the area of reaction surface. The lower chamber temperature (>350°C) is much higher then the water temperature (60°C) and the mass of the stainless steel lower chamber (7.8 kg) is much more than the mass of water (1.38 kg). Therefore we can neglect the effect of changing the water temperature within 30°C during the liquid metal/water interaction. We modified the test matrix to that shown in Table 5.1.

Table 5.1 Test Matrix of Experiments

Liquid Metal Temperature (°C)	Experiment Type	Reaction Time (Sec)	Initial Water Temperature (°C)	Liquid Metal Mass (gm)
350	Lithium-Lead Test	240	60	40
350	Control Test	240	60	45
400	Lithium-Lead Test	240	60	40
400	Control Test	240	60	45
500	Lithium-Lead Test	240	60	40
500	Control Test	240	60	45
600	Lithium-Lead Test	240	60	40
600	Control Test	240	60	45
650	Lithium-Lead Test	240	60	40
650	Control Test	240	60	45

B Modifications of Experimental Set-Up

The modifications were made in: (1) the experimental apparatus, (2) the data acquisition and control programs, (3) the water circulation system, (4) the vacuum system, and (5) the argon supply system. The modified experimental setup is shown in Figure 5.1

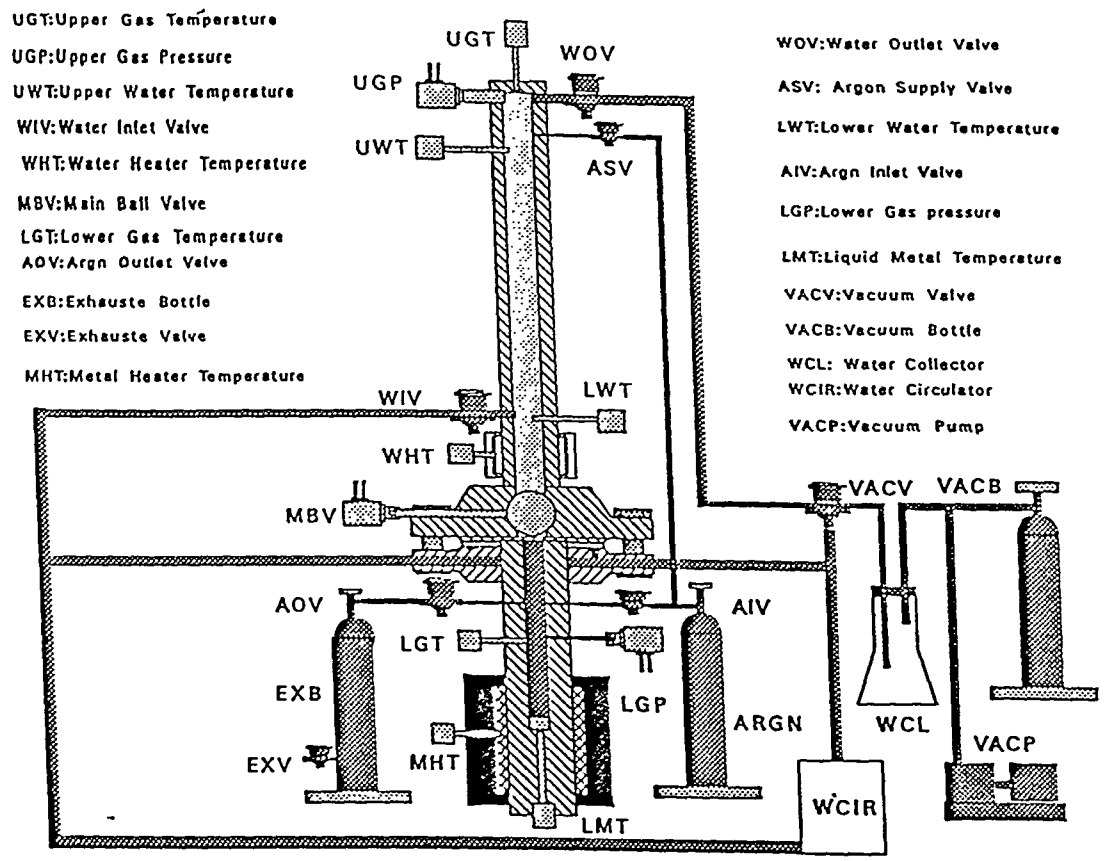


Figure.5.1 Modification of experimental Set-Up

The experimental apparatus is essentially a closed steel cylinder. To facilitate the loading of the reactants, the apparatus consists of two separable components; the upper portion of the apparatus with a pneumatic ball valve and the lower portion of the apparatus.

The upper portion of the apparatus that is placed on top of the ball valve contains 1385 cm^3 water. The upper portion of the apparatus also contains a convection coil connected to the water circulation system for use in controlling the water temperature while the experiment is being run.

The modification in this part included the disconnection of flow of water through the convection coil. The distilled water from the circulator was directly introduced into the upper chamber. The circulation was kept in the upper portion until the beginning of the countdown phase.

There was a furnace on the upper portion that helped to maintain the water temperature in the upper portion. But the position of the furnace is too high to heat the water at the bottom of upper chamber. This heater was replaced by a small flexible heater. The heater was wound near the ball valve to help keep the water temperature at the bottom of upper chamber. Two thermocouples were placed near the ball valve to measure the lower water and the heater temperatures. We added a vacuum system to the experimental setup. It included a vacuum pump, a vacuum reservoir bottle and a water collector. This system was used to provide induced boiling, thus removing all dissolved gases from the water.

Before the heating phase of the experiment, the lower portion was to be purged by the argon supply system. We added a argon balance line to the top of upper portion using the argon supply system to balance the pressures of upper and lower chambers after induced boiling.

The upper water and the lithium-lead temperatures are monitored and controlled by the PC based data acquisition and control system. When these temperatures attain their

predetermined values, the test is started by the system automatically. From this moment all the temperatures, pressures and time are recorded by this system until the end of the equilibrium phase of the test.

The modification in this part included using the interactive mode in the control program to help us choose the starting point of countdown phase. Before countdown the PC-DAS system will ask:"Do you want to continue?" If not, you can go back to change preset values or stop the test.

C Experimental Procedures

We developed an uncomplicated and consistent procedure to perform the experiment that is repeatable for all tests. A set of ordered steps was developed. The impetus behind these is our desire for safety and to eliminate as many extraneous variables as possible. The experiments are run in pairs, one with lithium-lead, and a control test using pure lead. Both of them are performed under identical conditions using the same procedure. Our intention is to use the liquid metal temperature difference of the lithium-lead test and control tests to calculate hydrogen generation per unit volume. For this reason, the apparatus is loaded and assembled in the same manner for both tests. The liquid metal and upper water temperatures are set and controlled by the PC-based data acquisition and control system for both the lithium and the lead tests. The main experimental variables are the initial liquid metal, time and the area of reaction surface. In this experimental set-up, the area of reaction surface is fixed. The amount of hydrogen generated is, therefore a function of the liquid metal temperature and time. Ultimately, this meant that the tests varied from one to the other only by choosing the different initial liquid metal temperature.

(i) Preparation of the Experiments

The $Li_{17}Pb_{83}$ alloy is supplied by the Fusion Technology Institute, Department of Nuclear Engineering and Engineering Physics, University of Wisconsin at Madison, in a reactor chamber shown in Figure 5.2.

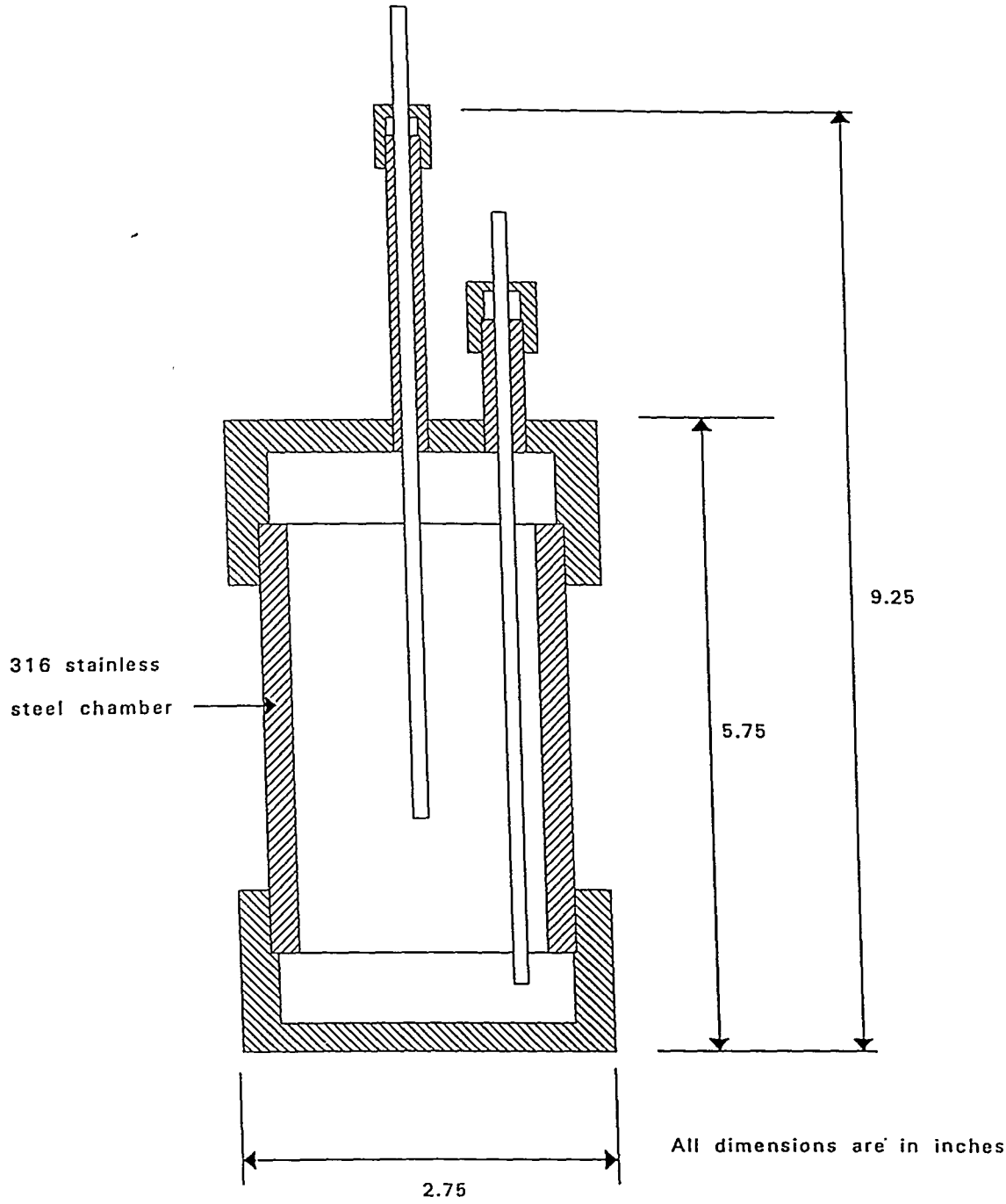


Figure 5.2 Reactor Chamber [11]

The reactor vessels are heated in a glove box under argon atmosphere and cast into small cylindrical test samples (D = 1.0 inch, L = 0.5 inch).

The sample is loaded into the lower portion of the system shown in Figure 5.1. The lithium-lead tests require a much more complicated procedure for loading. Because of the chemically reactive nature of the lithium-lead with many of the atmospheric gases, the lithium-lead had to be removed from its container and placed into the lower portion of the apparatus in a glove box under argon atmosphere.

The top of the lower portion is sealed by plastic film before being removed from the glove box. In the case of the control tests this involved nothing more than dropping a measured amount of lead shot into the lower chamber

Before the lower portion is bolted onto the bottom of the upper portion of the apparatus, we make sure that all the system is at room temperature (25°C). The thermocouples (LGT, LMT), pressure transducer(LGP), argon lines are connected to the inlet and outlet valves (AIV, AOV) at the lower portion of the apparatus.

The system is purged by argon for 5 minutes and the film is removed after the argon flow is initiated (open AIV, AOV, EXV). The main ball valve (MBV) is closed after this.

A vacuum pump (VACP) is used to evacuate the reservoir bottle (VACB) to an absolute pressure of 0.05 bar low enough to enable us perform the two minute induced boiling (P_{sat}=0.1994 bar) at 60°C.

The liquid metal furnace is raised and the lower chamber is enclosed by the lower furnace.

(ii) Procedure for Running the Experiments

When all the preparations are finished, the experiment is started by running a program LIPBTST4 (listed in Appendix A) that reads and controls the liquid metal temperature (LMT), Lower furnace temperature (MHT), upper and lower water temperature (UWT, LWT), Lower and upper gas temperature (LGT, UGT) and water heater temperature

(WHT), upper and lower gas pressure (UGP, LGP). It is also used to record these data at desired time intervals.

The heating phase of the experiment is initiated. This phase consists of simply running the program to turn on the liquid metal heater (LMH), upper water heater (UWH) and open the water inlet and outlet valves (WIV, WOV) to fill the upper portion of the apparatus with distilled water, and to circulate the water to control its temperature. the temperatures are controlled and maintained at their desired values by the PC-DAS. The water circulation system (WCIR) is able to heat the water to its desired temperature before the liquid metal furnace raises the liquid metal temperature to the given value. Since the furnace heater is always operated at 1500 W, the furnace temperature as a function of time is controlled by the PC-DAS identically for all the tests.

When the upper water temperature (UWT) and liquid metal temperature (LMT) are nearing their preset values, the dissolved air in the water is removed by closing water inlet valve (WIV) and opening vacuum valve (VACV) to induce boiling below 0.1994 bar. This is done by controlling vacuum valve to keep upper gas pressure below the saturated pressure corresponding to the water temperature (60°C) and maintaining the boiling for about two minutes. During this procedure, water vapor and liquid water come out from the upper chamber and condense in the water collector (WCL). Since the water temperature, vacuum pressure and induced boiling times are the same for all tests, the water volume in the water collector could approximately be controled to be the same for all the tests. This means that the water volume for all the tests is the same. An argon supply line is connected to the upper (ASV) and lower chamber (AIV) which is used to balance the pressure in the two chambers. Before balancing the pressure, the leakage is checked by pressurizing the system to 6 bar for 5 minutes to find out if there is any pressure decrease. After the leakage test, the argon supply line pressure is adjusted to the desired value by using a pressure regulator.

When liquid metal and upper water temperatures reach the desired value, a 30 second countdown phase is started manually on the PC-DAS. All the valves (WOV, ASV, WIV, AIV, AOV, EXV, VACV) are closed, and the system variables consisting of time (t), liquid metal temperature (LMT), upper gas temperature (UGT), upper water temperature (UWT), lower gas temperature (LWT), upper gas pressure (UGP), lower gas pressure (LGP), lower gas temperature (LGT), lower furnace temperature (LFT) are recorded. Since the system then becomes closed, the water and covering argon gas reach an equilibrium. The initial temperatures and pressures are measured to evaluate the mass of argon in the upper and lower chambers during this phase. At the end of the countdown phase, the initial water and liquid metal temperatures are still at desired values; the mass of argon, water and liquid metal are fixed; and the system pressure is known. The main ball valve (MBV) is ready to be opened for the initiation of the interaction.

When the main ball valve is opened, the reaction phase begins, without interference for a preset period of time (usually 4 minutes). After that, the main ball valve is closed and the argon outlet and exhaust valve (AOV, EXV) are opened two seconds after main ball valve is closed.

The upper chamber comes into equilibrium within 3.5 minutes after the ball valve is closed. During this period the lower chamber temperature increases a little. After this period the furnace heaters (UWH, LMH) are turned off.
After the last phase, the PC-DAS transfers all the data into three data files. They are COUNTD.DAT which contains the data for countdown period, REACTION.DAT which contains data for reaction period and EQUIL.DAT which contains data for equilibrium period.

When the system returns to room temperature, we measure the water volume trapped in vacuum line and in the water collection vessel which came out from the system when vacuum was produced during induced boiling.

The last step in the experimental procedure is to prepare the apparatus for the next test. The only noteworthy part of this process is the removal of the lower portion of the apparatus. Because the liquid metal is frozen into the lower chamber, it has to be drilled out.

VI. Results of The Experiments

A. Descriptions of The Raw Data

A graphical library of the data for 16 lithium-lead tests and 5 control tests is given in Appendix B. This collection of graphs shows the data from the pressure transducers and thermocouples during the interaction for each experiments.

We shall discuss the experimental results of lithium-lead test number L09 and lead test number N36 in detail. The discussion to be made on these selected experiments are typical of all the other fifteen lithium-lead and five pure lead experiments. These two tests were characterized by an initial water temperature of 60° C and an initial liquid metal temperature of 400° C. The system pressures of the two tests as functions of time are shown in Figure 6.1. Right after the main ball valve is opened, and the interaction is initiated, the system pressure rises continuously to a maximum value in about 50 sec. and then the pressure drops to an equilibrium value in about 190 seconds. The maximum pressure depends upon the initial conditions

The thermocouples' data from test L09 and N36 are plotted in Figures 6.2 and 6.3. In Figures 6.2, the lower gas temperature (LGT) is much higher then the lower water temperature (LWT) before the reaction phase. Right after the main ball value is opened, the lower water temperatures drops nearly to the lower water temperature. Then the lower gas temperature immediately rises to the saturation temperature (120^0C, system pressure of 2 bar). The lower water temperature rises a little slower than the lower gas temperature. The upper gas and water temperature (UGT, UWT) basically maintain at 60^0C during reaction phase.

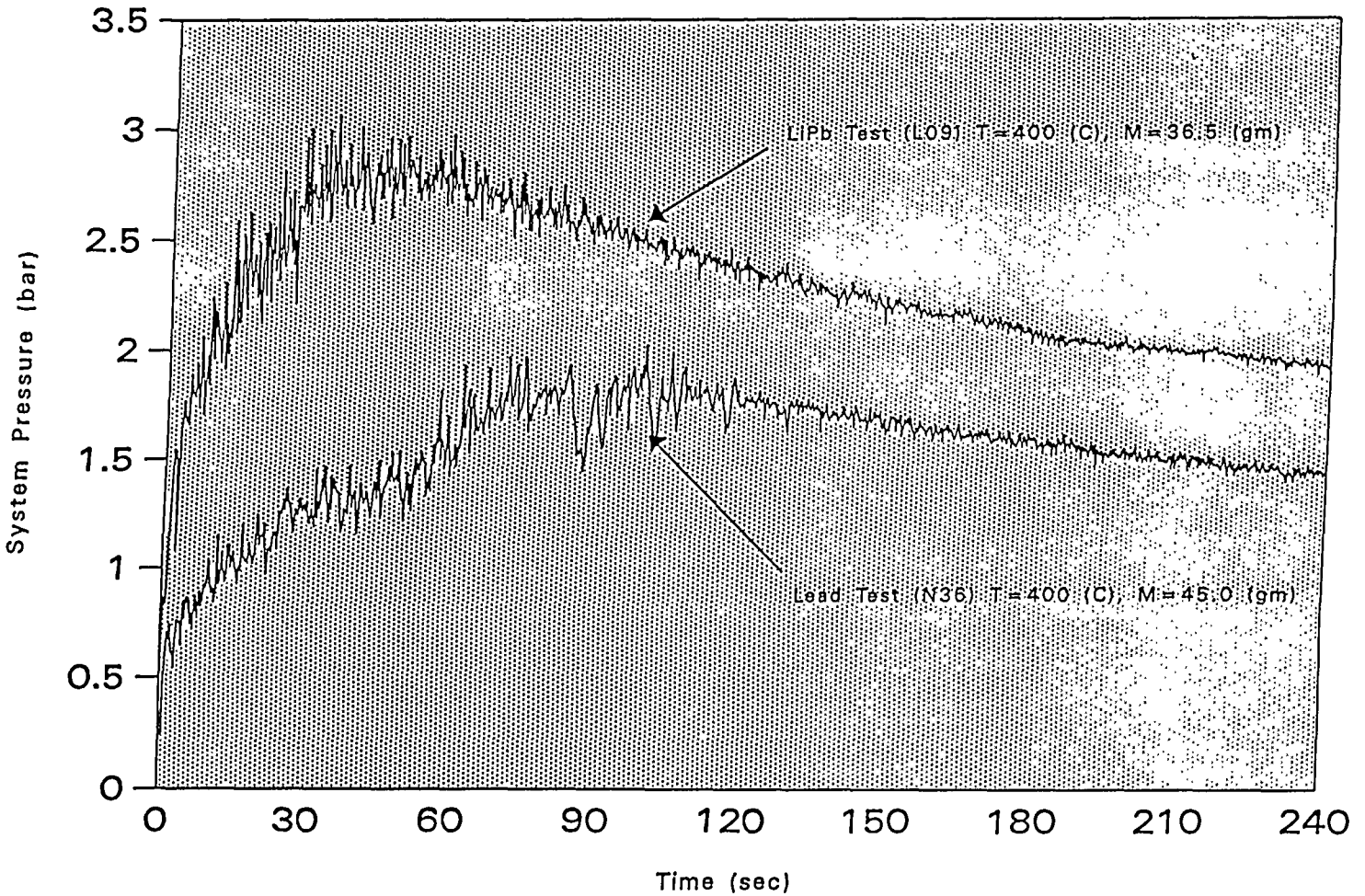


Figure 6.1 System Pressure as a Function of Time (L09 & N36)

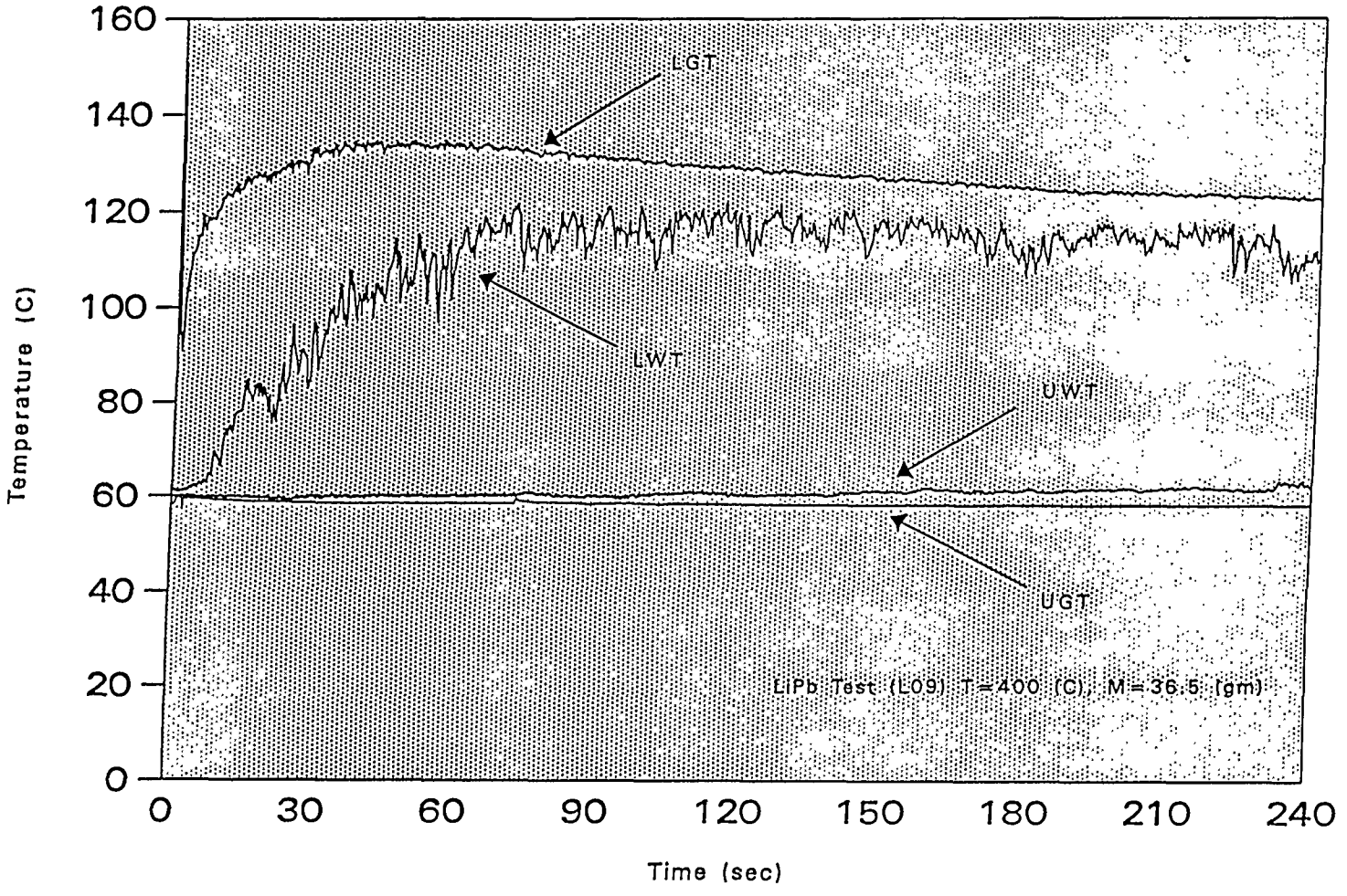


Figure 6.2 Gas and Water Temperature as a Function of Time (L09)

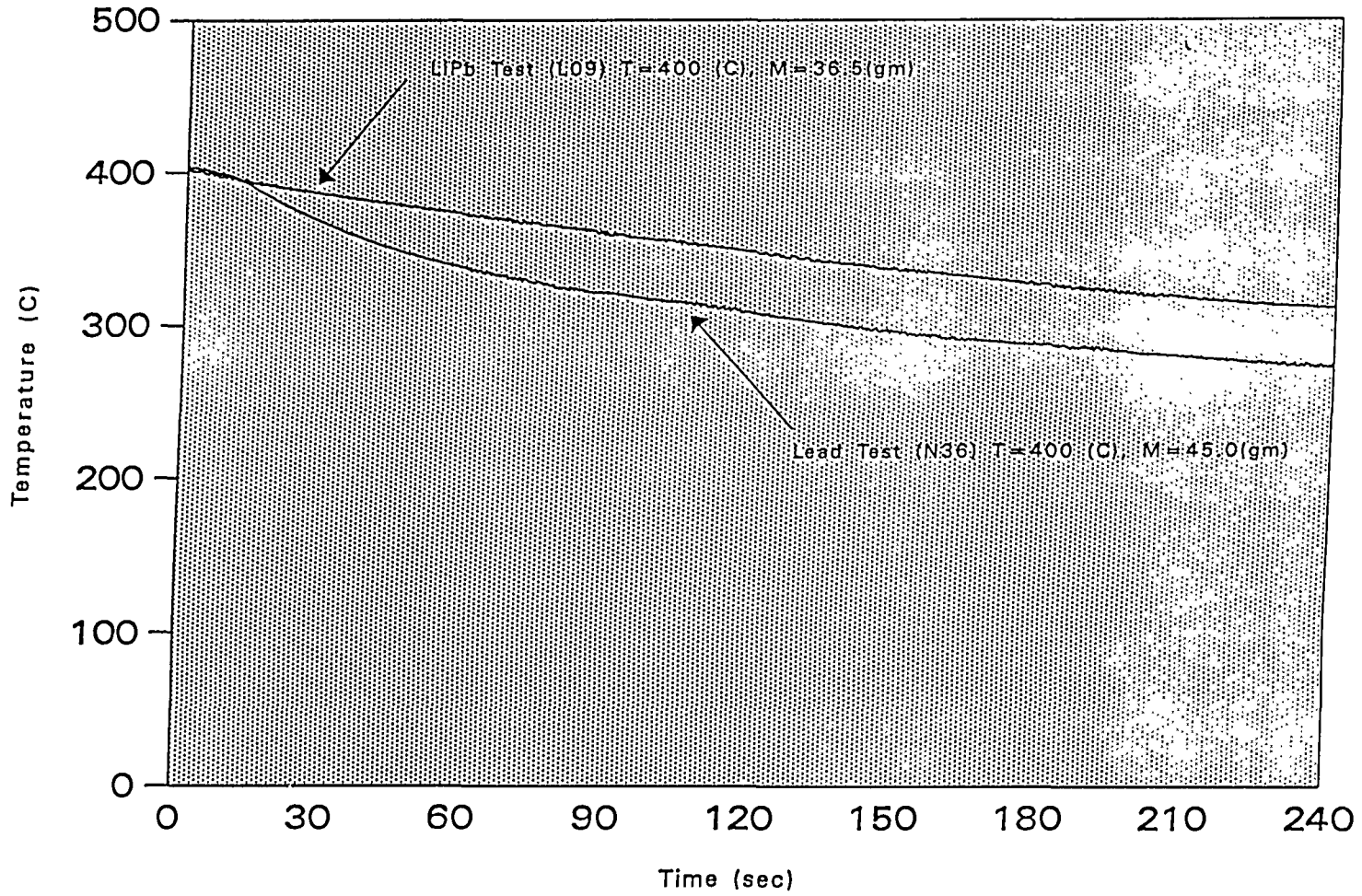


Figure 6.3 Liquid Metal Temperature as a Function of Time (L09 & N36)

All these phenomena are interpreted below. After the main ball valve is opened, the water comes to the lower chamber that causes the lower gas temperature drops to the lower water temperature. Then the water pours onto the liquid metal surface, the water begins to boil rapidly and a large burst of water vapor is formed that causes the system pressure (UGP, LGP), and the lower gas temperature to rise rapidly. At the same time, the higher temperature and pressure gas from the lower portion of the apparatus bubbles through the water column and rises to the top of the apparatus. The upper gas pressure is read by the transducer and the upper gas temperature read by thermocouple which are located on the top of the apparatus. Since the lower water temperature rises continuously and the upper gas and water temperatures basically remain at 60°C, we believe that the burst of vapor is cooled by the water and condensed after it bubbles through the water.

The graphs in Figure 6.3 show the responses of the liquid metal temperatures (LMT). They show that the liquid metal temperature of the lead test falls faster than lithium-lead test at the beginning, and become almost parallel after 60 sec. The liquid metal temperature differences between the two tests remain constant until the main ball valve is closed.

Before we discuss the calculation of the hydrogen mass, we compare the data graphs of lithium-lead test L09 shown in Figures 6.1, 6.2 and 6.3 to the data graphs from the corresponding lead test N36 shown in Figure 6.1 and 6.3, which were performed under the same initial conditions (60 °C water and 400 °C liquid metal temperature). Comparing the liquid metal temperature of the two tests shown in Figure 6.3, we notice that the liquid metal temperature of the lithium-lead test is consistently greater than the liquid metal temperature of the lead test. The gas and water temperature response are nearly the same for both tests. liquid metal temperature difference between the two tests is due to the heat generated during lithium-lead/water reaction . The temperature difference between the two tests depends upon the initial liquid metal temperature. At high initial liquid metal temperatures (650 °C) the difference is about 50°C. At low initial liquid metal temperatures (350 °C) the difference is about 30°C.

In Figure 6.1 and 6.2, we notice that the system pressure drops along with lower gas temperate from a maximum value to an equilibrium value after 50 seconds and the lower water temperature rises from 60°C to saturation temperature at the same time. We believe that the system pressure drop is due to the lower gas temperature drop. The thermal capacity of the lower portion is fixed by the initial liquid metal temperature. For low initial liquid metal temperature (350°C-500°C) experiments, after 50 seconds, the heat transferred from lower chamber to lower gas is less than the heat absorbed by water from lower gas.

B. Data Analysis

During the experiments, water is poured onto the exposed surface of a small lithium-lead pool. Since the experiments are small scale (e.g. the contact area is small), the result should provide the hydrogen generation rate per unit area. From the result of the experiment, we find that the system pressure, gas and water temperatures are functions of time. We need to find the partial pressure of hydrogen and the amount of hydrogen dissolved in the water. Then we can determine the rate of hydrogen generation as function of time during the lithium-lead/water reaction. We also need to determine the Arrhenius reaction rate constants in the equation (1) from the hydrogen generation curve.

$$D_{ii} = D_o \exp(-\frac{dE}{RT}) \qquad (1)$$

(i) Description of Analysis Method

The reaction equations for the lithium-lead and the lead/water interactions are given by.

$$Li + H_2O \rightarrow LiOH + \frac{1}{2}H_2 + 2.0*10^5 \text{ J/Mole Li} \qquad (2)$$

$$Lead + H_2O \rightarrow Lead + H_2O \qquad (3)$$

Two analysis method can be employed. These are: (1) Thermodynamics Method and (2) Heat Transfer Method. They are used to evaluate hydrogen generation rate during the reaction time by analyzing the raw pressure and temperature data from the experiments.

1. Thermodynamics Method

In the reaction phase, the moles of hydrogen generated can be expressed by using the ideal gas law. The schematic of this method is shown in Figure 6.4.

$$N_{H_2} = \frac{P_{H_2} V_{gas}}{R T_{gas}} + N_{H_2 sol} \qquad (4)$$

where

N_{H_2} is the total moles of hydrogen generated during the reaction phase,

P_{H_2} is the partial pressure (bar) of hydrogen during the reaction phase,

T_{gas} is the upper gas temperature (UGT) measured by thermocouple during the test,

R is molar gas constant (83.14395 bar cm^3/mole K),

$N_{H_2 sol}$ is the moles of hydrogen dissolved in the water during the reaction phase,

V_{gas} is the volume (cm^3) occupied by gases in the system during the reaction phase. It can be calculated using

$$V_{gas} = V_{tot} - V_{met} - V_{wat} \qquad (5)$$

where

V_{tot} is the total volume of the system (1523 cm^3) which is the sum of the volume in upper chamber (1385 cm^3) and lower chamber (138 cm^3) and

V_{wat} is the water volume in the system (1330 cm^3).

Before we initiate induced boiling, the upper chamber is completely filled with water (1385 cm^3). After induced boiling, the water volume in the collection vessel and vacuum line is measured to be 55 cm^3. In equation (5),

V_{met} is the liquid metal volume calculated using

$$V_{met} = \frac{M_{Li_{17}Pb_{83}}}{\rho_{Li_{17}Pb_{83}}} \qquad (6)$$

where

$\rho_{Li_{17}Pb_{83}}$ is the density of liquid metal (9.65 gm/cm^3) and

$M_{Li_{17}Pb_{83}}$ is the mass (gm) of the metal measured before the test.

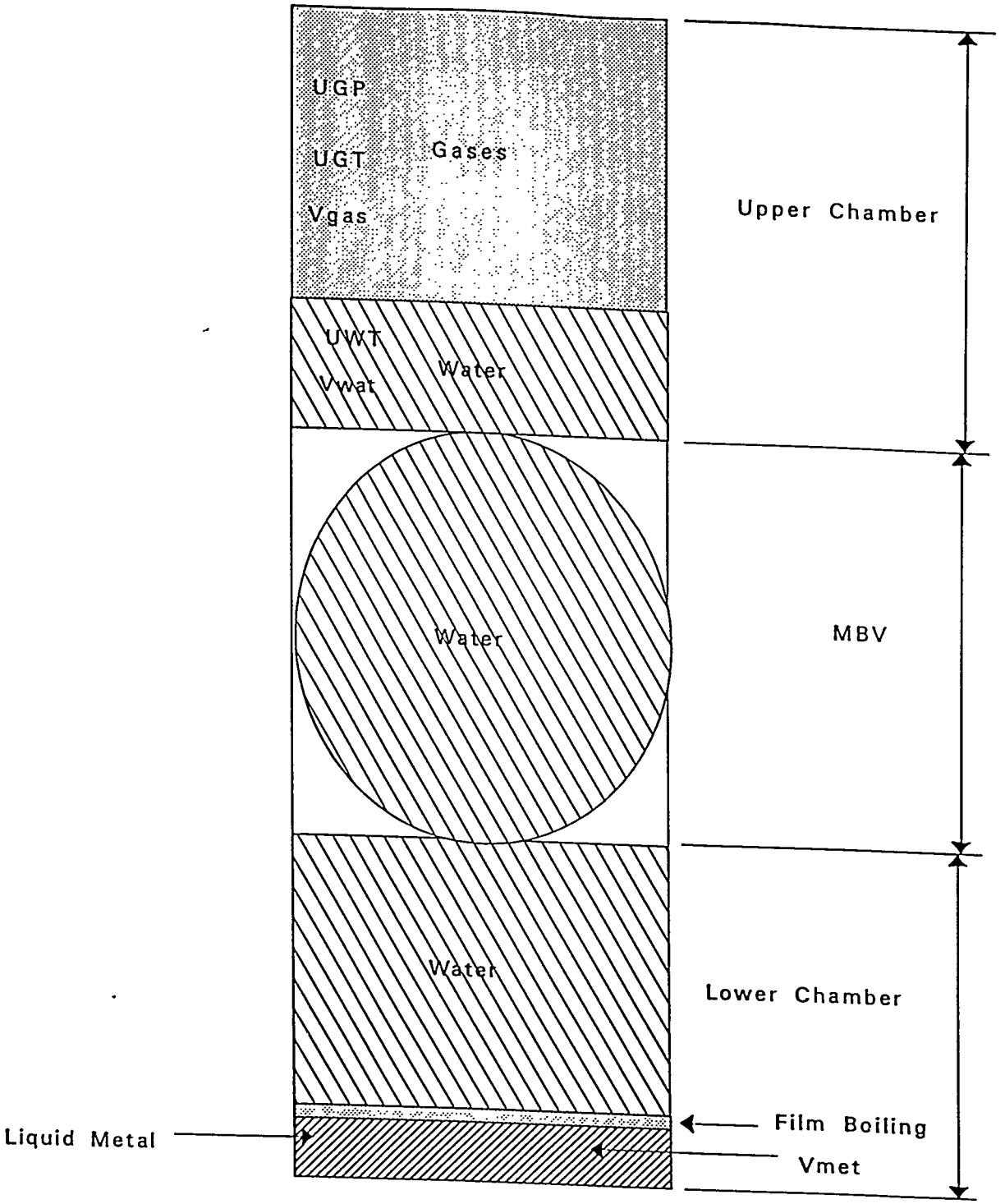


Figure 6.4 The Schematic of The Thermodynamics Method

In equation (4), the partial pressure of hydrogen P_{H_2} can be obtained from the measured system pressure P_{sys} which is composed of the partial pressures.

$$P_{sys} = P_{H_2} + P_{ar} + P_{H_2O} \quad (7)$$

Thus P_{H_2} is calculated using

$$P_{H_2} = P_{sys} - P_{ar} - P_{H_2O} \quad (8)$$

where

P_{sys} is the system pressure (UGP) measured during the test,

P_{H_2O} is the partial pressure of water vapor which is equal to the saturation pressure of water at the measured gas layer temperature (UGT) during the reaction phase and

P_{ar} is the partial pressure of argon which is calculated using the idea gas law.

$$P_{ar} = (N_{ar} - N_{arsol})\frac{RT_{gas}}{V_{gas}} \quad (9)$$

where V_{gas}, T_{gas} and R are as previously defined,

N_{arsol} is the moles of argon dissolved in the water during the reaction phase and

N_{ar} is the total moles of argon in the system.

The total moles of argon N_{ar} can be calculated from the system initial conditions. In the countdown phase, argon would fill the free volume above the liquid metal in the lower chamber and it would occupy the region above the water along with water vapor and a small amount would be dissolved in the water in the upper chamber. Using the ideal gas law, the moles of argon can mathematically be expressed as:

$$N_{ar} = N_{arup} + N_{ardn} \quad (10)$$

where

N_{arup} is the moles of argon in the upper chamber during the countdown phase,

N_{ardn} is the moles of argon in the lower chamber calculated using

$$N_{ardn} = \frac{P_{ardn}V_{gasdn}}{RT_{gasdn}} \quad (11)$$

where R is as previously defined,

T_{gasdn} is the lower gas temperature (LGT) measured during the countdown phase

V_{gasdn} is the gas volume in lower chamber calculated using

$$V_{gasdn} = V_{totdn} - V_{met} \tag{12}$$

where V_{met} is as previously defined,

V_{totdn} is the measured total volume of lower chamber (138 cm^3).

In equation (11),

P_{ardn} is the partial pressure of argon in the lower chamber measured during the countdown phase. Because argon is the only gas in the lower chamber during the countdown phase, the partial pressure of argon equals the measured lower region system pressure P_{sysdn} (LGP).

$$P_{ardn} = P_{sysdn} \tag{13}$$

We substitute equations (13) and (12) into equation (11) to get the moles of argon N_{ardn} in the lower chamber during the countdown phase.

In equation (10),

N_{arup} is the moles of argon in the upper chamber, it can be calculated using

$$N_{arup} = \frac{P_{arup} V_{gasup}}{R T_{gasup}} + N_{arsolup} \tag{14}$$

where R is as previously defined,

$N_{arsolup}$ - is the moles of argon dissolved in the water during the countdown phase,

T_{gasup} is the upper gas temperature (UGT) measured during the countdown phase,

V_{gasup} is the gas volume in the upper chamber during the countdown phase. It is the water volume (55 cm^3) which came out of the upper chamber during the induced boiling.

P_{arup} is the partial pressure of argon in the upper chamber. During the countdown phase, we have argon and water vapor in the upper chamber. The partial

pressure of argon can be obtained from the measured upper region system pressure P_{sysup} which is composed of the partial pressures.

$$P_{arup} = P_{sysup} - P_{H_2Oup} \tag{15}$$

where

P_{sysup} is the upper region system pressure (UGP) measured during the countdown phase and

P_{H_2Oup} is the partial pressure of water vapor which equals the saturation pressure of water at the measured gas layer temperature (UGT) during the countdown phase.

In equation (14), the moles of argon dissolved in the water $N_{arsolup}$ can be evaluated using the following equation,

$$N_{arsolup} = X_{arup} N_{H_2O} \tag{16}$$

where

N_{H_2O} is the moles of water in the system calculated using

$$N_{H_2O} = \frac{\rho_{H_2O} * V_{wat}}{m.wt_{H_2O}} \tag{17}$$

where

ρ_{H_2O} is the density of water and

$m.wt_{H_2O}$ is molecular weight of water.

In equation (16),

X_{arup} is the solubility of argon which is a function of the water temperature and the partial pressure of argon in upper chamber during the countdown phase. By Henry's law, the solubility of gas is directly proportional to the partial pressure of that gas [9]. Since at saturation temperature the solubility of a gas in a liquid equals 0, and since we know the solubility of argon in water at 25 °C and 1 atm only, then the solubility of argon in water can be expressed as:

$$X_{arup} = X_{ar}(25^\circ C, 1atm)\frac{(T_{satup} - T_{watup})}{(T_{satup} - 25^\circ C)}\frac{P_{arup}}{P_{atm}} \tag{18}$$

where P_{arup} is as previously defined in equation (15)

$X_{ar}(25^{o}C,1atm)$ is a constant ($3.7*10^{-7}$ $Mole_{ar}/Mole_{wat}$)

P_{atm} is the atmosphere pressure (1.013 bar),

T_{watup} is the water temperature measured during the countdown phase and

T_{satup} is the water saturation temperature evaluated at the measured upper region system pressure P_{sysup} during countdown phase.

$$T_{satup} = 373.998*(P_{sysup})^{0.07144015} - 273.15$$

where P_{sysup} is as previously defined. We substitute these back into equation (18), equation (17) and equation (16) step by step to get $N_{arsolup}$, then this and equation (15) can be substituted back into equation (14) to get the moles of argon N_{arup} in the upper chamber during countdown phase. By now, the moles of argon in upper chamber N_{arup} and lower chamber N_{ardn} are known. The total moles of argon N_{ar} is calculated using equation (10). With the initial moles of argon N_{ar} in the system known, the partial pressure of argon in the reaction phase can be calculated using equation (9). The only unknown in equation (9) is the moles of argon dissolved in the water N_{arsol} during reaction phase. It can be evaluated using the following equation

$$N_{arsol} = X_{ar} N_{H_2O} \qquad (19)$$

where N_{H_2O} is previously defined and

X_{ar} is the solubility of argon which is a function of the water temperature and the partial pressure of argon in all the system during the reaction phase. The solubility of argon in water can be expressed as:

$$X_{ar} = X_{ar}(25^{o}C,1atm)\frac{(T_{sat} - T_{wat})}{(T_{sat} - 25^{o}C)}\frac{P_{ar}}{P_{atm}} \qquad (20)$$

where $X_{ar}(25^{o}C,1atm)$ and P_{atm} is as previously defined,

T_{wat} is the water temperature measured during the reaction phase and

T_{sat} is the water saturation temperature evaluated at the measured system pressure P_{sys} during the reaction phase.

$$T_{sat} = 373.998*(P_{sys})^{0.07144015} - 273.15 \qquad (21)$$

We substitute them back into equation (20) and (19).

$$N_{arsol} = X_{ar}(25^{\circ}C, 1atm)\frac{(T_{sat} - T_{wat})}{(T_{sat} - 25^{\circ}C)}\frac{P_{ar}}{P_{atm}}N_{H_2O} \qquad (22)$$

The dissolved moles of argon becomes a function of the partial pressure of argon. This can be substituted into equation (9) to obtain the partial pressure of argon directly, because we only need to know the partial pressure of argon P_{ar}.

$$P_{ar} = \frac{N_{ar}\frac{RT_{gas}}{V_{gas}}}{1 + X_{ar}(25^{\circ}C, 1atm)\frac{(T_{sat} - T_{wat})}{(T_{sat} - 25^{\circ}C)}\frac{1}{P_{atm}}N_{H_2O}\frac{RT_{gas}}{V_{gas}}} \qquad (23)$$

After the partial pressure of argon P_{ar} is known, the partial pressure of hydrogen P_{H_2} is calculated using equation (8). With the partial pressure of hydrogen P_{H_2} known, the only unknown in equation (4) is the moles of hydrogen dissolved in the water N_{H_2sol} during the reaction phase. It can be evaluated using the following equation

$$N_{H_2sol} = X_{H_2}N_{H_2O} \qquad (24)$$

where N_{H_2O} is as previously defined and

X_{H_2} is the solubility of hydrogen which is a function of the water temperature and the partial pressure of hydrogen in all the system during reaction phase. The solubility of hydrogen in water can be expressed as:

$$X_{H_2} = X_{H_2}(25^{\circ}C, 1atm)\frac{(T_{sat} - T_{wat})}{(T_{sat} - 25^{\circ}C)}\frac{P_{H_2}}{P_{atm}} \qquad (25)$$

where P_{H_2}, P_{atm}, T_{wat} and T_{sat} are as previously defined and

$X_{H_2}(25^{\circ}C, 1atm)$ is a constant ($1.7*10^{-7}$).

We substitute P_{H_2}, P_{atm}, T_{wat} T_{sat} and $X_{H_2}(25^{\circ}C, 1atm)$ back into equation (25) and X_{H_2} N_{H_2O} into equation (24), then the dissolved moles of hydrogen N_{H_2sol} is known. By now, all the variables in equation (4): $P_{H_2}(t)$, $N_{H_2sol}(t)$, $T_{gas}(t)$ are known as function of time.

These can be substituted into equation (4) to obtain the hydrogen generation as function of time.

$$N_{H_2}(t) = \frac{P_{H_2}(t)V_{gas}}{RT_{gas}(t)} + N_{H_2sol}(t) \qquad (26)$$

The hydrogen generation rate as a function of time is calculated using

$$\frac{dN_{H_2}(t)}{dt} = \frac{N_{H_2}(t_2) - N_{H_2}(t_1)}{t_2 - t_1} \qquad (27)$$

where

$N_{H_2}(t_1)$ is the moles of hydrogen generation calculated at t_1 and

$N_{H_2}(t_2)$ is the moles of hydrogen generation calculated at t_2.

Finally the results of the hydrogen generation rate is divided by the area of the liquid metal surface to get the reaction rate per unit area.

All the variables are involved in the thermodynamics method of analysis, except the liquid metal temperature T_{LMT}.

2. Results of Thermodynamics Method of Analysis

We have developed a FORTRAN program named COMPUTE1 that is based on the equations (2) to (27) in the last section. The program listed in Appendix C, was used to analyze the raw data. We used the same program to calculate hydrogen generation for lithium-lead test and lead test. From equation (3), we know that there is no hydrogen generated in lead test. We used the hydrogen generation calaulated from lead test to calibrate the hydrogen generation calulated from lithium-lead test. This calibration is done using the hydrogen generation of lithium-lead test minus hydrogen generation caculated from lead test. A graphical library of the calibrated hydrogen generation computed by the program for 14 lithium-lead tests is given in Appendix D. This collection of graphs shows the moles of hydrogen generation for each tests. We shall discuss the experimental results of lithium-lead test number L14 in detail. The discussion to be made on this selected experiment is typical of all the other thirteen lithium-lead experiments. This test was characterized by an initial water temperature of 60° C and an initial liquid metal

temperature of 600° C. · The hydrogen generation of this test as a function of time is shown in Figure 6.5. Right after the main ball valve is opened, and the interaction is initiated, the hydrogen generation rises continuously to a maximum value in about 90 sec. and then the moles of hydrogen drops to an equilibrium value in about 150 sec. The maximum value of hydrogen generation depends upon the initial conditions exhibiting the same type of behavior as the system pressure shown in Figure 6.6. The calibrated hydrogen generation for each of the lithium-lead tests are summarized in Table 6.1

Table 6.1 Calibrated Hydrogen Generation for The Lithium-Lead Tests

Expt#	Type	T_{LiPb} (°C)	Mass (g)	$N_{H_2 Max}$ (Mole)
L01	Lithium-Lead Test	400	37.5	0.005994
L04	Lithium-Lead Test	350	46.5	0.008303
L05	Lithium-Lead Test	350	51.0	0.002034
L06	Lithium-Lead Test	350	56.0	0.007454
L07	Lithium-Lead Test	400	40.0	0.007384
L08	Lithium-Lead Test	500	53.5	0.008503
L09	Lithium-Lead Test	400	36.5	0.008248
L11	Lithium-Lead Test	600	44.0	0.008050
L12	Lithium-Lead Test	600	38.0	0.010726
L14	Lithium-Lead Test	600	49.0	0.012556
L15	Lithium-Lead Test	350	35.0	0.006410
L20	Lithium-Lead Test	650	41.0	0.005870
L21	Lithium-Lead Test	600	41.0	0.008760
L22	Lithium-Lead Test	600	35.0	0.011100
L23	Lithium-Lead Test	500	41.0	0.004820

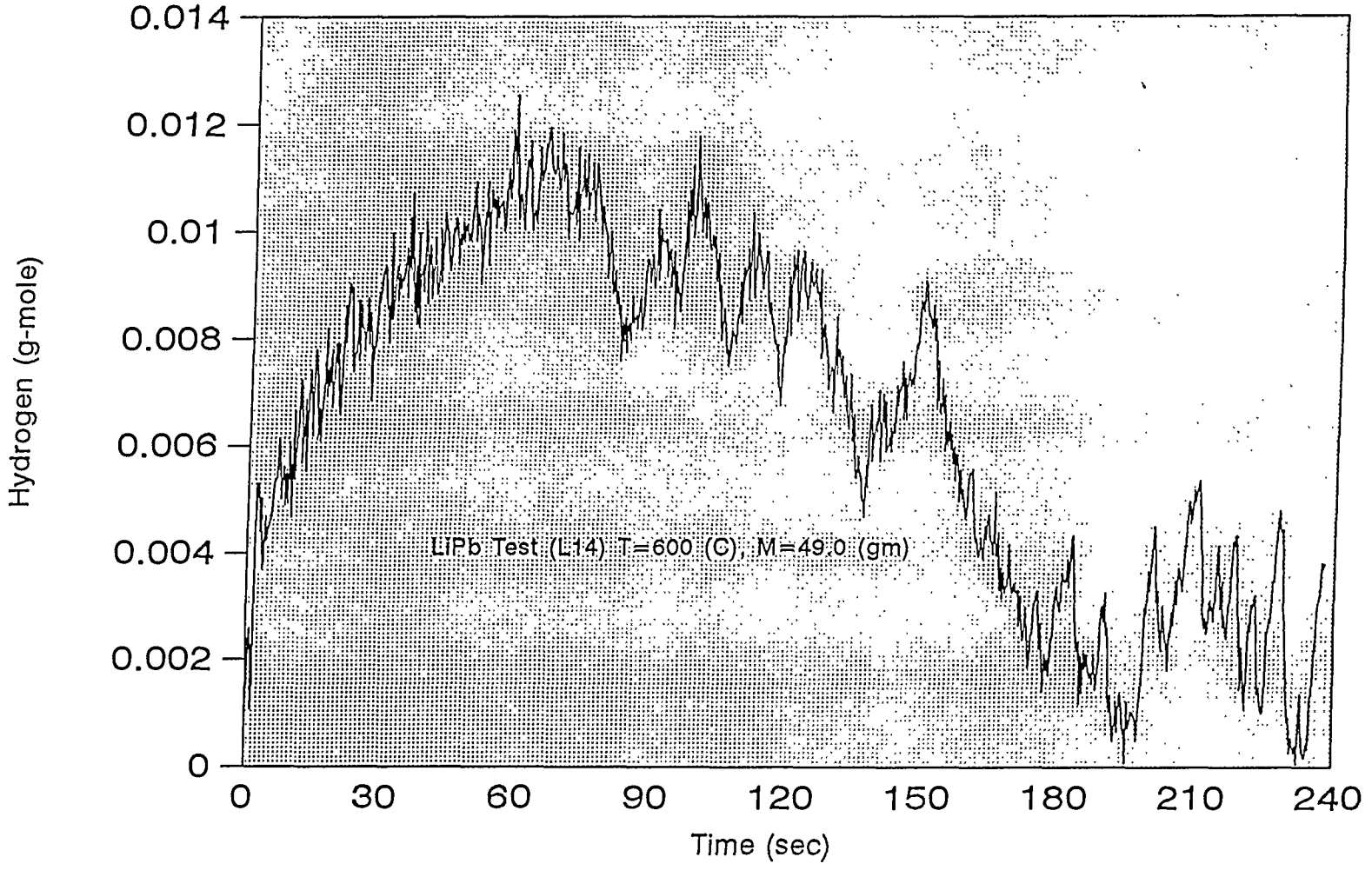


Figure 6.5 Corrected Hydrogen Generation as a Function of Time (L14)

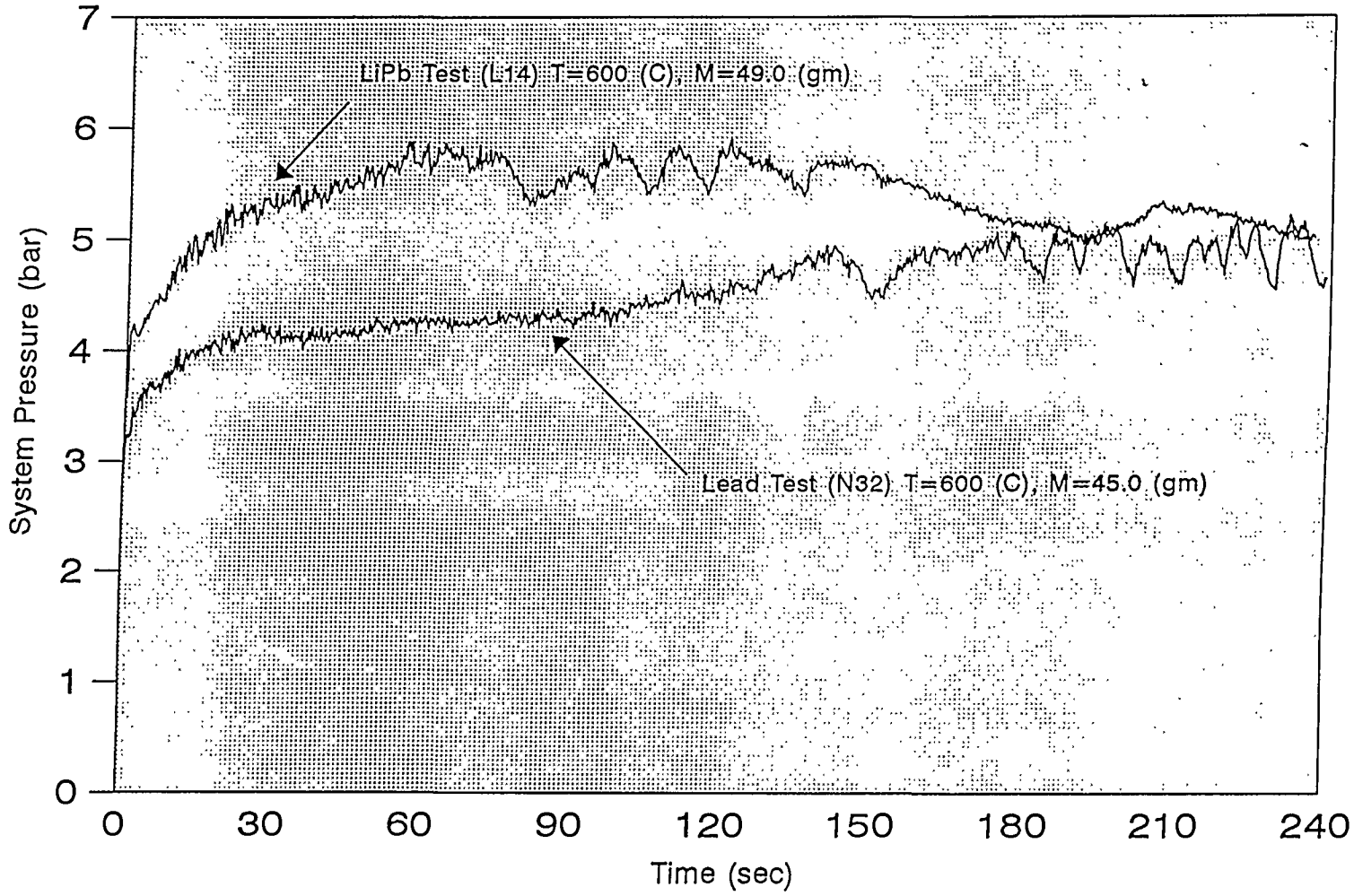


Figure 6.6 System Pressure as a Function of Time (L14 & N32)

3. Heat Transfer Method

From the reaction equation (2) and (3)

$$Li + H_2O \rightarrow LiOH + \frac{1}{2}H_2 + 2.0*10^5 \text{ J/Mole Li} \qquad (2)$$

$$Lead + H_2O \rightarrow Lead + H_2O \qquad (3)$$

it is seen that the hydrogen generation was accompanied by heat. Since the heat generation is proportional to moles of hydrogen generated, the relation between hydrogen generation and heat generation is represented as

$$N_{H_2} = C*Q \qquad (28)$$

where

$$C = 2.5*10^{-6} \quad \text{Mole /J} \qquad \text{at } 680°C \qquad (29)$$

The hydrogen generation rate is then given by

$$\frac{dN_{H_2}(t)}{dt} = C\frac{dQ(t)}{dt} \qquad (30)$$

We use a cylindrical control volume as Figure 6.7 to derive the necessary equations for this method. In the control volume, we can assume that the heat transfer is about Z axis symmetric. On the Z axis, the heat transfer occurs only along the Z direction. We can, therefore simplify the three dimension problem into one dimension problem. The energy equation in one dimension (Z) is given by

$$\frac{1}{\alpha}\frac{dT(Z,t)}{dt} = \frac{1}{k}\frac{dq}{dt} + \frac{d^2T(Z,t)}{dZ^2} \qquad (31)$$

where

k	is the thermal conductivity of $Li_{17}Pb_{83}$,
α	is the thermal diffusivity of $Li_{17}Pb_{83}$,
$T(Z,t)$	is the liquid metal temperature as a function of Z and time.
t	is time.
$\frac{dq}{dt}$	is unit volume heat generation.

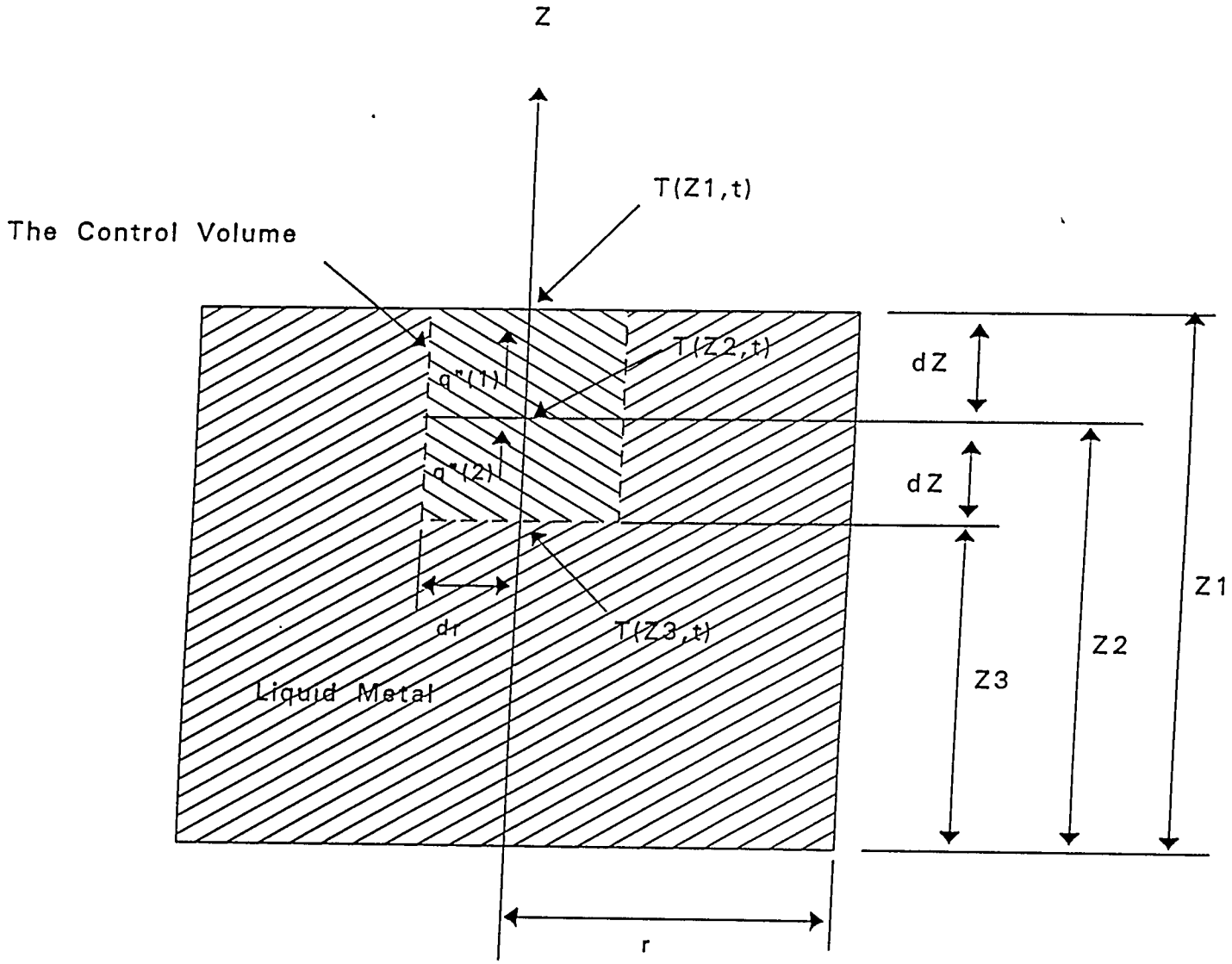


Figure 6.7 Heat Transfer Model

In equation (30)

$$\frac{dQ}{dt} = \frac{dq}{dt} V_{react} \tag{32}$$

where V_{react} is the reacted metal volume.

For Lithium-Lead test, we denote the variables by using the subscript L as show below

$$\frac{1}{\alpha}\frac{dT_L(Z,t)}{dt} = \frac{1}{k}\frac{dq}{dt} + \frac{d^2T_L(Z,t)}{dZ^2} \tag{33}$$

For Lead test, we denote the variables by using the subscript P as show below

$$\frac{1}{\alpha}\frac{dT_P}{dt} = 0 + \frac{d^2T_P}{dZ^2} \tag{34}$$

From the result of the experiment, we postulate that the liquid metal temperature difference between the lithium-lead and control test is due to the lithium-lead/water reaction. We subtract equation (34) from equation (33), and solve the resultant equation for dq/dt to get:

$$\frac{dq}{dt} = k[\frac{1}{\alpha}(\frac{dT_L}{dt} - \frac{dT_P}{dt}) - (\frac{d^2T_L}{dZ^2} - \frac{d^2T_P}{dZ^2})] \tag{35}$$

The first term in the bracket of equation (35) can be written in the form

$$\frac{1}{\alpha}(\frac{dT_L}{dt} - \frac{dT_P}{dt}) = \frac{1}{\alpha}\frac{d(T_L - T_P)}{dt} = \frac{1}{\alpha}\frac{dT_L - dT_P}{dt}$$

$$= \frac{1}{\alpha}\frac{[T_L(Z_2,t_2) - T_L(Z_2,t_1)] - [T_P(Z_2,t_2) - T_P(Z_2,t_1)]}{t_2 - t_1}$$

$$= \frac{1}{\alpha}\frac{[T_L(Z_2,t_2) - T_P(Z_2,t_2)] - [T_L(Z_2,t_1) - T_P(Z_2,t_1)]}{t_2 - t_1} \tag{36}$$

In the control volume shown in Figure 6.7, the liquid metal is uniform and the thermal conductivity of the liquid metal k is much higher than the thermal conductivity in the gas. We can assume that the temperature at the time t_1 along the Z axis has linear distribution. The temperature differences ΔT_L and ΔT_p along the Z axis are constant for lithium-lead test and lead test.

$$\Delta T_L = T_L(Z_3,t_1) - T_L(Z_2,t_1) = T_L(Z_2,t_1) - T_L(Z_1,t_1) \tag{37}$$

$$\Delta T_p = T_P(Z_3,t_1) - T_P(Z_2,t_1) = T_P(Z_2,t_1) - T_P(Z_1,t_1) \tag{38}$$

The heat flux in Z direction is calculated using equation

$$q''(Z,t) = -k\frac{dT(Z,t)}{dZ} \tag{39}$$

We substitute equation (37) and (38) into equation (39)

$$q_L''(2) = -k\frac{T_L(Z_3,t_1) - T_L(Z_2,t_1)}{\Delta Z} = -k\frac{\Delta T_L}{\Delta Z} \tag{40}$$

$$q_L''(1) = -k\frac{T_L(Z_2,t_1) - T_L(Z_1,t_1)}{\Delta Z} = -k\frac{\Delta T_L}{\Delta Z} \tag{41}$$

$$q_P''(2) = -k\frac{T_P(Z_3,t_1) - T_P(Z_2,t_1)}{\Delta Z} = -k\frac{\Delta T_P}{\Delta Z} \tag{42}$$

$$q_P''(1) = -k\frac{T_P(Z_2,t_1) - T_P(Z_1,t_1)}{\Delta Z} = -k\frac{\Delta T_P}{\Delta Z} \tag{43}$$

The heat flux is also a constant for identical test.

$$q_L''(2) = q_L''(1) \text{ and } q_P''(2) = q_P''(1) \tag{44}$$

The second term in the bracket of equation.(35) can be written in the form

$$\frac{d^2T_L}{dZ^2} - \frac{d^2T_P}{dZ^2} = \frac{d(\frac{dT_L}{dZ} - \frac{dT_P}{dZ})}{dZ} \tag{45}$$

Substitute equation (39) into equation (45) to get

$$\frac{-1}{k}\frac{d(q_L''-q_P'')}{dZ} = \frac{-1}{k}\frac{(dq_L''-dq_P'')}{dZ}$$

$$= \frac{-1}{k}\frac{[q_L''(2)-q_L''(1)]-[q_P''(2)-q_P''(1)]}{\Delta Z} \tag{46}$$

We substitute equation (44) into equation (46). Equation (46) is equal to zero and equation (35) becomes

$$\frac{dq(Z,t)}{dt} = \frac{k}{\alpha}[\frac{dT_L(Z,t)}{dt} - \frac{dT_P(Z,t)}{dt}] = \frac{k}{\alpha}\frac{d[T_L(Z,t)-T_P(Z,t)]}{dt}$$

$$= \frac{k}{\alpha}\frac{[T_L(Z_2,t_2)-T_P(Z_2,t_2)]-[T_L(Z_2,t_1)-T_P(Z_2,t_1)]}{t_2-t_1} \tag{47}$$

where

$$\frac{k}{\alpha} = \rho_{Li_{17}Pb_{83}} * C_{p_{Li_{17}Pb_{83}}} \tag{48}$$

where

$C_{p_{Li_{17}Pb_{83}}}$ is the heat capacity of $Li_{17}Pb_{83}$ (0.126 J/gm K) and

$\rho_{Li_{17}Pb_{83}}$ is the density of $Li_{17}Pb_{83}$ (9.65 gm/cm^3).

We substitute equation (48) into equation (47), equation (47) into equation (32), and equation (32) into equation (30) to get the moles of hydrogen generation rate directly. The moles of hydrogen generation rate is a function of time and initial liquid metal temperature.

$$\frac{dN_{H_2}(t)}{dt} = C\frac{dq(t)}{dt}V_{react}$$

$$= C*\rho*C_p*V_{react}\frac{[T_L(Z_2,t_2)-T_P(Z_2,t_2)]-[T_L(Z_2,t_1)-T_P(Z_2,t_1)]}{t_2-t_1}$$

$$= C*\rho*C_p*V_{react}\frac{[T_L(Z_2,t_2)-T_L(Z_2,t_1)]-[T_P(Z_2,t_2)-T_P(Z_2,t_1)]}{t_2-t_1}$$

$$= C*\rho*C_p*V_{react}\frac{d[T_L(t)-T_P(t)]}{dt} \qquad (49)$$

We integrate equation (49) to get the moles of hydrogen generation.

$$N_{H_2}(t) = C*\rho*C_p*V_{react}[T_L(t)-T_P(t)] \qquad (50)$$

If equation (50) is divided by V_{react}, the moles of hydrogen generation per unit reacted metal volume can be obtained directly by using the liquid metal temperature difference between the lithium-lead and control tests.

$$n_{H_2}(t) = C*\rho_{Li_{17}Pb_{83}}*C_p[T_L(t)-T_P(t)] \qquad (51)$$

4. Transformation of Results

We can transform the moles of hydrogen generation which is obtained by using the thermodynamics method to the moles of hydrogen generation per unit reacted metal volume. This will enable the results of the two independent methods to be compared. The transformation is accomplished using

$$n_{H_2}(t) = \frac{N_{H_2}(t)}{V_{react}} \qquad (52)$$

where

$N_{H2}(t)$ is the moles of hydrogen generation obtained using the thermodynamics method and

V_{react} is the reacted metal volume during the reaction phase (cm^3).

The reacted metal volume V_{react} is calculated using

$$V_{react} = \frac{M_{(Li_{17}Pb_{83})_{react}}}{\rho_{Li_{17}Pb_{83}}} \quad (53)$$

where $\rho_{Li_{17}Pb_{83}}$ is previously defined,

$M_{(Li_{17}Pb_{83})_{react}}$ is the mass of reacted lithium-lead.

The mass of reacted lithium-lead $M_{(Li_{17}Pb_{83})_{react}}$ is calculated using

$$M_{(Li_{17}Pb_{83})_{react}} = \frac{M_{(Li)_{react}}}{m_{f_{Li}}} \quad (54)$$

where

$M_{(Li)_{react}}$ is the reacted mass of lithium,

$m_{f_{Li}}$ is the mass fraction of lithium in the lithium-lead $Li_{17}Pb_{83}$.

The reacted lithium $M_{(Li)_{react}}$ is calculated using

$$M_{(Li)_{react}} = N_{Li} * m.w_{Li} \quad (55)$$

where

$m.w_{Li}$ is the molecular weight of lithium (6.941 gm/mole) and

N_{Li} is the reacted moles of lithium.

From the reaction equation (2), the reaction moles ratio of hydrogen to lithium is

$$\frac{N_{H_2}}{N_{Li}} = \frac{1}{2}$$

then

$$N_{H_2MAX} = 2N_{Li} \quad (56)$$

where N_{H_2Max} is the maximum moles of hydrogen generation listed in Table 1 obtained by thermodynamics method.

$N_{H_2 Max}$ is the maximum moles of hydrogen generation listed in Table 1 obtained by thermodynamics method.

In equation (54), the mass fraction of lithium $m_{f_{Li}}$ is calculated using

$$\frac{Y_{Li}}{Y_{Pb}} = \frac{\frac{m_{f_{Li}}}{m.w_{Li}}}{\frac{m_{f_{Pb}}}{m.w_{Pb}}} = \frac{17}{83} \qquad (57)$$

where

$\frac{Y_{Li}}{Y_{Pb}}$ is the atom ratio of the lithium-lead $Li_{17}Pb_{83}$ (17/83),

$m.w_{Pb}$ is the molecular weight of lead (207.2 gm/mole)

$m_{f_{Pb}}$ is the mass fraction of lead in the lithium-lead $Li_{17}Pb_{83}$.

The sum of the mass fractions is equal to 1

$$m_{f_{Li}} + m_{f_{Pb}} = 1 \qquad (58)$$

We substitute equate (55) into (54)

$$1 - m_{f_{Li}} = \frac{83}{17}\frac{m.w_{Pb}}{m.w_{Li}} m_{f_{Li}}$$

$$m_{f_{Li}} = \frac{1}{1 + \frac{83}{17}\frac{m.w_{Pb}}{m.w_{Li}}} = \frac{1}{1 + \frac{83}{17}\frac{207.2}{6.941}} = 0.0068145 \qquad (59)$$

We substitute equations (59) into (58), then (58) into (57), step by step to equation (53)

$$V_{react} = \frac{2 * N_{H_2 Max} * m.w_{Li}}{0.0068145 * \rho_{Li_{17}Pb_{83}}}$$

and V_{react} is listed in Table 6.2.

We substitute V_{react} and $N_{H_2}(t)$ which is calculated by the thermodynamics method into equation (52) to get the moles of hydrogen generation per unit reacted metal volume. We

will compare the results of the heat transfer method of analysis to the thermodynamics method in the following section.

Table 6.2 The Reacted Metal Volume from The Lithium-Lead Tests

Expt#	T_{LiPb} (°C)	Mass (g)	$N_{H_2 Max}$ (Mole)	V_{react} (cm^3)	V_{react}/V_{tot} 100%
L01	400	37.5	0.005994	1.26534	32.6
L04	350	46.5	0.008303	1.75277	36.4
L05	350	51.0	0.002034	0.42938	8.12
L06	350	56.0	0.007454	1.57355	27.1
L07	400	40.0	0.007384	1.55877	37.6
L08	500	53.5	0.008503	1.79499	32.4
L09	400	36.5	0.008248	1.74116	46.0
L11	600	44.0	0.008050	1.69936	37.3
L12	600	38.0	0.010726	2.26427	57.5
L14	600	49.0	0.012556	2.65059	52.2
L15	350	35.0	0.009810	2.07090	57.1
L20	650	41.0	0.005870	1.23916	29.2
L21	600	41.0	0.008760	1.84925	43.5
L22	600	35.0	0.011100	2.34322	64.6
L23	500	41.0	0.004820	1.01751	23.9

5. Results of Heat Transfer Method of Analysis

A program based on equation (51) in the last section, is used to analyze the liquid metal temperature difference between the lithium-lead test and lead test to obtain the hydrogen generation per unit reacted metal volume. We will discuss the experimental results of lithium-lead tests L05, L06 and lead test N34. These tests were characterized by an initial water temperature of 60° C and an initial liquid metal temperature of 350° C. The results of this calculation for three tests are shown in Figure 6.8 and 6.9, the moles of hydrogen generation per unit reacted metal volume is a functions of time. Right after the main ball valve is opened, and the interaction is initiated, the moles of hydrogen generation per unit reacted metal volume rises continuously to a maximum value in about 60 sec. and then remains at that value to the end of the reaction phase.

Another program based on equations from (52) to (58) in the last section is used to transform the moles of hydrogen generation which is the result of the first method to the moles of hydrogen generation per unit reacted metal volume. The results of test L05 and L06 are transformed and shown in Figure 6.10 and 6.11. The plots show that the moles of hydrogen generation per unit volume of reacted metal has the same behavior as the moles of hydrogen generation shown in Figure 6.12 and 6.13. By comparing Figures 6.8 and 6.9 with 6.10 and 6.11, the maximum values of hydrogen generated per unit volume between the two methods differ significantly. The differences between the two methods are believed to be due to two reasons: (1) The coefficient C in equation (28) was evaluated using lithium. The value of C should be much smaller than that using lithium-lead. The value of C is not known for lithium-lead. (2) The liquid metal temperature is measured indirectly. This temperature is measured by inserting a thermocouple into a thermocouple well at the bottom of the lower vessel. During the countdown phase, the temperature is uniform and constant in the region of liquid metal, thus there is no measurement error. In reaction phase, the response of the thermocouple is delayed by the thermocouple well. There is a temperature difference between the top of thermocouple well and the bottom of the liquid metal pool.

For the future experiment, we can use a lower chamber with two liquid metal pool, one for lithium-lead and another for lead to perform tests and use two thermocouples directly measure the two liquid metal temperatures simultaneously.

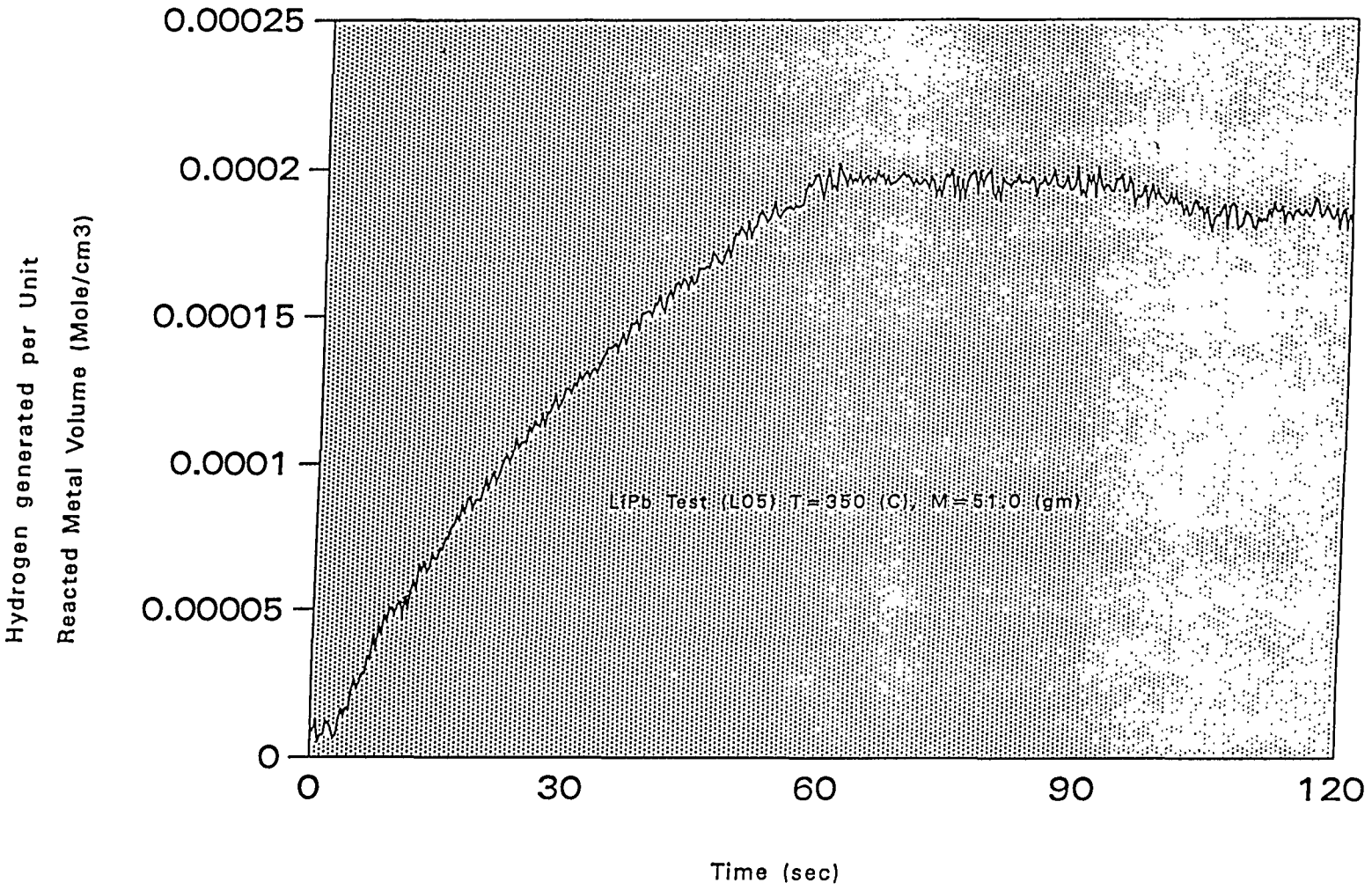


Figure 6.8 Hydrogen Generation as a function of Time

Analized by Heat Transfer Method (L05)

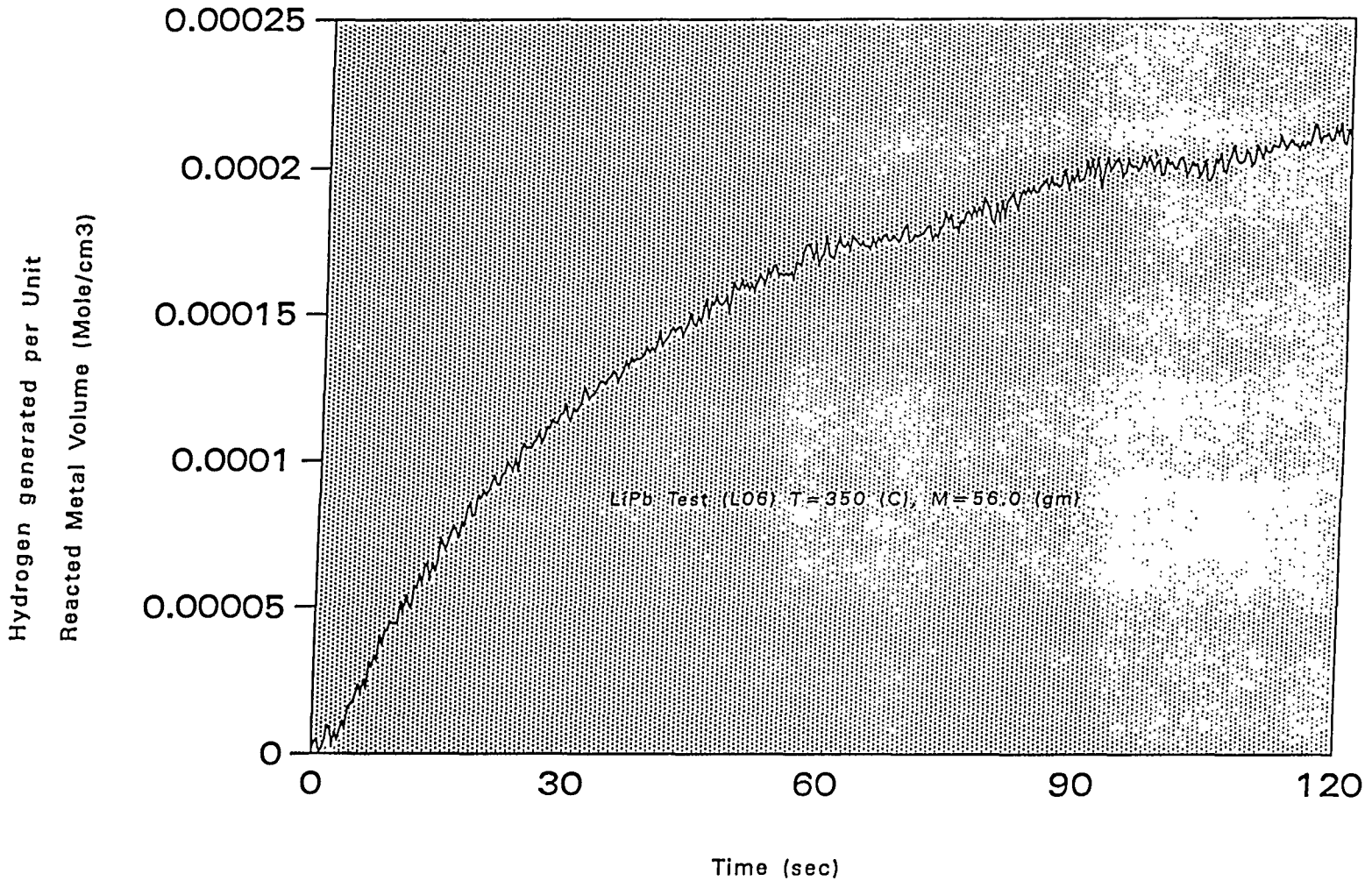


Figure 6.9 Hydrogen Generation as a function of Time

Analized by Heat Transfer Method (L06)

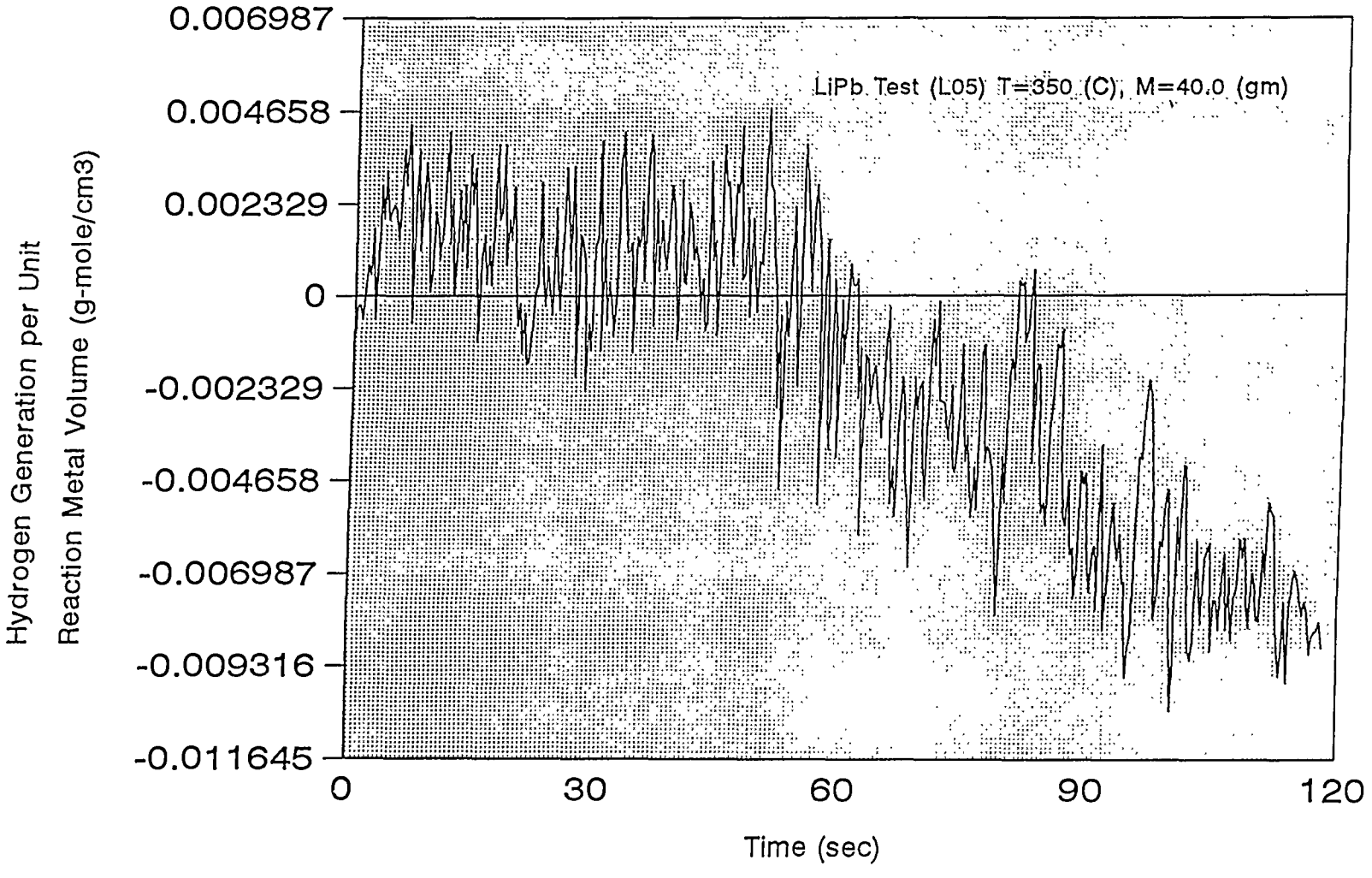


Figure 6.10 Corrected Hydrogen Generation as a Function of Time Transformed from Thermodynamics Method (L05)

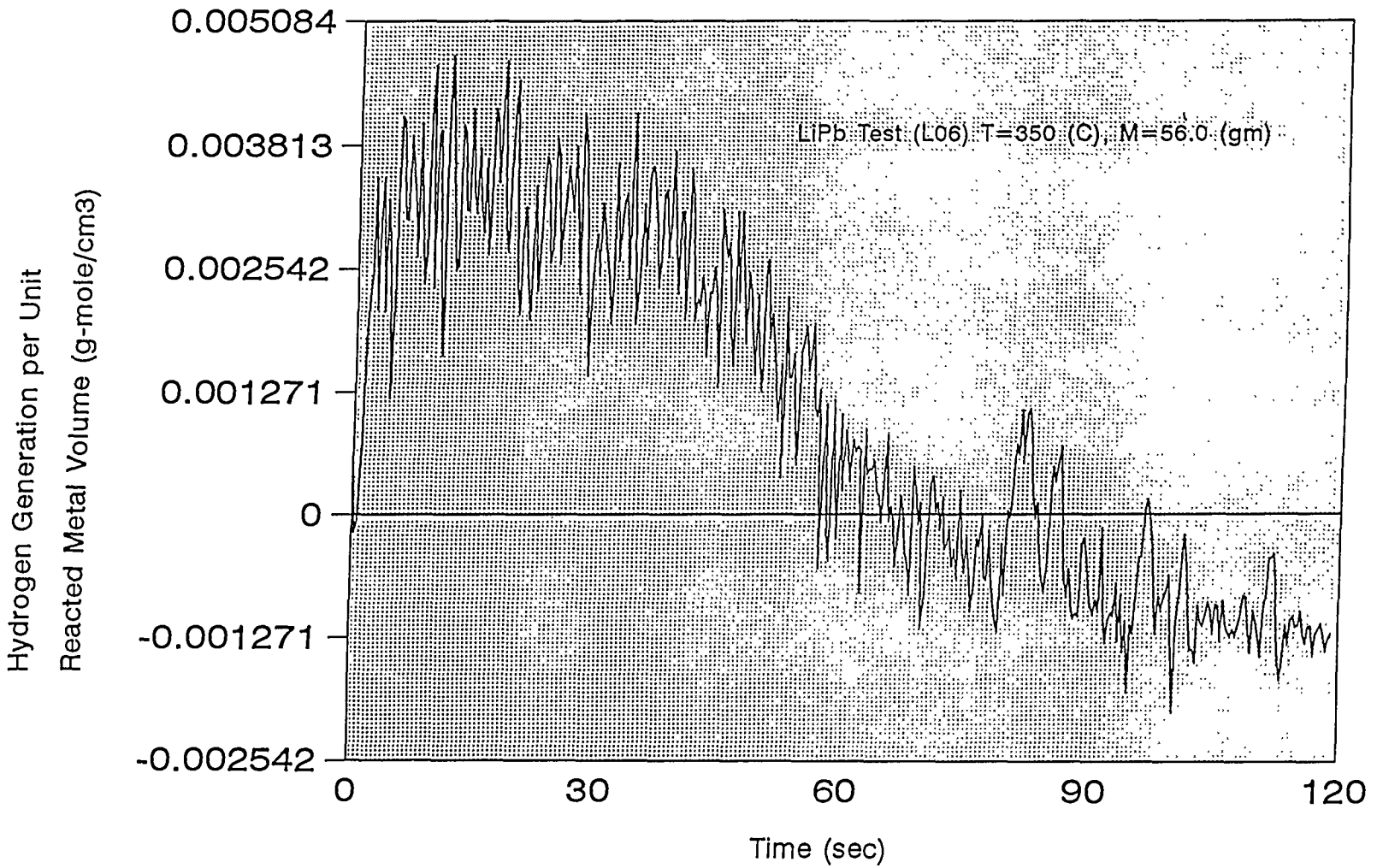


Figure 6.11 Corrected Hydrogen Generation as a Function of Time Transform from Thermodynamics Method (L06)

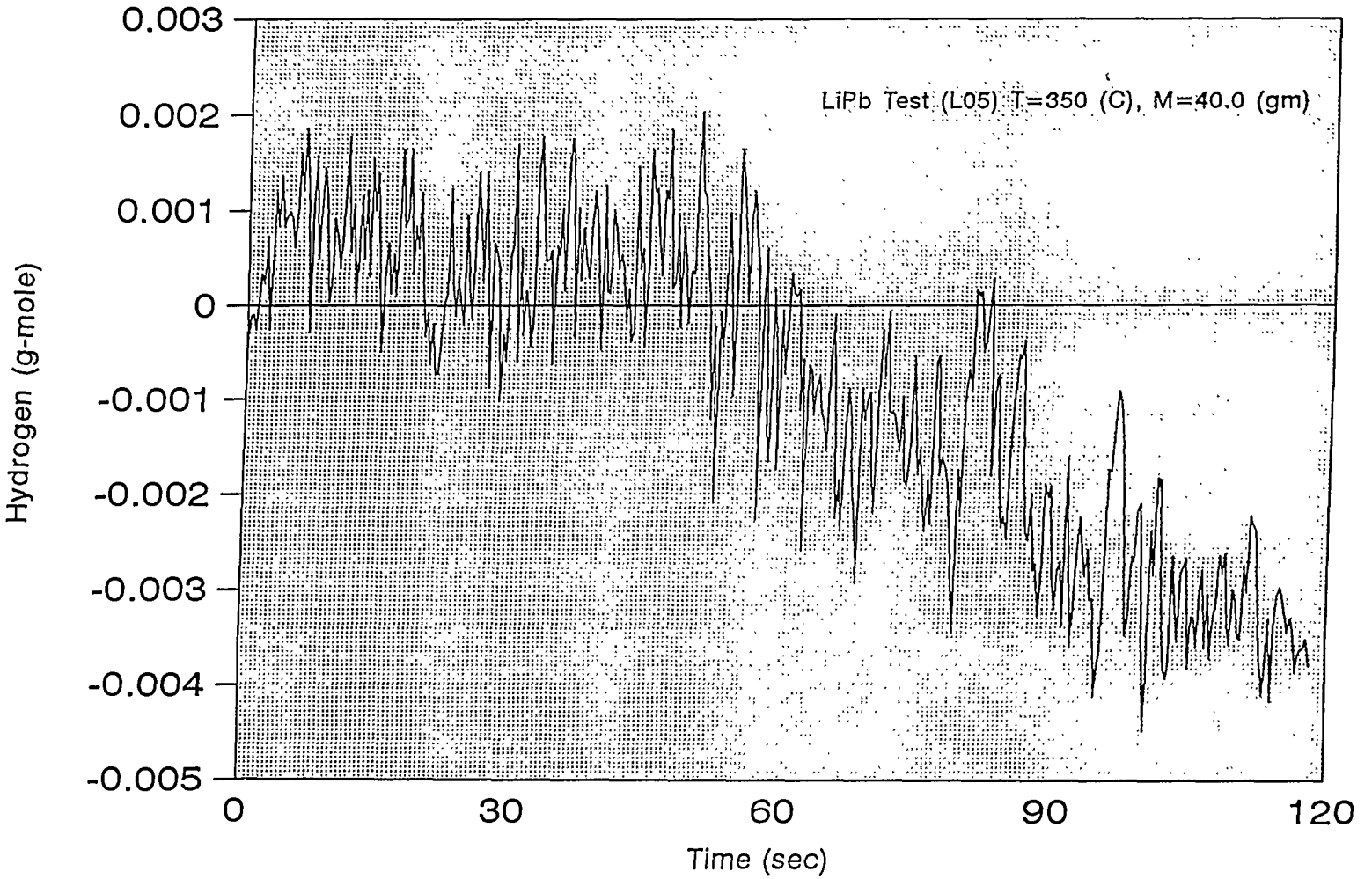


Figure 6.12 3 Corrected Hydrogen Generation as a Function of Time Analyzed by Thermodynamics Method (L05)

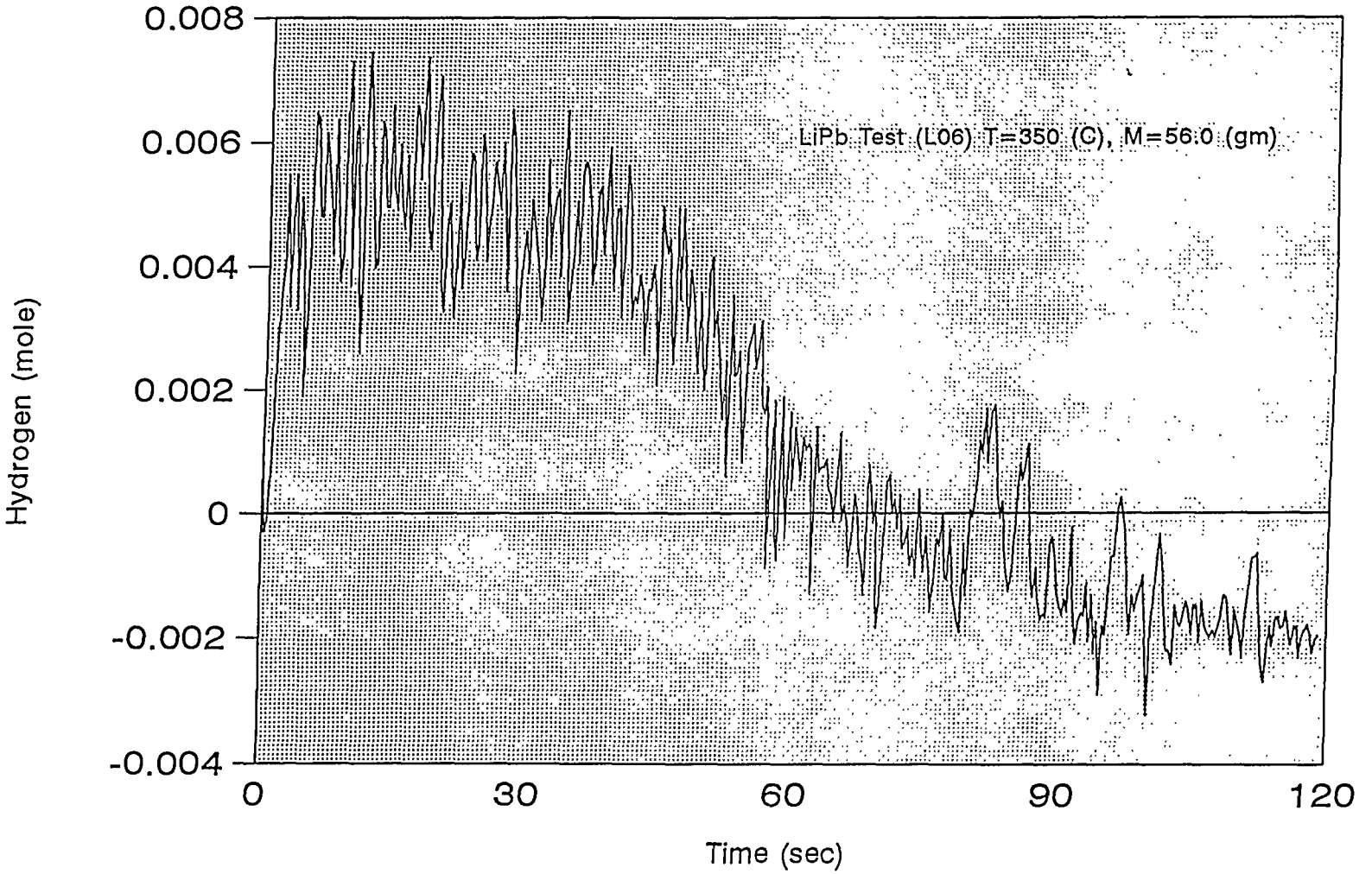


Figure 6.13 Corrected Hydrogen Generation as a Function of Time Analyzed by Thermodynamics Method (L06)

6. Determination of Reaction Rate Constants

The calculation results of hydrogen generation from the thermodynamics method of analysis will be used to derive the reaction coefficients B and ΔE in the parabolic rate equation :

$$\frac{dN_{H_2}(t)}{dt} = B * \exp(-\frac{\Delta E}{RT}) \qquad (60)$$

Where R is previously defined,

T is the initial liquid metal temperature.

One should note that mechanistically these constants B and ΔE are directly related to the D_o and dE in the liquid metal diffusivity equation.

$$D_{ii} = D_o \exp(-\frac{dE}{RT}) \qquad (61)$$

From equation (27) and (49), the hydrogen generation rate is a function of initial liquid metal temperature T and time t.

$$\frac{\partial(N_{H_2})}{\partial(t)} = \frac{\partial[N_{H_2}(T,t)]}{\partial(t)} \qquad (62)$$

We substitute equation (60) into equation (62)

$$\frac{\partial[N_{H_2}(T,t)]}{\partial(t)} = B * \exp(-\frac{\Delta E}{RT}) \qquad (63)$$

and integrate equation (63)

$$N_{H_2}(T,t) = \exp(-\frac{\Delta E}{RT}) * \int B * dt \qquad (64)$$

From the boundary condition:

$$N_{H_2}(T, t=0) = 0 \qquad (65)$$

$$\frac{\partial[N_{H_2}(T, t \to \infty)]}{\partial(t)} = 0 \qquad (66)$$

We assume

$$\int B * dt = A\{1 - \exp[-a(t^{\beta})]\} \qquad (67)$$

where a and β are constant to be determined

A is a constant.

The derivative of equation (67) is written in the form

$$B = A*a*\beta*(t^{\beta-1})*\exp[-a(t^{\beta})] \qquad (68)$$

Substitute equations (67) and (68) into equation (63) and (64), we get

$$\frac{\partial[N_{H_2}(T,t)]}{\partial(t)} = A*a*\beta*(t^{\beta-1})\exp[-a(t^{\beta})]\exp(-\frac{\Delta E}{RT}) \qquad (69)$$

$$N_{H_2}(T,t) = A*\{1-\exp[-a(t^{\beta})]\}\exp(-\frac{\Delta E}{RT}) \qquad (70)$$

Equation (69) and (70) are satisfied by the boundary conditions in equations (65), (66), and when

$$N_{H_2}(T,t\to\infty) = A*\exp(-\frac{\Delta E}{RT}) \qquad (71)$$

and the hydrogen generation is determined by the liquid metal temperature. In equation (71), the initial liquid metal temperature is fixed for each test. When time is infinite, the moles of hydrogen generation comes to the maximum value. In Table 6.1 and 6.2, the maximum hydrogen generation N_{H_2Max} is listed. That is calculated by using a program to select the maximum value of hydrogen generation from the results of thermodynamics method for each test. Equation (71) can be written in the form

$$N_{H_2Max}(T) = A*\exp(-\frac{\Delta E}{RT}) \qquad (72)$$

Equation (72) can be Linearized as

$$\ln[N_{H_2Max}(T)] = \ln(A) - \frac{\Delta E}{R}(\frac{1}{T}) \qquad (73)$$

The constants A and ΔE are evaluated by plotting $\ln[N_{H_2Max}(T)]$ versus $\frac{1}{T}$. The average maximum hydrogen generation data obtained from the results of the thermodynamics method listed in Table 6.3 is in computing $\ln[N_{H_2Max}(T)]$ through equation (73). The graph shown in Figure 6.14 is the results of plotting equation (73). A curve fitting program is used to determine the best line through the Linearized data.. The constants A and ΔE are determined from the best fitting equation.

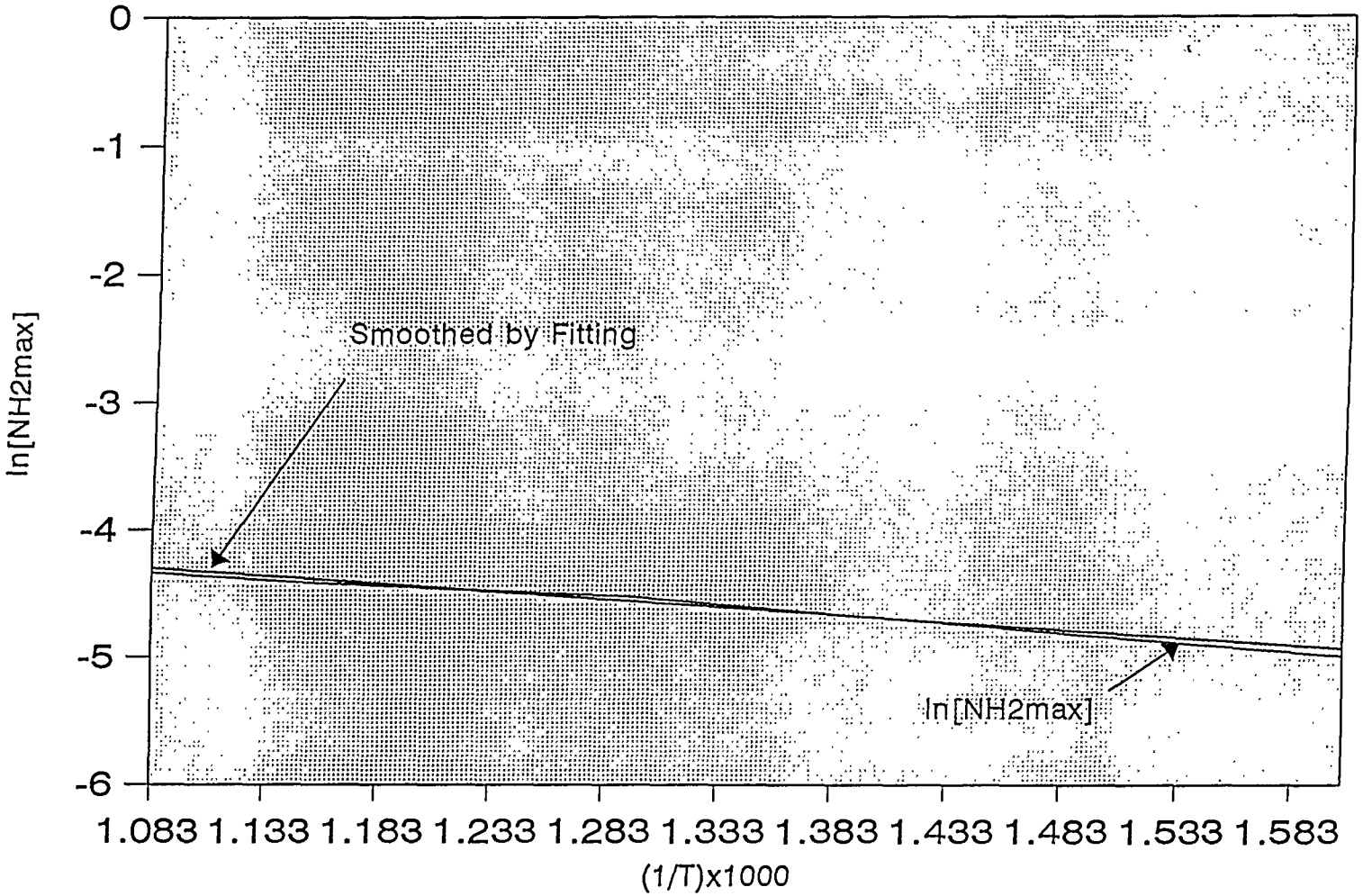


Figure 6.14 Linearization of Equation (73)and Fitting Equation

Table 6.3 The Average Moles of Hydrogen Generation

$T\ (^0K)$	$\overline{N_{H_2Max}}$ (mole)	$\ln[N_{H_2Max}(T)]$	$1/T$
350+273.15	0.0067	-5.005647753	0.001604750
400+273.15	0.0072	-4.933674253	0.001485552
600+273.15	0.0102	-4.585367559	0.001145278

From equation (73) and fitting equation

$$Y = -2.956027 - 1243.82X$$

where

$$Y = \ln[N_{H_2Max}(T)]$$

$$\ln A = -2.956027$$

$$\frac{\Delta E}{R} = 1243.82$$

the coefficients are

$$A = 0.052025203 \quad \text{(Mole)}$$

and

$$\Delta E = 1.03416*10^5 \quad \text{(J/Mole)}$$

where R is molar gas constant. Now we discuss the constants α and β in equation (70). We substitute equation (72) into equation (70) to get

$$\frac{N_{H_2}(T,t)}{N_{H_2Max}} = 1 - \exp[-\alpha(t^\beta)] \qquad (74)$$

Then

$$1 - \frac{N_{H_2}(T,t)}{N_{H_2Max}} = \exp[-\alpha(t^\beta)]$$

$$\ln[1 - \frac{N_{H_2}(T,t)}{N_{H_2Max}}] = -\alpha(t^\beta) \qquad (75)$$

where

$$\ln[1-\frac{N_{H_2}(T,t)}{N_{H_2Max}}]<0 \qquad (76)$$

finally equation (70) is Linearized to get

$$\ln\{-\ln[1-\frac{N_{H_2}(T,t)}{N_{H_2Max}}]\}=\ln a+\beta\ln(t) \qquad (77)$$

When the initial liquid metal temperature is known, the left side of equation (77) is a function of time. Let

$$Y(t)=\ln\{-\ln[1-\frac{N_{H_2}(T,t)}{N_{H_2Max}}]\} \qquad (78)$$

then

$$Y(t)=\ln a+\beta\ln(t) \qquad (79)$$

The constants a and β are evaluated by plotting Y(t) versus ln(t). The hydrogen generation data obtained from the results of the thermodynamics method is used in computing Y(t) through equation (76). A graph shown in Figure 6.15 is the results of Linearization of test L20. Results for the other tests are shown in Appendix E. A curve fitting program is used to determine the best line through the linearization. The constants a and β are determined from the best fitting equation. The results are listed in Table 6.4

Table 6.4 Coefficients Calculated from The Lithium-Lead Tests

Expt#	T_{LiPb} (°C)	N_{H_2Max} (Mole)	$\ln a$	a	β
L01	400	0.005994	-1.2	0.3	0.78
L06	350	0.007454	-0.3	0.74	0.29
L07	400	0.007384	-1.0	0.37	0.63634
L09	400	0.008248	-0.9	0.41	0.6788
L11	600	0.008050	-1.2	0.3	0.78
L12	600	0.010726	-1.6	0.2	0.82
L14	600	0.012556	-1.32	0.30	0.56
L15	350	0.009810	-1.5	0.22	0.86
L20	650	0.005870	-1.8	0.17	0.63
L23	500	0.004820	-2.2	0.11	0.57
Average				0.28	0.68

The constants α and β are plotted along T axis shown in Figure 6.16a and 6.16b.

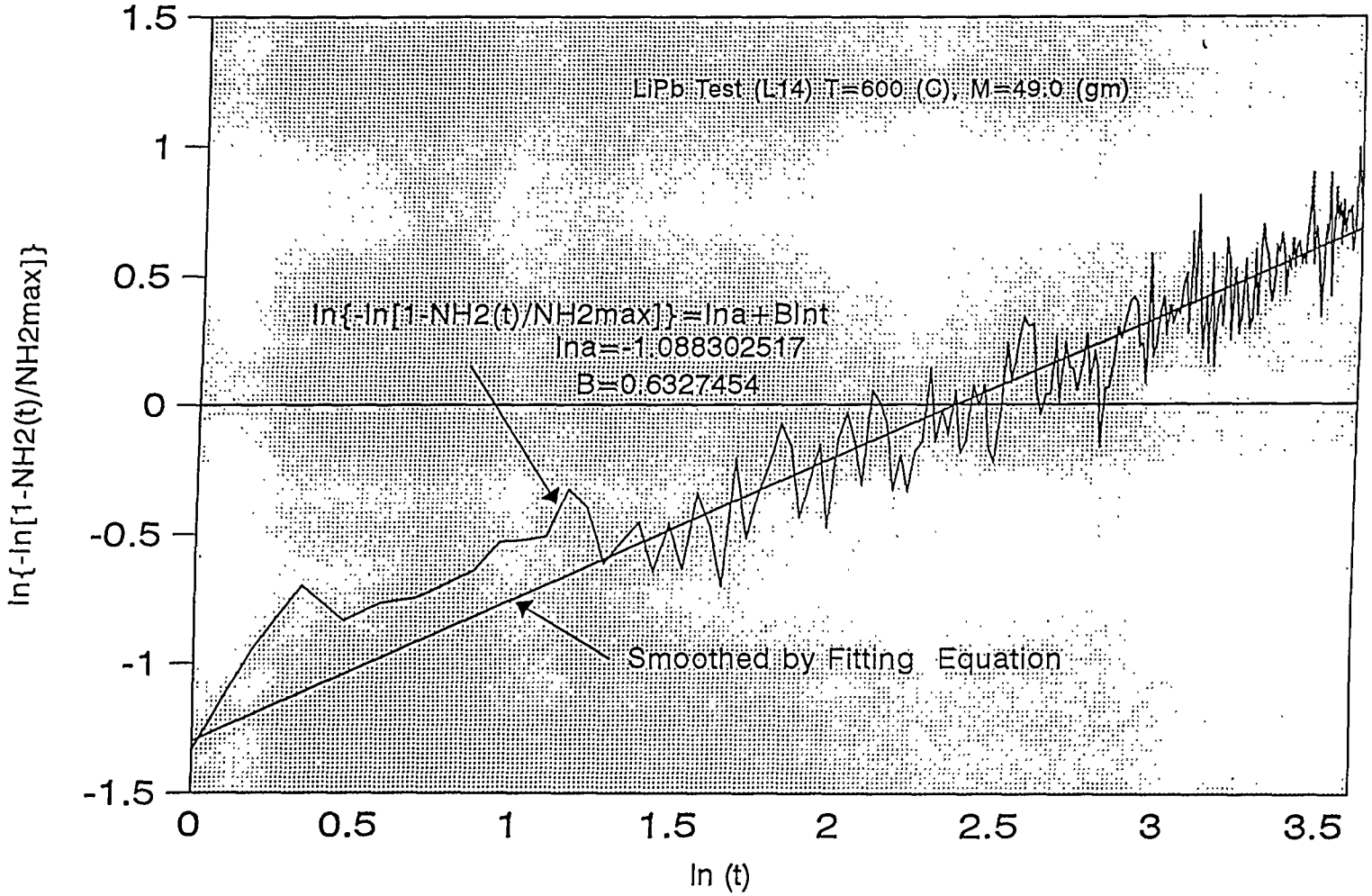


Figure 6.15 Hydrogen Generation Linearized by Equation (78) for Test (L14)

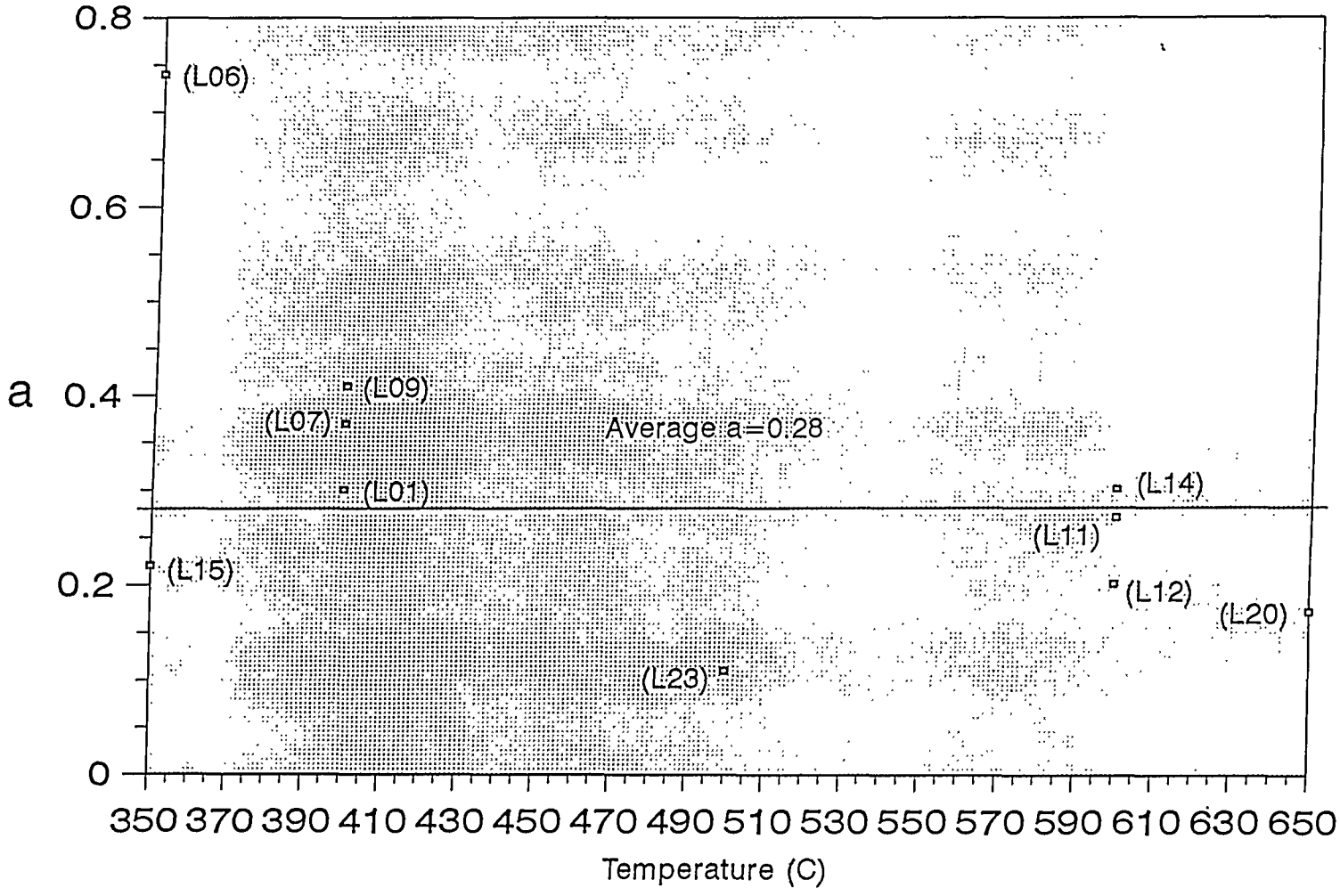


Figure 6.16a Constant (a) Distrabution along Temperature Axis

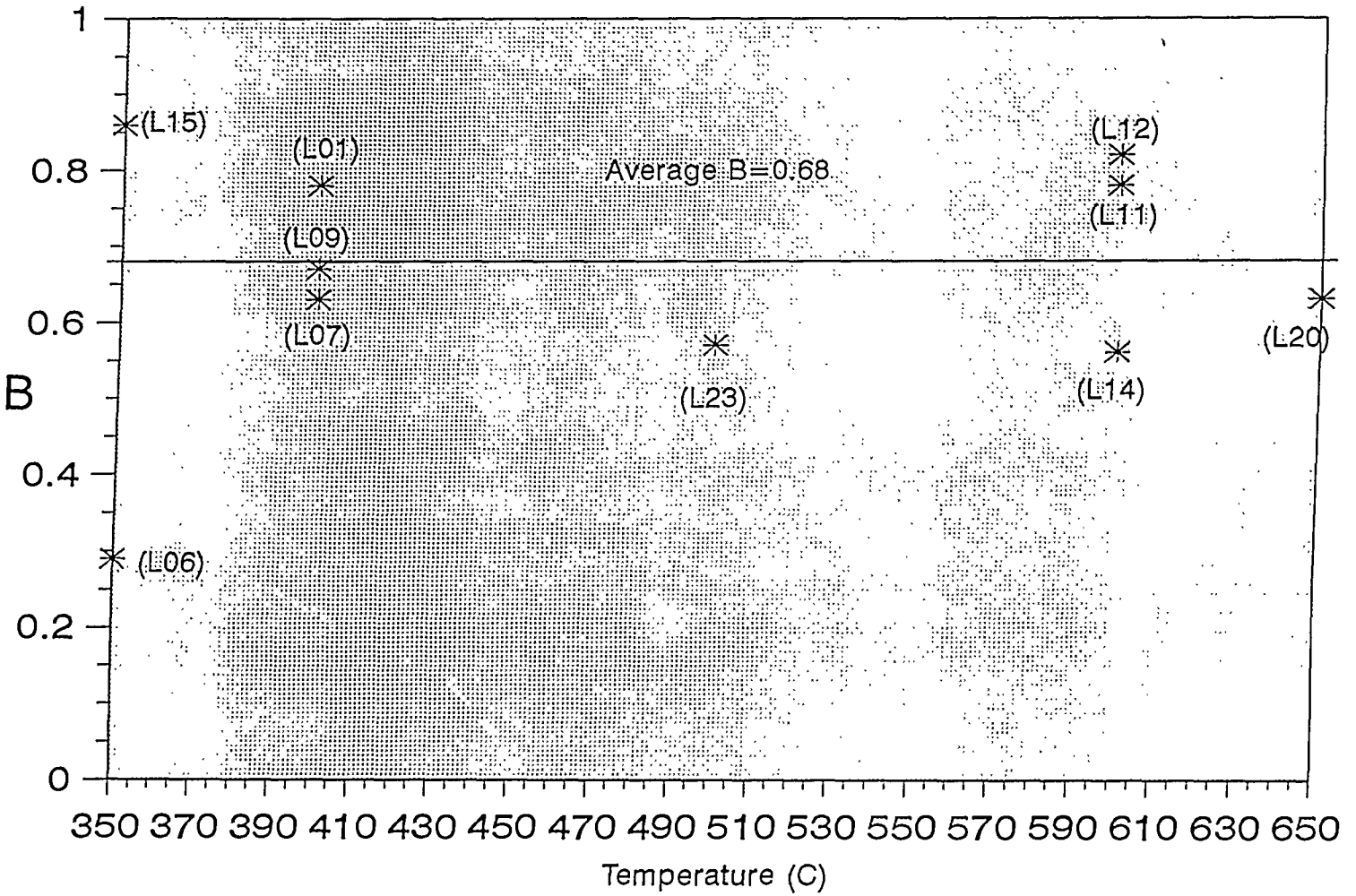


Figure 6.16b Constant (B) Distrabution along Temperature Axis

From the two graphs, we notice that the constants α and β are independent of temperature. We remove the discrete points and calculate the average of the constant α and β listed in Table 6.4

7. Determination of the Hydrogen Generation Equation

The average of the constants α and β listed in Table 6.3, are used to determine the hydrogen generation equation. All the terms in equation (70) are known, the moles of hydrogen generation equation is:

$$N_{H_2}(T,t) = 0.052*\{1-\exp[-0.28(t^{0.68})]\}\exp(-\frac{1.2438*10^3}{T}) \qquad (80)$$

The hydrogen generation are calculated using equation (80) with different liquid metal temperature (350°C-600°C) and within 240 sec. The results are shown in Figure 6.17,6.18, and 6.19. These figures also show the hydrogen generation as evaluated with test L14, L07, L15. Equation (80) reproduces the general shape of the test data, except for the hydrogen leakage.

8. Determination of the Hydrogen Generation Rate Equation

All the coefficients in equate (80) are substituted into equation (69).

$$\frac{\partial[N_{H_2}(T,t)]}{\partial(t)}$$

$$= 0.052*0.28*0.68*(t^{-0.32})\exp[-0.28(t^{0.68})]\exp(-\frac{1.2438*10^3}{T}) \qquad (81)$$

Three figures shown in Figure 6.20, 6.21 and 6.22, are calculated using equation (81) with different temperature (350°C-600°C) and within 240 sec. These figures also show the hydrogen generation rate as evaluated with test L14, L07, L15. Finally the results of the hydrogen generation rate should be divided by the area of the liquid metal surface to get the reaction rate per unit area.

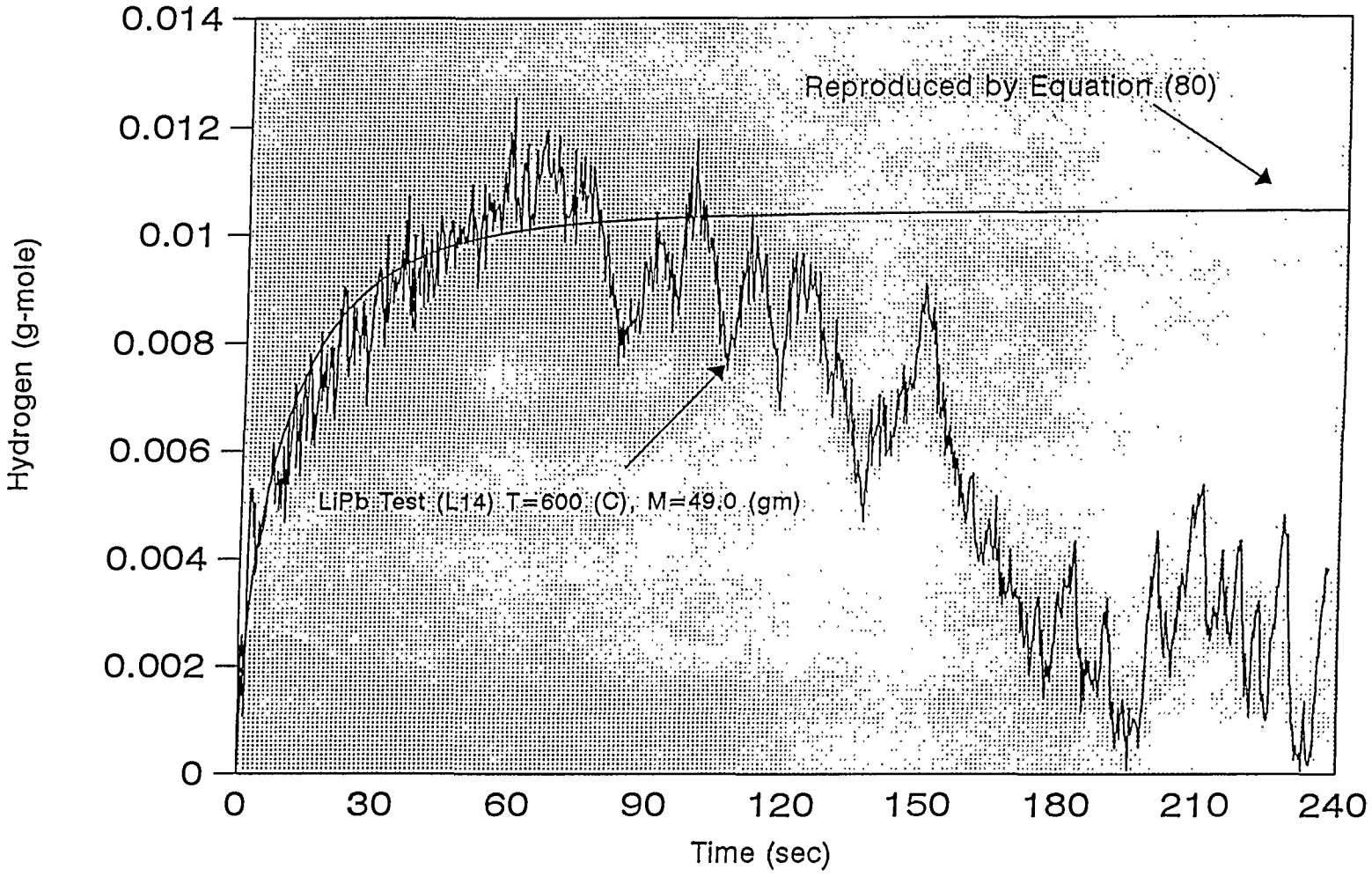


Figure 6.17 Corrected Hydrogen Generation as a Function of Time (L14)

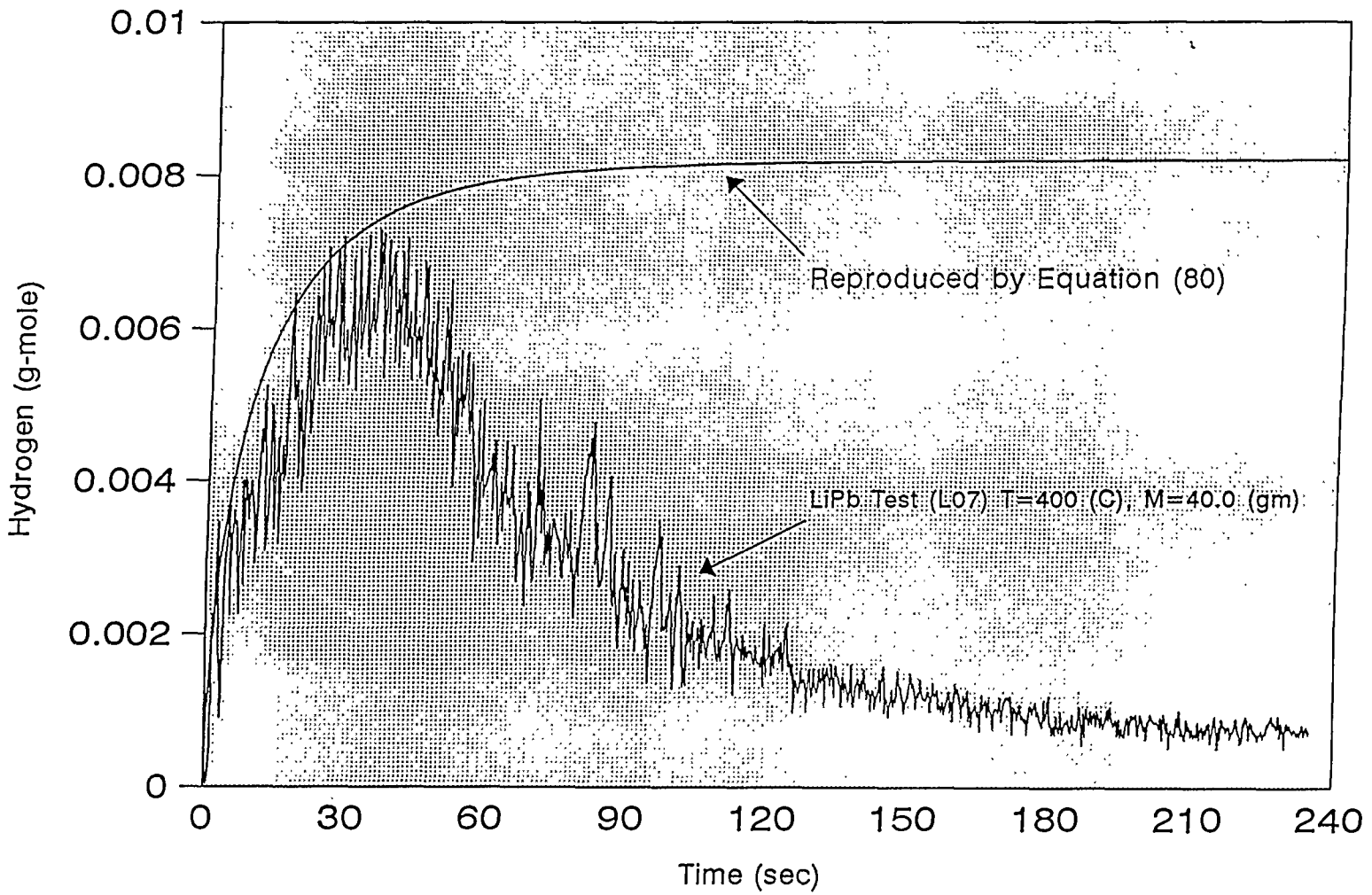


Figure 6.18 Corrected Hydrogen Generation as a Function of Time (L07)

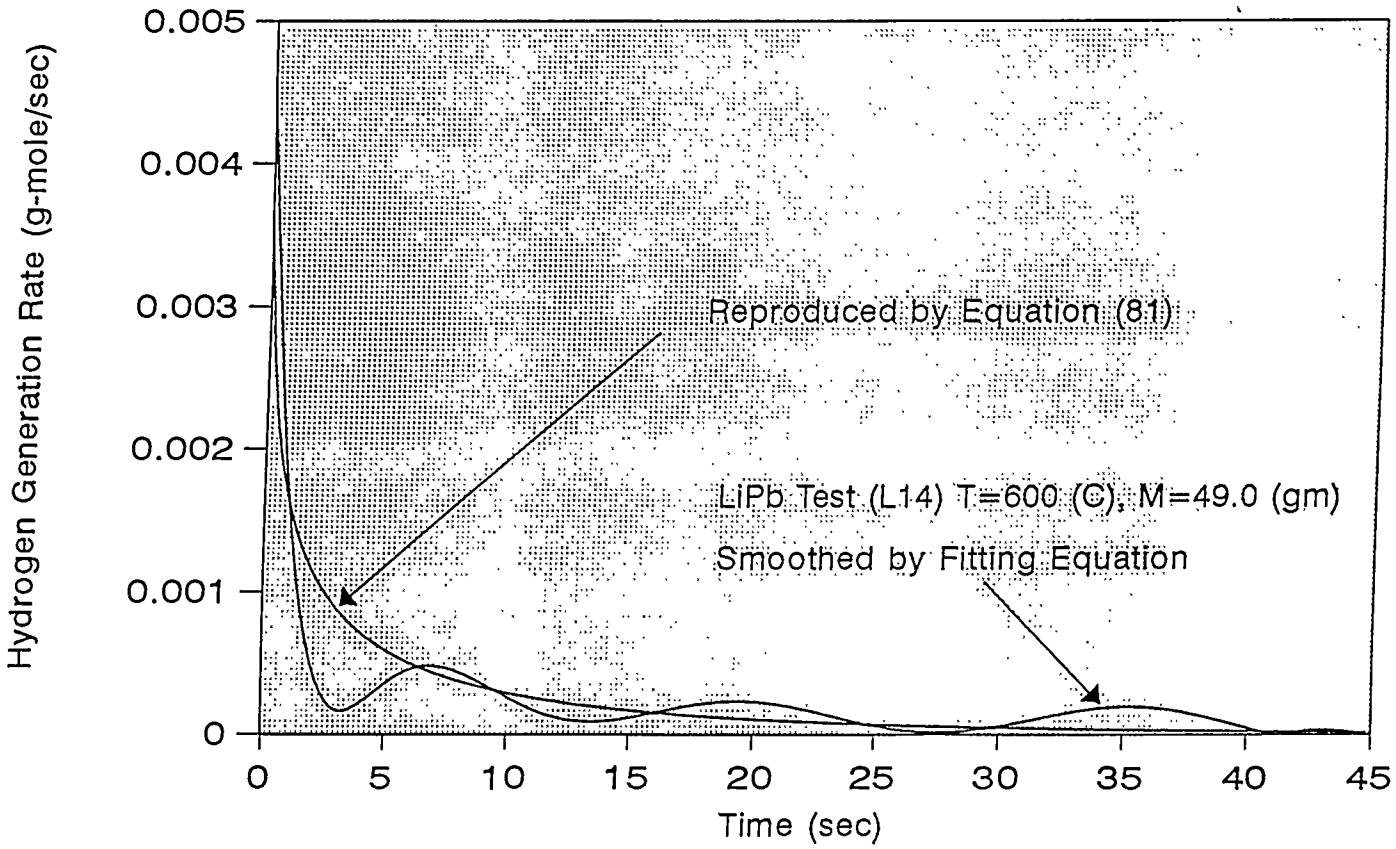


Figure 6.20 Hydrogen Generation Rate as a Function of Time (L14)

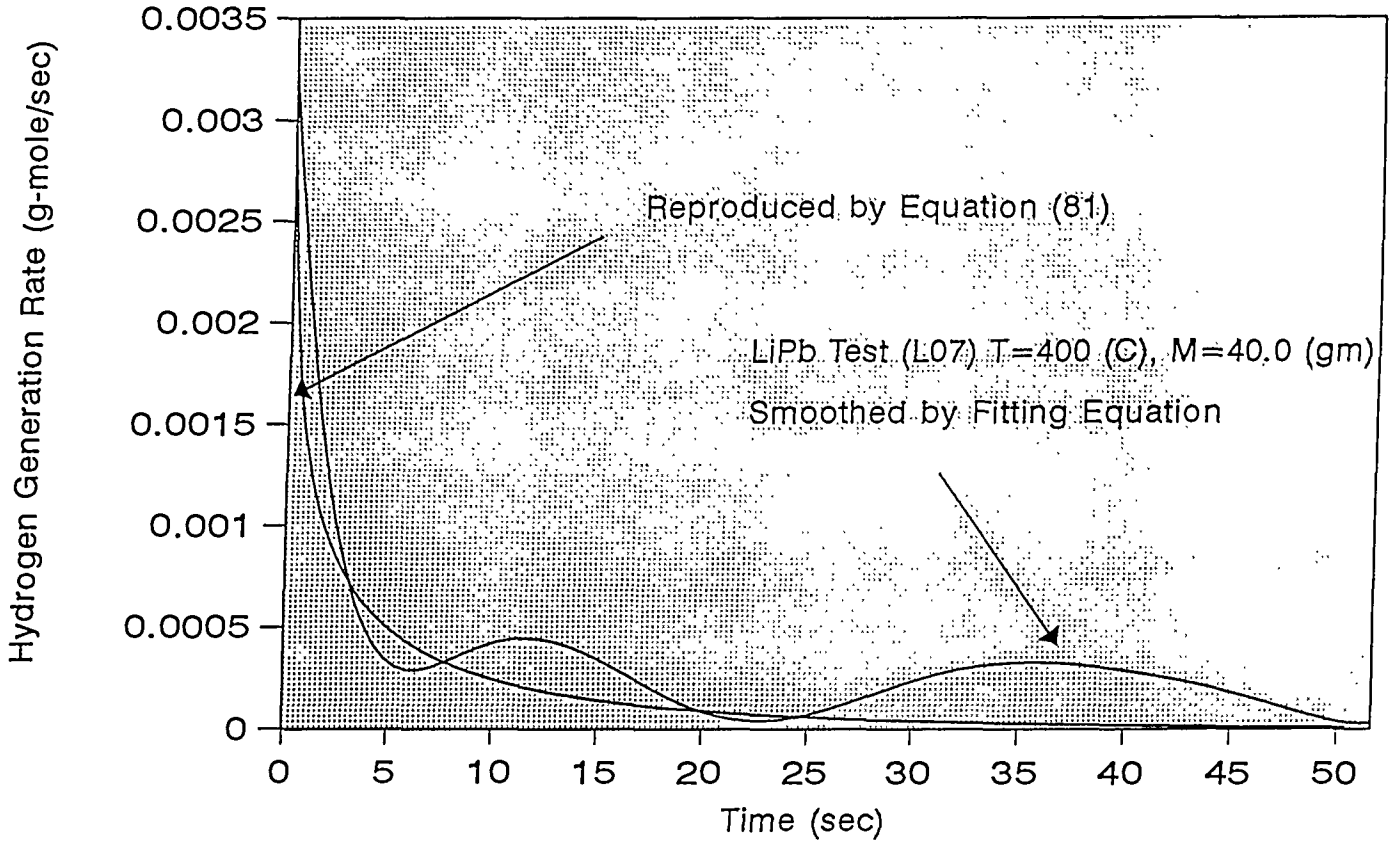


Figure 6.21 Hydrogen Generation Rate as a Function of Time (L07)

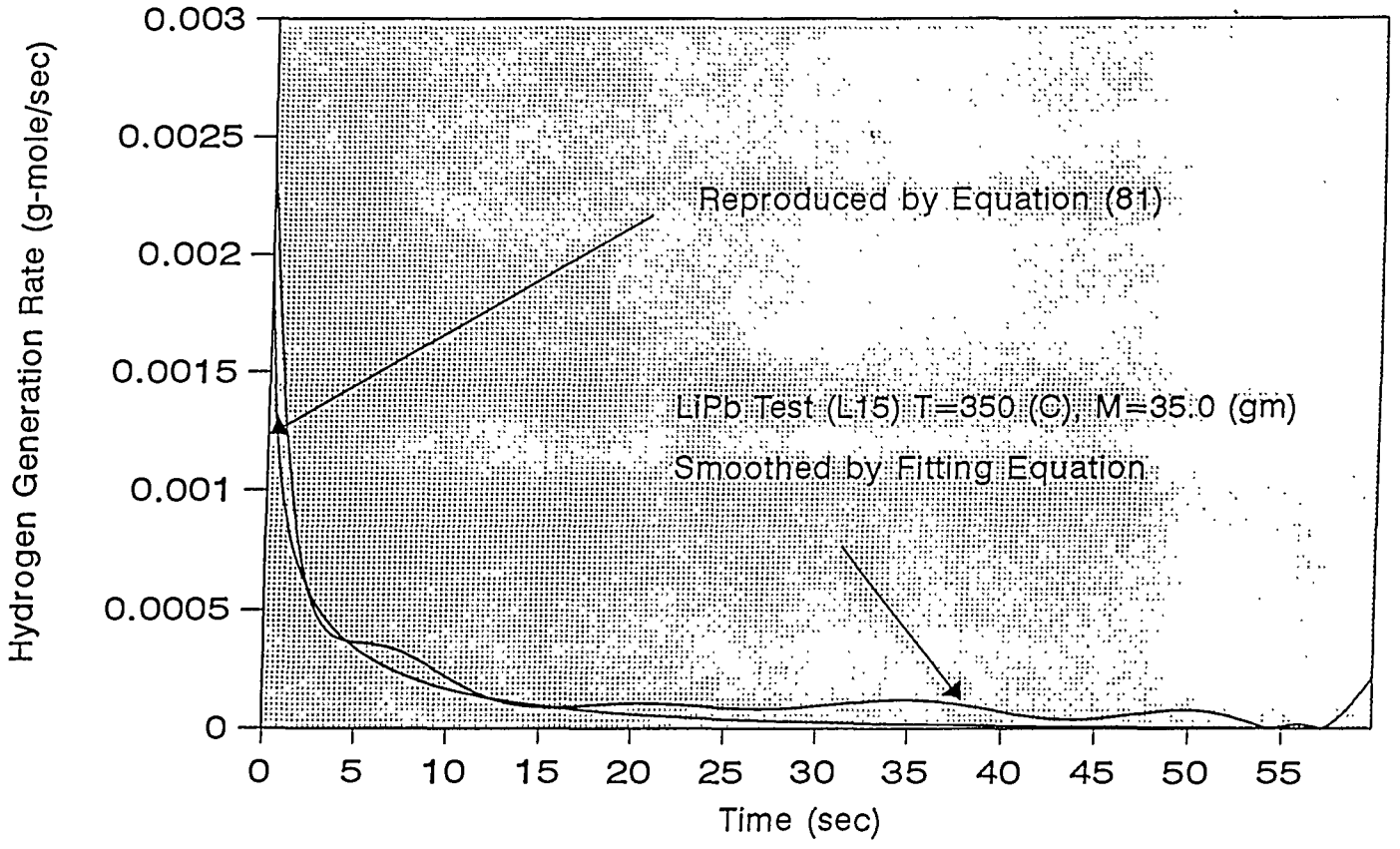


Figure 6.22 Hydrogen Generation Rate as a Function of Time (L15)

VII. Error Analysis

A. Measurement System Errors

Errors introduced by measurement system can be estimated by analytical method. This method requires an estimate of the fixed and random components of error from each componentt of system, usually based on the menufacturer's specifications and uses root-sum-square combination method to combine them for multiple-sample analysis. In this method, the error propagation formula [10] is expressed as:

$$\varepsilon_Y = \sqrt{\sum_{i=1}^{K} \left(\frac{\partial Y}{\partial X_i}\right)^2 * (\varepsilon_{X_i})^2} \qquad (82)$$

where

Y is the result of the experiment. It is a function of each variable X_i,

ε_Y is error of the result due to the error of measurement system,

ε_{X_i} is the error of the components given by the manufacturer's specifications and calibrations.

The error in the calculated moles of hydrogen can be found by applying equation (82) to equation (4) of the themodynanics method, which is used to evaluate the moles of hydrogen generated by the teaction. The error of the moles of hydrogen is given by:

$$(\varepsilon_{N_{H_2}})^2 = \left(\frac{\partial N_{H_2}}{\partial P_{H_2}}\right)^2 * (\varepsilon^2{}_{P_{H_2}} + \varepsilon^2{}_P) + \left(\frac{\partial N_{H_2}}{\partial V_{gas}}\right)^2 * (\varepsilon_{V_{gas}})^2 + \left(\frac{\partial N_{H_2}}{\partial T_{gas}}\right)^2 * (\varepsilon^2{}_{T_{gas}} + \varepsilon^2{}_T) \quad (83)$$

Our analysis of the experiment depended upon the data from four measurement devices and their supporting electronics; the pressure transducer (UGP), the liquid metal thermocouple (LMT), the water thermocouple (UWT), and the gas layer thermocouple (UGT). These devices and their supporting electronics are calibrated and the maximum errors in the full measurement ranges are listed in Table 7.1

Table 7.1 The Errors in Measurement System

Devices	Type	Maximum Error
Pressure transducer (UGP)	Setra 204	$\varepsilon_{P_{H_2}} = 1.4*10^{-2}$ (bar)
Liquid Metal Thermocouple (LMT)	K	$\varepsilon_{T_{LMT}} = 3.05$ (°C)
Water Thermocouple (UWT)	K	$\varepsilon_{T_{wat}} = 2.2$ (°C)
Gas Thermocouple (UGT)	E	$\varepsilon_{T_{gas}} = 1.7$ (°C)
Graduated Cylinder	TEKK	$\varepsilon_{V_{gas}} = 1.0$ (cm^3)
DAS for Temperature Measurement	AIM7	$\varepsilon_T = 0.25$ (°C)
DAS for Pressure Measurement	AMM2	$\varepsilon_P = 1.4*10^{-3}$ (bar)
Leakage		$\varepsilon_{P_L} = 1.16*10^{-4}$ (bar)

From equation (4)

$$\frac{\partial N_{H_2}}{\partial P_{H_2}} = \frac{V_{gas}}{RT_{gas}} + X_{H_2}(25^oC, 1atm)\frac{(T_{sat} - T_{wat})}{(T_{sat} - 25^oC)}\frac{1}{P_{atm}}\frac{\rho_{H_2O} * V_{wat}}{m.wt_{H_2O}} \qquad (84)$$

where

V_{gas} is the gas volume in system (193 cm^3)

R is the gas constant (83.14395 bar cm^3/mole K)

T_{gas} is the gas temperature (60+273.15°K)

$X_{H_2}(25^oC, 1atm)$ is constant ($1.7*10^{-7}$)

T_{sat} is the water saturation temperature (160°C, at 6 bar)

T_{wat} is the water temperature (60°C)

P_{atm} is the atmosphere pressure (1.03 bar)

ρ_{H_2O} is the density of water ($1.0098-4.86871*10^{-4}*60^oC$)

V_{wat} is the water volume (1330 cm^3)

$m.wt_{H_2O}$ is the molecular weight of water (18.02 gm/mole)

Substitute them into equation (84)

$$(\frac{\partial N_{H_2}}{\partial P_{H_2}})^2 * (\varepsilon^2{}_{P_{H_2}} + \varepsilon^2{}_P + \varepsilon^2{}_{P_L}) = 1.1*10^{-8} \qquad \text{(g-mole}^2\text{)}$$

From equation (4)

$$\frac{\partial N_{H_2}}{\partial T_{gas}} = \frac{V_{gas}}{R}\frac{(-1)}{(T_{gas})^2} \qquad (85)$$

$$(\frac{\partial N_{H_2}}{\partial T_{gas}})^2 * (\varepsilon^2{}_{T_{gas}} + \varepsilon^2{}_T) = 7.8*10^{-8} \qquad \text{(g-mole}^2\text{)}$$

and

$$\frac{\partial N_{H_2}}{\partial V_{gas}} = \frac{P_{H_2}}{RT_{gas}} \qquad (86)$$

where

P_{H_2} is the maximum partial pressure of hydrogen measured in the system (6bar),

$$(\frac{\partial N_{H_2}}{\partial V_{gas}})^2 * (\varepsilon_{V_{gas}})^2 = 4.6*10^{-8} \qquad \text{(g-mole}^2\text{)}$$

then

$$(\varepsilon_{N_{H_2}})^2 = 1.1*10^{-8} + 7.8*10^{-8} + 4.6*10^{-8} = 1.35*10^{-7} \qquad \text{(g-mole}^2\text{)}$$

Finally, the maximum error of hydrogen generation due to measuremental devices is:

$$\varepsilon_{N_{H_2}} = 0.000367 \qquad \text{(g-mole)}$$

B. The Error in Experimental Results

The propagation formula [10] can be used to evaluate the error of the mean moles of hydrogen for the group of tests at each initial liquid metal temperature. The error in the mean moles of hydrogen is related to the errors in the moles of hydrogen from each test by:

$$\varepsilon_{H_2 mean} = \frac{1}{K}\sqrt{\sum_{i=1}^{K}[\varepsilon_{H_2}(i)]^2} \tag{87}$$

where

$\varepsilon_{H_2 mean}$ is error of the mean moles of hydrogen from tests,

K is the numbers of tests,

$\varepsilon_{H_2}(i)$ is error of the moles of hydrogen from the (i)th test calculated using

$$\varepsilon_{H_2}(i) = N_{H_2 Max}(i) - \overline{N}_{H_2 Max} \tag{88}$$

where

$N_{H_2 Max}(i)$ is the maximum moles of hydrogen from the (i)th test,

$\overline{N}_{H_2 Max}$ is average of the maximum moles of hydrogen from K tests calculated using

$$\overline{N}_{H_2 Max} = \frac{1}{K}\sum_{i=1}^{K} N_{H_2 Max}(i) \tag{89}$$

Referring to the maximum moles of hydrogen from the (i)th test $N_{H_2 Max}(i)$ listed in Table 6.1 and the average of the maximum moles of hydrogen from K tests $\overline{N}_{H_2 Max}$ listed in Table 6.3, the error of the mean moles of hydrogen is calculated using equation (86) from the results of the thermodynamics method and listed in Table 7.2.

Table 7.2 The Error of Calibrated Hydrogen Generation

LMT	Average	Error	Experiment Error	Equipment Error	Combined Error
T (^0C)	$\overline{N}_{H_2 Max}$ (mole)	$\varepsilon_{H_2 mean}$ (mole)	$\frac{\varepsilon_{H_2 mean}}{\overline{N}_{H_2 Max}} * 100\%$	$\frac{\varepsilon_{H_2}}{\overline{N}_{H_2 Max}} * 100\%$	$\frac{\sqrt{\varepsilon^2_{H_2 mean} + \varepsilon^2_{H_2}}}{\overline{N}_{H_2 Max}} * 100\%$
350	0.0067	0.00147	22.0%	3.34%	22.6%
400	0.0072	0.00053	7.4%	2.45%	8.95%
600	0.0102	0.00158	15.5%	3.59%	15.9%

VIII. Summary of Results and Conclusions

A. Summary of Results

One experimental setup was used to perform 17 lithium-lead and 15 lead experiments in the hydrogen generation rate study. The mass range of lithium-lead samples was from 35.0 gm to 56.0 gm. The initial liquid metal temperature range was from 350°C to 650°C. The initial water temperature was 60°C. The maximum amount of hydrogen generation ranged from 0.0067±0.00147 g-mole at 350 °C to 0.0102±0.00158 g-mole at 600 °C over a time period of 240 seconds. The average hydrogen generation per unit area ranged from 13.2 g-mole/m^2 at 350 °C to 20.1 g-mole/m^2 at 600 °C. The maximum amount of hydrogen generation rate range was from 0.0025 mole/sec (350°C) to 0.0045 mole/sec (600°C) at the beginning of the reaction phase. The average hydrogen flux ranged from 0.0551 g-mole/m^2 sec (350°C) to 0.0838 g-mole/m^2 sec (600°C) over a time period of 240 second.

Two methods were developed to analyze the raw data from the experiments. The thermodynamics method was the main method used in the analysis to determine the hydrogen generation, hydrogen generation rate, and the reaction rate constants. The heat transfer method is simpler then the thermodynamics. However it needs an accurate value of the C evaluated using lithium-lead. Since this condition was not satisfied, we did not get reasonable result from the heat transfer method.

Three graphical libraries were plotted to show the results of experiments and analysis in Appendix B, D and E.

Four reaction coefficients were determined from the hydrogen generation curve. In the parabolic rate equation,

$$\frac{dN_{H_2}(t)}{dt} = B * \exp(-\frac{\Delta E}{RT})$$

where the constants B actually is a function of time,

$$B = A * \alpha * \beta * (t^{\beta-1}) * \exp[-\alpha(t^{\beta})]$$

and the values of A, α and β determined from the experimental results are

$A = 0.052025$ (g-mole),

$\alpha = 0.28$ (sec^{-1}),

$\beta = 0.68$ (constant)

and

$\Delta E = 1.0336 * 10^5$ (J/g-mole)

This reaction coefficient ($\Delta E = 1.03 * 10^5$) is compared with the modified reaction constant ($\Delta E = 1.09 * 10^5$) which is introduced in the literature review. They are nearly the same. The hydrogen flux are compared with the Herzog's results which is introduced in the literature review. They are in the same range shown in Figure C.1.

B. Conclusions:

1. The modified experimental setup can be used to determine the extent of the lithium-lead/water reaction by measuring water, gas and liquid metal temperature and gas pressure. From the results of analysis, the experiments can be repeated under identical conditions in this system.

2. The extent of reaction was found to vary over the range of initial liquid metal temperatures between 350° C and 650° C. The g-moles of hydrogen generation is a function of time and liquid metal temperature.

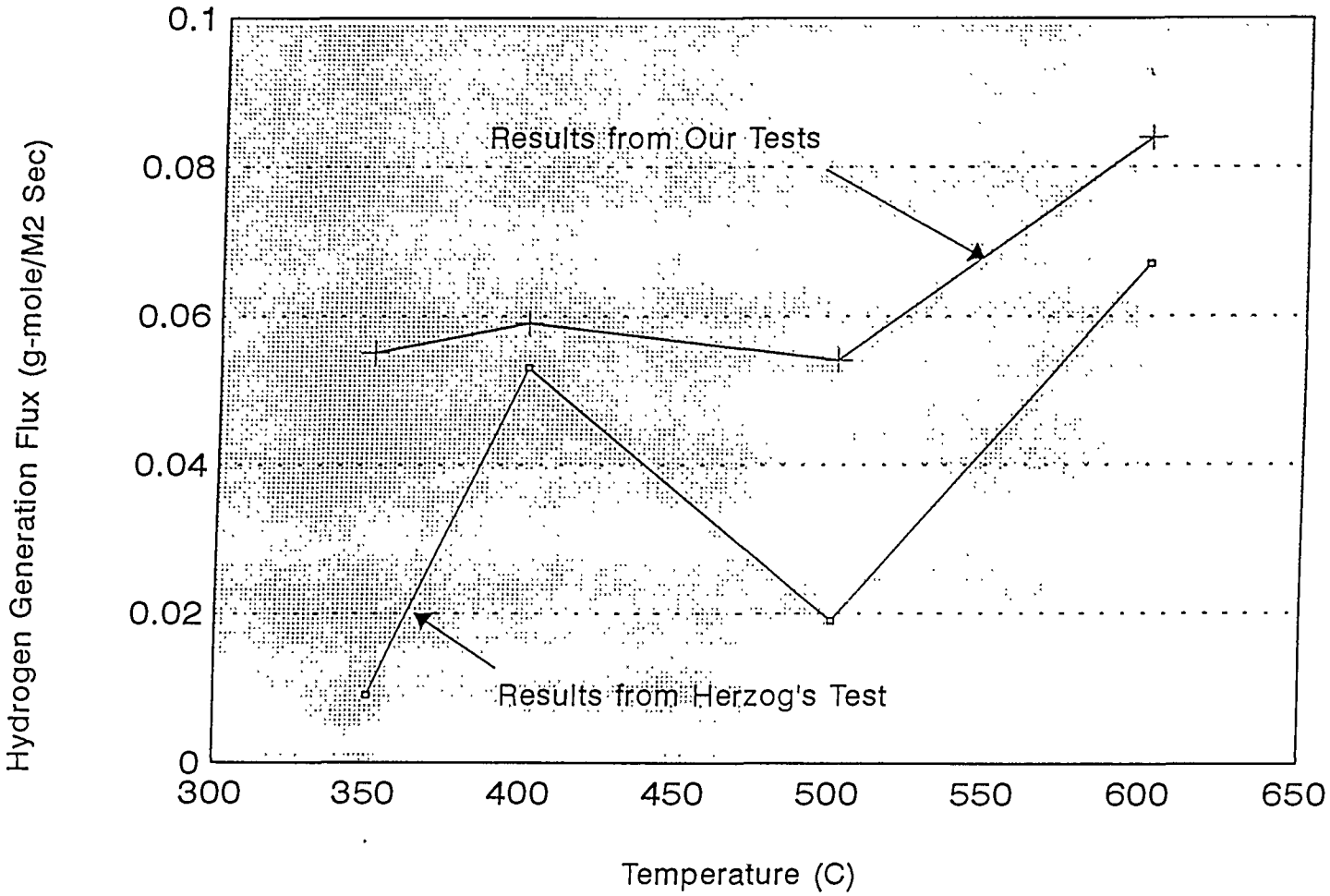


Figure C 1 Average Hydrogen Generation Flux for LiPb and Water Reaction [7]

3. Analysis of the g-moles of hydrogen data about 240 seconds from the lithium-lead tests showed that the hydrogen generation equation and the Arrhenius reaction rate constants can be determined from the g-moles of hydrogen generation curve.

4. The developed hydrogen generation and hydrogen generation rate equations can be used to predicate the hydrogen generation and hydrogen generation rate during $Li_{17}Pb_{83}$/water reaction.

C. Recommendations:

1. It is recommended that the further experiments be done using a lower chamber with two liquid metal pool, one for lithium-lead and another for lead. Two thermocouples should be used to directly measure the two liquid metal temperatures simultaneously. In this way, we can use two methods to evaluate hydrogen generation and the coefficient C in equation (28).

2. It is recommended that before and after each experiment, the samples of the metal should be analyzed by chemical method to find how many lithium reacted. The result of chemical analysis can be used to correct the maximum value of hydrogen generation from the thermodynamics and heat transfer methods of analysis.

IX. PROBLEMS ENCOUNTERED DURING PERIOD OF RESEARCH

Problems Encountered

Two major problems were encountered during the first six month of the project, all being the result of the project contract date occurring almost a month after beginning of the semester. The principal investigator was unable to obtain release time to actively work on the project in the Fall Semester of 1990 (August 28-December 31, 1990) because of the late contract date. A College technician could not be assigned to work on the project in the Fall Semester of 1990 as result of the late contract date. We could also not get the college technician to work on the project in the Spring Semester of 1991 (January-May 1991) due to heavy work load already being assigned by the college. In the summer of 1992, a technician was assigned to the project. By this time all the design and equipment acquisition had been completed. The complete system (including lower and upper chambers, all heaters, solenoid valves, butterfly valve and the data acquisition system) was assembled. In July 1992, pressure leakage test was conducted on the vessels and the butterfly valve was found to be leaking in the closed position. Also the cooling coil had defective welding joint. Upon discussion with the valve manufacturer, the butterfly valve was returned, and a zero leakage all metal valve was ordered in august 1992 for replacement. The valve size for this valve had to be charged to 1" due to cost. The valve was not received until January 15 1993. The change in the valve size necessitated redesign of the upper chamber and modifications in the lower chamber. The modifications and assembly of the new system were completed in march, 1993 and successfully tested. A Supply of lithium-lead was received from Oakridge National Lab in July 1993. From August through October 1993, a set up for melting and pouring the $Li_{17}Pb_{83}$ was constructed. In November 1993, a faulty valve in the $Li_{17}Pb_{83}$ melt-pouring set up resulted

in spill of the metal causing the metal to contaminated. Several unsuccessful attempts were made to get a new $Li_{17}Pb_{83}$ supply from Oakridge. A supple of $Li_{17}Pb_{83}$ was not received until we made arrangement with Fusion Technology Institute at the University of Wisconsin in October 1994. Dr. Lioyd Nelson delivered the much needed quality supple of the lithium-lead metal in November 1994. Actual experiments was started in November 1994 and completed in May 1995. Experimental analysis and final report preparation was completed in August 1995.

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APPENDIX A

LISTING OF DATA ACQUISITION AND CONTROL PROGRAM

```
10 REM ************************************************************************
20 REM *    DATA ACQUISITION AND CONTROL PROGRAM FOR  LITHIUM-LEAD/WATER    *
30 REM *                REACTION EXPERIMENTAL RESEARCH                      *
40 REM *                       DEVELOPED BY                                 *
50 REM *                  DR. PAUL ORLEANS BINEY                            *
60 REM *                      JANUARY 1993                                  *
65 REM *                        MODIFIED BY
*
67 REM *                     QING-YUAN LI
*
69 REM *                      JANUARY 1995                                  *
70 REM ************************************************************************

100 REM *  SET RELAY NUMBERS FOR DIGITAL RELAY CONTROLLED EQUIPMENT          *
110 REM *  ALL RELAYS ARE ON PCM3, WHICH IS THE 16 CHANNEL AC/DC POWER       *
120 REM *  CONTROL BOARD.                                                    *

140 REM *   RELAY #    IONAME      DESCRIPTION OF EQUIPMENT ATTACHED         *
144 REM *     0         UWH        UPPER WATER HEATER                        *
150 REM *     1         LMH        LOWER LIQUID METAL HEATER                 *
160 REM *     2         CWV        COOLING WATER SOLENOID VALVE              *
170 REM *     3         AIV        ARGON INLET SOLENOID VALVE (LOWER)
*
180 REM *     4         AOV        ARGON OUTLET SOLENOID VALVE               *
190 REM *     5         USV        UPPER SOLENOID VALVE (ASV FOR UPPER)*
200 REM *     6         MBV        MAIN BALL VALVE ACTUATOR
210 REM *     7         VAC        VACUUM VALVES
220 REM *     9         WIV        WATER INLET VALVE

230 REM *  THERMOCOUPLES DESCRIPTION AND IONAMES ASSIGNED

240 REM *  ALL THERMOCOUPLES ARE ON AIM7 BOARD
250 REM *  IONAME:  IS THE INPUT/OUTPUT NAME ASSIGNED IN CONFIGURATION FILE
260 REM *  TYPE   :  IS THE THERMOCOUPLE TYPE
270 REM *  GAIN   :  IS THE PRODUCT OF LOCAL GAIN (100) AND GLOBAL GAIN
280 REM *  WTMAX  :  IS THE ANTICIPATED MAXIMUM WORKING TEMPERATURE
290 REM *  VMAX   :  IS THE MAXIMUM OUTPUT VOLTAGE FROM TC AFTER GAIN IS
300 REM *            APPLIED. THE VOLTAGE CORRESPONDS TO THAT AT WTMAX
310 REM *                              AIM7

320 REM *     DESCRIPTION      IONAME CHANNEL TYPE GAIN  WTMAX    VMAX
340 REM *  UPPER GAS TEMP.       UGT     1      E   1000   150C   9.8680V
350 REM *  LOWER GAS TEMP.       LGT     4      K    200  1000C   8.2536V
360 REM *  UPPER WATER TEMP.     UWT     2      K   1000   150C   6.1370V
370 REM *  LOWER WATER TEMP.     LWT     3      E   1000   150C   9.8680V
380 REM *  UPPER FURNACE TEMP.   UFT     6      K    200  1200C   9.7656V
390 REM *  LOWER FURNACE TEMP.   LFT     7      K    200  1200C   9.7656V
400 REM *  LIQUID METAL TEMP.    LMT     5      K    200  1000C   8.2536V

420 REM * PRESSURE TRANSDUCER DESCRIPTION AND IONAMES ASSIGNED IN
430 REM * CONFIGURATION FILE
440 REM *                              AMM2
450 REM *     DESCRIPTION      IONAME CHANNEL TYPE GAIN  WPMAX    VMAX
460 REM *    ---------------------------------------------------------
470 REM *  UPPER GAS PRESSURE    UGP     1    ABS   2   100 PSI  10.00V
475 REM *  LOWER GAS PRESSURE    LGP     2    ABS   2   100 PSI  10.00V
477 REM * ************************************************************************

481 REM *   THE EXPERIMENT HAS FIVE MAJOR PHASES. THE DATA ACQUISITION       *
483 REM *   AND CONTROL SYSTEM HAS BEEN SET UP TO AUTOMATICALL CONTROL       *
485 REM *   ALL EVENTS AND GO THROUGH ALL FIVE PHASES WITHOUT OPERATOR       *
487 REM *   INTERFACE. THE FOLLOWING ARE THE MAJOR VARIABLES THAT CAN        *
```

```
489 REM *    BE CHANGED IN THE PROGRAM IF NECESSARY BEFORE RUNNING          *
491 REM *    THE PROGRAM.                                                   *
492 REM *                                BACKGROUND BACKGROUND NUMBER    NUMBER *
493 REM * PHASE  DESCRIPTION            INTERVAL   INTERVAL  OF DATA   OF DATA*
494 REM *                               VARIABLE   VALUE     VARIABLE   VALUE  *
495 REM *   1  UPPER WATER HEATING       FGROUND    30SEC                      *
496 REM *   2  LIQUID METAL HEATING      FGROUNG    30SEC                      *
497 REM *   3  COUNTDOWN TO REACTION     BINT3%      10       NDP3!       60.  *
498 REM *   4  CHEMICAL REACTION         BINT4%       2       NDP4!      100.  *
499 REM *   5  EQUILIBRIUM PERIOD        BINT5%     200       NDP5!       90.  *
500 REM *                                                                   *
501 REM *********************************************************************
502 REM  TIME INTERVAL  BETWEEN DATA=BINT*IR*0.001 SECONDS

506 BINT3%=10      : REM BACKGROUND INTERVAL FOR COUNTDOWN PHASE
507 BINT4%=2       : REM BACKGROUND INTERVAL FOR REACTION PHASE
508 BINT5%=10    : REM BACKGROUND INTERVAL FOR EQUILIBRIUM PHASE
512 NDP3!=100!     : REM NUMBER OF DATAPOINTS FOR COUNTDOWN PHASE
513 NDP4!=1200!    : REM NUMBER OF DATAPOINTS FOR REACTION PHASE
514 NDP5!=200!    : REM NUMBER OF DATAPOINTS FOR EQUILIBRIUM PHASE
515 LP3!=1!      : REM NUMBER OF DATAPOINTS FOR COUNTDOWN PHASE
516 LP4!=1!     : REM NUMBER OF DATAPOINTS FOR REACTION PHASE
517 LP5!=1!     : REM NUMBER OF DATAPOINTS FOR EQUILIBRIUM PHASE
518 DTSV=1          : REM TIME INTERVAL FOR CLOSURE/OPENING OF VALVES( SEC)
519 BOILT=10.!       : REM WATER BOILING TIME
520 RCDT=20.        : REM COUNTDOWN TIME PERIOD
521 EQT=120.         : REM EQUILIBRIUM TIME PERIOD

523 REM * DEFINE  EXPERIMENTAL VARIABLES

541 IR%=100         : REM INTERRUPT RATE (FIXED FOR PROGRAM AT 100MSEC INTERVAL
542 ITESTNO=1       : REM TEST NUMBER (NEEDS TO BE CHANGED FOR EACH EXPERIMENT)

548 RTIME%=160.   : REM REACTION TIME FOR PARTICULAR EXPERIMENT
549 UWDT=2           : REM MAXIMUM ALLOWABLE ERROR IN UPPER WATER TEMPERATURE
550 LMDT=2           : REM MAXIMUM ALLOWABLE ERROR IN LIQUID METAL TEMPERATURE
551 REM DTUH=25      : REM MAXIMUM ALLOWABLE ERROR IN UPPER FURNACE TEMPERATURE
552 UFDT=2          : REM MAXIMUM ALLOWABLE ERROR IN UPPER FURNACE TEMPERATURE
553 LFDT=2          : REM MAXIMUM ALLOWABLE ERROR IN LOWER FURNACE TEMPERATURE
554 PTIME%=20       : REM PAUSETIME IN SECONDS FOR FOREGROUND INTERVAL
555 PTIMEC%=20        : REM PAUSETIME IN SECONDS FOR CONTROL TIME INTERVAL

556 CALL KDINIT
600 DIM ONN%(1): DIM OFFF%(1): DIM TIM%(8): DIM TM#(8)
602 DIM  SIG1!(6),SIG2!(3),SIG3!(2)
603 DIM UWH1A(1), UWH1B(1), UWH1C(1), UWH1D(1), UWH1E(1): PRINT LP!
604 DIM LGH1A(1), LGH1B(1), LGH1C(1), LGH1D!(1)
610 ONN%(0)=0: OFFF%(0)=1: ST%=10: LP!=1!
620 UGP$="UGP": WIV$="WIV"
622 CWV$="CWV": USV$="USV": UWH$="UWH": AIV$="AIV": AOV$="AOV"
623 USV$="USV": UGT$="UGT": LGT$="LGT": LFT$="LFT": LMT$="LMT"
624 LMH$="LMH": UFT$="UFT": LGP$="LGP": UWT$="UWT": LWT$="LWT"
626 MBV$="MBV": CJUWLWT$="CJN,UWT,LWT": CJUGT$="CJN,UGT": VAC$="VAC"
628 CJUFT$="CJN,UFT": CJLGT$="CJN,LGT": CJLMT$="CJN,LMT": CJLFT$="CJN,LFT"

630 REM  CREATE DIGITAL ARRAYS FOR CONTROLLING VALVES AND HEATERS

650 CALL ARMAKE'("CWVOPEN%",1.,CWV$)
660 CALL ARMAKE'("CWVCLOSE%",1.,CWV$)
670 CALL ARMAKE'("USVOPEN%",1.,USV$)
680 CALL ARMAKE'("USVCLOSE%",1.,USV$)
690 CALL ARMAKE'("UWHONN%",1.,UWH$)
700 CALL ARMAKE'("UWHOFFF%",1.,UWH$)
702 CALL ARMAKE'("LMHONN%",1.,LMH$)
705 CALL ARMAKE'("LMHOFFF%",1.,LMH$)
710 CALL ARMAKE'("AIVOPEN%",1.,AIV$)
720 CALL ARMAKE'("AIVCLOSE%",1.,AIV$)
```

```
730 CALL ARMAKE'("AOVOPEN%",1.,AOV$)
740 CALL ARMAKE'("AOVCLOSE%",1.,AOV$)
744 CALL ARMAKE'("MBVOPEN%",1.,MBV$)
746 CALL ARMAKE'("MBVCLOSE%",1.,MBV$)
747 CALL ARMAKE'("VACONN%",1.,VAC$)
748 CALL ARMAKE'("VACOFFF%",1.,VAC$)
749 CALL ARMAKE'("WIVOPEN%",1.,WIV$)
750 CALL ARMAKE'("WIVCLOSE%",1.,WIV$)

760 REM PUT DIGITAL VALUES OF ON/OFF INTO KDAC ARRAYS FOR DIGITAL CONNTROL
770 REM OF VALVES AND HEATERS.

800 CALL ARPUT'("CWVOPEN%",1.,1.,CWV$,1,ONN%(),"C.RAW.INT")
810 CALL ARPUT'("CWVCLOSE%",1.,1.,CWV$,1,OFFF%(),"C.RAW.INT")
820 CALL ARPUT'("USVOPEN%",1.,1.,USV$,1,ONN%(),"C.RAW.INT")
825 CALL ARPUT'("USVCLOSE%",1.,1.,USV$,1,OFFF%(),"C.RAW.INT")
830 CALL ARPUT'("UWHONN%",1.,1.,UWH$,1,ONN%(),"C.RAW.INT")
840 CALL ARPUT'("UWHOFFF%",1.,1.,UWH$,1,OFFF%(),"C.RAW.INT")
845 CALL ARPUT'("AIVOPEN%",1.,1.,AIV$,1,ONN%(),"C.RAW.INT")
850 CALL ARPUT'("AIVCLOSE%",1.,1.,AIV$,1,OFFF%(),"C.RAW.INT")
860 CALL ARPUT'("AOVOPEN%",1.,1.,AOV$,1,ONN%(),"C.RAW.INT")
870 CALL ARPUT'("AOVCLOSE%",1.,1.,AOV$,1,OFFF%(),"C.RAW.INT")
880 CALL ARPUT'("MBVOPEN%",1.,1.,MBV$,1,ONN%(),"C.RAW.INT")
890 CALL ARPUT'("MBVCLOSE%",1.,1.,MBV$,1,OFFF%(),"C.RAW.INT")
891 CALL ARPUT'("LMHONN%",1.,1.,LMH$,1,ONN%(),"C.RAW.INT")
892 CALL ARPUT'("LMHOFFF%",1.,1.,LMH$,1,OFFF%(),"C.RAW.INT")
893 CALL ARPUT'("VACONN%",1.,1.,VAC$,1,ONN%(),"C.RAW.INT")
894 CALL ARPUT'("VACOFFF%",1.,1.,VAC$,1,OFFF%(),"C.RAW.INT")
895 CALL ARPUT'("WIVOPEN%",1.,1.,WIV$,1,ONN%(),"C.RAW.INT")
896 CALL ARPUT'("WIVCLOSE%",1.,1.,WIV$,1,OFFF%(),"C.RAW.INT")

897 PRINT "*****************************************"
898 PRINT "* INPUT UPPER WATER SETPOINT TEMPERATURE *"
899 PRINT "*****************************************"

900 INPUT UWSETPT

901 PRINT "*****************************************"
902 PRINT "* INPUT LIQUID METAL SETPOINT TEMPERATURE *"
903 PRINT "*****************************************"

904 INPUT LMSETPT
905 PRINT "UWSETPT,LMSETPT";UWSETPT;LMSETPT
906 PRINT "DO YOU WANT TO CHANGE? Y OR N?"
907 INPUT ANS$
908 IF (ANS$="Y" OR ANS$="y") THEN GOTO 897
909 LFSETPT=LMSETPT+150    : REM LOWER FURNACE SETPOINT TEMPERATURE
910 TSAT!=UWSETPT    : REM BOILING TEMPERATURE AT LOWERED PRESSURE
911 UFSETPT=UWSETPT    : REM UPPER FURNACE SETPOINT TEMPERATURE

912 REM BEGIN DATA ACQUISITION AND CONTROL
921 PRINT " ***************************************************************"
922 PRINT " * THE ARGON INLET VALVE IS BEING CHECKED AND OPENED            *"
923 PRINT " * THEN AFTER 2 INTONS  THE ARGON OUTLET VALVE IS CHECKED/OPENED*"
924 PRINT " * THE COOLING WATER SOLENOID VALVE IS BEING CLOSED              *"
925 PRINT " ***************************************************************"

930 TNH=0: TIM%(0)=1
932 CALL KDTIMER'(TIM%(),"NT","")
940 CALL INTON'(IR%,"MIL")
943 CALL BGWRITE'("AIVOPEN%",AIV$,1,1,"NT","AIVSTAT")
945 CALL KDTIMERRD'(TM#())
947 IF TM#(0)*IR%/1000<DTSV GOTO 945
948 CALL BGWRITE'("AOVOPEN%",AOV$,1,1,"NT","AOVSTAT")
949 CALL BGWRITE'("CWVOPEN%",CWV$,1,1,"NT","CWVSTAT")
950 CALL BGWRITE'("WIVOPEN%",WIV$,1,1,"NT","WIVSTAT")
953 PRINT " ***********************************************************"
```

```
954 PRINT " * THE UPPER WATER HEATER AND LIQUID METAL HEATER ARE     *"
955 PRINT " * BEING TURNED ON TO BEGIN THE INITIAL HEATING PHASE.   *"
956 PRINT " ************************************************************"

960 CALL BGWRITE'("UWHONN%",UWH$,1,1,"NT","UWHSTAT")
961 CALL BGWRITE'("LMHONN%",LMH$,1,1,"NT","LMHSTAT")
962 UHST%=1
970 CALL BGSTATUS'("CWVSTAT",ST%)
982 IF ST% <> 0 GOTO 970
983 PRINT "STATUS OF CWV IS ", ST%
984 REM CALL INTOFF
990 REM

992 PRINT " ************************************************************"
994 PRINT " * ACQUIRING DATA FOR HEATING OF UPPER WATER AND LIQUID METAL *"
995 print " *      AND SIMULTANEOUS DATA ACQUISITION ON FOREGROUND.      *"
996 PRINT " ************************************************************"
998 CALL KDPAUSE'(PTIME%,"SEC")
1000 CALL FGREAD'("CJN,UWT,UFT,LGT,LMT,LFT","NONE", SIG1!(),"C.THCU.K","NT")
1010 CALL FGREAD'("CJN,LWT,UGT","NONE", SIG2!(),"C.THCU.E","NT")
1020 CALL FGREAD'("UGP,LGP","NONE", SIG3!(),"C.VOLTS","NT")
1176 REM ************ PRINT DATA *******
1178 UFT1=SIG1!(2): LWT1=SIG2!(1): UWT1=SIG1!(1):UWAVG=0.5*(UWT1+LWT1)
1179 UGP1=SIG3!(0)*20*6.8948E-2 : LGP1=SIG3!(1)*20*6.8948E-2: UGT1=SIG2!(2)
1180 LGT1=SIG1!(3): LMT1=SIG1!(4): LFT1=SIG1!(5)
1181 PRINT "UWT,LWT,UGT,UFT,UGP ARE ";UWT1;LWT1;UGT1;UFT1;UGP1;"bar"
1182 PRINT "LFT1;LMT1;LGT1;LGP1";LFT1;LMT1;LGT1;LGP1;" bar"
1183 IF( UFT1>UFSETPT+UFDT AND UHST%=1) THEN GOSUB 4000
1184 IF( UFT1<UFSETPT-UFDT AND UHST%=0) THEN GOSUB 5000
1185 IF( LFT1>LFSETPT+LFDT AND LHST%=1) THEN GOSUB 4500
1186 IF( LFT1<LFSETPT-LFDT AND LHST%=0) THEN GOSUB 5500

1200 REM  *********      PERFORM TEST TO DETERMINE IF WATER AND          ***
1210 REM  ********* LIQUID METAL SETPOINT TEMPERATURES HAVE BEEN ATTAINED ***
1212 IF (UWT1 >UWSETPT-UWDT AND UWT1<UWSETPT+UWDT) THEN PRINT "UPPER WATER
TEMPERATURE IS WITHIN SETPOINT RANGE"
1214 IF (LMT1 >LMSETPT-LMDT AND LMT1<LMSETPT+LMDT) THEN PRINT "LIQUID METAL
TEMPERATURE IS WITHIN SETPOINT RANGE"
1300 REM    *** PERFORM MAJOR TEST TO CHECK IF BOTH WATER AND ***
1310 REM    ***          METAL TEMPS ARE WITHIN RANGE        ****
1315 IF ABS(UWT1-UWSETPT)<UWDT AND ABS(LMT1-LMSETPT)<LMDT GOTO 1325
1320 GOTO 998
1325 PRINT " LIQUID METAL AND UPPER WATER ARE AT PRESET TEMPS"
1330 PRINT   "UWT, LWT, LMT,UGP ARE ";UWT1;LWT1;LMT1;UGP1*20.0*6.8948E-2
1335 PRINT " THE UPPER  AND WATER INLET SOLENOID VALVES ARE BEING CLOSED"
1340 PRINT "      TO READY SYSTEM FOR INDUCED BOILING BY VACUUM PUMP    "
1360 CALL BGWRITE'("WIVCLOSE%",WIV$,1,1,"NT","WIVSTAT2")
1370 CALL BGWRITE'("CWVOPEN%",CWV$,1,1,"NT","CWVSTAT2")
1380 PRINT "CLOSE ALL MANUAL VALVES ON CHAMBER EXCEPT THE UPPER BALL VALVE"
1400 PRINT "CLOSE ALL MANUAL VALVES ON CHAMBER EXCEPT THE UPPER BALL VALVE"
1411 PRINT "  *****  2 MINUTE BOILING, ACTIVATED BY DRAWING VACUUM *******"
1412 PRINT "  *****  OVER THE UPPER GAS SPACE IS BEING INITIATED ******"
1414 PRINT "************************************************"
1415 PRINT "* DO YOU CLOSE WATER INLET AND OUTLET VALVE?    *"
1416 PRINT "* DO YOU OPEN UPPER VALVE AND VAC VALVE?        *"
1422 PRINT "* DO YOU WANT CONTINUE THE EXPERIMENT? Y OR N? *"
1424 PRINT "************************************************"
1426 INPUT ANS$
1428 IF (ANS$="Y" OR ANS$="y") THEN GOTO 1465
1430 GOTO 897
1470 TIM%(1)=1
1480 CALL KDTIMER'(TIM%(),"NT","")
1490 CALL KDTIMERRD'(TM#())
1500 CALL KDPAUSE'(PTIMEC%,"SEC")
1510 CALL FGREAD'("CJN,UWT,UFT,LGT,LMT,LFT","NONE", SIG1!(),"C.THCU.K","NT")
1520 CALL FGREAD'("CJN,LWT,UGT","NONE", SIG2!(),"C.THCU.E","NT")
1530 CALL FGREAD'("UGP,LGP","NONE", SIG3!(),"C.VOLTS","NT")
```

```
1540 REM ************ PRINT DATA *******
1550 UFT1=SIG1!(2): LWT1=SIG2!(1): UWT1=SIG1!(1):UWAVG=0.5*(UWT1+LWT1)
1560 UGP1=SIG3!(0)*20*6.8948E-2 : LGP1=SIG3!(1)*20*6.8948E-2: UGT1=SIG2!(2)
1570 LGT1=SIG1!(3): LMT1=SIG1!(4): LFT1=SIG1!(5)
1572 PRINT "CONTROL THE VACUUM VALVE"
1580 PRINT "UWT,LWT,UGT,UFT,UGP ARE ";UWT1;LWT1;UGT1;UFT1;UGP1;"bar"
1582 PRINT "LFT1;LMT1;LGT1;LGP1";LFT1;LMT1;LGT1;LGP1;" bar"
1584 IF( UFT1>UFSETPT+UFDT AND UHST%=1) THEN GOSUB 4000
1586 IF( UFT1<UFSETPT-UFDT AND UHST%=0) THEN GOSUB 5000
1588 IF( LFT1>LFSETPT+LFDT AND LHST%=1) THEN GOSUB 4500
1590 IF( LFT1<LFSETPT-LFDT AND LHST%=0) THEN GOSUB 5500
1592 TK=UWT1+273.15
1593 X1=10.81166+8.897199E-3*TK-1.93160E-5*TK*TK+1.341150E-8*TK*TK*TK-
4127.204/(TK-32.82)
1594 PSAT=EXP(X1)
1597 IF TM#(1)*IR%/1000 < BOILT GOTO 1490
1598 REM
1600 PRINT "  ***  INDUCED BOILING COUNTDOWN TIME IS OVER "
1610 PRINT "BEEPING TO REMIND OPERATOR TO SHUT UPPER BALL VALVE
1612 PRINT " MANUALLY WITHIN ONE MINUTE
1614 PRINT "************************************************"
1615 PRINT "* DO YOU CLOSE UPPER VALVE AND VAC VALVE?       *"
1616 PRINT "* DO YOU CHECK THE VOLAGE OF MBV? IS IT 12 V?   *"
1622 PRINT "* DO YOU WANT CONTINUE THE EXPERIMENT? Y OR N? *"
1624 PRINT "************************************************"
1626 INPUT ANS$
1628 IF (ANS$="Y" OR ANS$="y") THEN GOTO 1630
1629 GOTO 1411
1645 CALL BGWRITE'("AOVCLOSE%",AOV$,1,1,"NT","AOVSTAT2")
1660 PRINT "CLOSE UPPER BALL VALVE MANUALLY"
1934 PRINT " *   A 60 SECONDS COUNTDOWN TIME IS BEING STARTED TO ACQUIRE   * "
1936 PRINT " *   DATA FOR CALCULATING THE LOWER ARGON MASS AND FOR         * "
1938 PRINT " *   ESTABLISHING INITIAL CONDITIONS                          * "
1940 PRINT " ************************************************************ "
2030 PRINT " ****** ACQUIRE DATA FOR COUNTDOWN *******"
2040 PRINT " ****** PHASE ON BACKGROUND GO **********"
 2050 REM ****** ACQUIRE UPPER DATA ******
2052 TIM%(4)=1
2054 CALL KDTIMER'(TIM%(),"NT","")
2060 CALL BGREAD'("UWHEAT3A",NDP3!,CJUWLWT$,BINT3%,"NONE",1,"NT","UWHDAT3A")
2070 CALL BGREAD'("UWHEAT3B",NDP3!,CJUGT$,BINT3%,"NONE",1,"NT","UWHDAT3B")
2080 CALL BGREAD'("UWHEAT3C",NDP3!,CJUFT$,BINT3%,"NONE",1,"NT","UWHDAT3C")
2090 CALL BGREAD'("UWHEAT3D",NDP3!,UGP$,BINT3%,"NONE",1,"NT","UWHDAT3D")
2100 REM  ****** ACQUIRE LOWER DATA  ********
2120 CALL BGREAD'("LDAT2A",NDP3!,CJLGT$,BINT3%,"NONE",1,"NT","LDATA2A")
2130 CALL BGREAD'("LDAT2B",NDP3!,CJLMT$,BINT3%,"NONE",1,"NT","LDATA2B")
2140 CALL BGREAD'("LDAT2C",NDP3!,LGP$,BINT3%,"NONE",1,"NT","LDATA2C")
2142 CALL BGREAD'("LDAT2D",NDP3!,LFT$,BINT3%,"NONE",1,"NT","LDATA2D")
2144 CALL KDTIMERRD'(TM#())
2146 IF TM#(4)*IR%/1000 < RCDT GOTO 2144
2147 CALL ARLASTP'("LDAT2D",LP3!)
2200 REM
2210 PRINT : PRINT "  ***  COUNTDOWN TIME IS OVER******"
2220 PRINT "  ***  THE MAIN BALL VALVE IS BEING OPENED ****"
2221 REM
2222 CALL ARLASTP'("LDAT2C",LP3!)
2230 CALL BGWRITE'("MBVOPEN%",MBV$,1,1,"NT","MBVSTAT1")
2240 CALL BGHALT'("UWHDAT3A,UWHDAT3B,UWHDAT3C,UWHDAT3D","NT","HALT3")
2250 CALL BGHALT'("LDATA2A,LDATA2B,LDATA2C,LDATA2D","NT","HALT4")
2290 PRINT : PRINT " ****** ACQUIRING DATA FOR REACTION****"
2300 PRINT " ****** PHASE ON BACKGROUND GO ****"
2310 REM ****** ACQUIRE UPPER DATA ******
2313 TIM%(5)=1
2314 CALL KDTIMER'(TIM%(),"NT","")
2315 CALL KDTIMERRD'(TM#())
2320 CALL BGREAD'("UWHEAT4A",NDP4!,CJUWLWT$,BINT4%,"NONE",1,"NT","UWHDAT4A")
2330 CALL BGREAD'("UWHEAT4B",NDP4!,CJUGT$,BINT4%,"NONE",1,"NT","UWHDAT4B")
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2340 CALL BGREAD'("UWHEAT4C",NDP4!,CJUFT$,BINT4%,"NONE",1,"NT","UWHDAT4C")
2350 CALL BGREAD'("UWHEAT4D",NDP4!,UGP$,BINT4%,"NONE",1,"NT","UWHDAT4D")
2360 REM  ****** ACQUIRE LOWER DATA  ********
2363 CALL BGREAD'("LDAT3A",NDP4!,CJLGT$,BINT4%,"NONE",1,"NT","LDATA3A")
2364 CALL BGREAD'("LDAT3B",NDP4!,CJLMT$,BINT4%,"NONE",1,"NT","LDATA3B")
2365 CALL BGREAD'("LDAT3C",NDP4!,LGP$,BINT4%,"NONE",1,"NT","LDATA3C")
2366 CALL BGREAD'("LDAT3D",NDP4!,LFT$,BINT4%,"NONE",1,"NT","LDATA3D")
2430 CALL KDTIMERRD'(TM#())
2440 IF TM#(5) * IR%/1000 < RTIME% GOTO 2430
2442 CALL ARLASTP'("LDAT3D",LP4!)
2444 CALL BGHALT'("UWHDAT4A,UWHDAT4B,UWHDAT4C,UWHDAT4D","NT","HALT4")
2446 CALL BGHALT'("LDATA3A,LDATA3B,LDATA3C,LDATA3D","NT","HALT5")
2460 PRINT " ***  REACTION IS OVER "
2470 PRINT " ***  THE MAIN BALL VALVE IS BEING CLOSED "
2480 PRINT " ***  LIQUID METAL HEATER IS BEING TURNED OFF "
2490 PRINT " ***  UPPER WATER HEATER  IS BEING TURNED OFF "
2500 PRINT " ***  ARGON OUTLET VALVE IS BEING OPENED 2 SEC AFTER BALL VALVE
CLOSURE"
2510 PRINT " ***  SETTING-UP TO ACQUIRE UPPER CHAMBER DATA UNTIL EQUILIBRIUM"
2520 PRINT " ***  IS ACHIEVED "
2540 TIM%(6)=1
2550 CALL KDTIMER'(TIM%(),"NT","")
2560 CALL BGWRITE'("MBVCLOSE%",MBV$,1,1,"NT","MBVSTAT3")
2565 CALL BGWRITE'("AOVOPEN%",AOV$,1,1,"NT","AOVSTAT3")
2570 CALL KDTIMERRD'(TM#())
2580 IF TM#(6)*IR% < 2*DTSV GOTO 2570
2600 CALL BGWRITE'("LMHOFFF%",LMH$,1,1,"NT","LMHSTAT3")
2610 CALL BGWRITE'("UWHOFFF%",UWH$,1,1,"NT","UWHSTAT3")
2670 PRINT " **** SETTING UP TO ACQUIRE DATA UNTIL EQUILIBRIUM IS ATTAINED"
2680 PRINT " ****** IN THE UPPER CHAMBER"
2690 REM ****** ACQUIRE UPPER DATA ******
2691 TIM%(7) = 1
2692 CALL KDTIMER'(TIM%(),"NT","")
2693 CALL KDTIMERRD'(TM#())
2700 CALL BGREAD'("UWHEAT5A",NDP5!,CJUWLWT$,BINT5%,"NONE",1,"NT","UWHDAT5A")
2710 CALL BGREAD'("UWHEAT5B",NDP5!,CJUGT$,BINT5%,"NONE",1,"NT","UWHDAT5B")
2720 CALL BGREAD'("UWHEAT5C",NDP5!,CJUFT$,BINT5%,"NONE",1,"NT","UWHDAT5C")
2730 CALL BGREAD'("UWHEAT5D",NDP5!,UGP$,BINT5%,"NONE",1,"NT","UWHDAT5D")
2740 REM  ****** ACQUIRE LOWER DATA  ********
2750 CALL BGREAD'("LDAT4A",NDP5!,CJLGT$,BINT5%,"NONE",1,"NT","LDATA4A")
2751 CALL BGREAD'("LDAT4B",NDP5!,CJLMT$,BINT5%,"NONE",1,"NT","LDATA4B")
2753 CALL BGREAD'("LDAT4C",NDP5!,LGP$,BINT5%,"NONE",1,"NT","LDATA4C")
2754 CALL BGREAD'("LDAT4D",NDP5!,LFT$,BINT5%,"NONE",1,"NT","LDATA4D")
2795 CALL KDTIMERRD'(TM#())
2797 IF TM#(7)*IR%/1000 < EQT GOTO 2795
2798 CALL ARLASTP'("LDAT4D",LP5!)
2799 CALL BGHALT'("UWHDAT5A,UWHDAT5B,UWHDAT5C,UWHDAT5D","NT","HALT6")
2800 CALL BGHALT'("LDATA4A,LDATA4B,LDATA4C,LDATA4D","NT","HALT7")

2801 REM
2802 PRINT "          REACTION IS OVER FOLKS!  "
2810 PRINT " ****************************************************"
2820 PRINT " *   TRANSFERRIN ALL KDAC DATA ARRAYS TO DISK        *"
2830 PRINT " ****************************************************"
2840 REM
2850 REM  ******  REACTION IS OVER
3220 PRINT
3230 PRINT " LITHIUM-LEAD TEST NO ", ITESTNO, " IS OVER"
3240 PRINT " RELOAD THE LOWER CHAMBER AND BEGIN A NEW TEST"
3260 PRINT "TRANSFERRING DATA ARRAYS FOR PHASES 3,4 AND 5 TO DISK FILE"
3270 REM

3280 OPEN "COUNTD.DAT" FOR OUTPUT AS #1
3290 OPEN "REACTION.DAT" FOR OUTPUT AS #2
3300 OPEN "EQUIL.DAT" FOR OUTPUT AS #3
3301 PRINT "LP3,LP4,LP5";LP3!;LP4!;LP5!
3302 FOR I=1 TO LP3
```
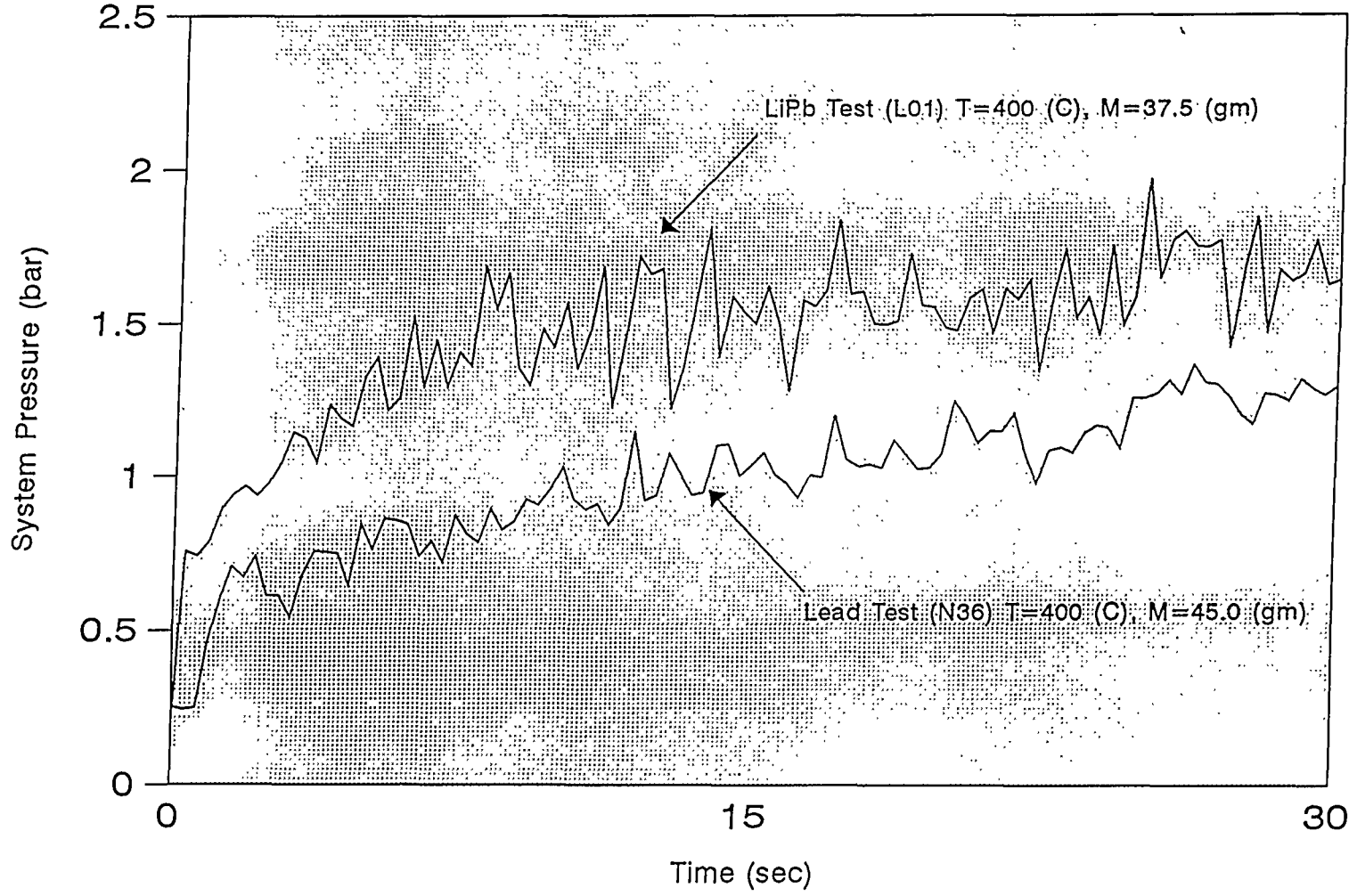

```
3304 CALL ARGET'("UWHEAT3A",I!,I!,UWT$,1,UWH1A!(),"C.THCU.K")
3306 CALL ARGET'("UWHEAT3A",I!,I!,LWT$,1,UWH1B!(),"C.THCU.E")
3308 CALL ARGET'("UWHEAT3B",I!,I!,UGT$,1,UWH1C!(),"C.THCU.E")
3310 CALL ARGET'("UWHEAT3C",I!,I!,UFT$,1,UWH1D!(),"C.THCU.K")
3312 CALL ARGET'("UWHEAT3D",I!,I!,UGP$,1,UWH1E!(),"C.VOLTS")
3314 CALL ARGET'("LDAT2A",I!,I!,LGT$,1,LGH1A!(),"C.THCU.K")
3316 CALL ARGET'("LDAT2B",I!,I!,LMT$,1,LGH1B!(),"C.THCU.K")
3318 CALL ARGET'("LDAT2C",I!,I!,LGP$,1,LGH1C!(),"C.VOLTS")
3322 UFT1=UWH1D!(0): LWT1=UWH1B!(0): UWT1=UWH1A!(0):UWAVG=0.5*(UWT1+LWT1)
3324 UGP1=UWH1E!(0)*20*6.8948E-2 : LGP1=LGH1C!(0)*20*6.8948E-2: UGT1=UWH1C!(0)
3326 LGT1=LGH1A!(0): LMT1=LGH1B!(0): LFT1=LGH1D!(0):UFT1=UWH1D!(0)
3328 TIME3=BINT3%*(I-1)*IR%/1000
3330 PRINT #1, USING "###.##### "; TIME3; UGT1; LGT1; UWT1;LWT1; LMT1;
UFT1;LFT1;UGP1;LGP1
3332 NEXT I

3340 FOR I=1 TO LP4
3342 CALL ARGET'("UWHEAT4A",I!,I!,UWT$,1,UWH1A!(),"C.THCU.K")
3344 CALL ARGET'("UWHEAT4A",I!,I!,LWT$,1,UWH1B!(),"C.THCU.E")
3346 CALL ARGET'("UWHEAT4B",I!,I!,UGT$,1,UWH1C!(),"C.THCU.E")
3348 'CALL ARGET'("UWHEAT4C",I!,I!,UFT$,1,UWH1D!(),"C.THCU.K")
3350 CALL ARGET'("UWHEAT4D",I!,I!,UGP$,1,UWH1E!(),"C.VOLTS")
3352 CALL ARGET'("LDAT3A",I!,I!,LGT$,1,LGH1A!(),"C.THCU.K")
3354 CALL ARGET'("LDAT3B",I!,I!,LMT$,1,LGH1B!(),"C.THCU.K")
3360 TIME4=BINT4%*(I-1)*IR%/1000
3362 UFT1=UWH1D!(0): LWT1=UWH1B!(0): UWT1=UWH1A!(0):UWAVG=0.5*(UWT1+LWT1)
3364 UGP1=UWH1E!(0)*20*6.8948E-2 : LGP1=LGH1C!(0)*20*6.8948E-2: UGT1=UWH1C!(0)
3366 LGT1=LGH1A!(0): LMT1=LGH1B!(0): LFT1=LGH1D!(0):UFT1=UWH1D!(0)
3368 PRINT #2, USING "###.##### "; TIME4; UGT1; LGT1; UWT1;LWT1; LMT1;
UFT1;LFT1;UGP1;LGP1
3369 NEXT I

3370 FOR I=1 TO LP5
3372 CALL ARGET'("UWHEAT5A",I!,I!,UWT$,1,UWH1A!(),"C.THCU.K")
3374 CALL ARGET'("UWHEAT5A",I!,I!,LWT$,1,UWH1B!(),"C.THCU.E")
3376 CALL ARGET'("UWHEAT5B",I!,I!,UGT$,1,UWH1C!(),"C.THCU.E")
3378 CALL ARGET'("UWHEAT5C",I!,I!,UFT$,1,UWH1D!(),"C.THCU.K")
3380 CALL ARGET'("UWHEAT5D",I!,I!,UGP$,1,UWH1E!(),"C.VOLTS")

3382 REM ****** GET LOWER DATA *******
3384 CALL ARGET'("LDAT4A",I!,I!,LGT$,1,LGH1A!(),"C.THCU.K")
3386 CALL ARGET'("LDAT4B",I!,I!,LMT$,1,LGH1B!(),"C.THCU.K")
3388 CALL ARGET'("LDAT4C",I!,I!,LGP$,1,LGH1C!(),"C.VOLTS")
3392 TIME5=BINT5%*(I-1)*IR%/1000
3393 UFT1=UWH1D!(0): LWT1=UWH1B!(0): UWT1=UWH1A!(0):UWAVG=0.5*(UWT1+LWT1)
3394 UGP1=UWH1E!(0)*20*6.8948E-2 : LGP1=LGH1C!(0)*20*6.8948E-2: UGT1=UWH1C!(0)
3395 LGT1=LGH1A!(0): LMT1=LGH1B!(0): LFT1=LGH1D!(0):UFT1=UWH1D!(0)

3396 PRINT #3, USING "###.##### "; TIME5; UGT1; LGT1; UWT1;LWT1; LMT1;
UFT1;LFT1;UGP1;LGP1
3397 NEXT I
3398 CALL INTOFF

3460 PRINT " THAT'S THE END OF DATA ACQUISITION, FOLKS!"
3480 END

4000 CALL BGWRITE'("UWHOFFF%",UWH$,1,1,"NT","ST1")
4100 UHST%=0
4200 RETURN

4500 CALL BGWRITE'("LMHOFFF%",LMH$,1,1,"NT","ST2")
4600 LHST%=0
4700 RETURN

5000 CALL BGWRITE'("UWHONN%",UWH$,1,1,"NT","ST1")
5100 UHST%=1
5200 RETURN
```

```
5500 CALL BGWRITE'("LMHONN%",LMH$,1,1,"NT","ST1")
5600 LHST%=1
5700 RETURN

6000 CALL BGWRITE'("VACONN%",VAC$,1,1,"NT","ST1")
6100 UPST%=1
6200 RETURN

6500 CALL BGWRITE'("VACOFFF%",VAC$,1,1,"NT","ST1")
6600 UPST%=0
6700 RETURN
```

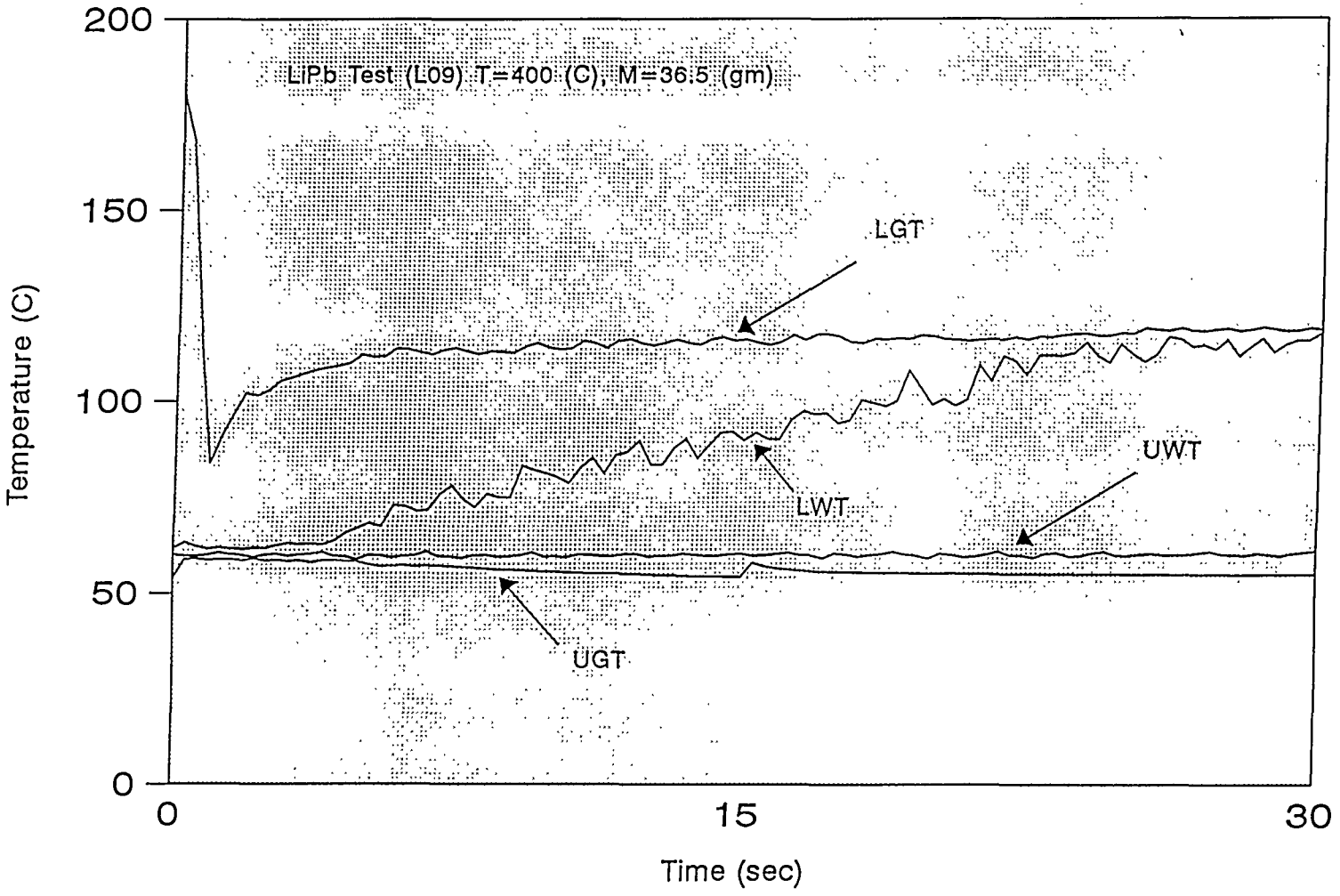
APPENDIX B

GRAPHICAL PRESENTATION OF EXPERIMENTAL RESULTS

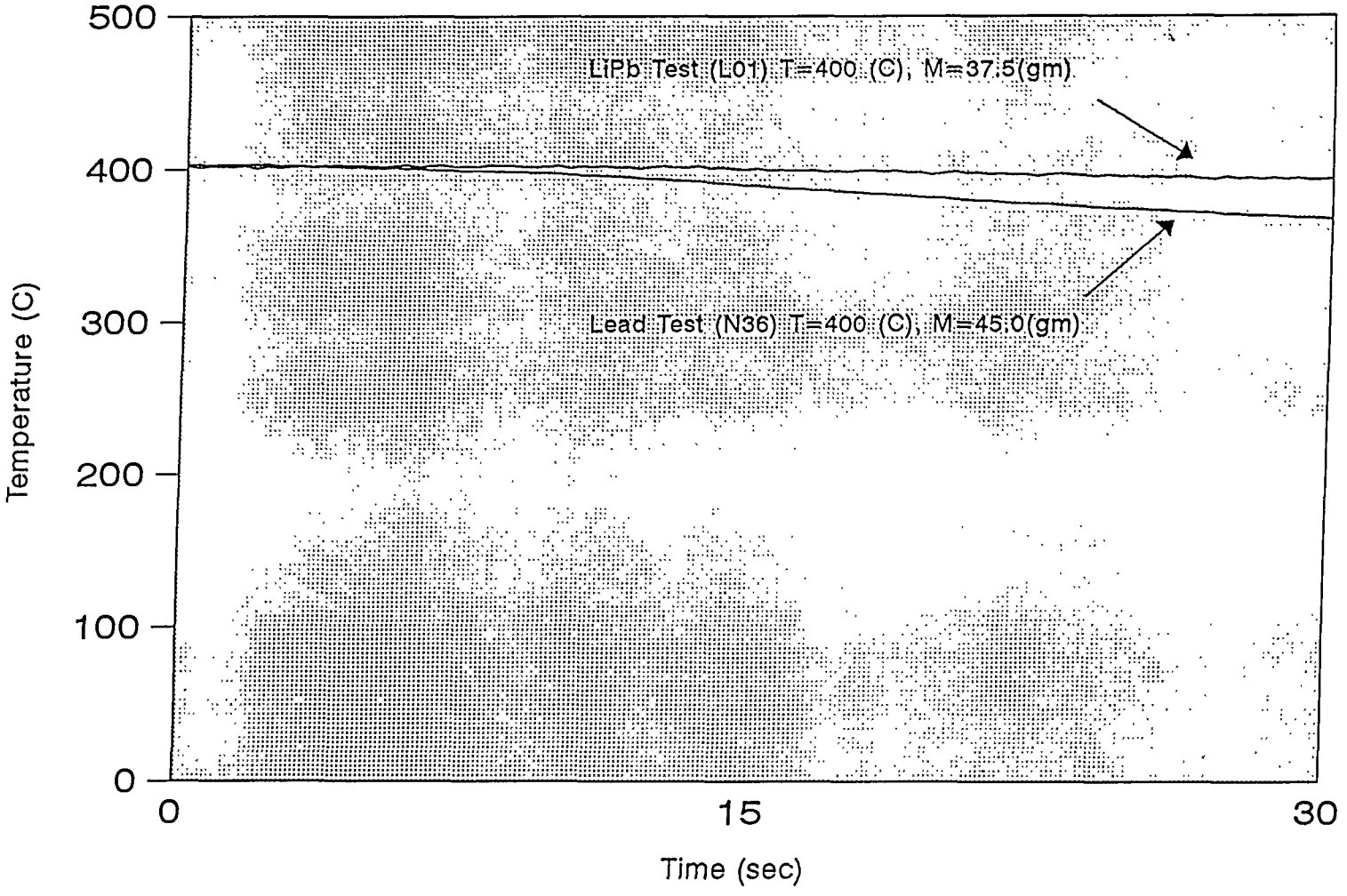
The following 52 graphs contain a complete representation of the data drawn from 16 lithium-lead tests and 5 lead tests. The graphs are listed in the following table. The table gives the page numbers in groups of the test. In each group, the order of the graphs are: 1. System Pressure. 2. Water and Gas Temperature. 3. Liquid Metal Temperature.



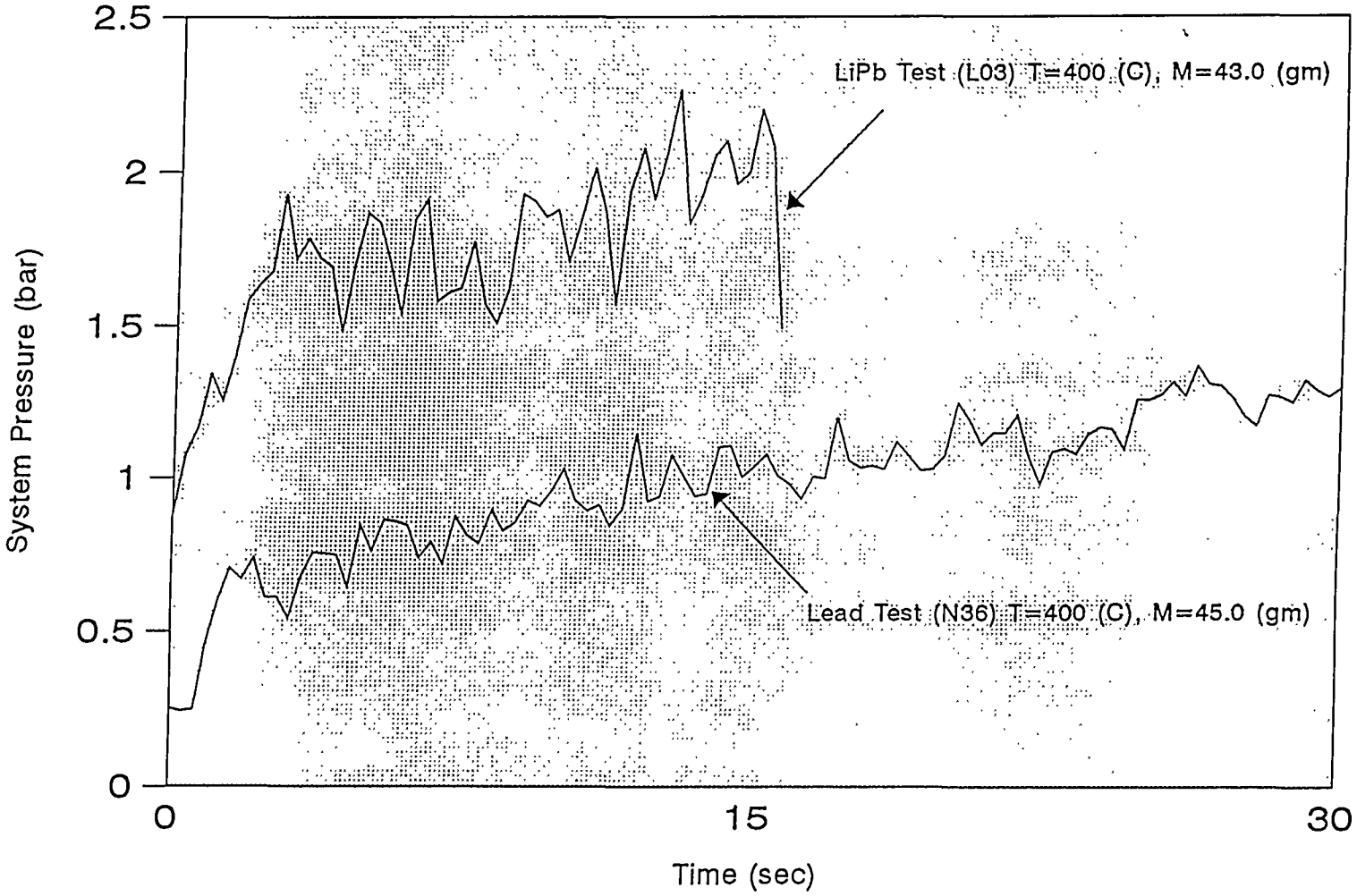
Appendix B Figure 1.1 System Pressure as a Function of Time (L01 & N36)



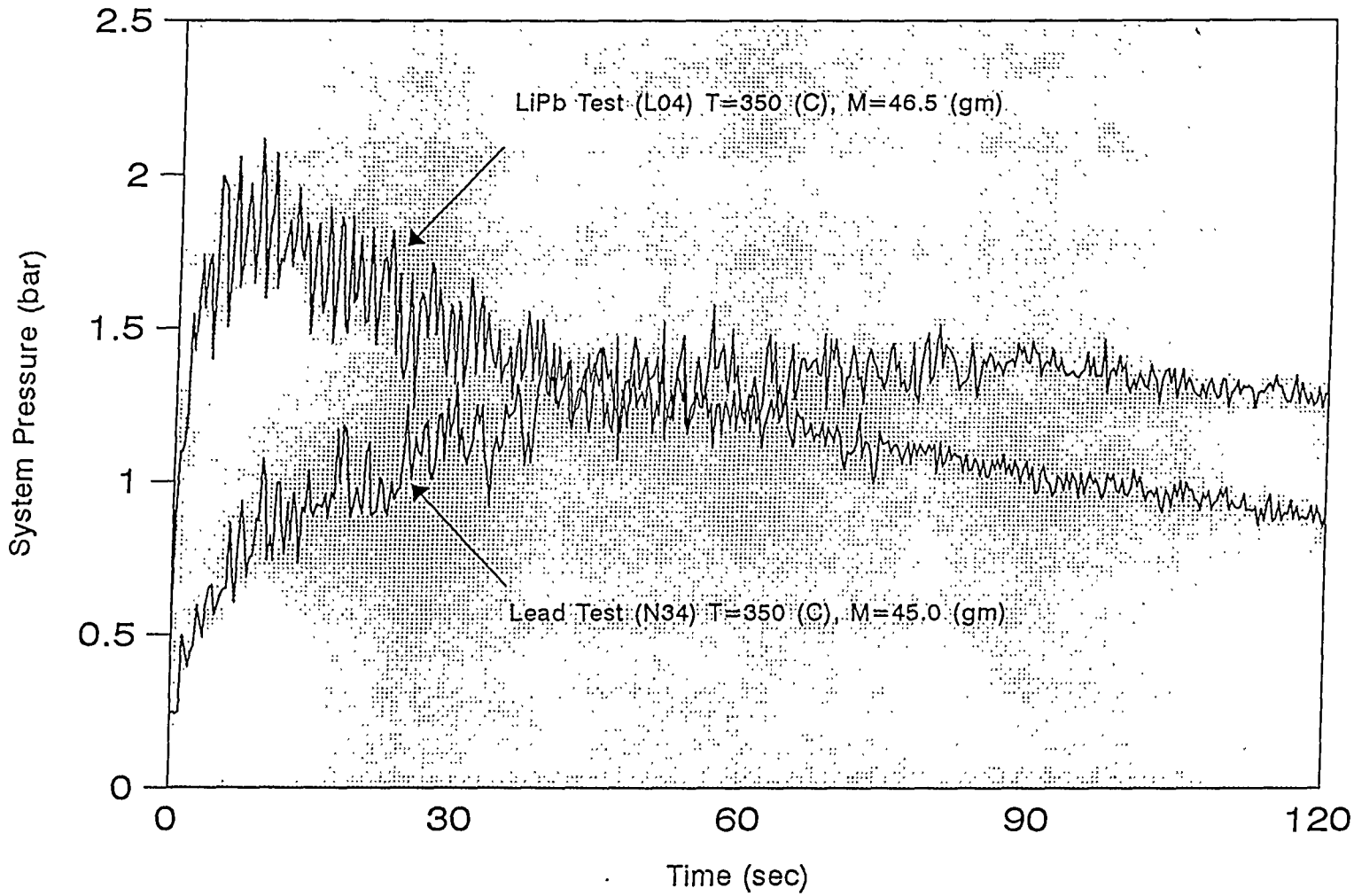
Appendix B Figure 1.2 Gas and Water Temperature as a Function of Time (L01)



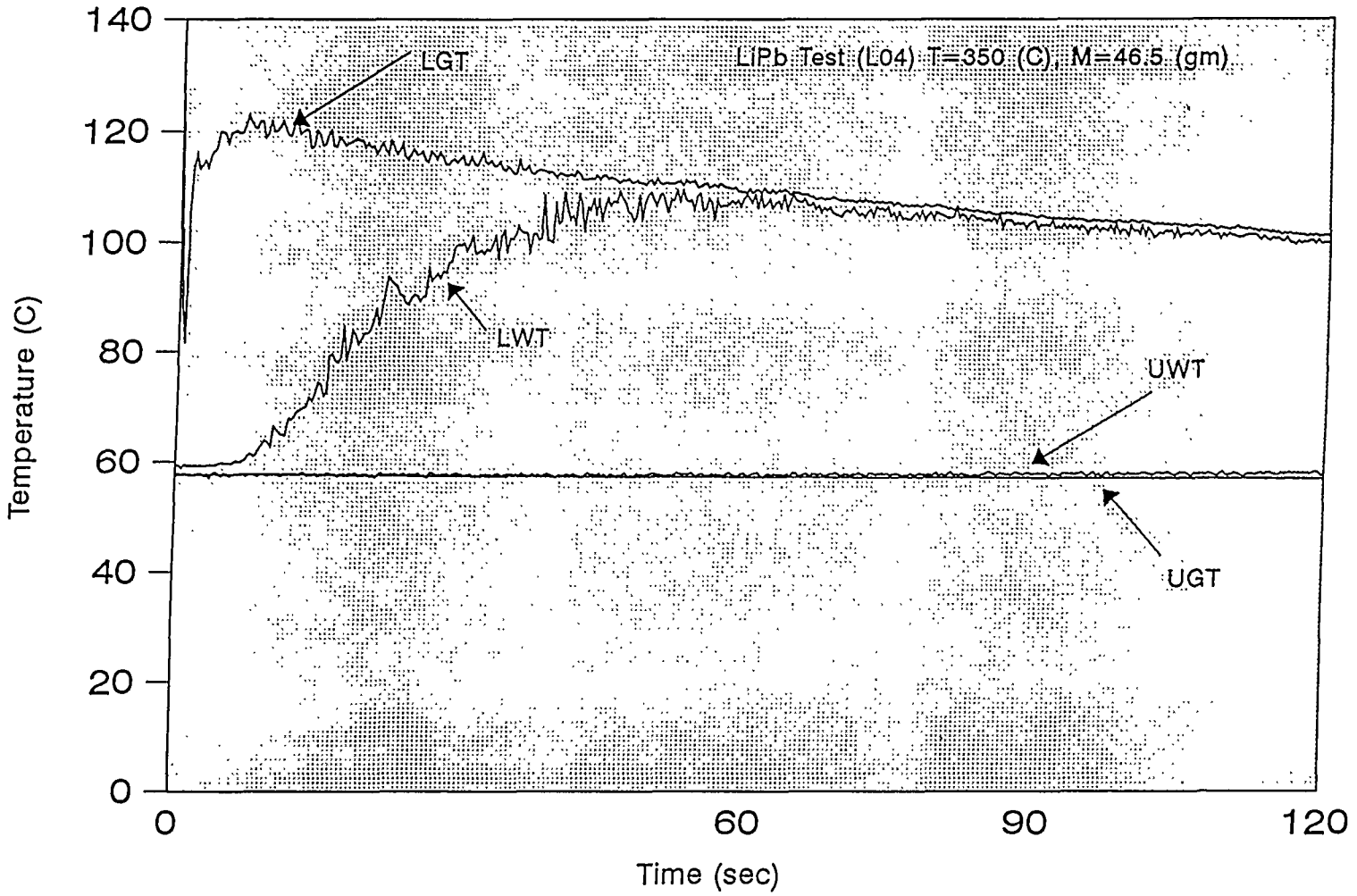
Appendix B Figure 1.3 Liquid Metal Temperature as a Function of Time (L01 & N36)



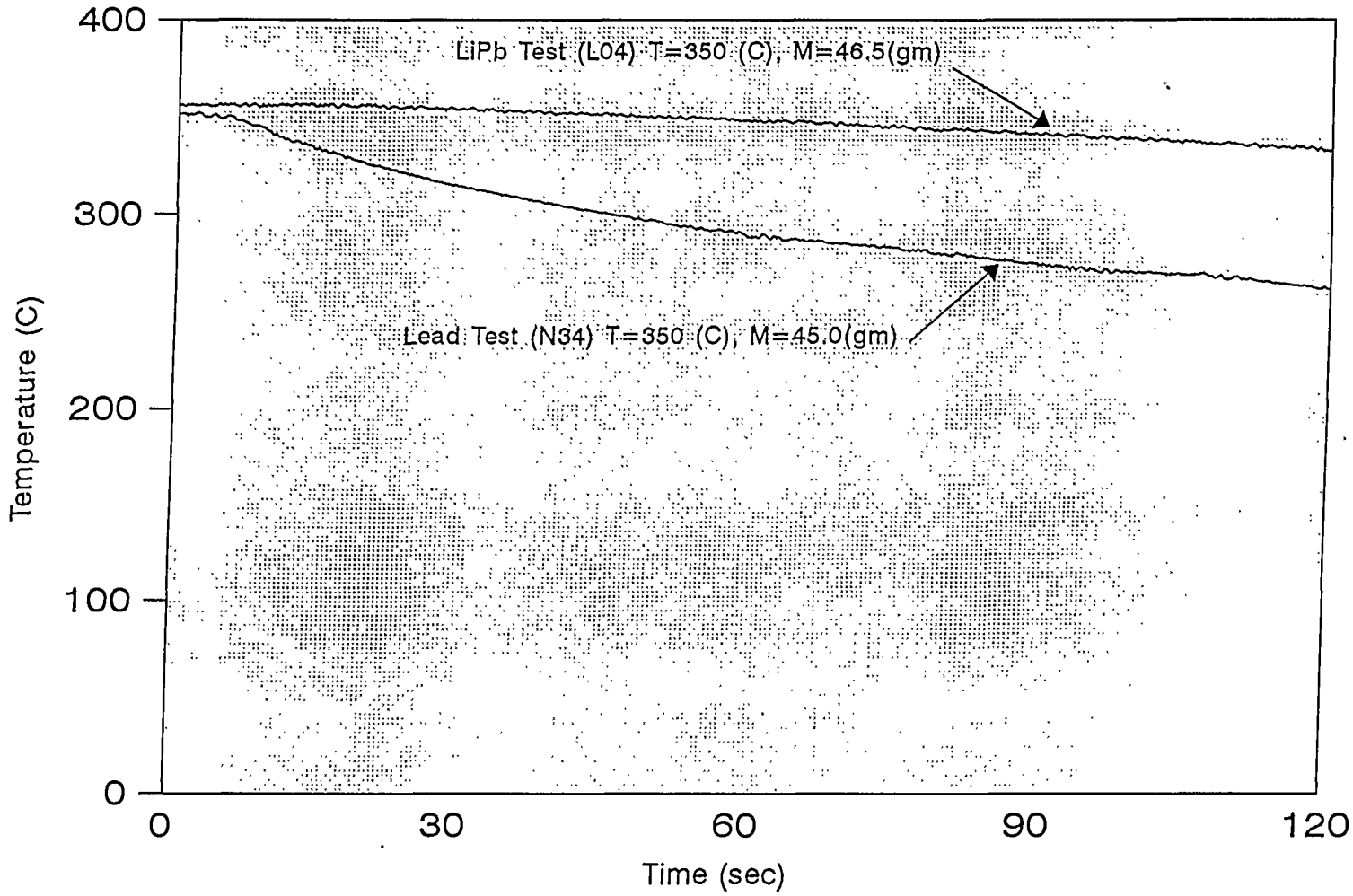
Appendix B Figure 2.1 System Pressure as a Function of Time (L03 & N36)



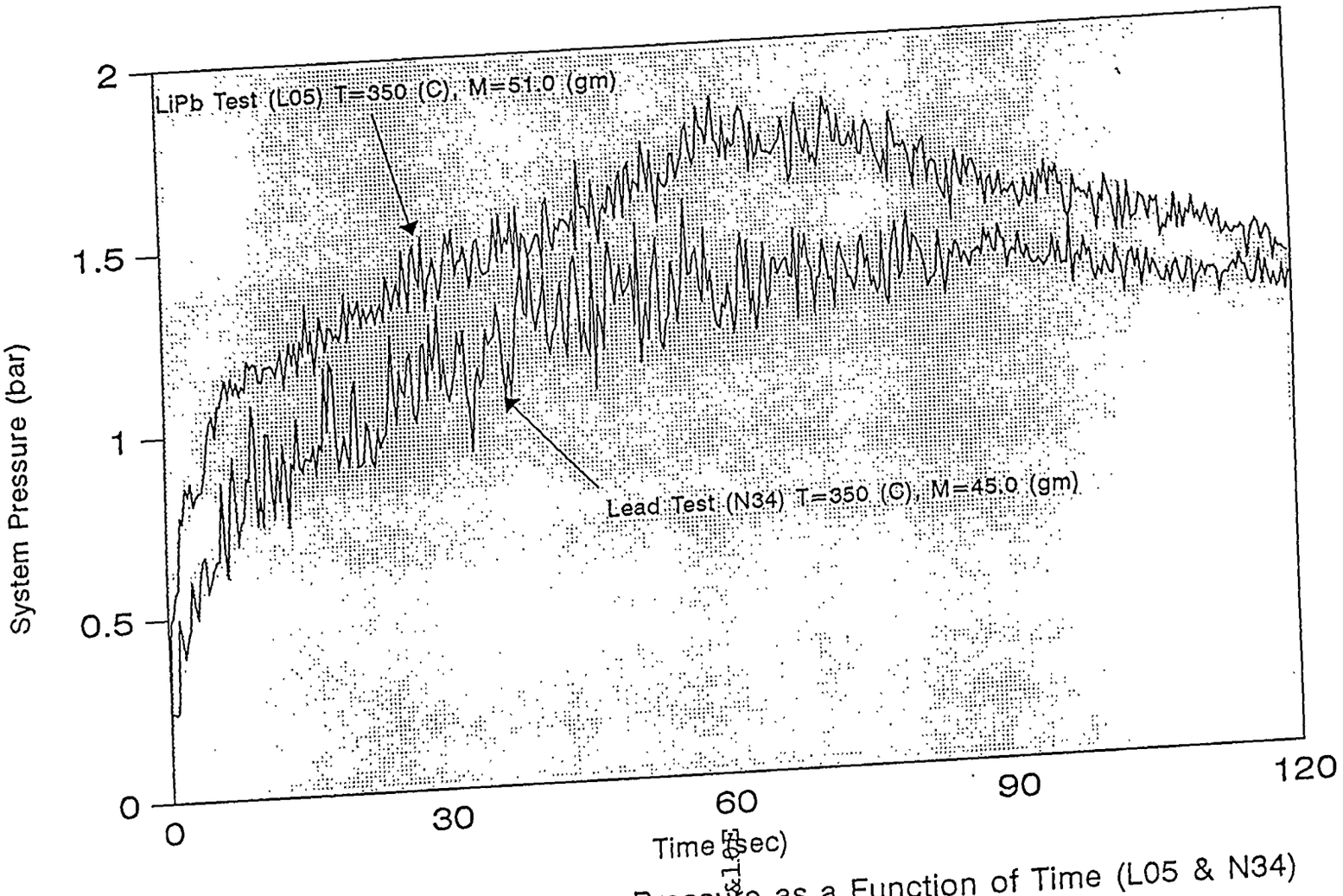
Appendix B Figure 3.1 System Pressure as a Function of Time (L04 & N34)



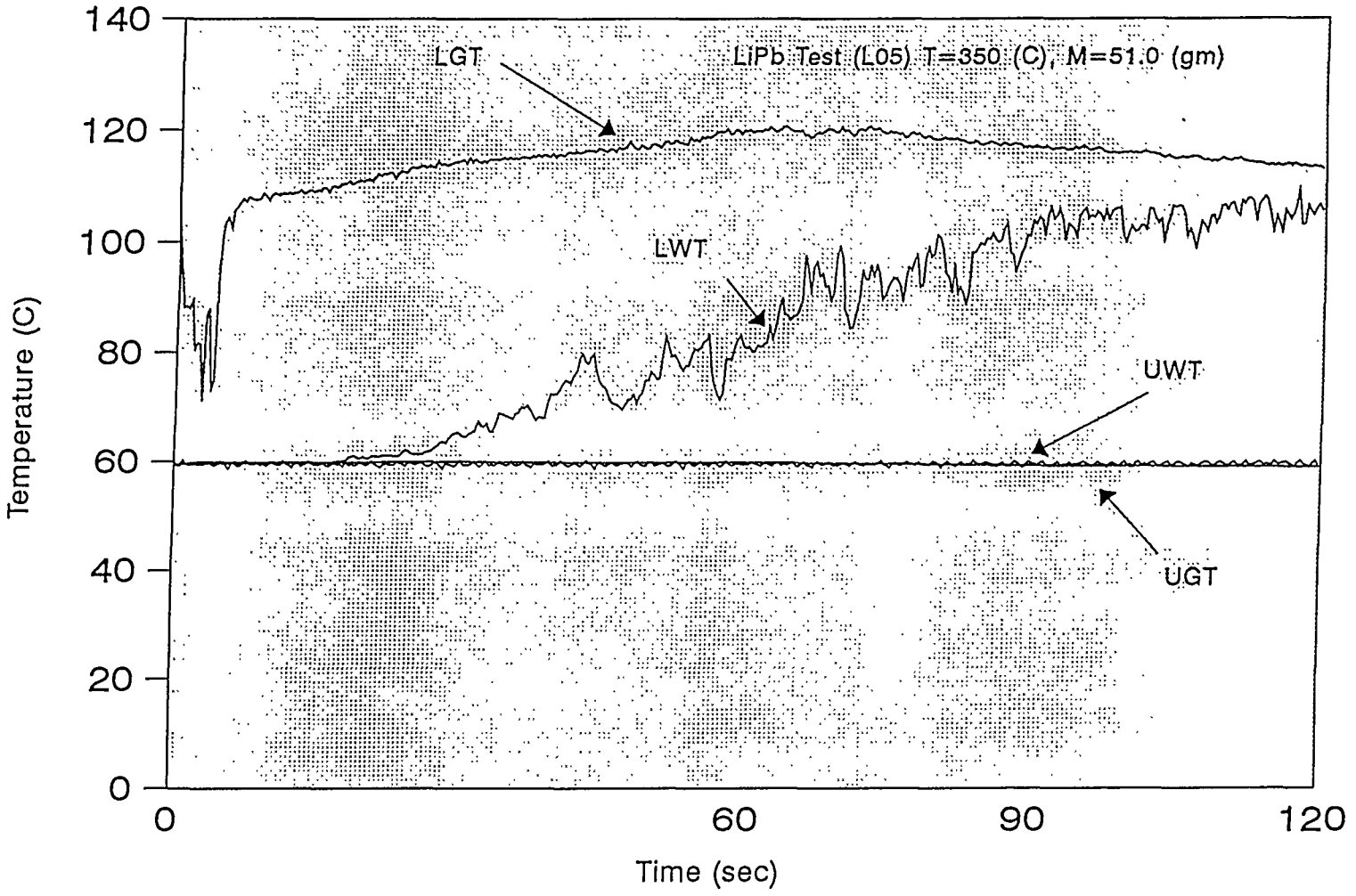
Appendix B Figure 3.2 Gas and Water Temperature as a Function of Time (L04)



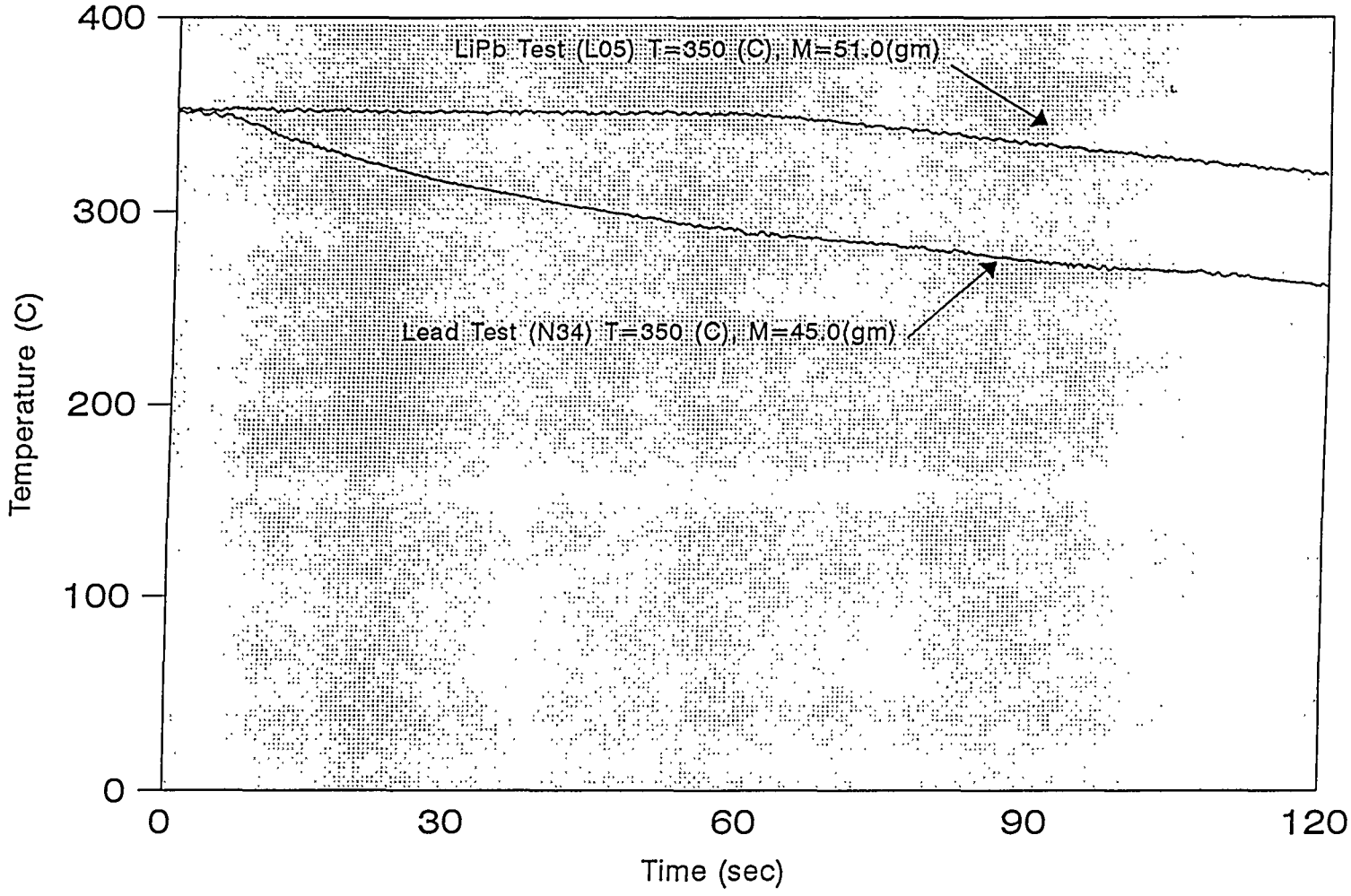
Appendix B Figure 3.3 Liquid Metal Temperature as a Function of Time (L04 & N34)



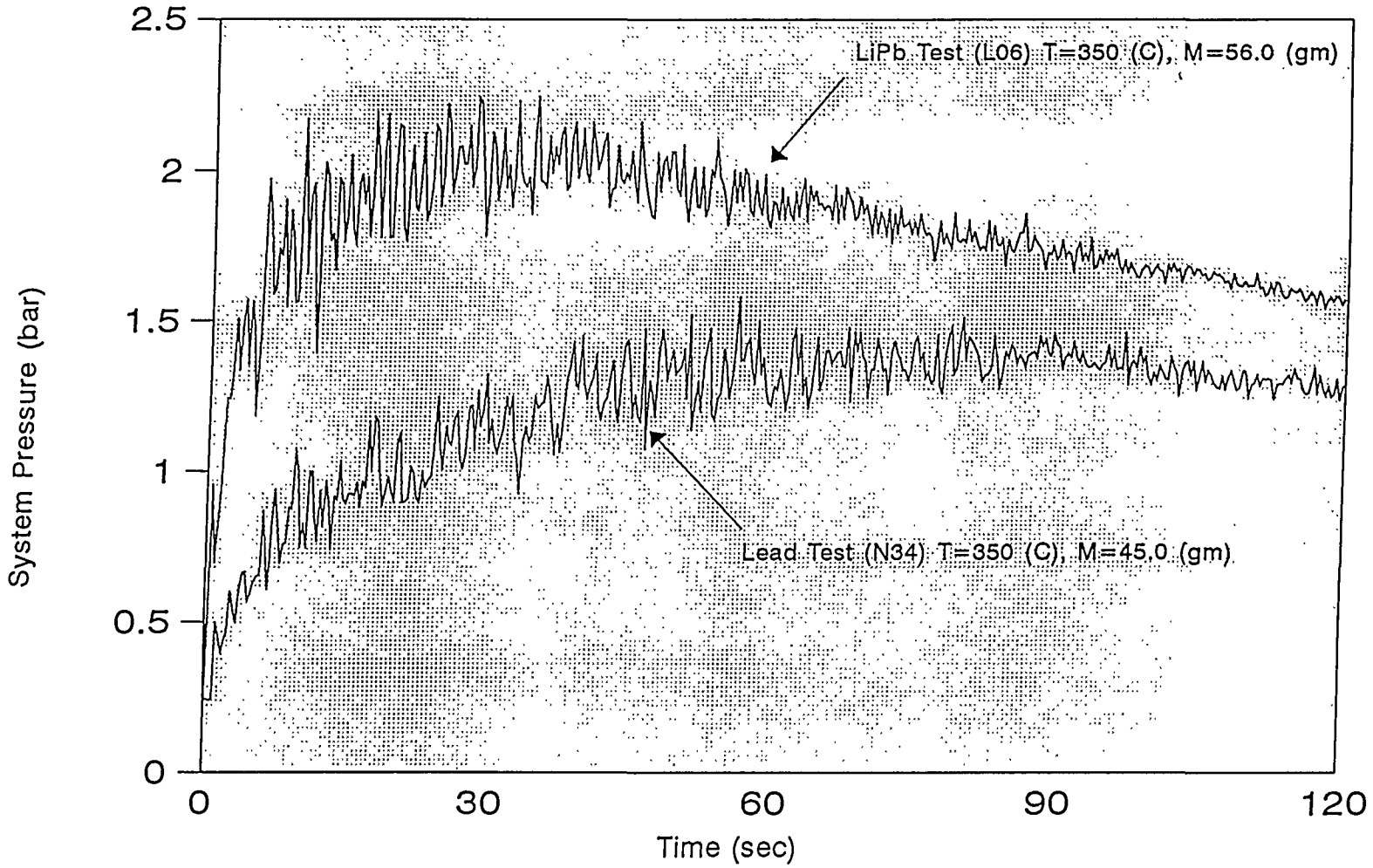
Appendix B Figure 4.1 System Pressure as a Function of Time (L05 & N34)



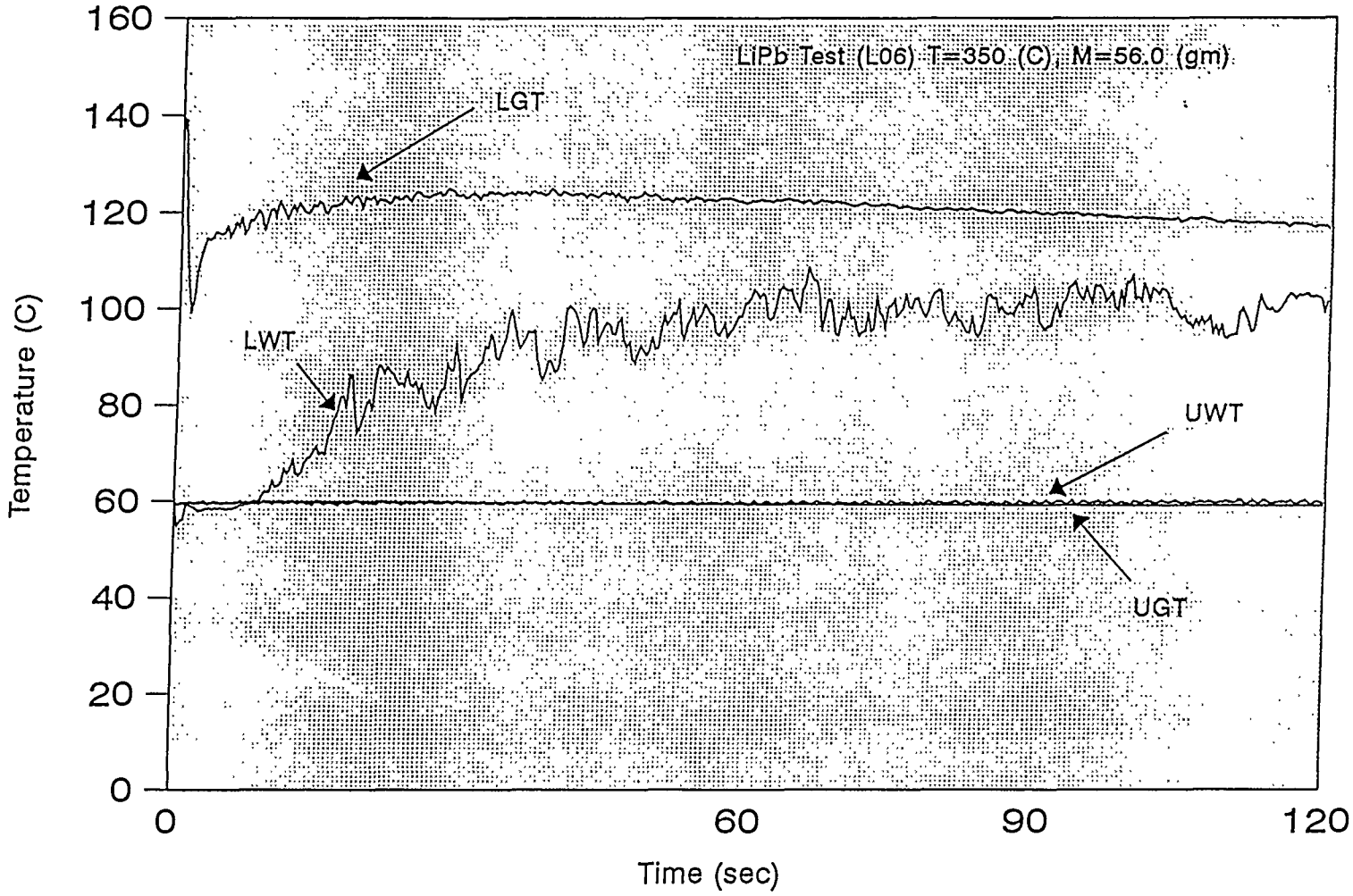
Appendix B Figure 4.2 Gas and Water Temperature as a Function of Time (L05)



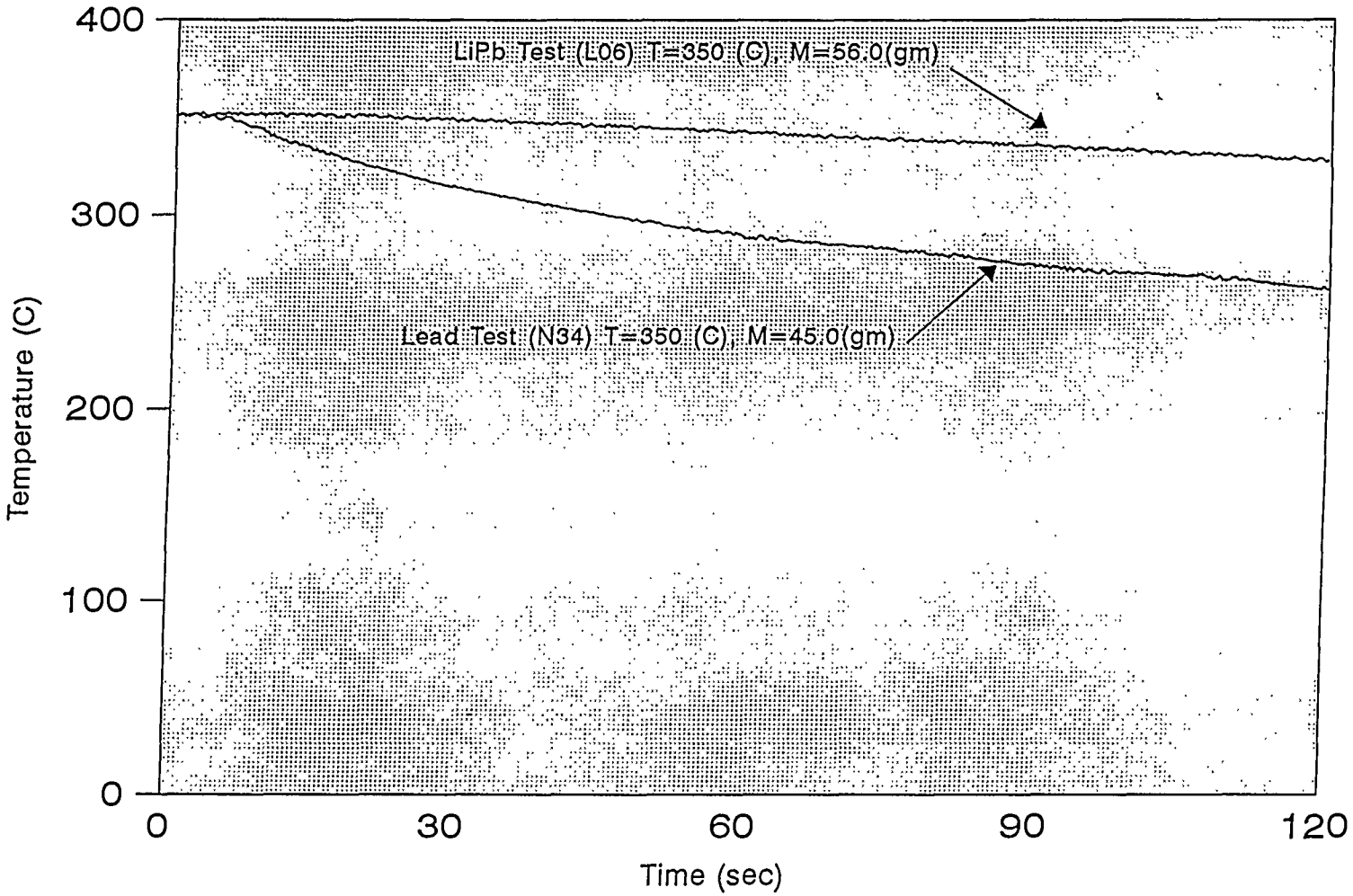
Appendix B Figure 4.3 Liquid Metal Temperature as a Function of Time (L05 & N34)



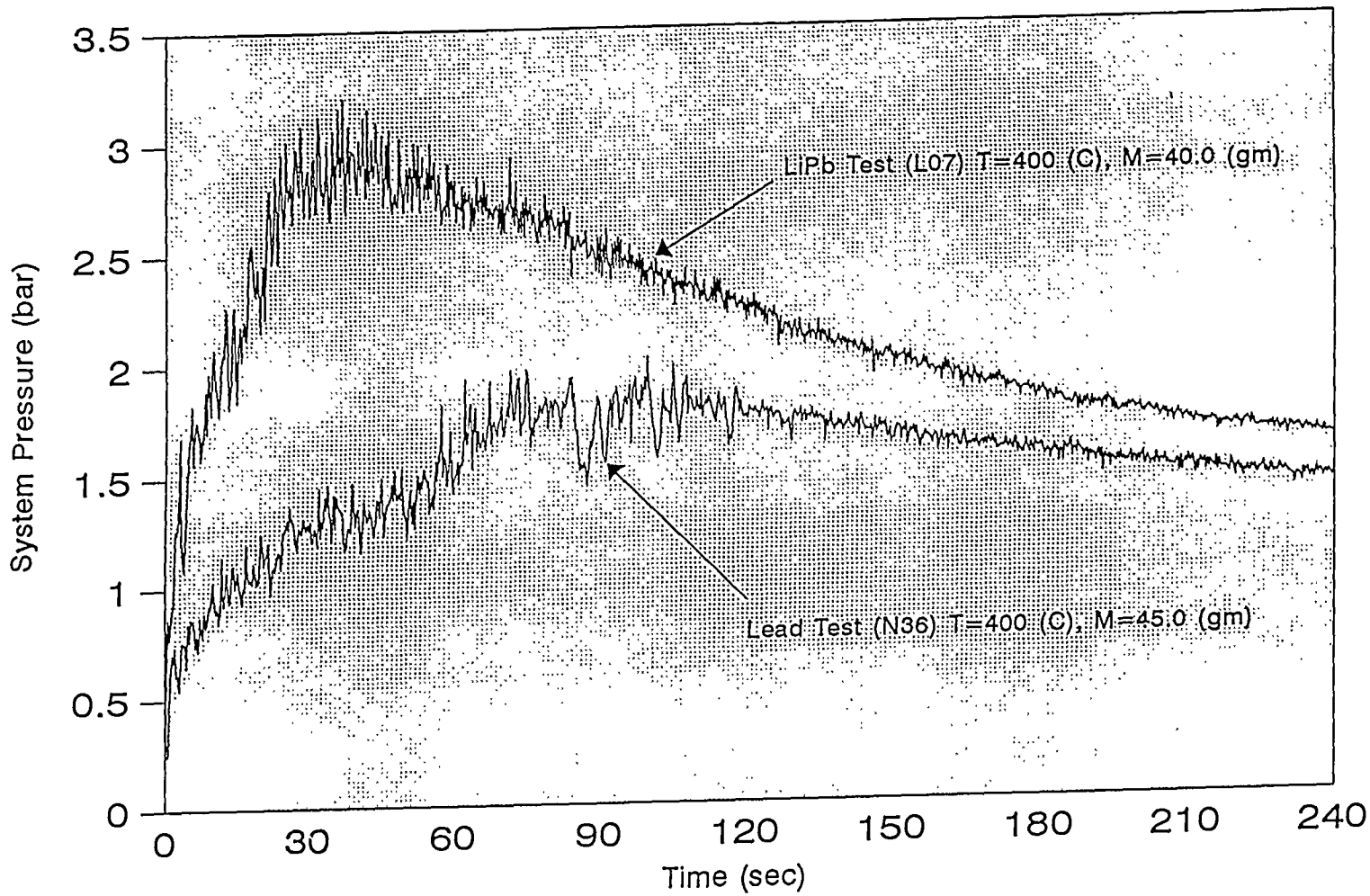
Appendix B Figure 5.1 System Pressure as a Function of Time (L06 & N34)



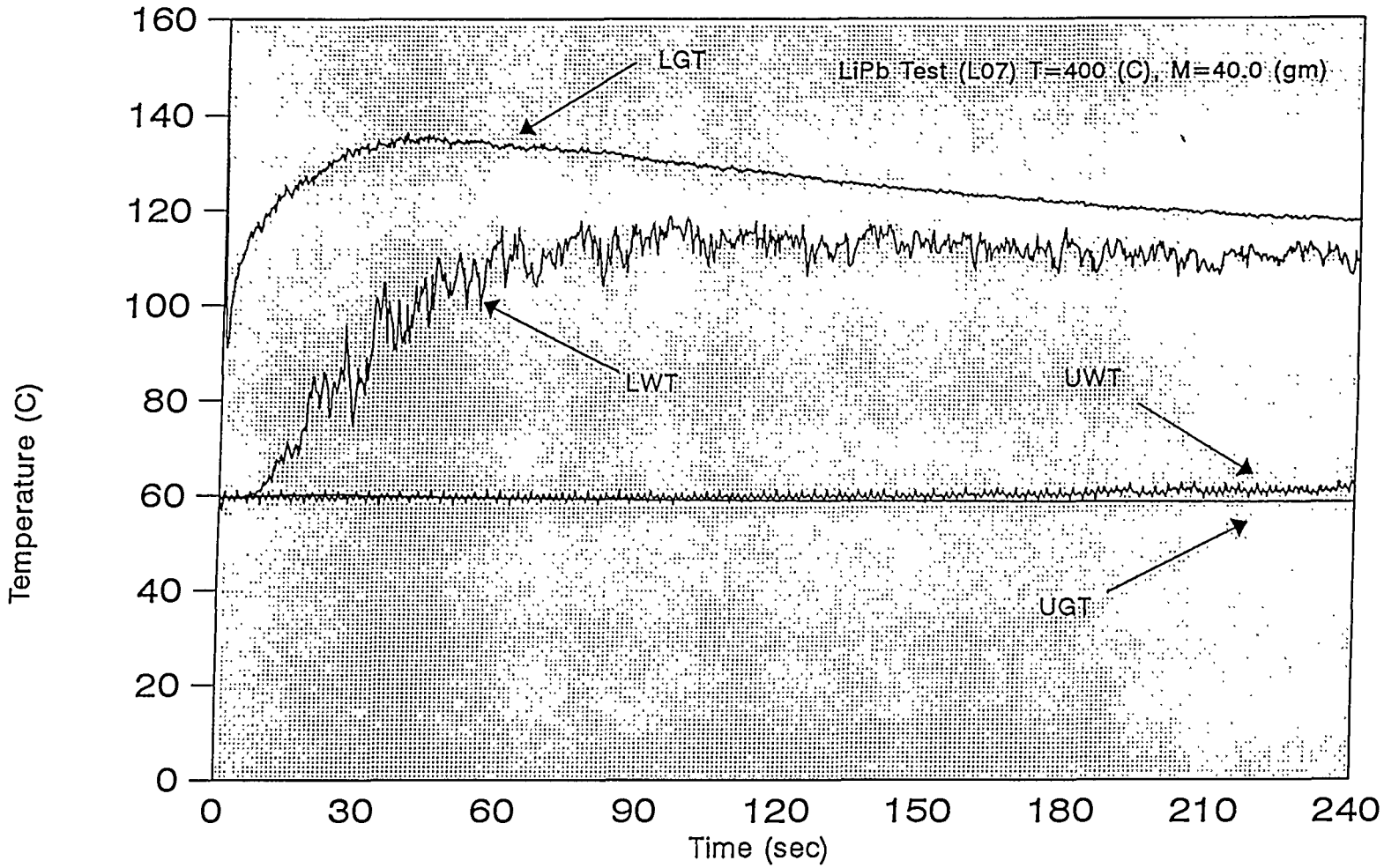
Appendix B Figure 5.2 Gas and Water Temperature as a Function of Time (L06)



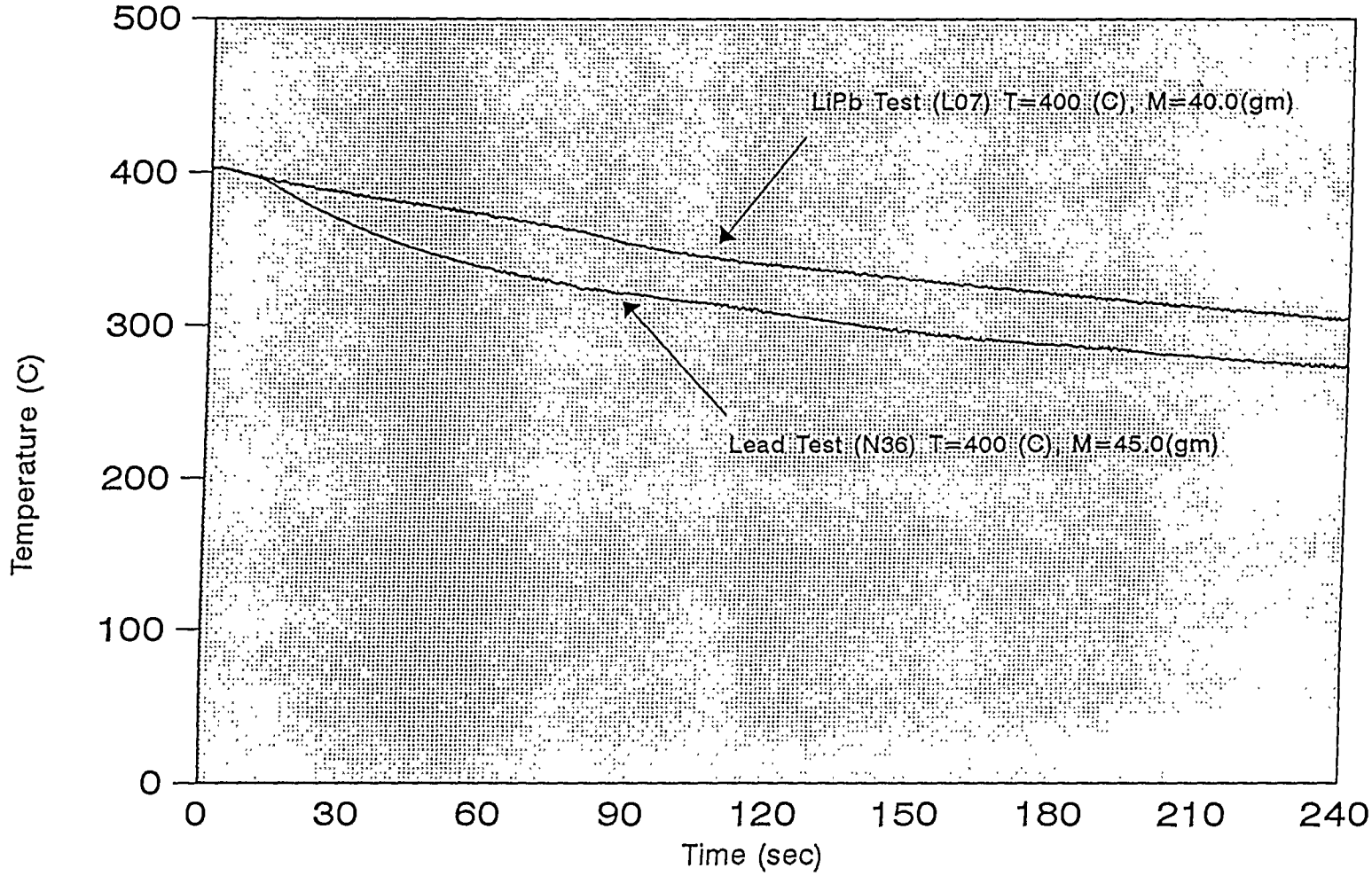
Appendix B Figure 5.3 Liquid Metal Temperature as a Function of Time (L06 & N34)



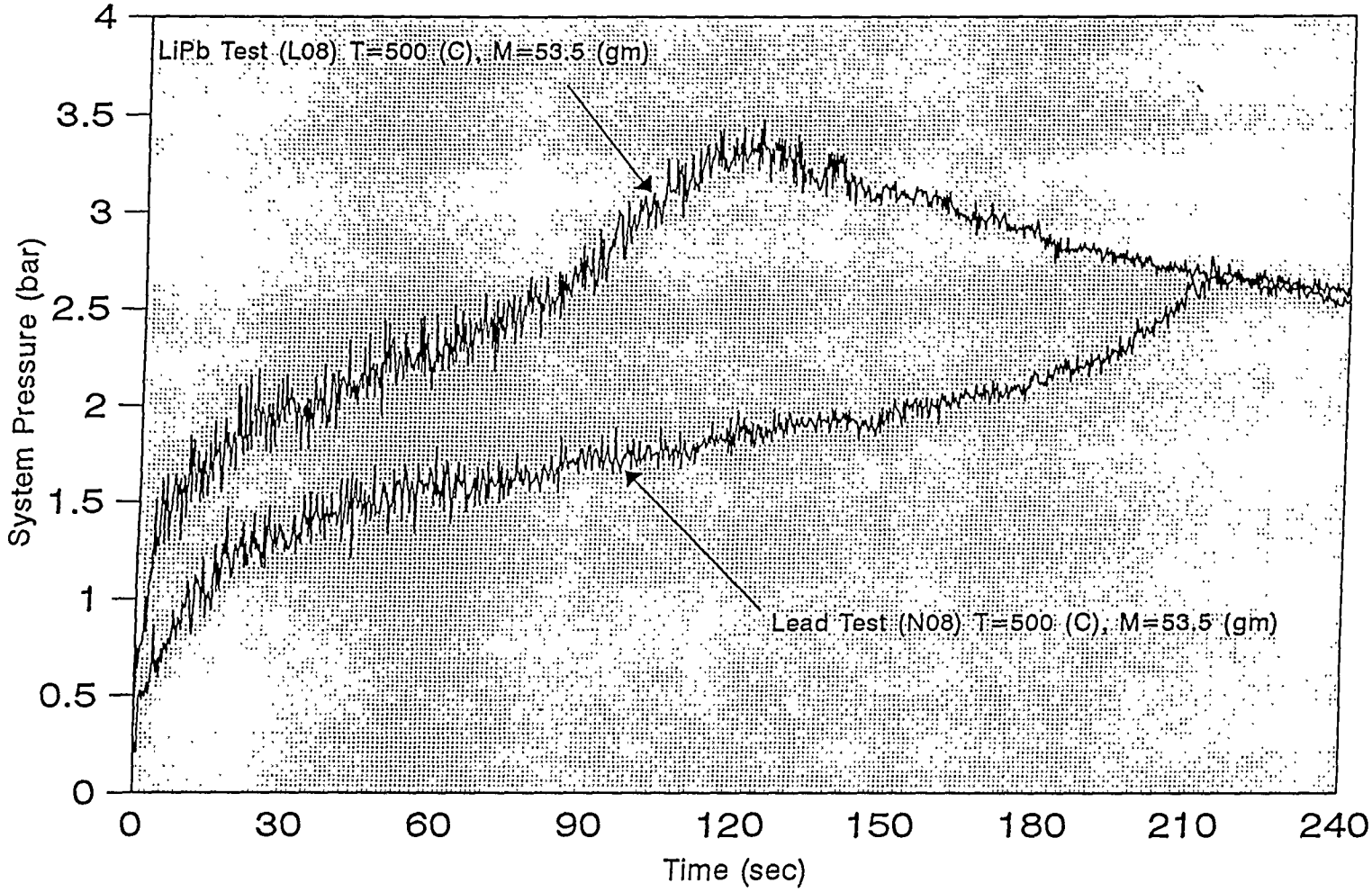
Appendix B Figure 6.1 System Pressure as a Function of Time (L07 & N36)



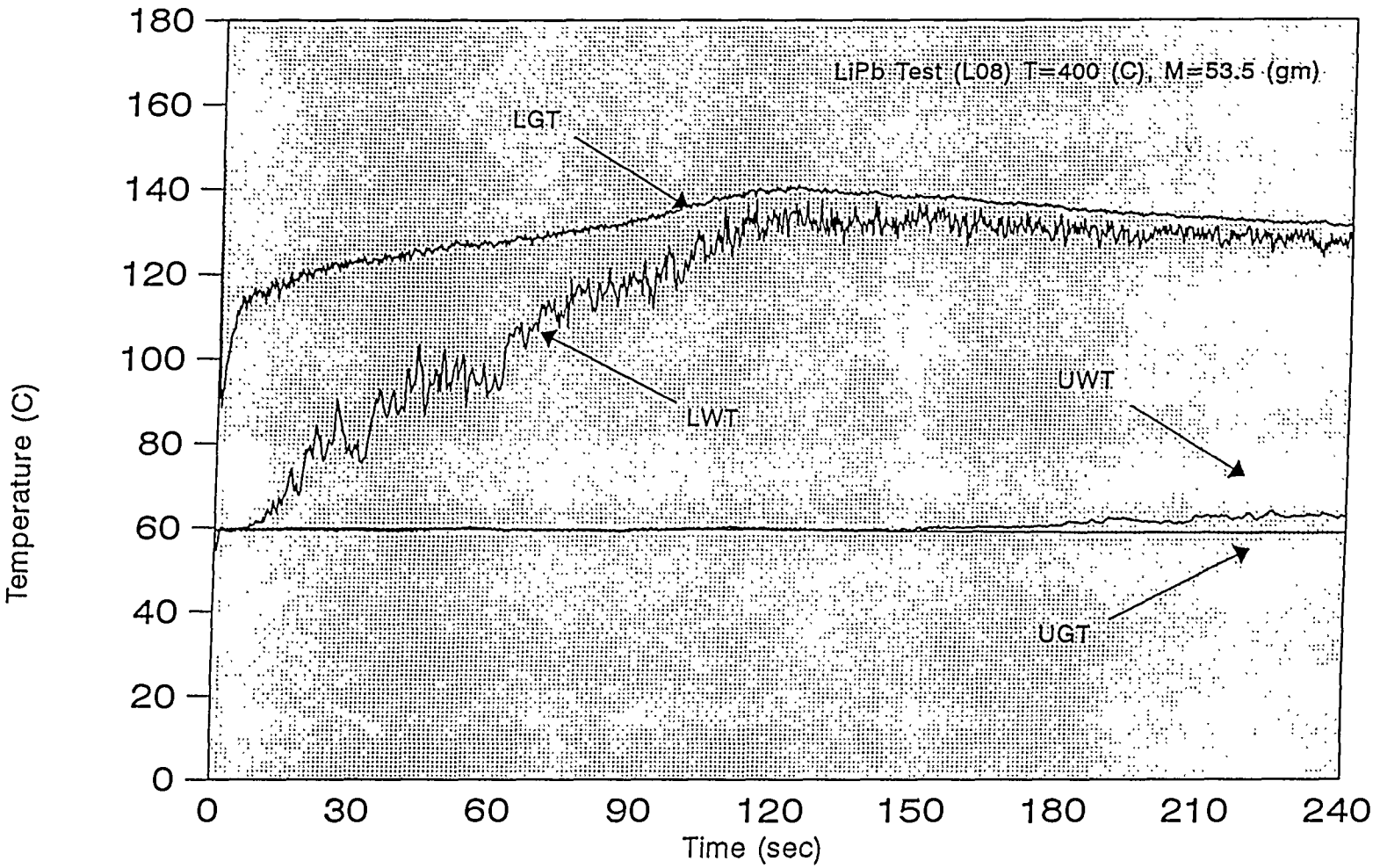
Appendix B Figure 6.2 Gas and Water Temperature as a Function of Time (L07)



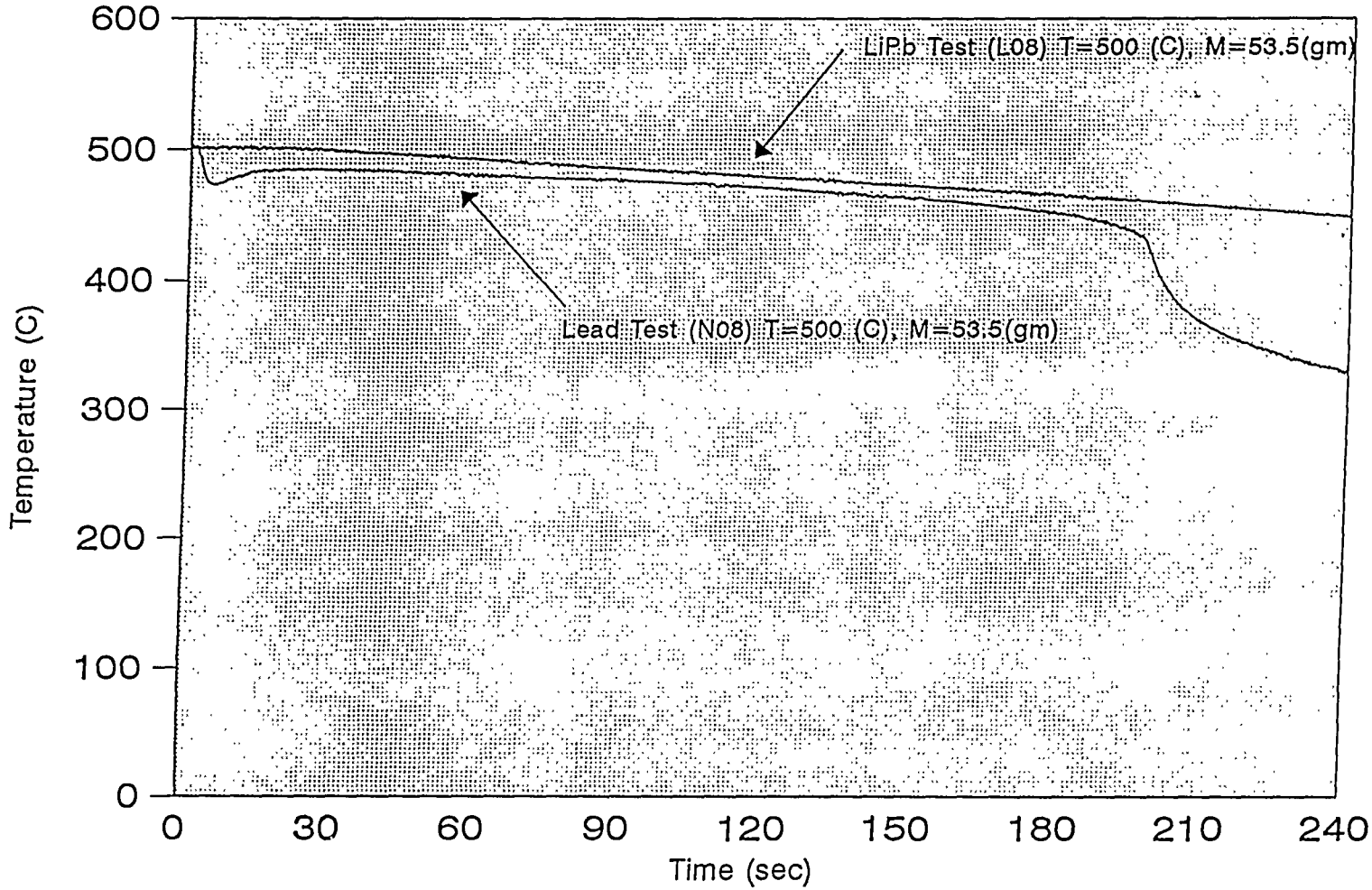
Appendix B Figure 6.3 Liquid Metal Temperature as a Function of Time (L07 & N36)



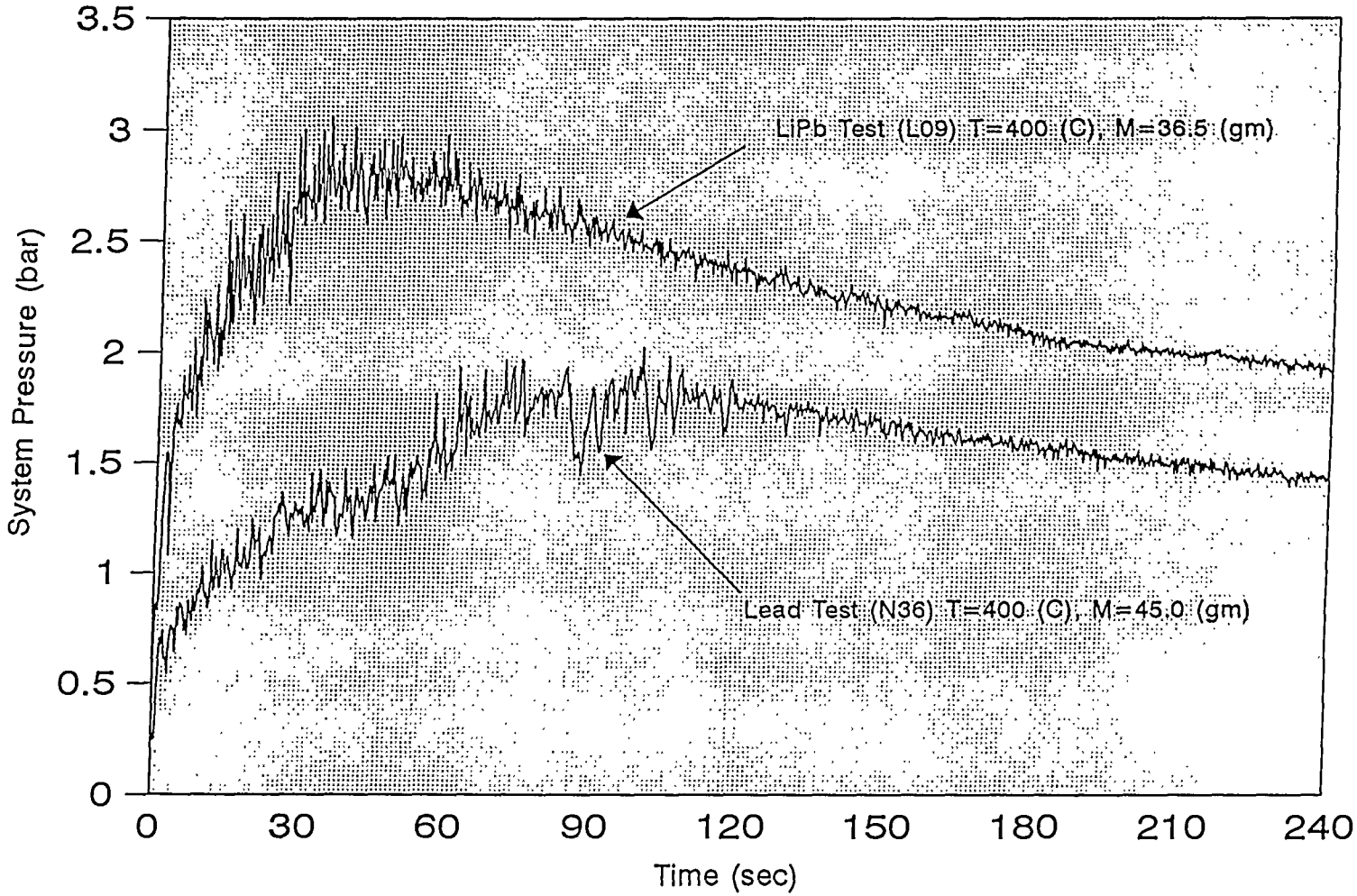
Appendix B Figure 7.1 System Pressure as a Function of Time (L08 & N08)



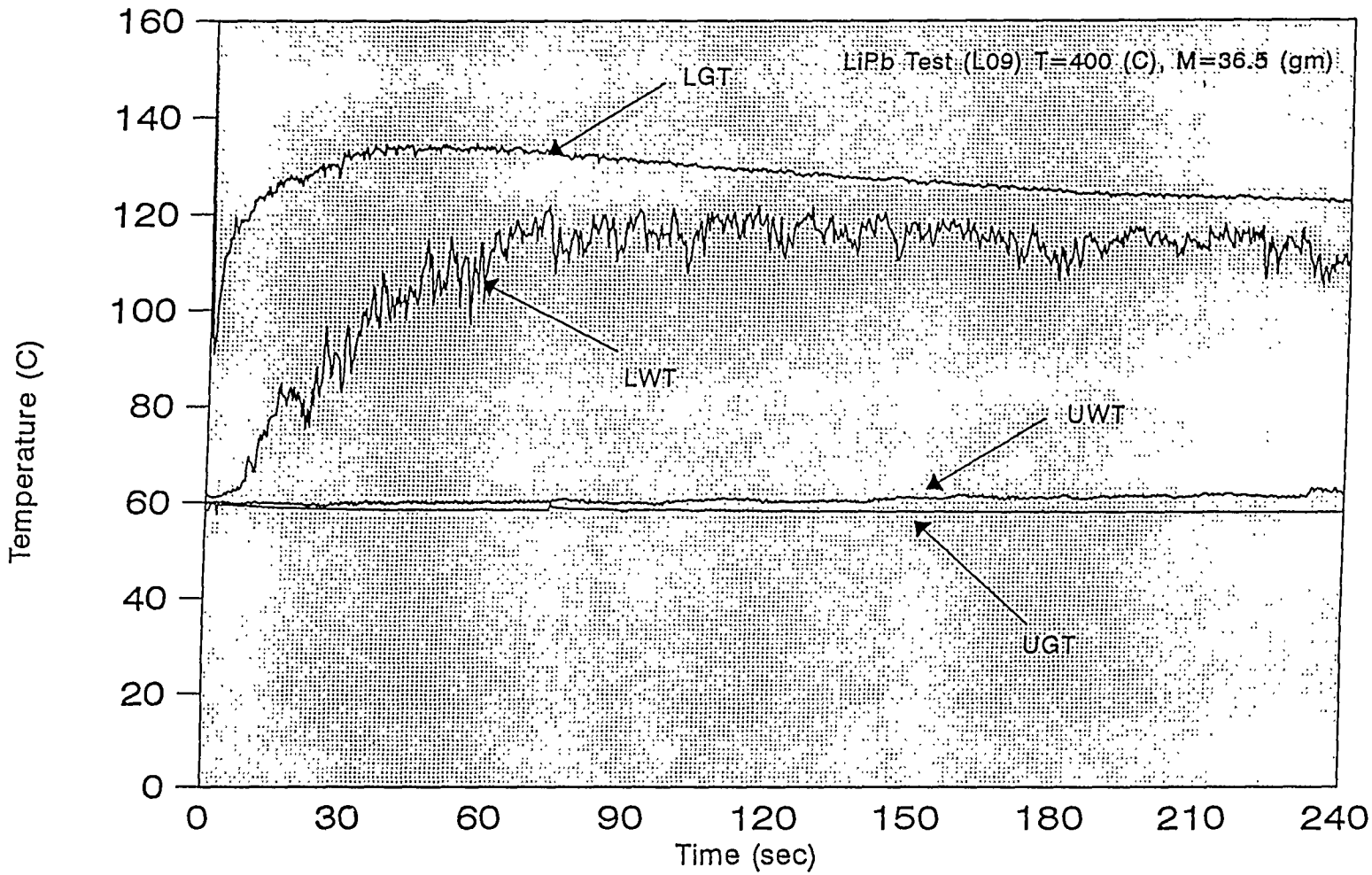
Appendix B Figure 7.2 Gas and Water Temperature as a Function of Time (L08)



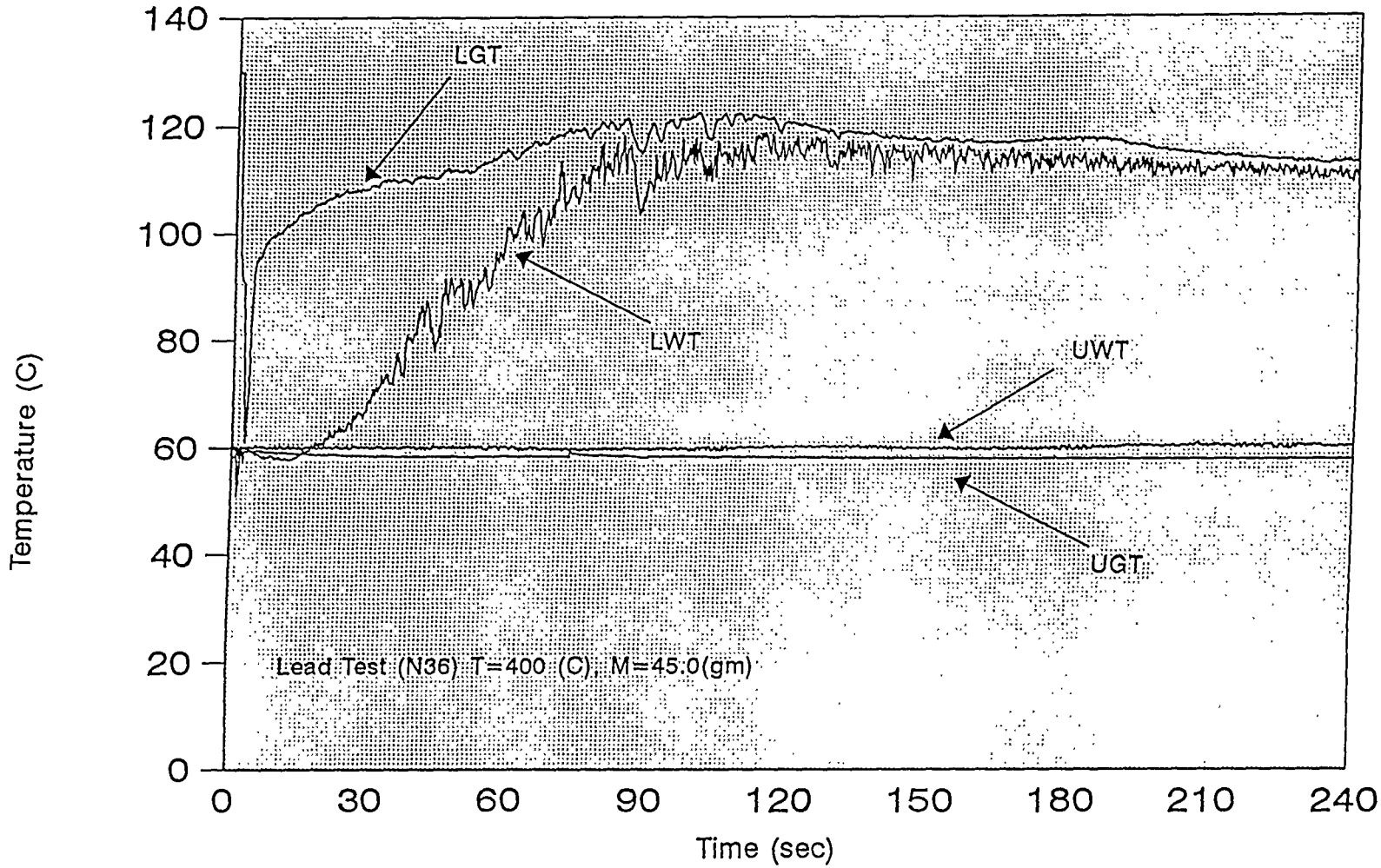
Appendix B Figure 7.3 Liquid Metal Temperature as a Function of Time (L08 & N08)



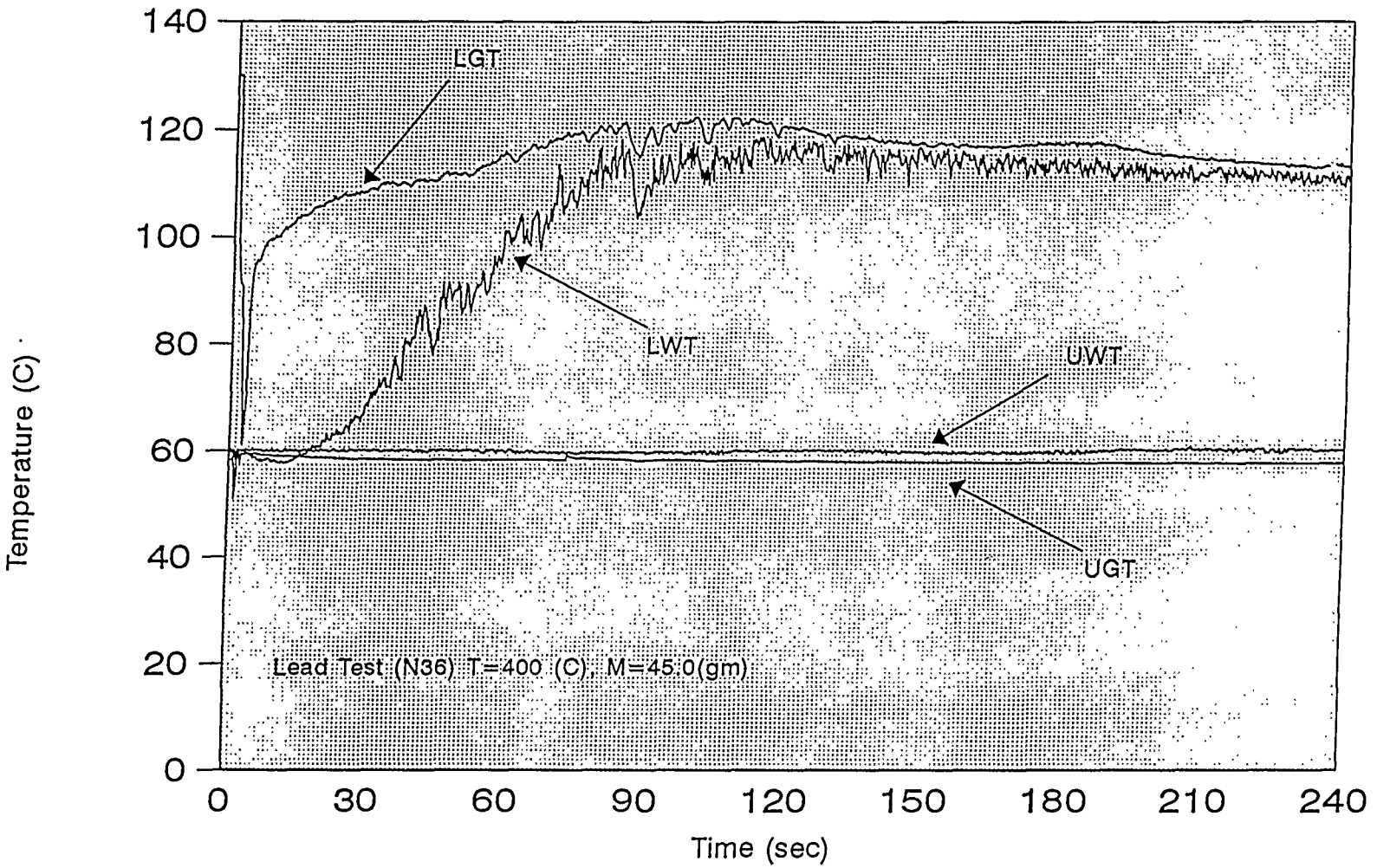
Appendix B Figure 8.1 System Pressure as a Function of Time (L09 & N36)



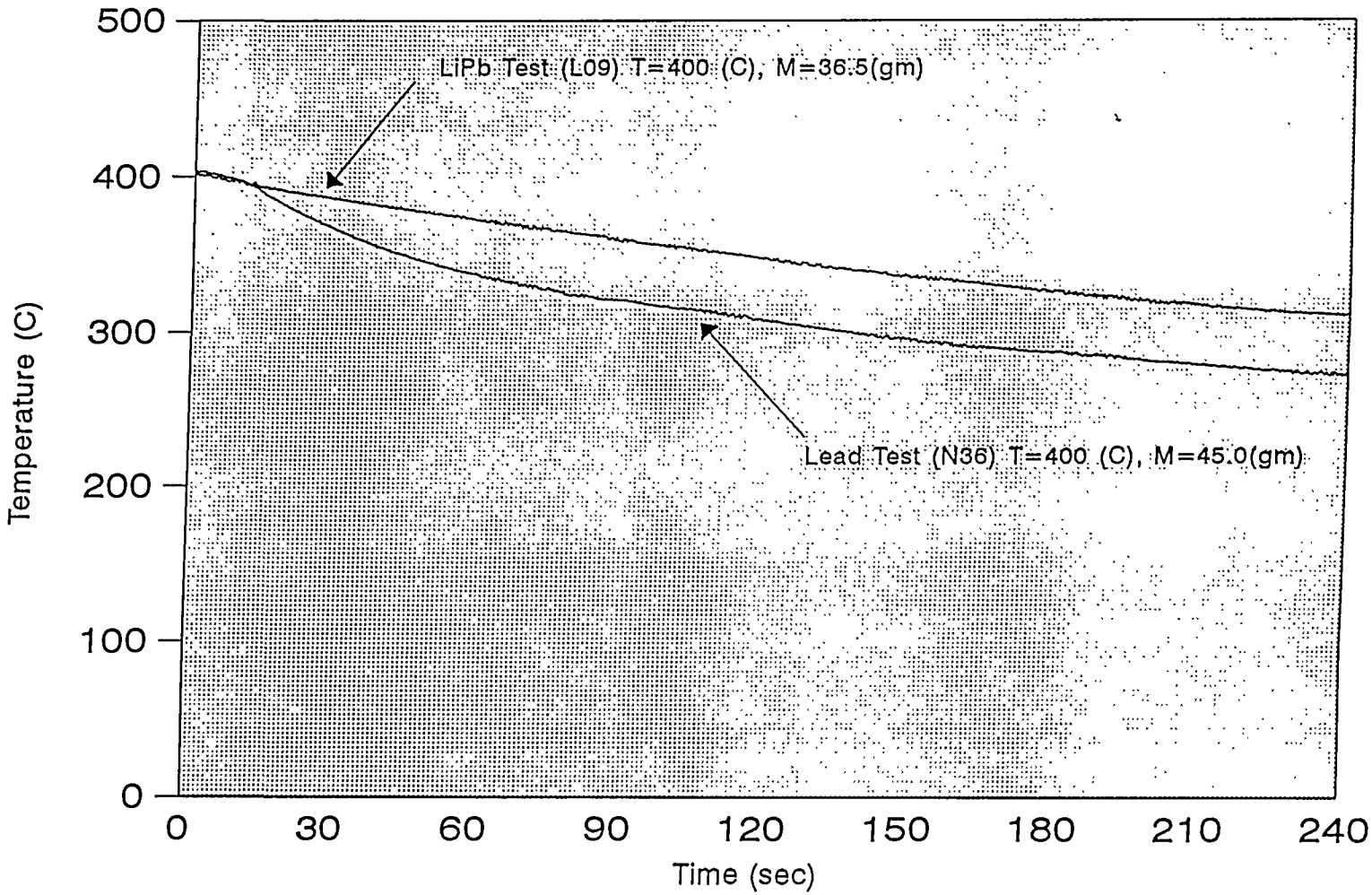
Appendix B Figure 8.2 Gas and Water Temperature as a Function of Time (L09)



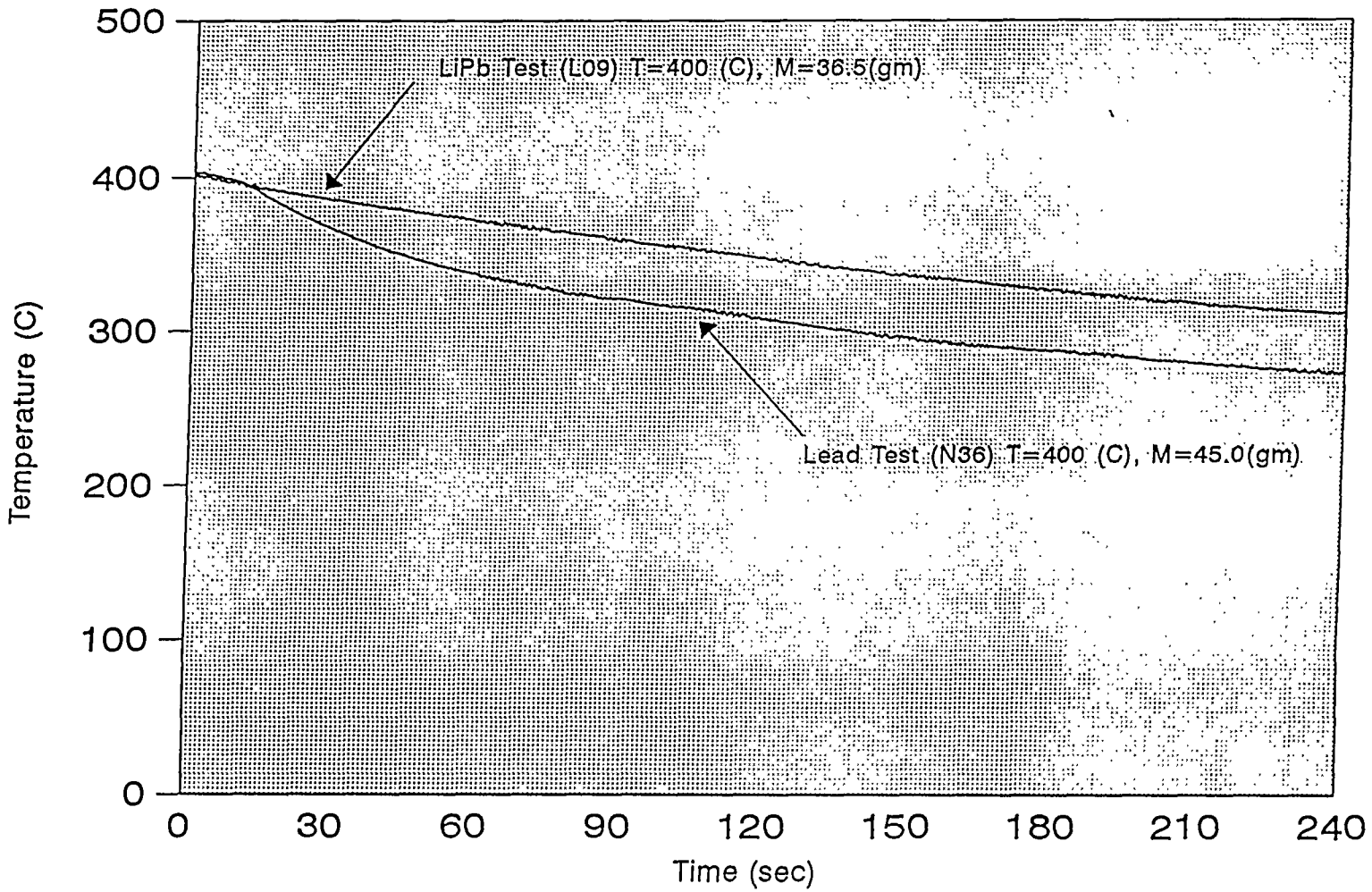
Appendix B Figure 8.3 Gas and Water Temperature as a Function of Time (N36)



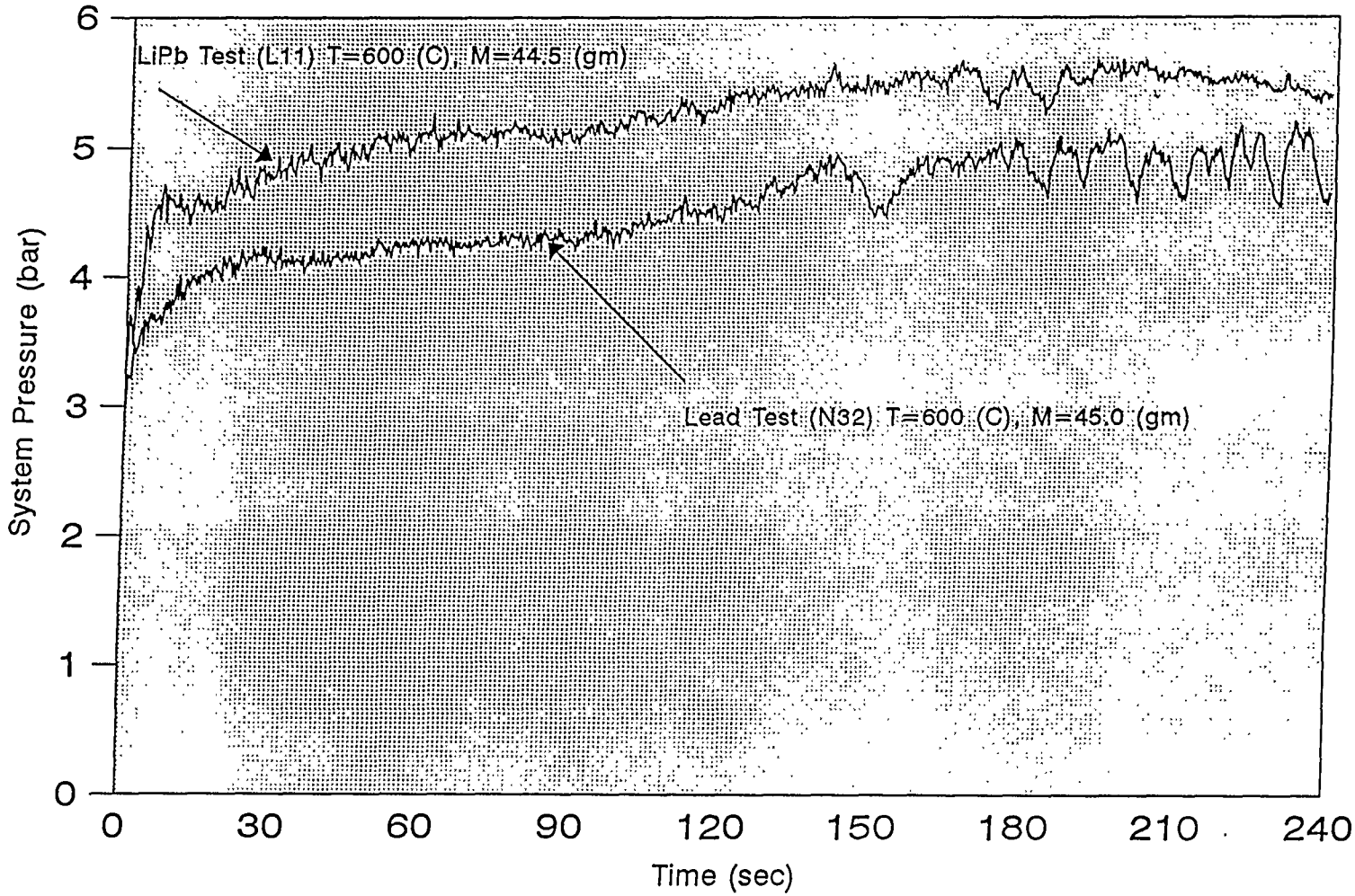
Appendix B Figure 8.3 Gas and Water Temperature as a Function of Time (N36)



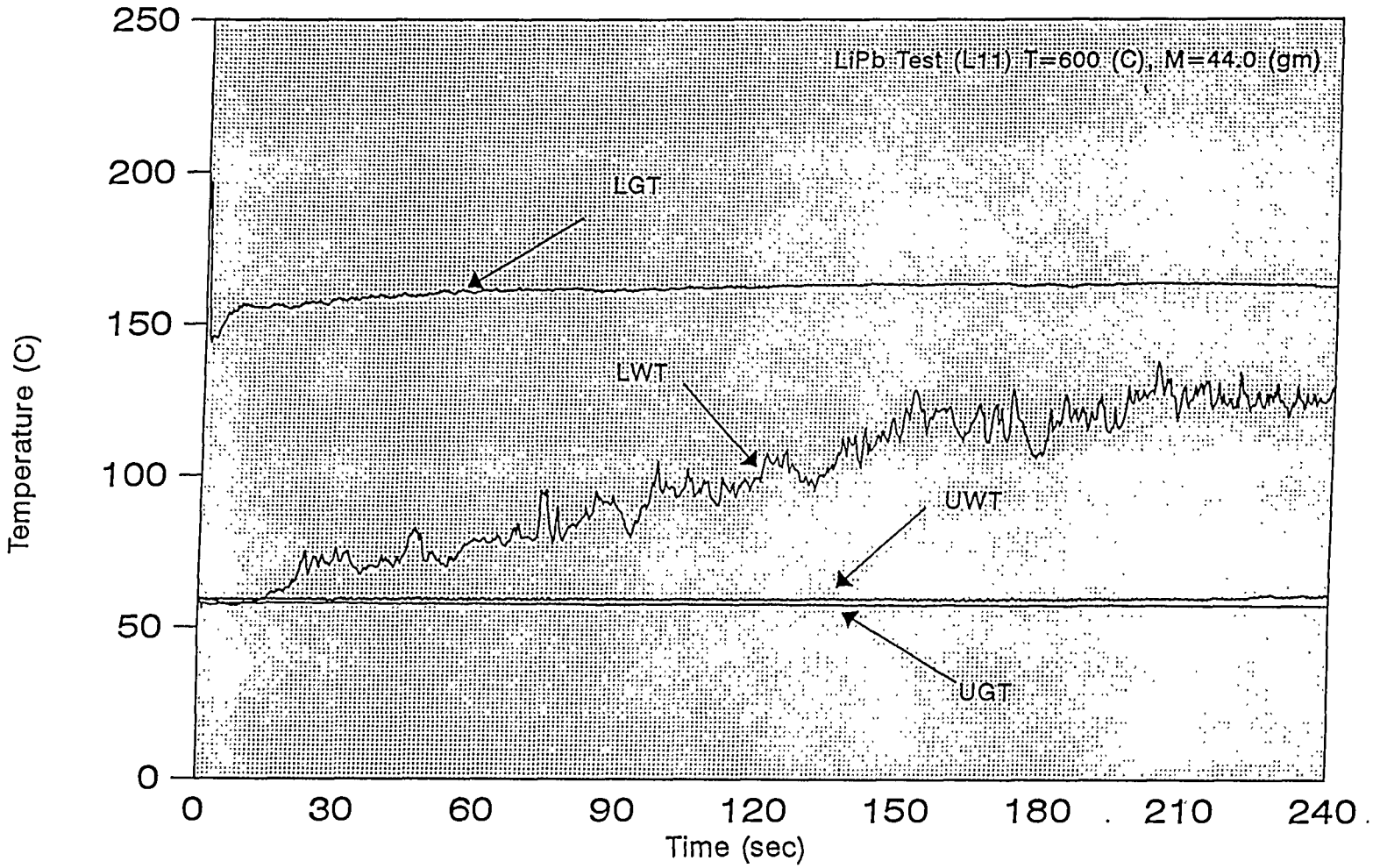
Appendix B Figure 8.4 Liquid Metal Temperature as a Function of Time (L09 & N36)



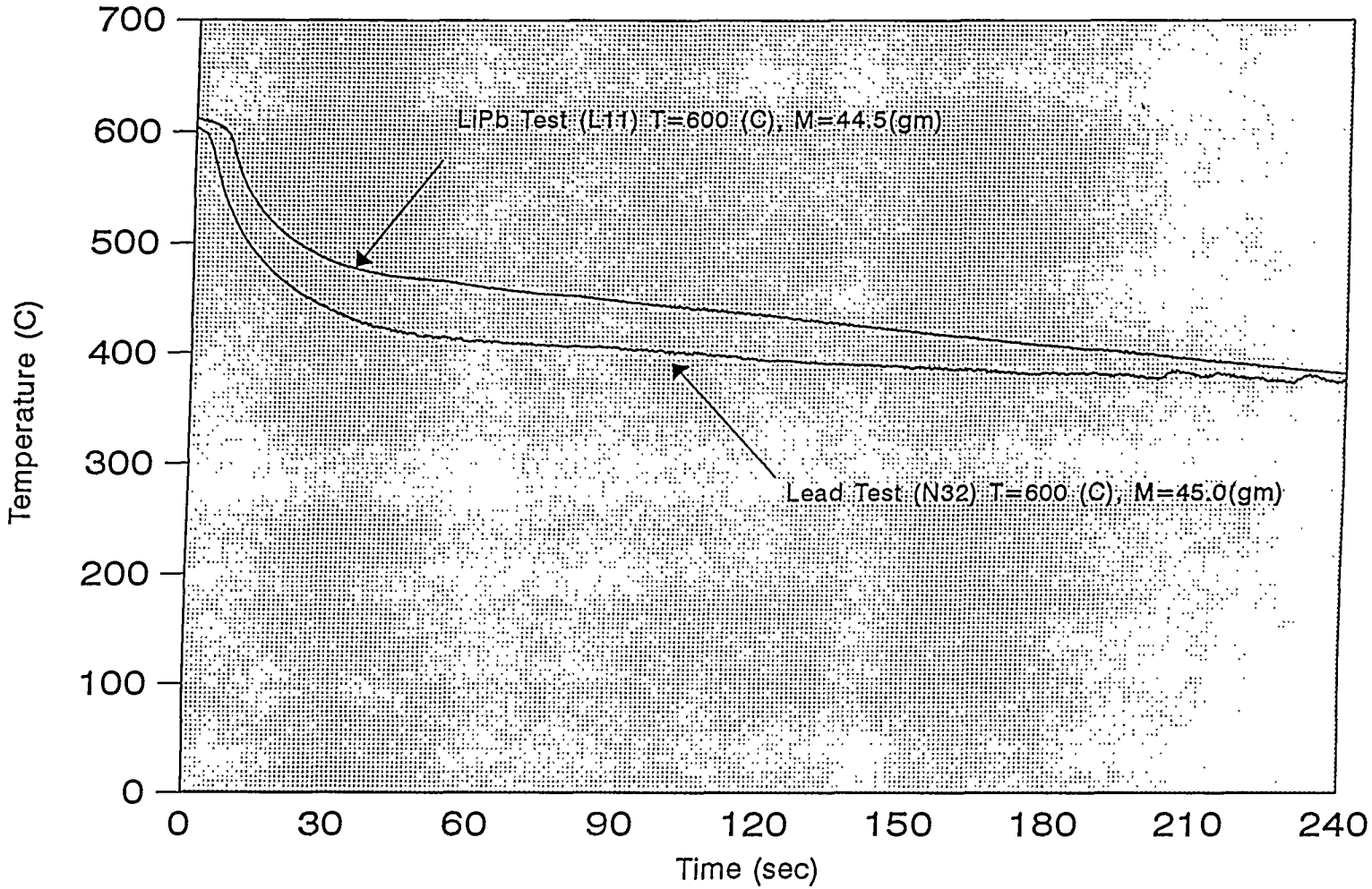
Appendix B Figure 8.4 Liquid Metal Temperature as a Function of Time (L09 & N36)



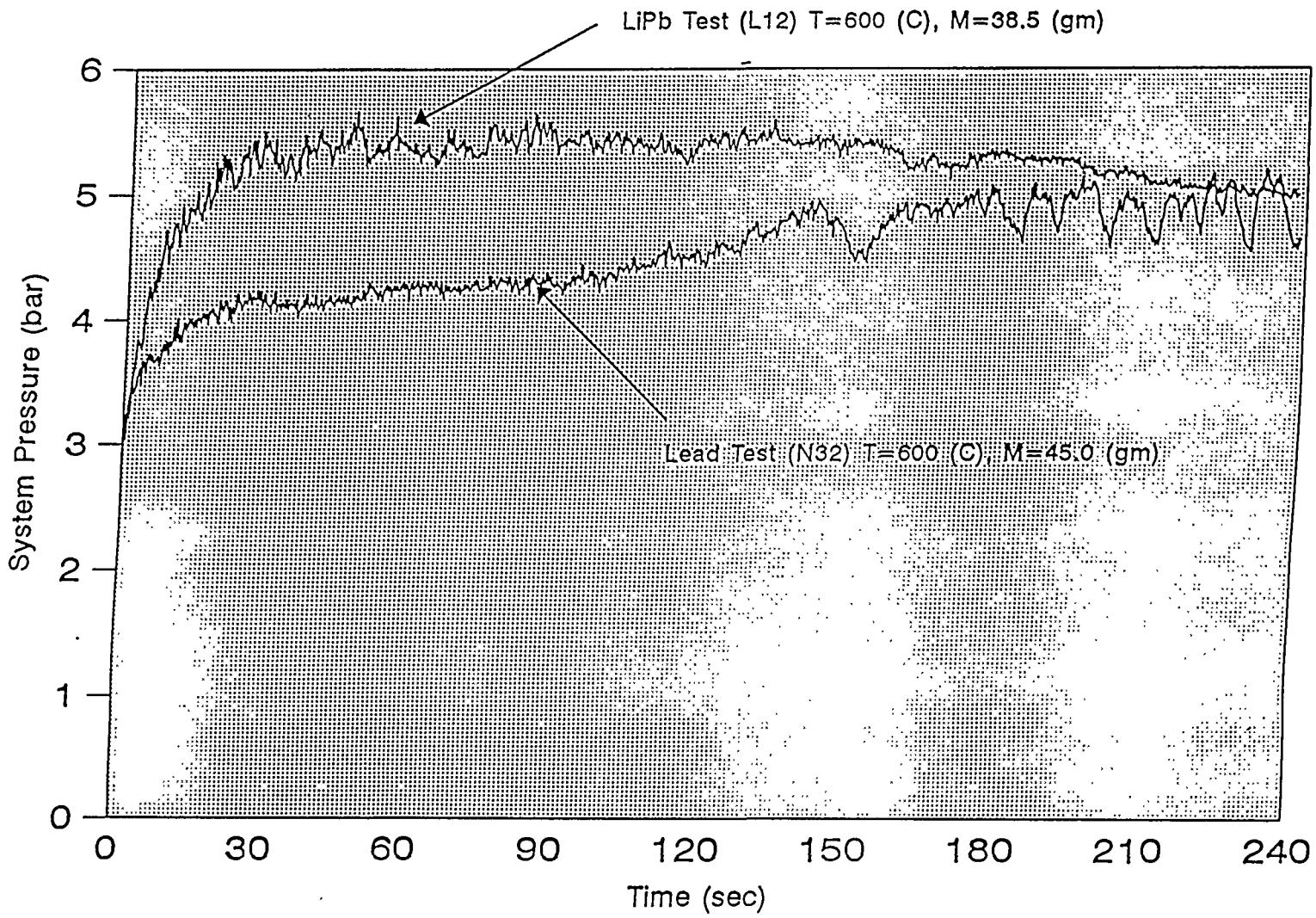
Appendix B Figure 9.1 System Pressure as a Function of Time (L11 & N32)



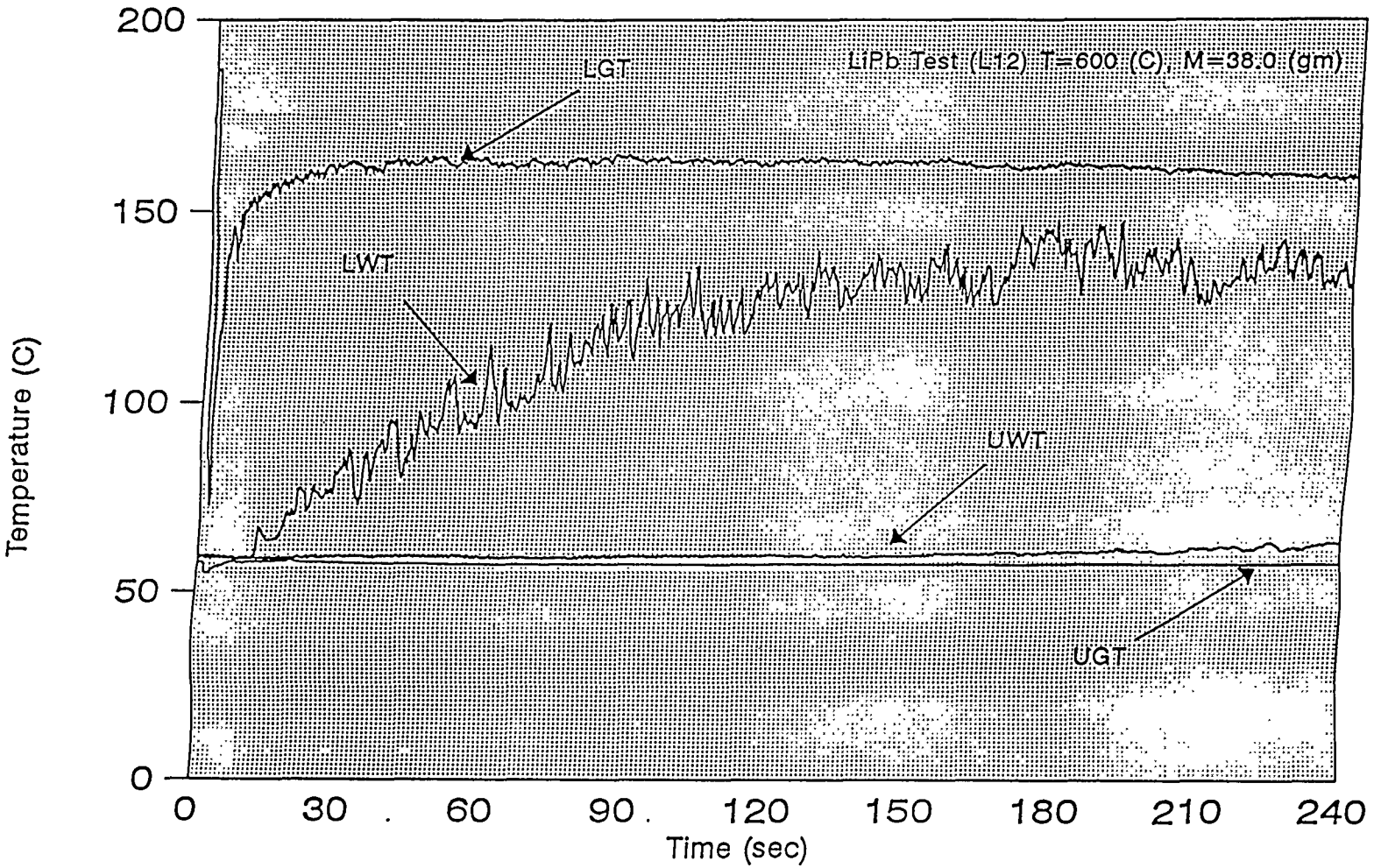
Appendix B Figure 9.2 Gas and Water Temperature as a Function of Time (L11)



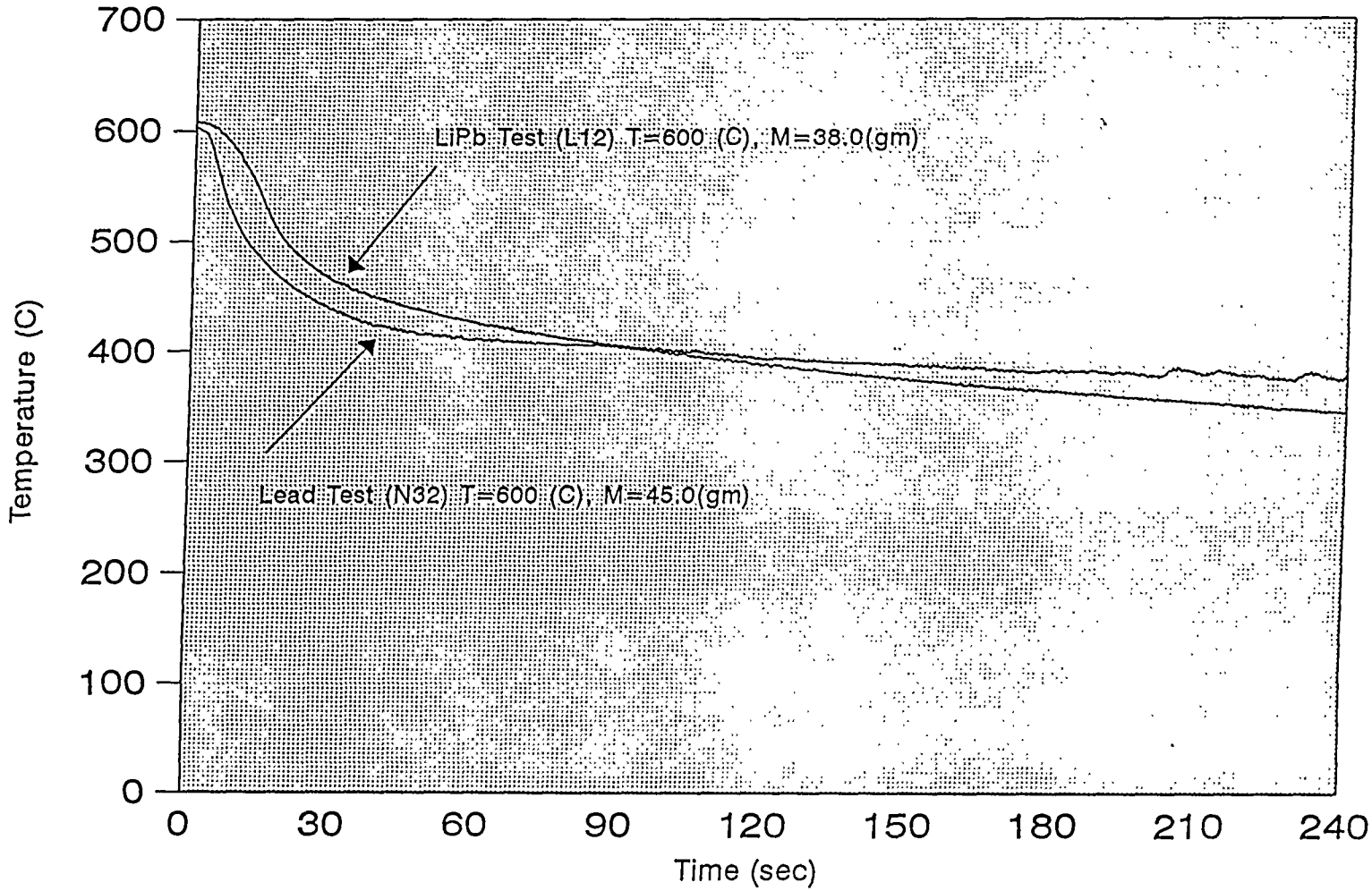
Appendix B Figure 9.3 Liquid Metal Temperature as a Function of Time (L11 & N32)



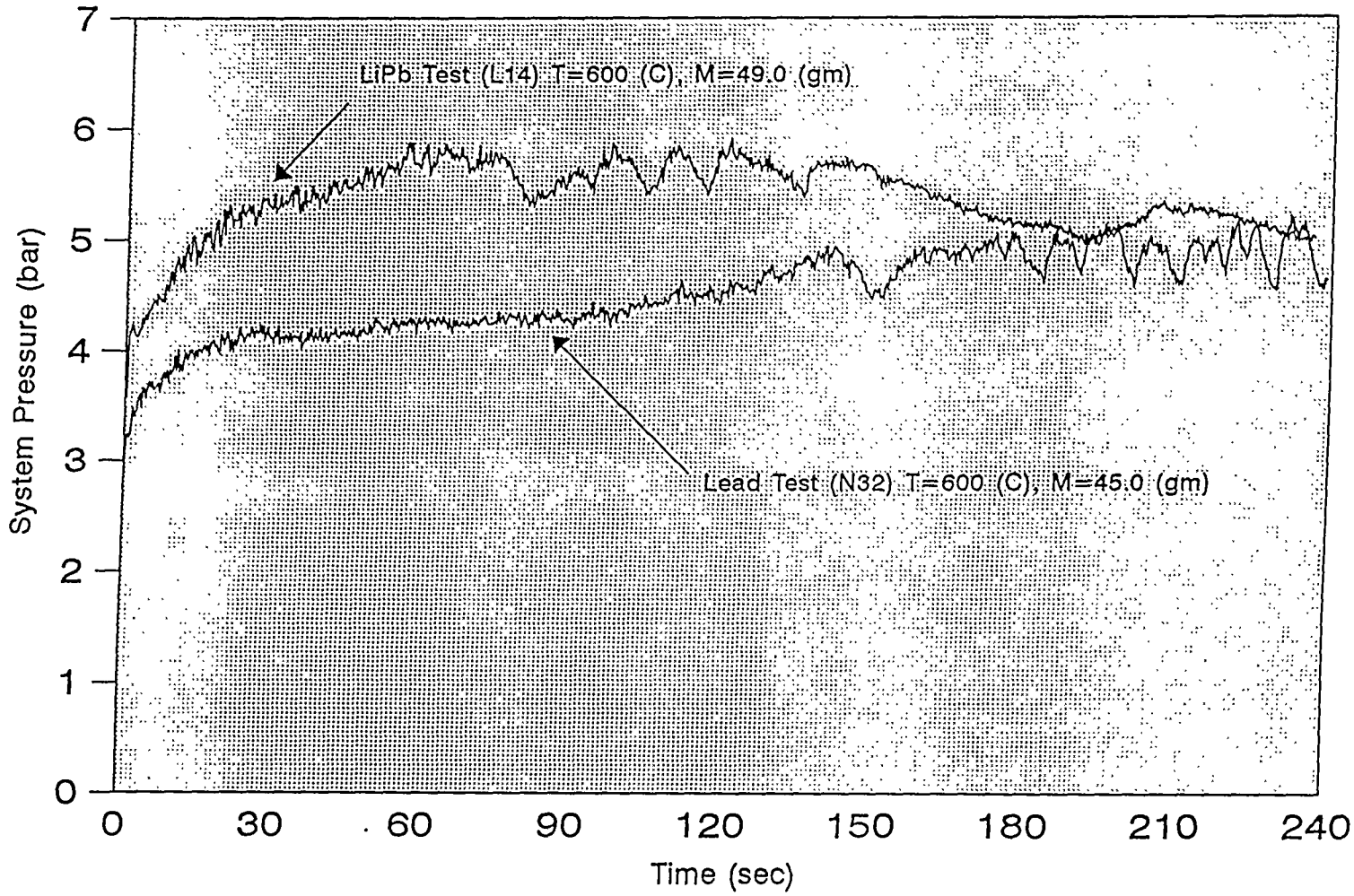
Appendix B Figure 10.1 System Pressure as a Function of Time (L12 & N32)



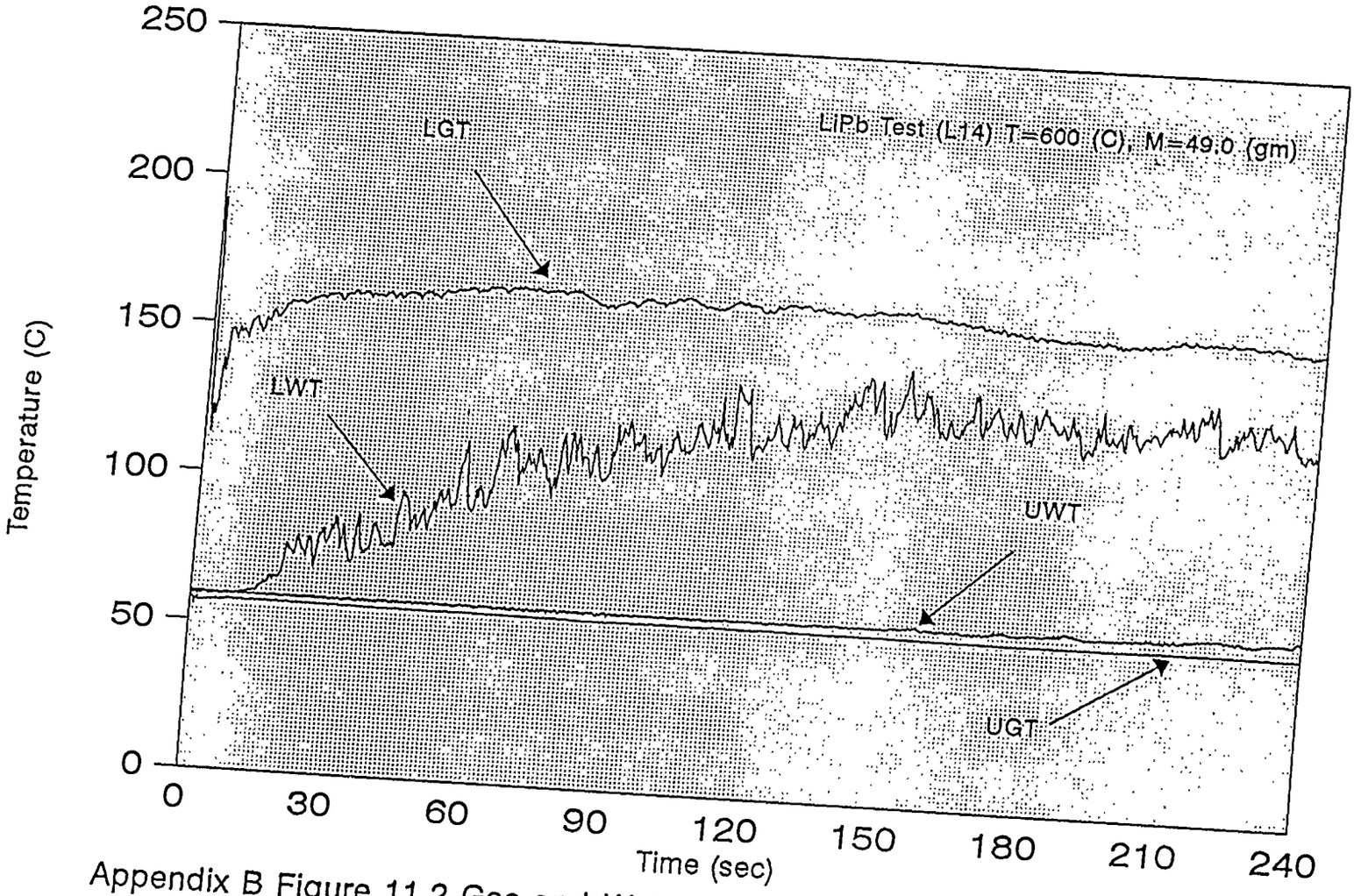
Appendix B Figure 10.2 Gas and Water Temperature as a Function of Time (L12)



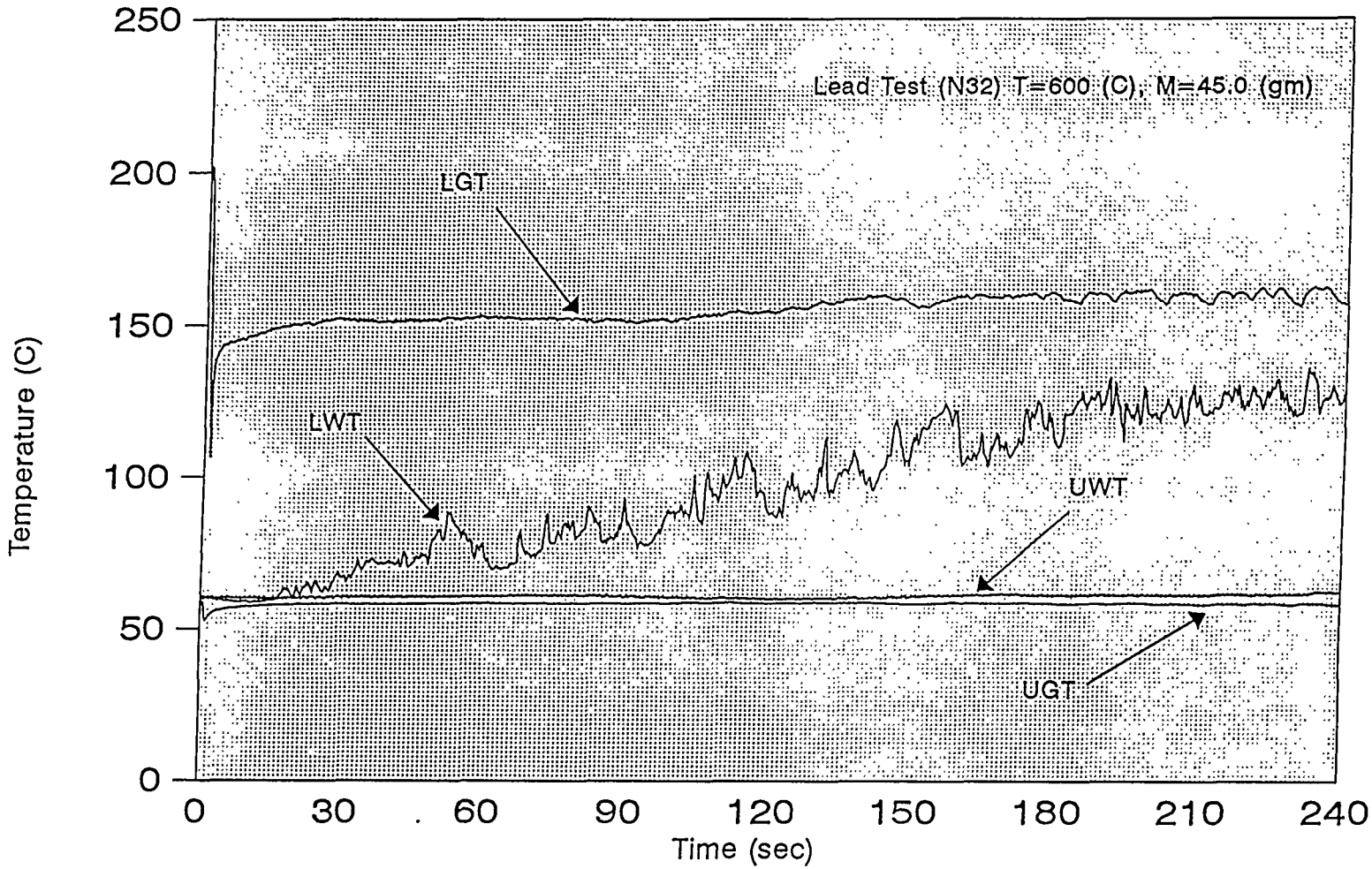
Appendix B Figure 10.3 Liquid Metal Temperature as a Function of Time (L12 & N32)



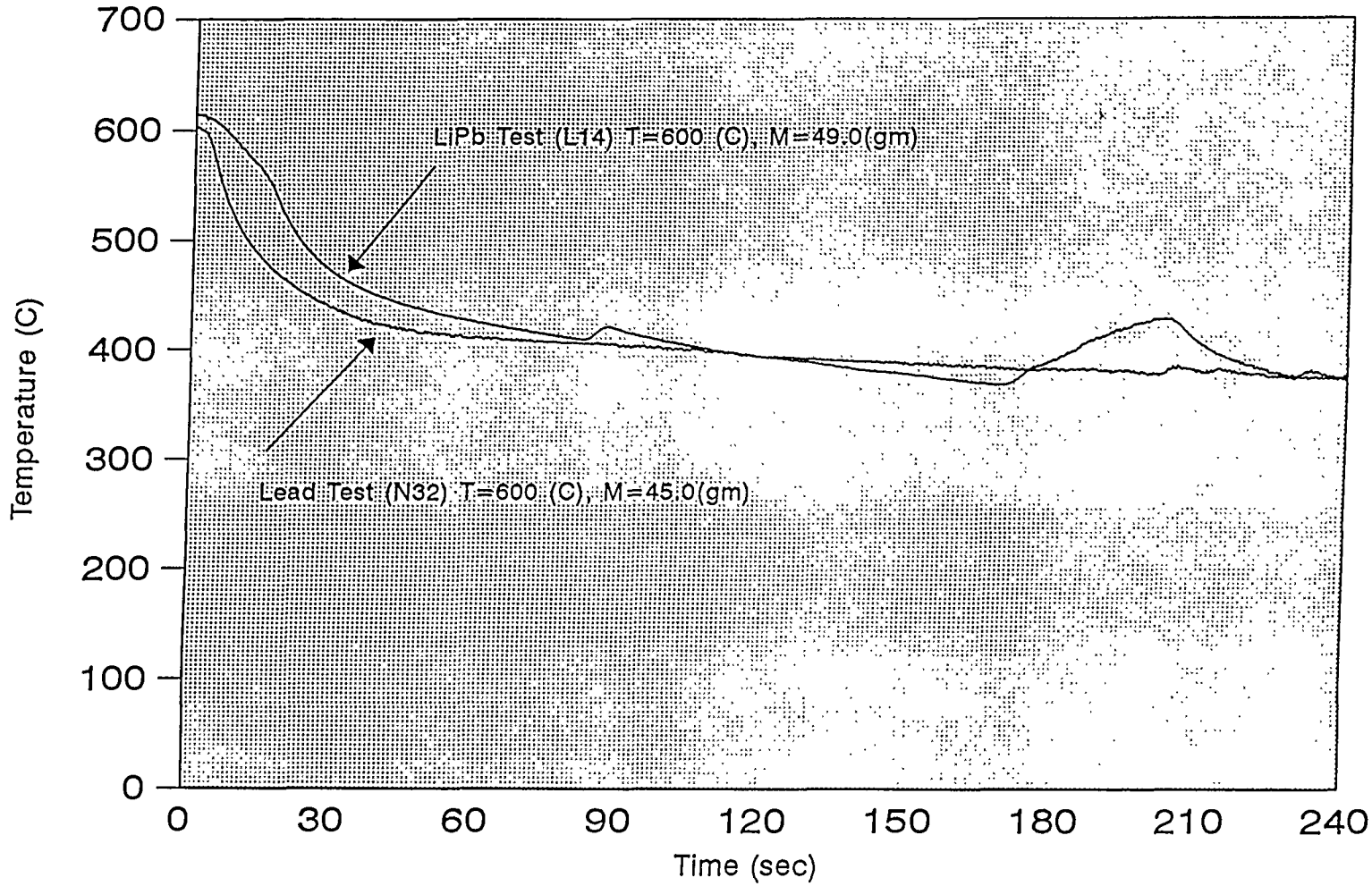
Appendix B Figure 11.1 System Pressure as a Function of Time (L14 & N32)



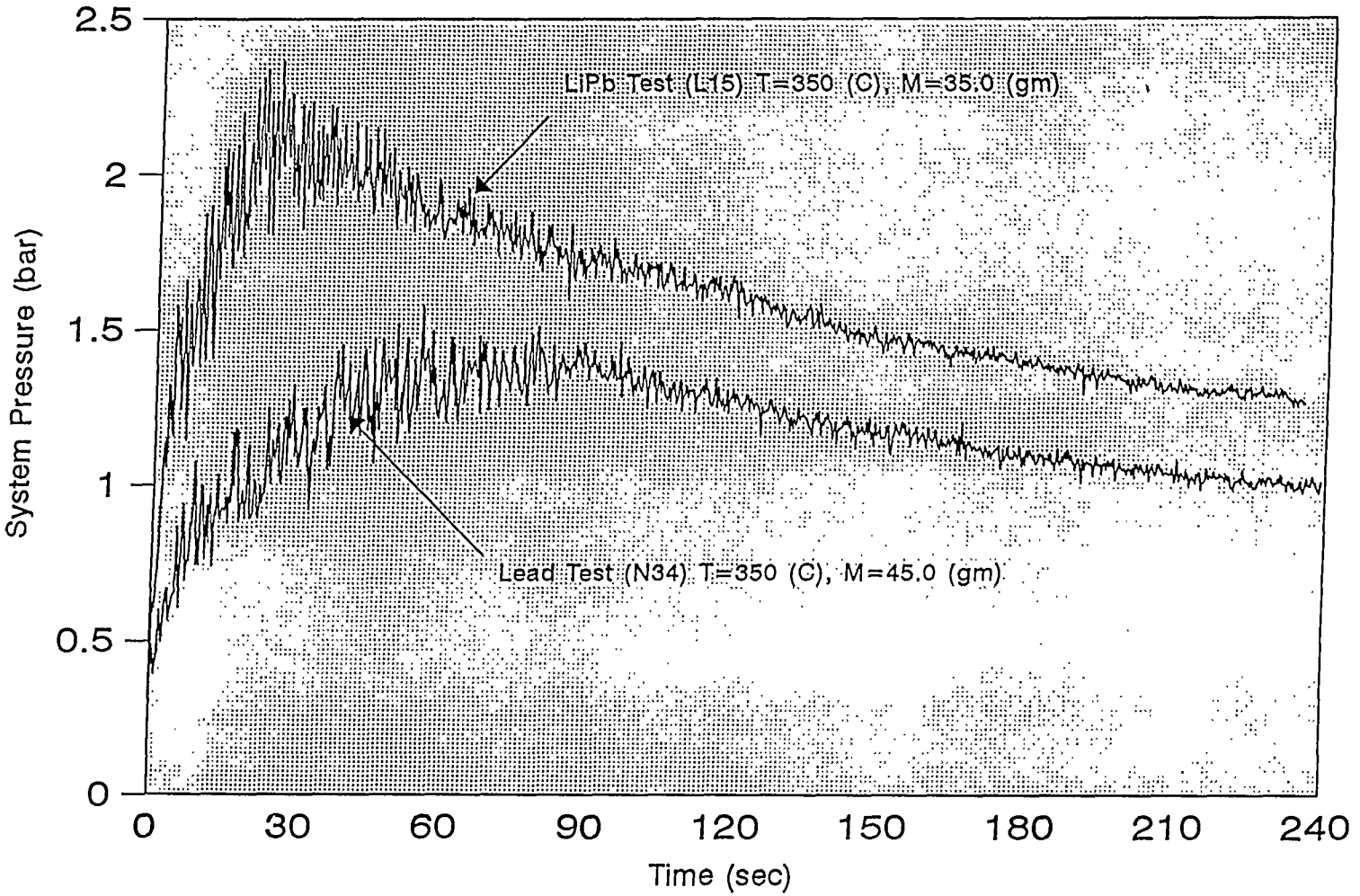
Appendix B Figure 11.2 Gas and Water Temperature as a Function of Time (L14)



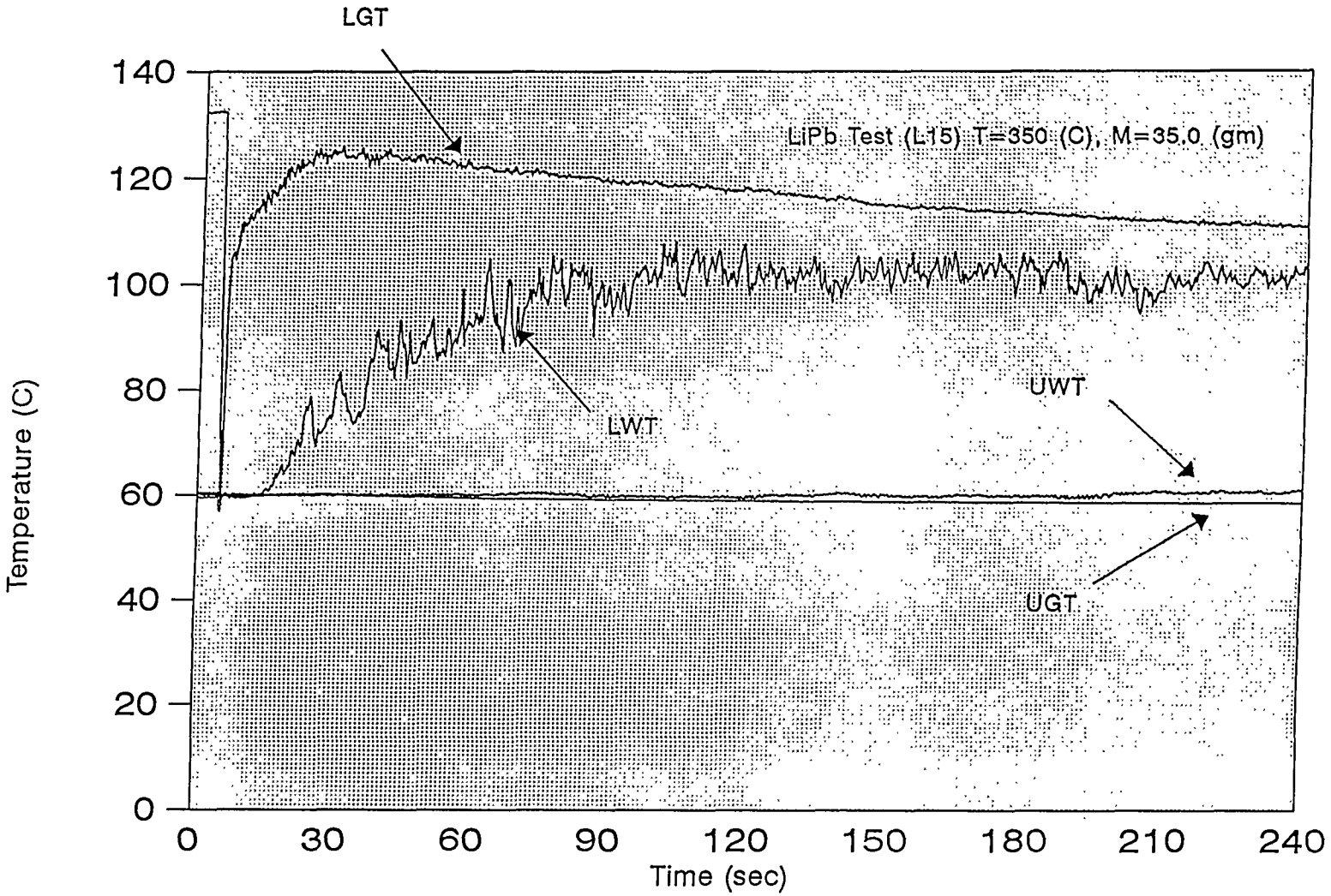
Appendix B Figure 11.3 Gas and Water Temperature as a Function of Time (N32)



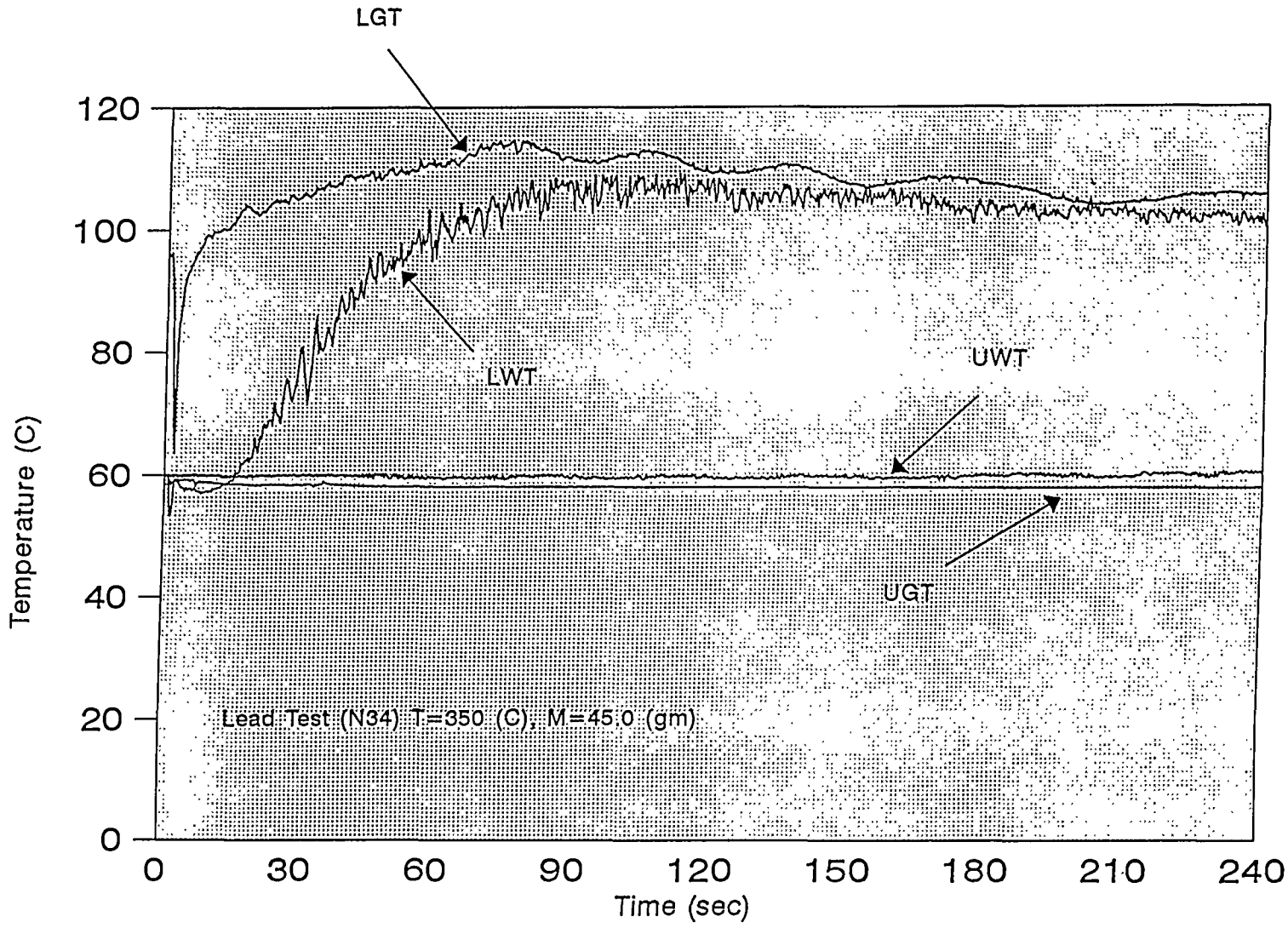
Appendix B Figure 11.4 Liquid Metal Temperature as a Function of Time (L14 & N32)



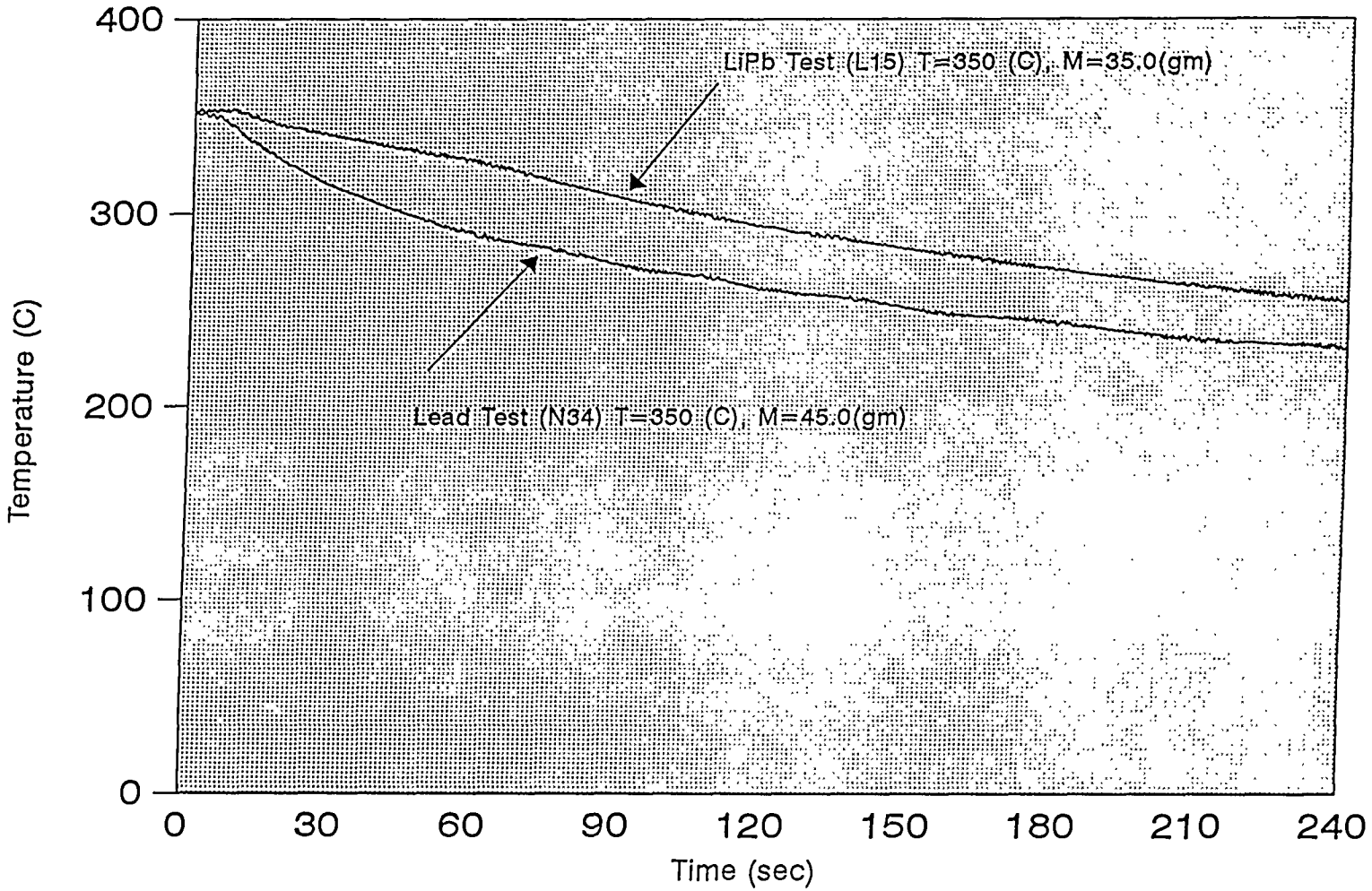
Appendix B Figure 12.1 System Pressure as a Function of Time (L15 & N34)



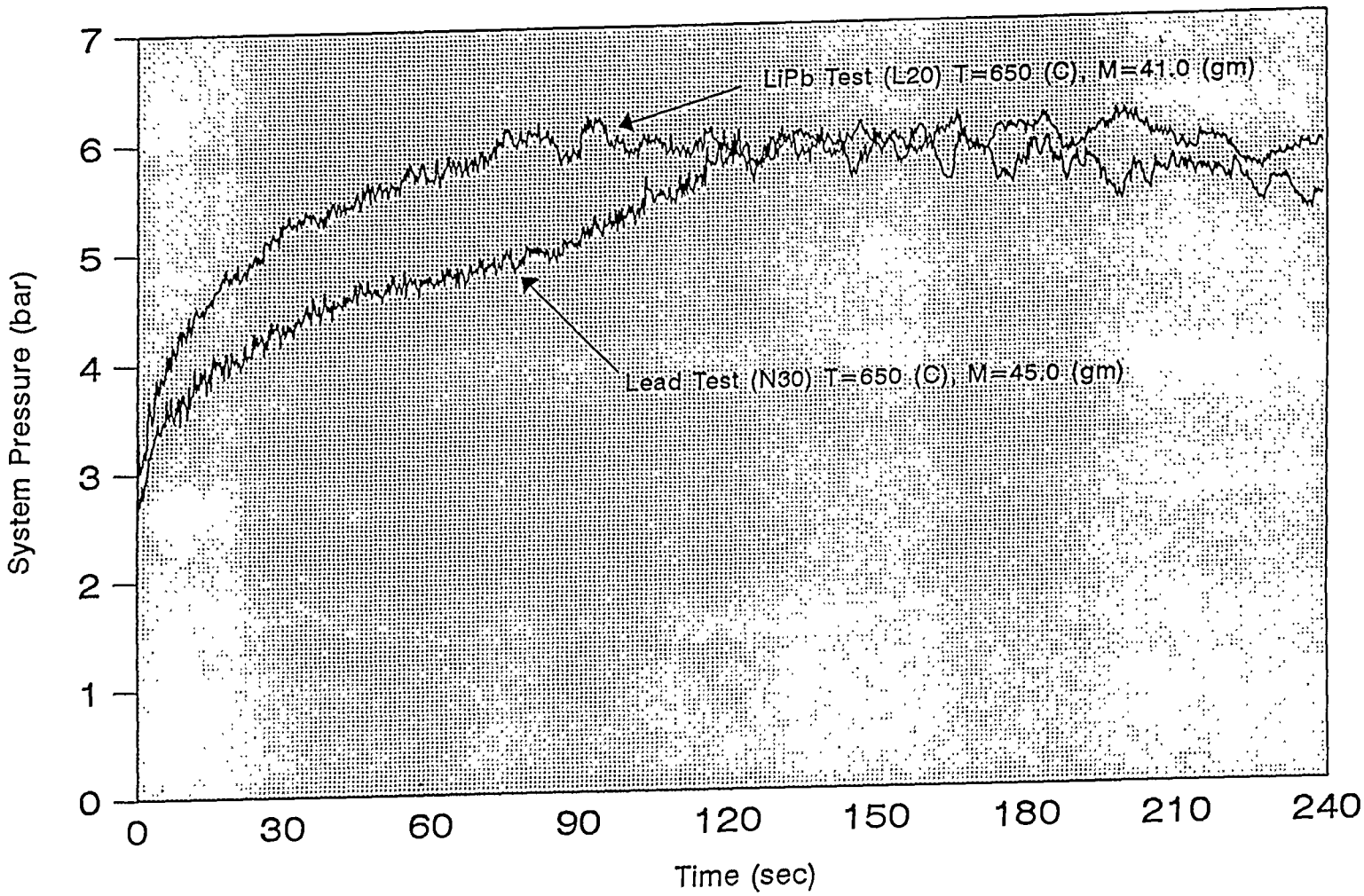
Appendix B Figure 12.2 Gas and Water Temperature as a Function of Time (L15)



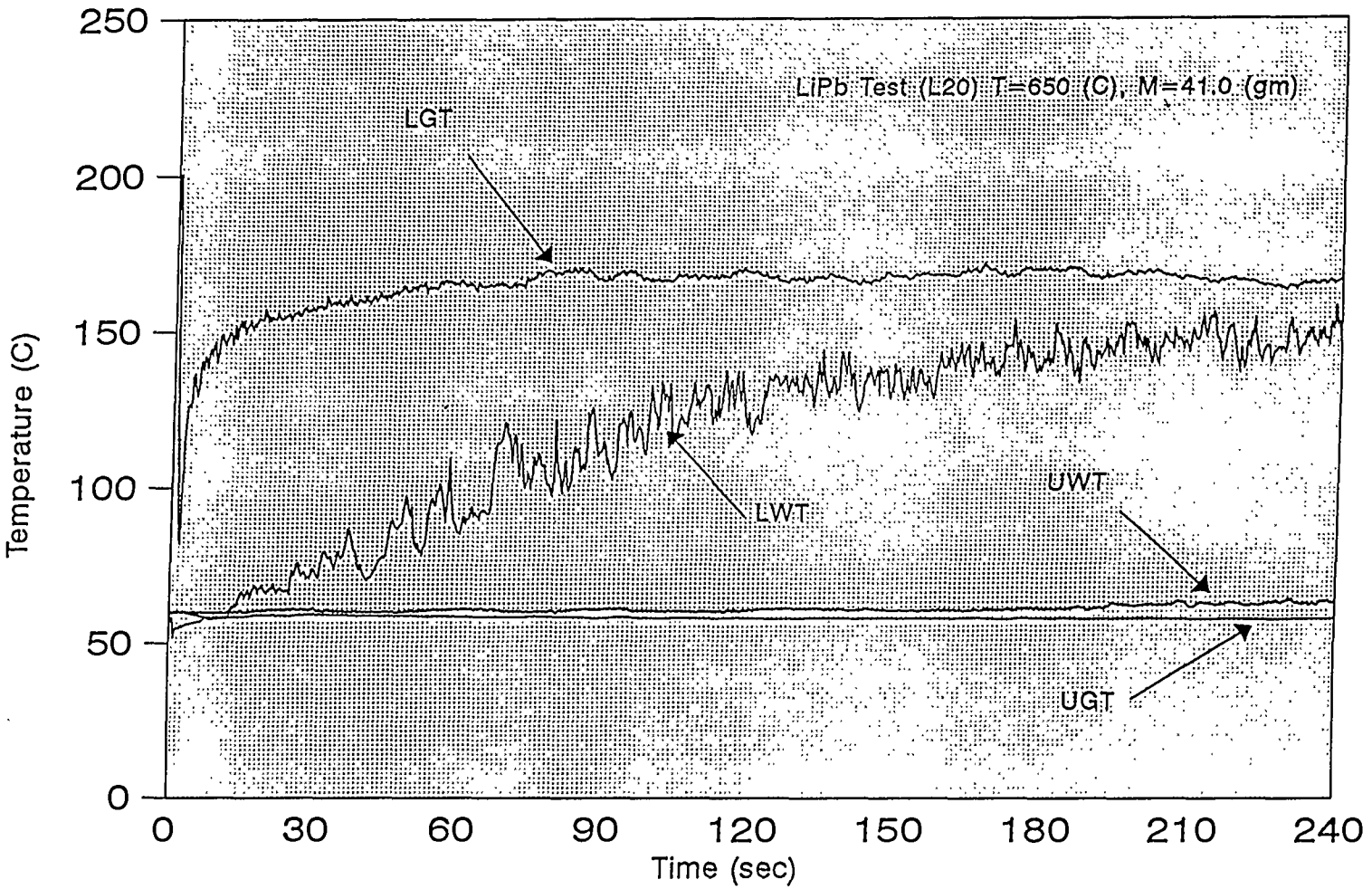
Appendix B Figure 12.3 Gas and Water Temperature as a Function of Time (N34)



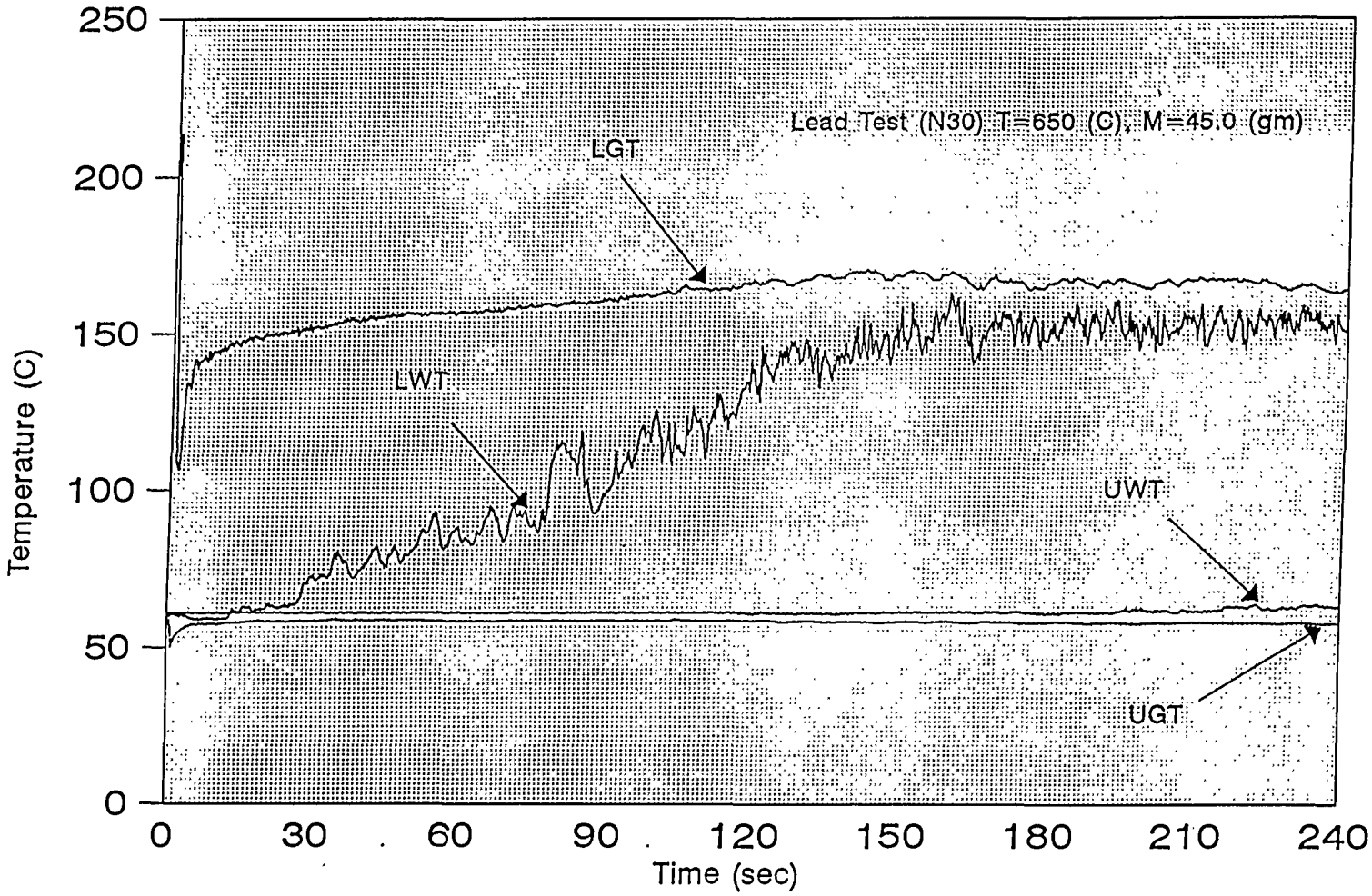
Appendix B Figure 12.4 Liquid Metal Temperature as a Function of Time (L15 & N34)



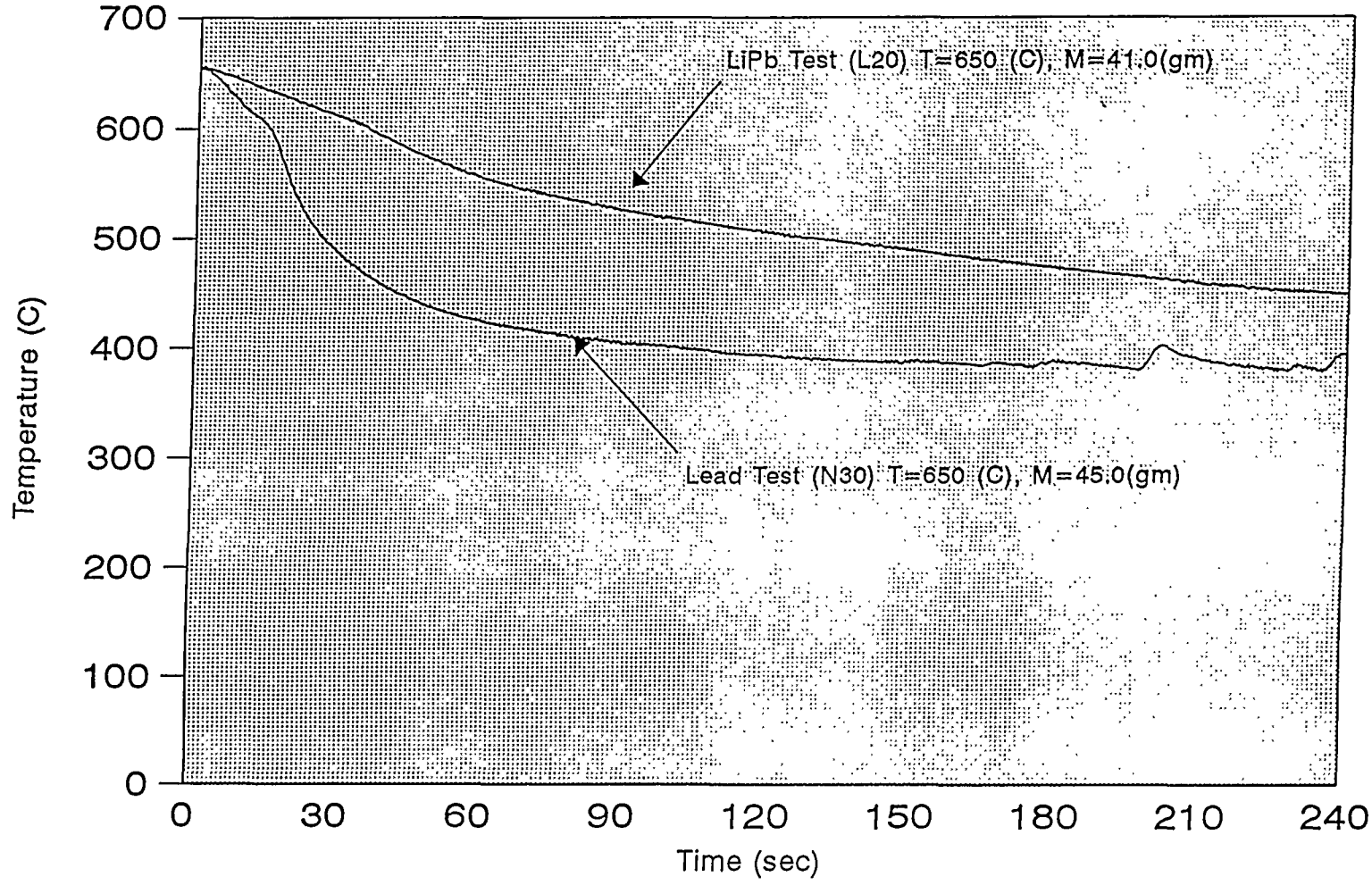
Appendix B Figure 13.1 System Pressure as a Function of Time (L20 & N30)



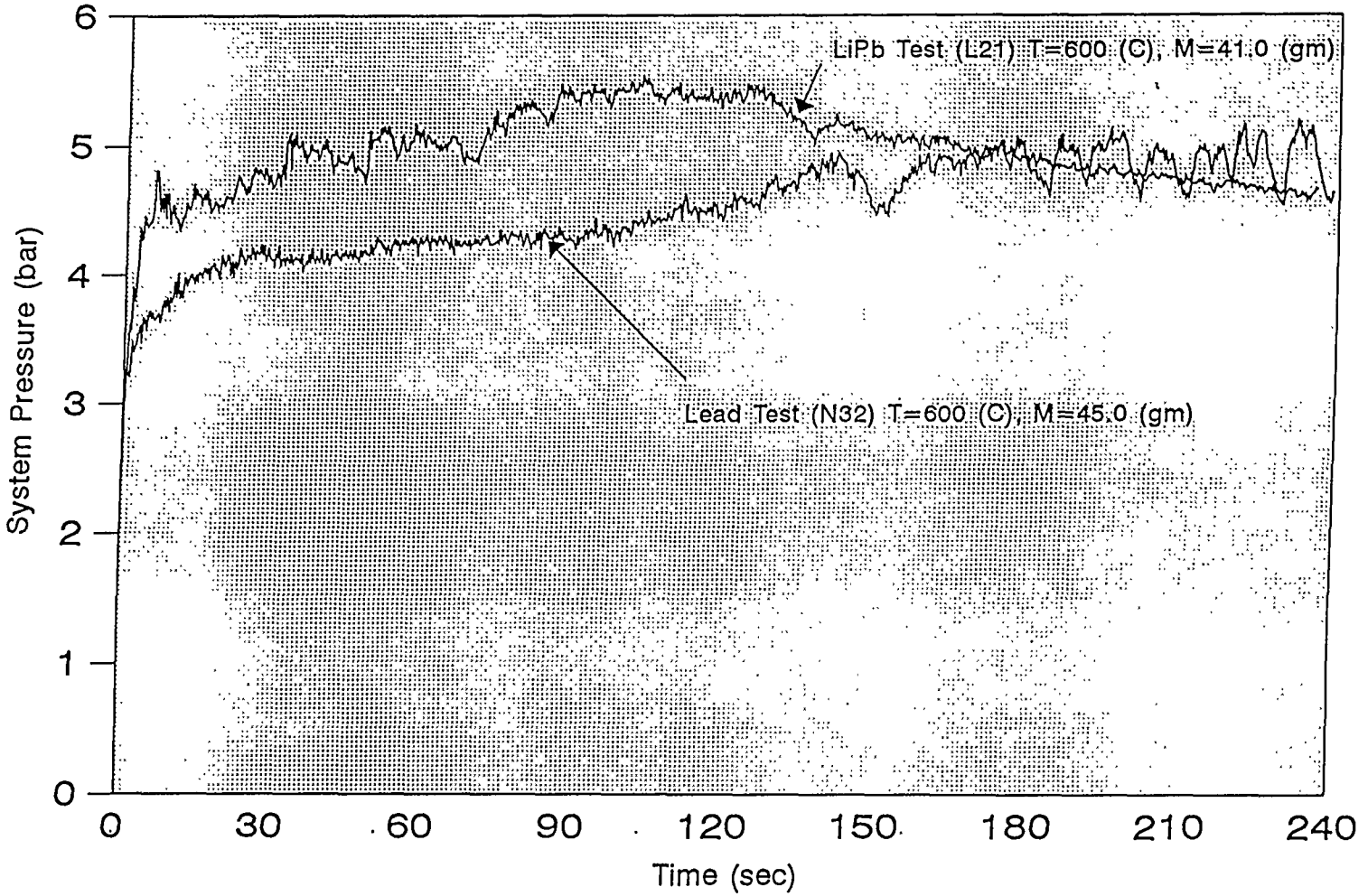
Appendix B Figure 13.2 Gas and Water Temperature as a Function of Time (L20)



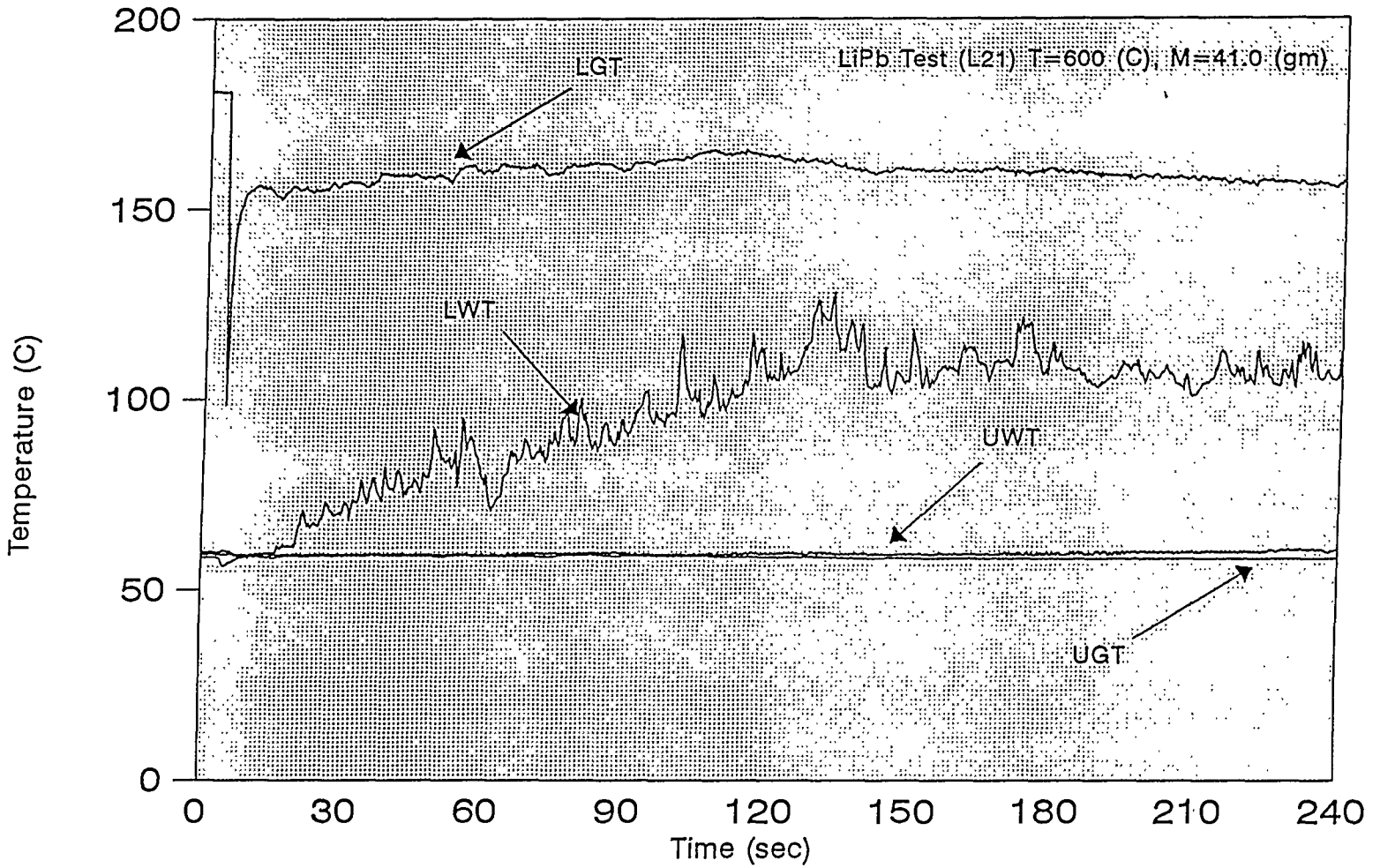
Appendix B Figure 13.3 Gas and Water Temperature as a Function of Time (N30)



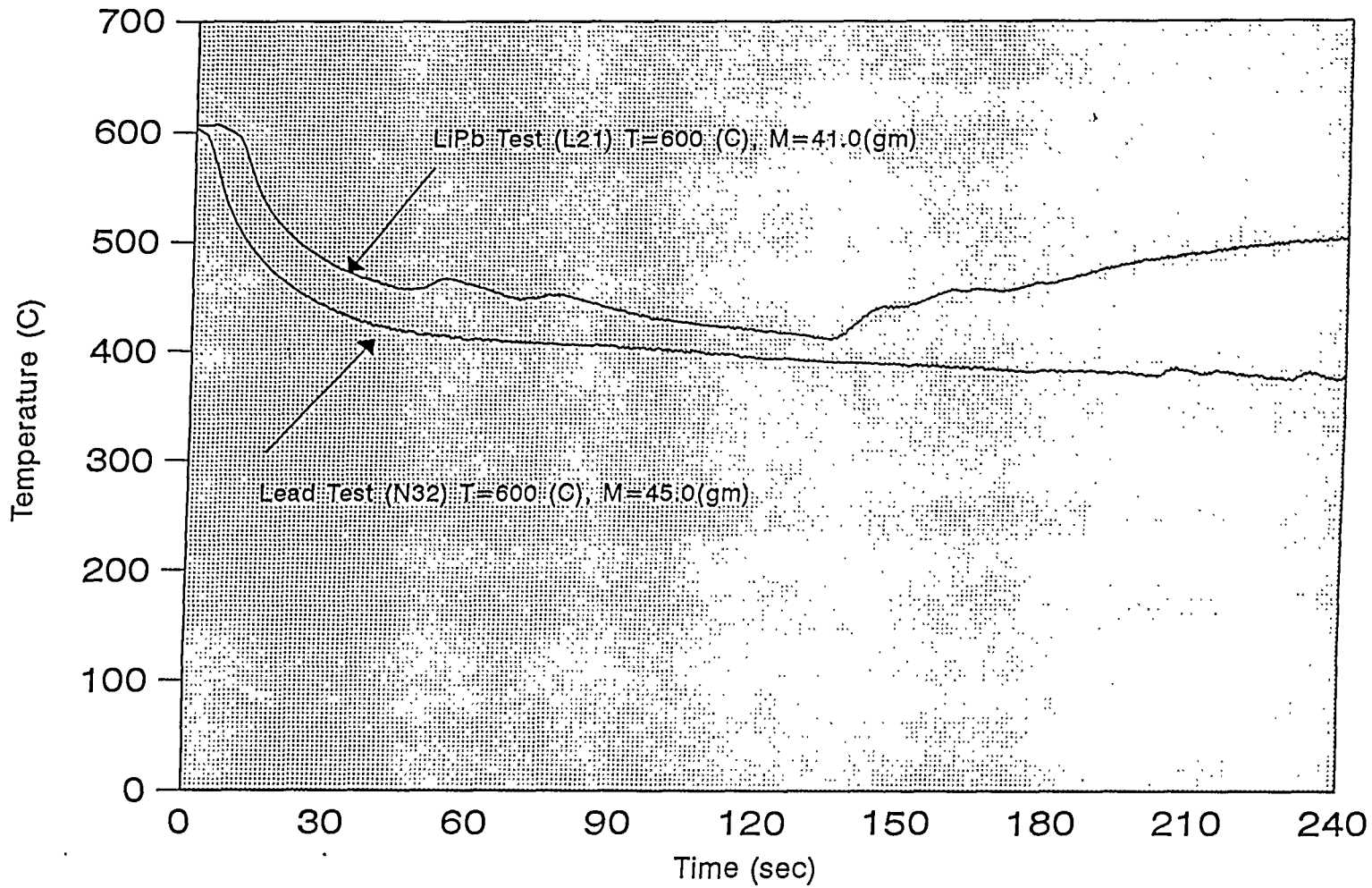
Appendix B Figure 13.4 Liquid Metal Temperature as a Function of Time (L20 & N30)



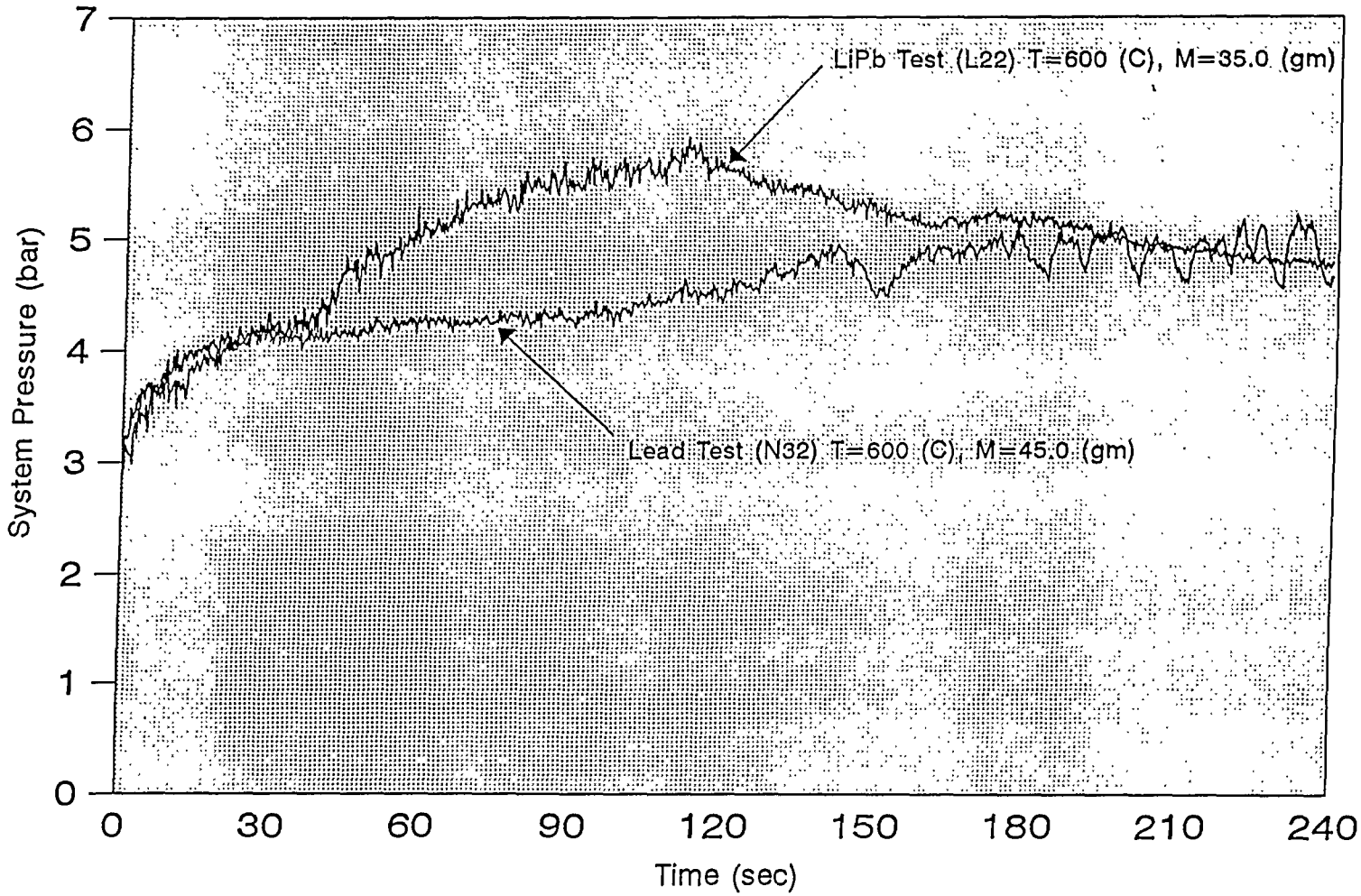
Appendix B Figure 14.1 System Pressure as a Function of Time (L21 & N32)



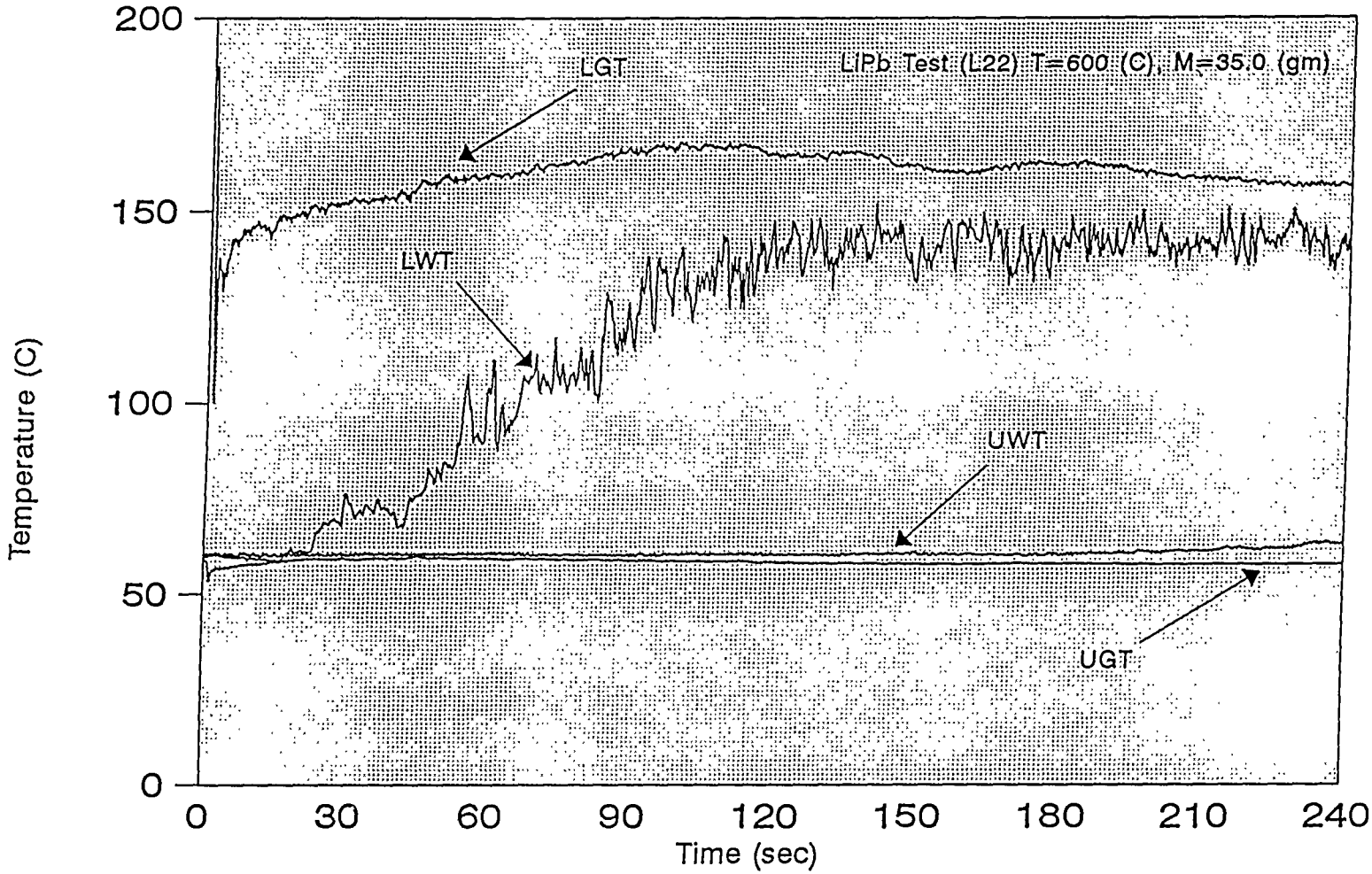
Appendix B Figure 14.2 Gas and Water Temperature as a Function of Time (L21)



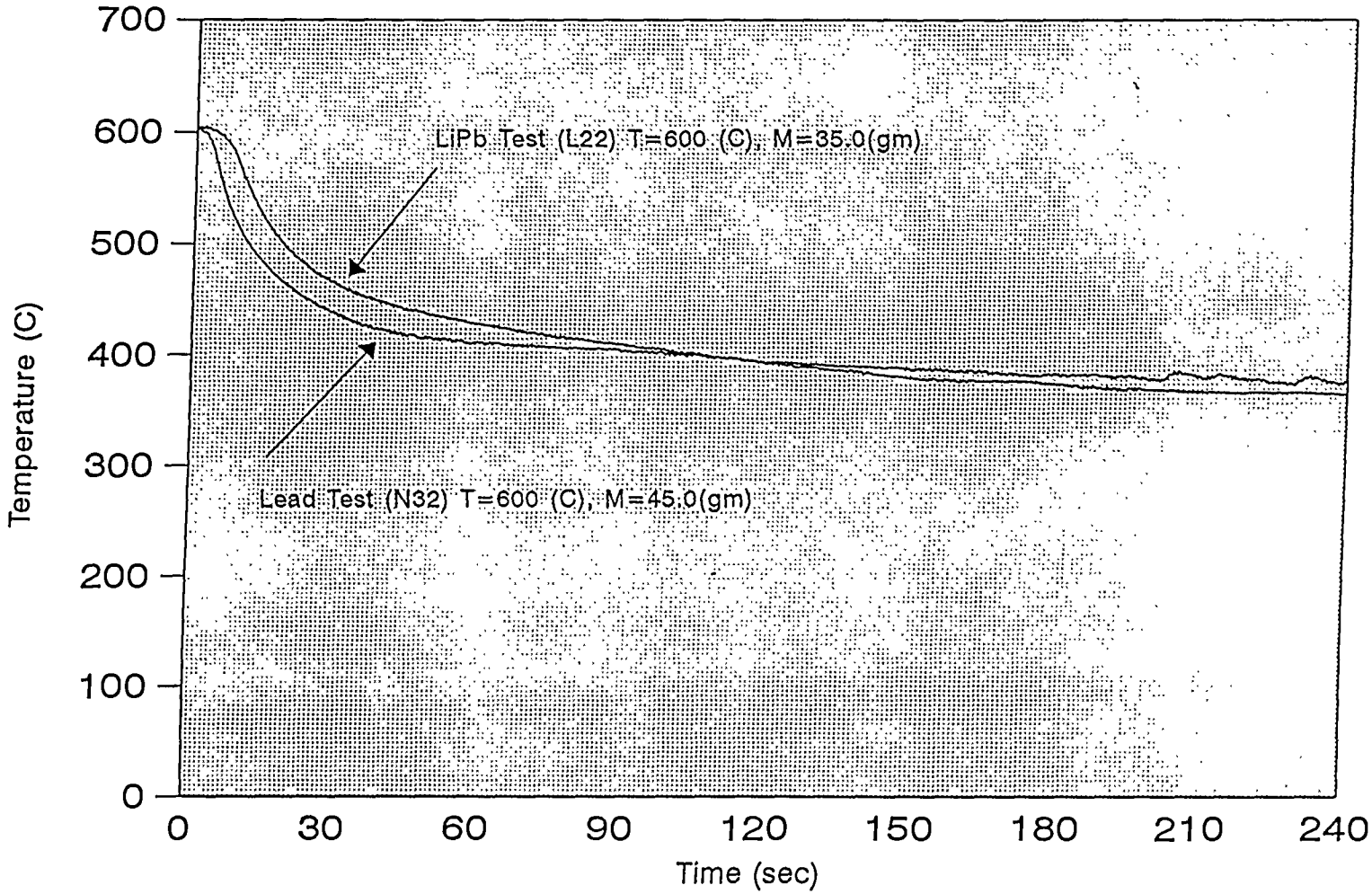
Appendix B Figure 14.3 Liquid Metal Temperature as a Function of Time (L21 & N32)



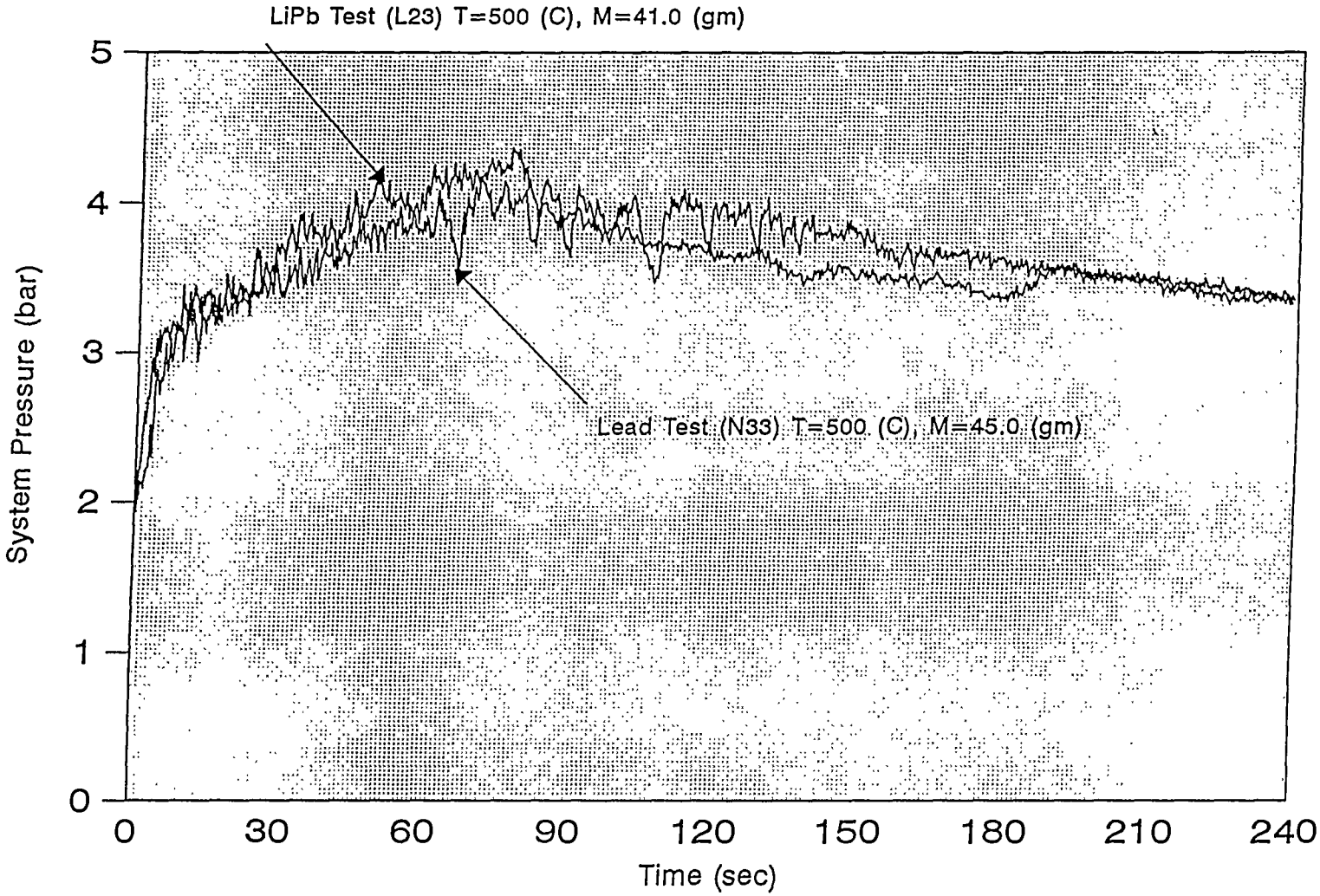
Appendix B Figure 15.1 System Pressure as a Function of Time (L22 & N32)



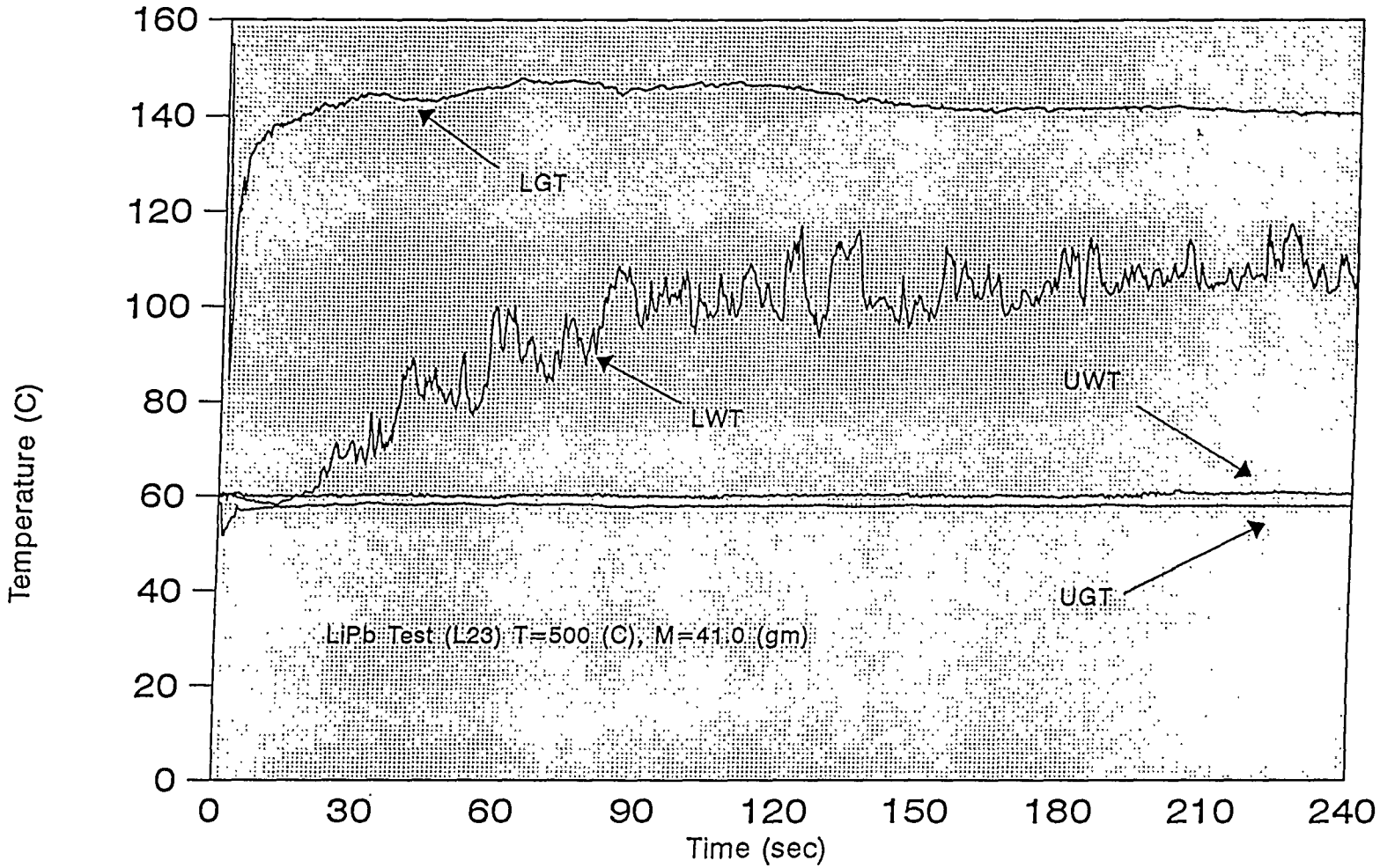
Appendix B Figure 15.2 Gas and Water Temperature as a Function of Time (L22)



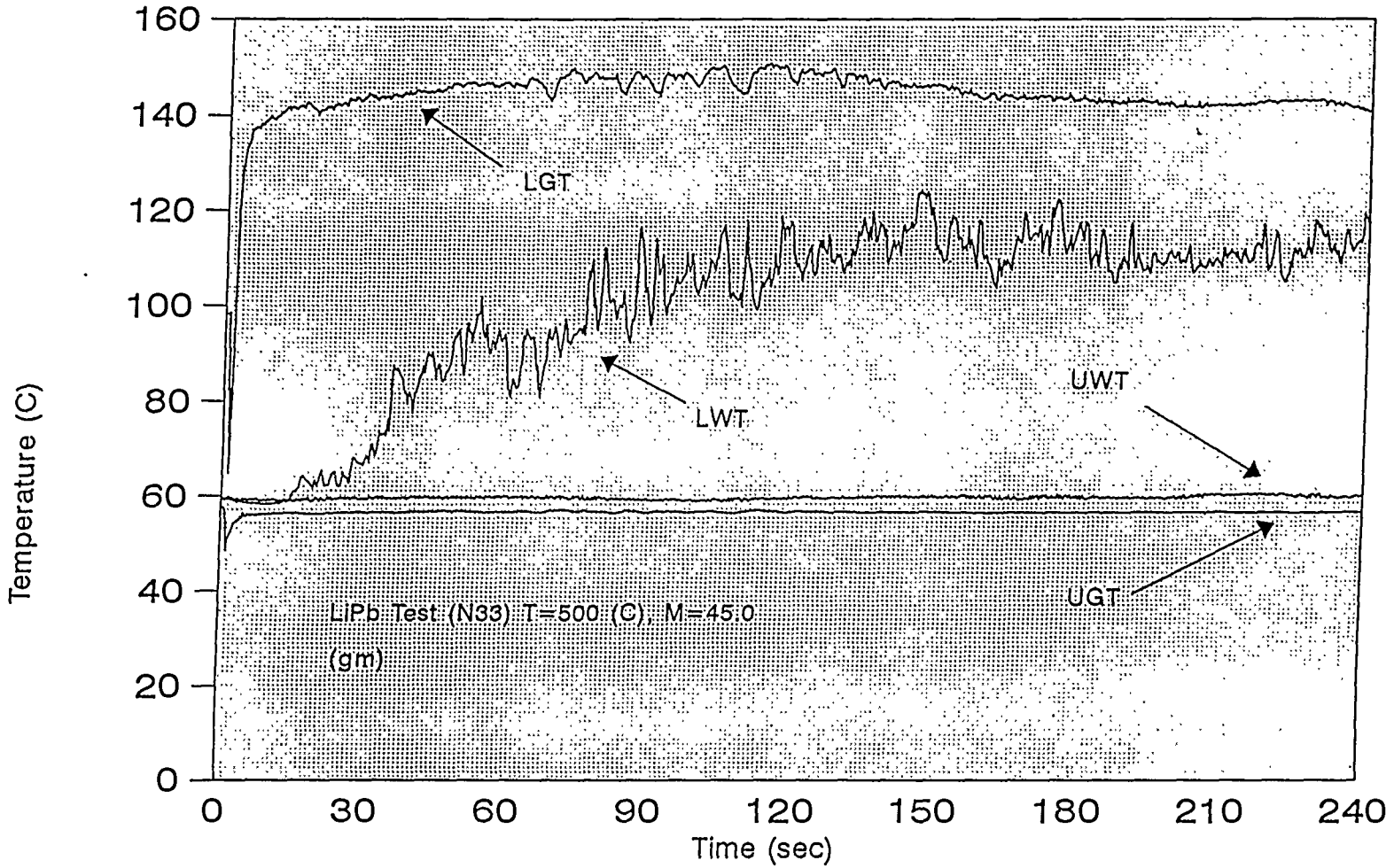
Appendix B Figure 15.3 Liquid Metal Temperature as a Function of Time (L22 & N32)



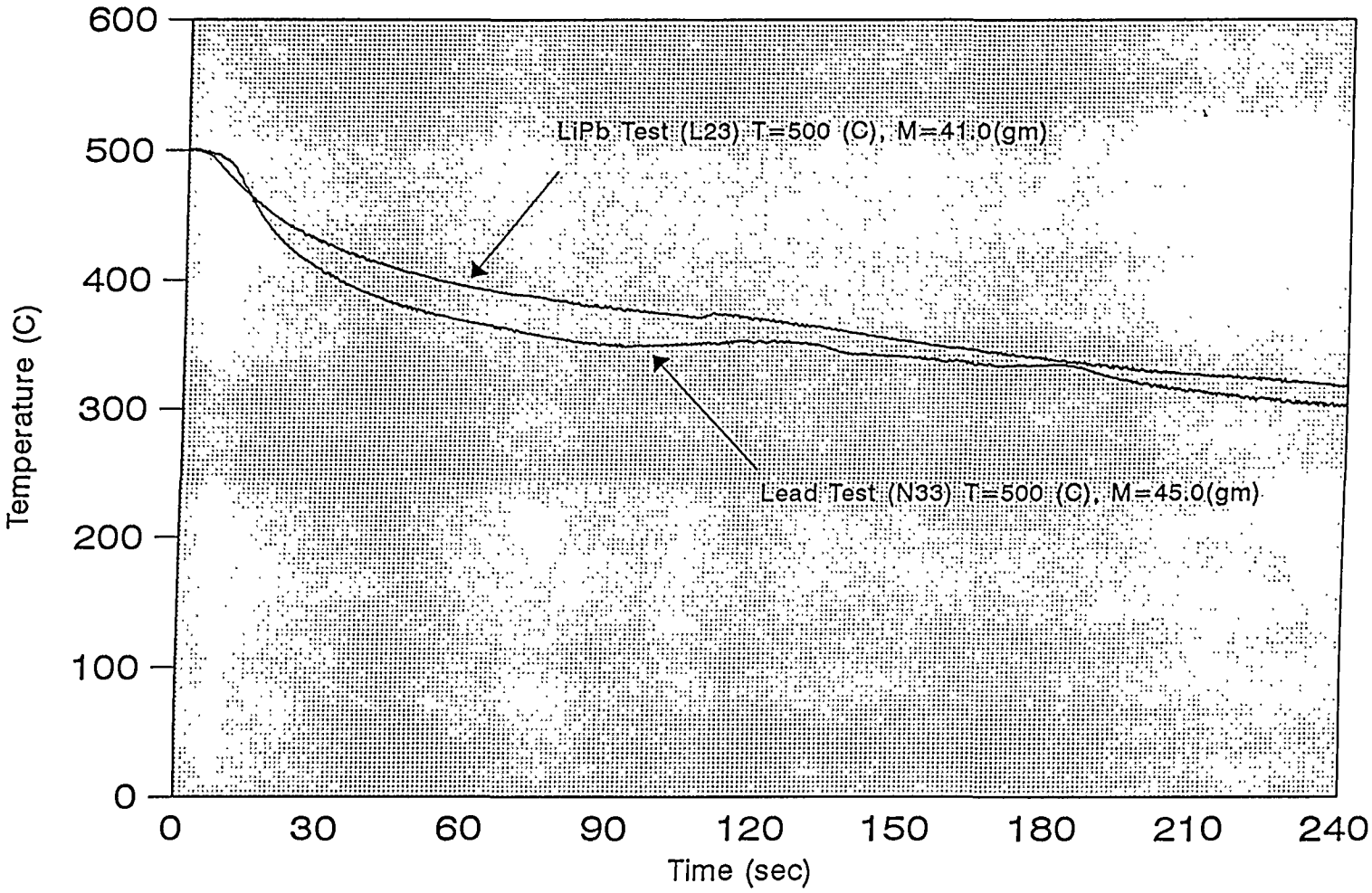
Appendix B Figure 16.1 System Pressure as a Function of Time (L23 & N33)



Appendix B Figure 16.2 Gas and Water Temperature as a Function of Time (L23)



Appendix B Figure 16.3 Gas and Water Temperature as a Function of Time (N33)



Appendix B Figure 16.4 Liquid Metal Temperature as a Function of Time (L23 & N33)

APPENDIX C

LISTING OF DATA ANALYSIS PROGRAM

COMPUTE 1

```
C                              PROGRAM
C
C     This program analyzes the experiment output.  It reads in the
C  data from the countdown phase, the reaction phase and the equilibrium
C  phase from the datafiles COUNTD.DAT, REACTION.DAT and EQUIL.DAT
C  respectively.
C
C  It then calculates the initial pressure and temperatures in the upper
C  and lower chambers. It calculates the mass of argon initially in the
lower
C  chamber at the start of the experiment.  The program then
C  calculates the system pressure due to the water vapor
C  pressure and Argon pressure.
C
C
C
      IMPLICIT  DOUBLE PRECISION  ( A-H, M-Z )
      IMPLICIT  INTEGER  ( I-L )
C      REAL *8 TLM,PLG,TLW,TLG
C


      DIMENSION TIME(500),UGT(500),TLG(500),UWT(500),TLW(500)
      DIMENSION TLM(500),TUF(500),TLF(500),UGP(500),PLG(500)
      COMMON/FACTOR/C(9)

      CHARACTER*15  FILENM1
      CHARACTER*15  FILENM2
      CHARACTER*15  FILENM3
      CHARACTER*15  FILEDP
      CHARACTER*1   RESPON
C
C
C*****  PROGRAM CONSTANTS  *****
C***** VUPFINAL IS THE FINAL GAS SPACE ABOVE LIQUID LEVEL AFTER EXPT.
C***** MEASURED FROM THE LIQUID LEVEL GAUGE AFTER THE EXPERIMENT.
C***** VDN = VOLUME OF THE LOWER CHAMBER BELOW THE LOWER FLANGE
C***** VDEAD1 = VOLUME OF DEAD SPACE IN VALVE
C***** VDEAD2 = VOLUME OF DEAD SPACE IN FLANGES AND THROUGH GASKET
THICKNESS
C***** BELOW BALL OF CLOSED VALVE
C***** VUPTOTAL = TOTAL VOLUME OF THE UPPER CHAMBER
C***** FWL = FINAL WATER LEVEL IN INCHES
C
      VDEAD1=22.86D0
      VDEAD2= 25.17D0
      VDN=90.09
      VUPTOTAL = 1385.D0
      ILEAK=0

C
C****CURVE FIT COEFFICIENTS FOR UPPER VOLUME AS FUNCTION OF WATER LEVEL
C      ZO= -2.23958
```

```
C       Z1= 28.9583
        UGV=55.00
C*** EQUATION FOR UPPER VOLUME AS A FUNCTION OF FINAL WATER LEVEL
C
 115   FORMAT(A)
       WRITE (*,145)
 145   FORMAT(10X,'The default initial upper gas volume is 55 cm3'
     3         / 10X, 'Do you want to change this (y/n)?' )
       READ (*,115)  RESPON
       IF  ( ( RESPON .EQ. 'Y' ) .OR. ( RESPON .EQ. 'y' ) )  THEN
       WRITE (*,150)
 150       FORMAT ( 10X, 'Enter the new final water level (in)')
       READ (*,*) UGV
       ENDIF

C       VUPFINAL=ZO+Z1*FWL
C
C **** INPUT THE LIQUID METAL MASS *****
C
       WRITE (6,125)
 125     FORMAT ( 10X, 'Enter the liquid metal mass (gm)' )
       READ (*,*)  MASLIQ
       DLIQ = 9.
       VGASDN = VDN -  MASLIQ / DLIQ + VDEAD2
C      VGASUPI = VUPFINAL - (VGASDN + VDEAD1)
C      VGASUPF = VUPFINAL
C      VH2O=VUPTOTAL-VGASUPI
       VGASUPI = UGV
       VH2O=VUPTOTAL-VGASUPI
       VGASUPF = UGV + (VGASDN + VDEAD1)
       RGAS = 83.14395
C     Universal Gas Constant     (bar/mole K)
       MWH2O = 18.02
C*****  SATURATION PRESSURE FORMULA FACTORS  *****
       C(1) = -7.691234564
       C(2) = -26.08023696
       C(3) = -168.1706546
       C(4) =  64.23285504
       C(5) = -118.9646225
       C(6) =  4.167117320
       C(7) =  20.97506760
       C(8) =  1.D9
       C(9) =  6.
C*****  LOGICAL UNIT NUMBERS  *****
C       IWRITE = 6
C       IREAD = 6
       IDATA1 =9
       IDATA2 = 10
       IDATA3 = 11
       IDELTP = 12
       ITH2O = 13
       ITLM = 14
       IPRES = 15
       ISYST = 16
       IPCOMP = 17
       IDOUT = 18
       IPH2 = 19
       IMH2 = 20
C*****  OUTPUT FILES  *****
       OPEN  ( ITH2O, FILE = 'TH2O.DAT')
```

```
      OPEN  ( ITLM, FILE = 'TLM.DAT')
      OPEN  ( IPRES, FILE = 'PRES.DAT')
      OPEN  ( ISYST, FILE = 'SYSTEM.TXT')
      OPEN  ( IPH2, FILE = 'PH2.DAT')
      OPEN  ( IMH2, FILE = 'MH2.DAT')
C*****  INPUT SECTION  *****
      FILENM1='COUNTD.DAT'
      FILENM2='REACTION.DAT'
      FILENM3='EQUIL.DAT'
      FILEDP='DELTP.DAT'
C      FILENM='P.DAT'
      OPEN  ( IDATA1, FILE = FILENM1)
      OPEN  ( IDATA2, FILE = FILENM2)
      OPEN  ( IDATA3, FILE = FILENM3)
C
      IDTP = 1
      AREA = 5.0671
      STOT = MASLIQ / ( DLIQ * AREA )
C
      TEQ = 600.
      WRITE (*,165)  TEQ
 165    FORMAT ( 10X, 'The time at which the mass of hydrogen is aver',
     1           'aged = ', 1P1G11.4, ' sec' / 10X, 'Do you want to ',
     2           'change it (y/n)?' )
      READ (*,115)  RESPON
      IF  ( ( RESPON .EQ. 'Y' ) .OR. ( RESPON .EQ. 'y' ) )  THEN
      WRITE (*,170)
 170      FORMAT ( 10X, 'Enter the new value of TEQ ' )
      READ (*,*)  TEQ
      END IF
      IMHAVE = 0
      IFLAG = 0
      MH2SUM = 0.
C
      IPOUT = 0
      WRITE (*,175)
 175    FORMAT ( 5X, 'Do you want the components of the pressure ',
     1               'saved (y/n)?' )
      READ (*,115)  RESPON
      IF  ( ( RESPON .EQ. 'Y' ) .OR. ( RESPON .EQ. 'y' ) )  THEN
      OPEN  ( IPCOMP, FILE = 'PCOMP.DAT')
      IPOUT = 1
      END IF
C
 200  CONTINUE
C
C*************************************************************************
C     INITIAL EXPERIMENTAL DATA
C*************************************************************************
C
C     In this section we read in the data for the countdown phase before
the
C  valve is opened.  We then calculate the average initial  temperatures
and
C  pressure in both the upper and lower chambers.
      I = 0
 250  CONTINUE
C
      I = I + 1
C
```

```
      READ (IDATA1,*,END=251)TIME(I),UGT(I),TLG(I),UWT(I),TLW(I)
     1,TLM(I),TUF(I),TLF(I),UGP(I),PLG(I)
C
C******* CONVERT PRESSURE FROM VOLTS TO BARS
C
C         UGP(I)=UGP(I)*20.D0*6.8948D-2
C         PLG(I)=PLG(I)*20.D0*6.8948D-2
C
C
WRITE(*,*)TIME(I),UGT(I),TLG(I),UWT(I),TLW(I),TLM(I),UGP(I),PLG(I)

       GO TO 250
C
  251 ICOUNT = I
      JCOUNT = ICOUNT - 1
C*****  EVALUATE INITIAL LOWER GAS PRESSURE AND TEMPERATURE ******
C*****  AND THE INITIAL UPPER GAS PRESSURE AND TEMPERATURE  *****
C*****  AND THE INITIAL LIQUID METAL TEMPERATURE **********
C ***** USING DATA FROM THE COUNTDOWN PHASE *****
       L = 0
       SUMPLG=0.
       SUMTLG=0.
       SUMUGP = 0.
       SUMUGT = 0.
       SUMUWT = 0.
       SUMTLM = 0.
C
C  EVALUATE SUMS
C
       DO 300  I = 1, JCOUNT
         SUMPLG = SUMPLG + PLG(I)
         SUMTLG = SUMTLG + TLG(I)
C
         SUMUGP = SUMUGP + UGP(I)
         SUMUGT = SUMUGT + UGT(I)
         SUMUWT = SUMUWT + UWT(I)
         SUMTLM = SUMTLM + TLM(I)
C

  300  CONTINUE
C
C   EVALUATE MEAN VALUES
C
       L=JCOUNT
       PDN = SUMPLG / DBLE( L )
       TDN = SUMTLG / DBLE( L )
       PUP = SUMUGP / DBLE( L )
       TUP = SUMUGT / DBLE( L )
       TH2OI = SUMUWT / DBLE( L )
       TLMI = SUMTLM / DBLE( L )
 C*****  EVALUATE STANDARD DEVIATIONS OF AVERAGED QUANTITIES  *****
       SDVPDN = 0.
       SDVTDN = 0.
C
       SDVPUP = 0.
       SDVTUP = 0.
       SDVTH2 = 0.
       SDVTLM = 0.
C
       DO 350  I = 1,JCOUNT
```

```
      SDVPDN = SDVPDN  +  ( PDN - PLG(I) ) * ( PDN - PLG(I) )
      SDVTDN = SDVTDN  +  ( TDN - TLG(I) ) * ( TDN - TLG(I) )
C
      SDVPUP = SDVPUP  +  ( PUP -UGP(I) ) * ( PUP - UGP(I) )
      SDVTUP = SDVTUP  +  ( TUP - UGT(I) ) * ( TUP - UGT(I) )
      SDVTH2 = SDVTH2  +  ( TH2OI - UWT(I) ) * ( TH2OI - UWT(I) )
      SDVTLM = SDVTLM  +  ( TLMI - TLM(I) ) * ( TLMI - TLM(I) )

 350  CONTINUE
      SDVPDN = DSQRT( SDVPDN / DBLE( JCOUNT ) )
      SDVTDN = DSQRT( SDVTDN / DBLE( JCOUNT ) )
C
      SDVPUP = DSQRT( SDVPUP / DBLE( JCOUNT ) )
      SDVTUP = DSQRT( SDVTUP / DBLE( JCOUNT ) )
      SDVTH2 = DSQRT( SDVTH2 / DBLE( JCOUNT ) )
      SDVTLM = DSQRT( SDVTLM / DBLE( JCOUNT ) )
C
C*****  EVALUATE INITIAL WATER VAPOR PRESSURE  *****
      TUPK = TUP + 273.15
      TDNK = TDN + 273.15
C
      CALL PSAT  (TUPK, PVAPI  )
C
C*****  EVALUATE INITIAL ARGON MASS IN SOLUTION  *****
C
C      First we evaluate the initial Ar solubility and water density.
      TSATK = 373.998 * ( PUP**(.07144015) )
      TSAT = TSATK - 273.15
      XAR = 3.7D-7 * (TSAT - TH2OI)*(PUP-PVAPI)/(TSAT-25.0)/1.013
      IF(XAR .LT.0.0) XAR=0.0
      DENH2O = 1.0098  -  4.86871D-4 * TH2OI
C
      MARSOL = XAR * VH2O * DENH2O / MWH2O
C
      MARUP = ( PUP - PVAPI ) * VGASUPI / (RGAS*TUPK)
      MARDOWN =  PDN * VGASDN / (RGAS*TDNK )
      MAR = MARUP + MARDOWN + MARSOL
C*****  OUTPUT INITIAL VALUES  *****
C
C     First we output problem parameters to the screen.
      WRITE (*,400)  FILENM1,FILENM2,FILENM3
      WRITE (ISYST,401)   FILENM1,FILENM2,FILENM3
  400   FORMAT ( /// 5X, 'For the system pressure files ', 3A12 / )
  401   FORMAT ( 5X, 'For the system pressure files ', 3A12 / )
C
      IF  ( IDTP .EQ. 0 )  THEN
C        WRITE (*,405)  FILEDP
C        WRITE (ISYST,405)  FILEDP
  405     FORMAT ( 5X, 'And the DELTAP pressure file ', A12 / )
      END IF
C
      WRITE (*,410)  TLMI, SDVTLM, TH2OI, SDVTH2, MASLIQ, STOT
      WRITE (ISYST,410)  TLMI, SDVTLM, TH2OI, SDVTH2, MASLIQ, STOT
  410   FORMAT( 5X, 'The experimental parameters are: '/
     1          5X, 'initial liquid metal temp. = ', 1P1G11.4, ' +/- ',
     2              1P1G11.4, ' C ' /
     3          5X, 'initial water temperature  = ', 1P1G11.4, ' +/- ',
     4              1P1G11.4, ' C ' /
     5          5X, 'liquid metal mass          = ', 1P1G11.4, ' gm  '/
     6          5X, 'and the metal has a depth  = ', 1P1G11.4, ' cm  '/)
```

```
C
      WRITE (*,415)  TUP, SDVTUP, VGASUPI, TDN, VGASDN
      WRITE (ISYST,415)  TUP, SDVTUP, VGASUPI, TDN, VGASDN
 415    FORMAT(10X, 'with initial upper Ar temp = ', 1P1G11.4, ' +/- ',
     1              1P1G11.4, ' C  ' /
     2         10X, 'the upper gas layer volume = ', 1P1G11.4, ' cm3 '/
     3         10X, 'with initial lower Ar temp = ', 1P1G11.4, ' C   '/
     4         10X, 'the lower gas layer volume = ', 1P1G11.4, ' cm3 '/)
C
      WRITE (*,420)  PUP, SDVPUP, PDN, SDVPDN
      WRITE (ISYST,420)  PUP, SDVPUP, PDN, SDVPDN
 420    FORMAT(10X, 'the initial upper pressure = ', 1P1G11.4, ' +/- ',
     2               1P1G11.4, ' bar ' /
     3         10X, 'the initial lower pressure = ', 1P1G11.4, ' +/- ',
     4               1P1G11.4, ' bar ' //)
C
      WRITE (*,425)  MAR, MARUP, MARDOWN, MARSOL
      WRITE (ISYST,425)  MAR, MARUP, MARDOWN, MARSOL
 425    FORMAT(10X, 'the total argon mass       = ', 1P1G11.4, ' mole'/
     1         10X, 'the  upper chamb argon mass= ', 1P1G11.4, ' mole'/
     1         10X, 'the lower chamb argon mass = ', 1P1G11.4, ' mole'/
     1         10X, 'the argon mass in solution = ', 1P1G11.4, ' mole'/)


C
C     Now to output the initial values to the data files.
      PAR = PUP - PVAPI
      MHLEAK = 0.
      IF  ( IPOUT .EQ. 1 )  THEN
      WRITE (IPCOMP,998)  TIME(JCOUNT), PAR, PVAPI, MARSOL, MHLEAK
      END IF
      PH2 = 0.
      MH2TOT = 0.
C      WRITE (IPH2,999)  TIME(JCOUNT), PH2
C     WRITE (IMH2,999)  TIME(JCOUNT), MH2TOT
C
      TIME0 = 0.0
C
C*********************************************************************
C             MAIN CALCULATIONAL LOOP
C   THIS SECTION READS IN THE DATA FOR THE REACTION PHASE AND CALCULATES
C   THE MASS OF HYDROGEN GENERATED DURING THE PHASE AS A FUNCTION OF
C   TIME. CORRECTION FOR LEAKAGE IS MADE USING LEAKAGE INFORMATION
C   FROM A SEPARATE FILE
C*********************************************************************
C*********************************************************************
C           INNER LOOP
C*********************************************************************
C
C*****  DATA INPUT SECTION  *****
C
      K=0

 2000 CONTINUE
C
      K=K+1

       READ (IDATA2,*,END=2500)TIME1,TGAS1,TLG1,TH2O1,TLW1,TLM1
     1 ,TUF1,TLF1,PRES1,PLG1
C
```

```
C ******* CONVERT PRESSURE FROM VOLTS TO BARS *******
C
C       PRES1=PRES1*20.D0*6.8948D-2
C       PLG1 =PLG1*20.D0*6.8948D-2

C         READ (IDATA,*,END=2500)  TIME1, PRES1, TGAS1, TH2O1, TLM1
C
C
C*****  EVALUATE PVAP(TGAS1)  *****
       TGASK = TGAS1 + 273.15
C
       CALL PSAT  (TGASK,PVAP )
C
C*****  EVALUATE ARGON MASS IN SOLUTION  *****
C
C      This is the argon that stays in solution as it
c      bubbles to the upper chamber.
C
       TSATK = 373.998 * ( PRES1**(.07144015) )
       TSAT = TSATK - 273.15
       XAR = 3.7D-7 *(TSAT - TH2O1)*(PRES1-PVAP)/(TSAT-25.0)/1.013
       DENH2O = 1.0098  -  4.86871D-4 * TH2O1
       IF(K.EQ.1) THEN
       XAR=0.D0
       ENDIF
C
       MARSOL = XAR * VH2O * DENH2O / MWH2O
C*****  EVALUATE HYDROGEN MASS IN SOLUTION  *****
C
C      This is the hydrogen in solution.
       XH2 = 1.7D-7 *(TSAT-TH2O1)*PH2/(TSAT-25.0)/1.013
       MH2SOL = XH2 * VH2O * DENH2O / MWH2O
C*****  EVALUATE NEW ARGON MASS  *****
C
C      Here we calculate the new argon mass, which is lower due to leak-
C  age.  But first we must estimate the leakage rate at the system pres-
C  sure.
C ***************** SET CONSTANTS TO ZERO ************
       A1=0.0
       B1=0.0
       C1=0.0
       IF(ILEAK .GT. 0 ) THEN
       DPDT = A1  +  B1 * PRES1  +  C1 * PRES1 * PRES1
       IF  ( DPDT .LT. 0. )  DPDT = 0.
C
       MAR = MAR  -  ( DPDT * ( PAR / ( PAR + PH2+PVAP ) ) * ( TIME1
      1                   - TIME0 ) * VGASUPF / ( RGAS * TGASK ) )
C
C*****  EVALUATE TOTAL HYDROGEN MASS TO HAVE LEAKED FROM SYSTEM  *****
       MHLEAK = MHLEAK  +  ( DPDT * ( PH2 / ( PAR + PH2+PVAP ) ) *
      1            ( TIME1 - TIME0 ) * VGASUPF / ( RGAS * TGASK ) )
       ENDIF
C
C*****  UPDATE ARGON PRESSURE  *****
       PAR = ( MAR - MARSOL ) * RGAS * TGASK / VGASUPF
C
C*****  EVALUATE HYDROGEN PRESSURE  *****

       PH2 = PRES1 - PAR - PVAP
```

```
C         PH2 = PRES1 - PAR - PVAP - DELPC - ( MH2SOL * RGAS * TGASK
C     1         / VGASUPF )
C
C*****  EVALUATE TOTAL HYDROGEN MASS  *****
      MH2TOT = ( PH2 * VGASUPF / ( RGAS * TGASK ) )  +  MH2SOL  +
     1             MHLEAK
C
C
C*****  OUTPUT NON-EQUILIBRIUM DATA  *****
      WRITE (ITH2O,997)  TIME1, TH2O1, TGAS1
      WRITE (ITLM,999)  TIME1, TLM1
      WRITE (IPRES,999)  TIME1, PRES1
      WRITE (IPH2,999)  TIME1, PH2
      WRITE (IMH2,999)  TIME1, MH2TOT
      IF  ( IDTP .EQ. 0 )  THEN
C          WRITE (IDOUT,999)  TIME1, DELPC
      END IF
      IF  ( IPOUT .EQ. 1 )  THEN
        WRITE (IPCOMP,998)  TIME1, PAR, PVAP, MARSOL, MHLEAK
      END IF
C
      TIME0 = TIME1
C*****  END OF INNER LOOP  *****
C
      GO TO 2000
C
C*****  END OF DELTAP COMPARISON LOOP  *****
C
 2500 CONTINUE
C



C
C**********************************************************************
C             MAIN CALCULATIONAL LOOP FOR EQUILIBRIUM PHASE
C   THIS SECTION READS IN THE DATA FOR THE EQUILIBRIUM PHASE AND
CALCULATES
C   THE MASS OF HYDROGEN INVENTORY DURING THE PHASE AS A FUNCTION OF
C   TIME. CORRECTION FOR LEAKAGE IS MADE USING LEAKAGE INFORMATION
C   FROM A SEPARATE FILE
C**********************************************************************
C**********************************************************************
C           INNER LOOP
C**********************************************************************
C
C*****  DATA INPUT SECTION  *****
C
      TIME0=0.0
 3000 CONTINUE
C
      READ (IDATA3,*,END=3500)TIME1,TGAS1,TLG1,TH2O1,TLW1,TLM1
     1 ,TUF1,TLF1,PRES1,PLG1
C
C ******* CONVERT PRESSURE FROM VOLTS TO BARS *******
C
C       PRES1=PRES1*20.D0*6.8948D-2
C       PLG1 =PLG1*20.D0*6.8948D-2
```

```
C       WRITE(ISYST,*)TIME,TGAS1,TLG1
C         READ (IDATA,*,END=2500)  TIME1, PRES1, TGAS1, TH2O1, TLM1
C
C
C*****  EVALUATE PVAP(TGAS1)  *****
       TGASK = TGAS1 + 273.15
C
       CALL PSAT  (TGASK,PVAP )
C*****  EVALUATE ARGON MASS IN SOLUTION  *****
C
C      This is the argon that comes out of solution due to the rising
C  water temperature.
       VH2O=VUPTOTAL-VGASUPF
       TSATK = 373.998 * ( PRES1**(.07144015) )
       TSAT = TSATK - 273.15
       XAR = 3.7D-7 *(TSAT-TH2O1)*PAR/(TSAT-25.0)/1.013
       DENH2O = 1.0098  -  4.86871D-4 * TH2O1
C
       MARSOL = XAR * VH2O * DENH2O / MWH2O
C*****  EVALUATE HYDROGEN MASS IN SOLUTION  *****
C
C      This is the hydrogen in solution.
       XH2 = 1.7D-7 *(TSAT-TH2O1)*PH2/(TSAT-25.0)/1.013
       MH2SOL = XH2 * VH2O * DENH2O / MWH2O
C*****  EVALUATE NEW ARGON MASS  *****
C
C      Here we calculate the new argon mass, which is lower due to leak-
C  age.  But first we must estimate the leakage rate at the system pres-
C  sure.
C ***************** SET CONSTANTS TO ZERO ************
       A1=0.0
       B1=0.0
       C1=0.0
       IF(ILEAK .GT. 0 ) THEN
       DPDT = A1  +  B1 * PRES1  +  C1 * PRES1 * PRES1
       IF  ( DPDT .LT. 0. )  DPDT = 0.
C
       MAR = MAR  -  ( DPDT * ( PAR / ( PAR + PH2+PVAP ) ) * ( TIME1
      1                  - TIME0 ) * VGASUPF / ( RGAS * TGASK ) )
C
C*****  EVALUATE TOTAL HYDROGEN MASS TO HAVE LEAKED FROM SYSTEM  *****
       MHLEAK = MHLEAK  +  ( DPDT * ( PH2 / ( PAR + PH2+PVAP ) ) *
      1           ( TIME1 - TIME0 ) * VGASUPF / ( RGAS * TGASK ) )
       ENDIF

C*****  UPDATE ARGON PRESSURE  *****
       PAR = ( MAR - MARSOL ) * RGAS * TGASK / VGASUPF
C
C*****  EVALUATE HYDROGEN PRESSURE  *****
C
       PH2 = PRES1 - PAR - PVAP
       WRITE(*,*)"PRES1, PAR, PVAP, PH2",PRES1,PAR,PVAP,PH2
C
C        PH2 = PRES1 - PAR - PVAP - DELPC - ( MH2SOL * RGAS * TGASK
C     1        / VGASUPF )
C
C*****  EVALUATE TOTAL HYDROGEN MASS  *****
       MH2TOT = ( PH2 * VGASUPF / ( RGAS * TGASK ) )  +  MH2SOL  +
      1             MHLEAK
```

```
C       WRITE(*,*)"MADE IT THIS FAR"
C       STOP
C
C*****  EVALUATE AVERAGE HYDROGEN MASS AT TEQ  *****
C***** THIS IS DONE BY AVERAGING THE TOTAL MASS BETWEEN ******
C***** THE TIME INTERVAL TEQ-DTEQ AND TEQ
C         DTEQ=2.0
C         IF  ( ( TIME1 .GE. ( TEQ - DTEQ ) )  .AND.  ( TIME1 .LE.
C     1         ( TEQ + DTEQ ) ) )  THEN
          IMHAVE = IMHAVE + 1
          MH2SUM = MH2SUM + MH2TOT
C           WRITE(ISYST,*)TIME1,MH2SUM
C         ELSE
C         IF ( ( TIME1 .GT. ( TEQ  ) ) .AND. (IFLAG .EQ.
C     1       0 ))  THEN
C           IFLAG = 1
C           MH2AVE = MH2SUM / DBLE( IMHAVE )
C
C           WRITE (*,450)  TEQ, MH2AVE
C           WRITE (ISYST,450)  TEQ, MH2AVE
C 450         FORMAT(10X, 'at time                        = ', 1P1G11.4,
C     1                 ' sec ' /
C     2             5X, 'the total mass of hydrogen = ', 1P1G11.4,
C     3                 ' mole' )
C
C         END IF
C         END IF
C
C*****  OUTPUT DATA  FROM NON-EQUILIBRIUM TO EQUILIBRIUM STATE *****
        WRITE (ITH2O,997)  TIME1, TH2O1, TGAS1
        WRITE (ITLM,999)  TIME1, TLM1
        WRITE (IPRES,999)  TIME1, PRES1
        WRITE (IPH2,999)  TIME1, PH2
        WRITE (IMH2,999)  TIME1, MH2TOT
        IF  ( IDTP .EQ. 0 )  THEN
C           WRITE (IDOUT,999)  TIME1, DELPC
        END IF
        IF  ( IPOUT .EQ. 1 )  THEN
          WRITE (IPCOMP,998)  TIME1, PAR, PVAP, MARSOL, MHLEAK
        END IF
C
        TIME0 = TIME1
C*****  END OF INNER LOOP  *****
C
        GO TO 3000
C
C*****  END OF DELTAP COMPARISON LOOP  *****
C
 3500 CONTINUE
C
          MH2AVE = MH2SUM / DBLE( IMHAVE )
C
          WRITE (*,450)  TIME1, MH2AVE,MH2SOL,MHLEAK
          WRITE (ISYST,450)  TIME1, MH2AVE,MH2SOL,MHLEAK
  450     FORMAT(10X, 'at time                                = ', 1P1G11.4,
     1                ' sec ' /
     2           5X, 'the total mass of hydrogen          = ', 1P1G11.4,
     3                ' mole' /
     2           5X, 'the total mass of hydrogen IN SOL   = ', 1P1G11.4,
     3                ' mole' /
```

```
     2          5X, 'the total mass of hydrogen LEAKEED = ', 1P1G11.4,
     3                  ' mole' )
C
C
C*************************************************************************
C          END OF PROGRAM
C*************************************************************************
C
 997  FORMAT ( 3(2X,1P1G11.4) )
 998  FORMAT ( 5(2X,1P1G11.4) )
 999  FORMAT ( 2(2X,1P1G11.4) )

C*****  OUTPUT FILES  *****
      CLOSE ( ITH2O)
      CLOSE ( ITLM)
      CLOSE ( IPRES)
      CLOSE ( ISYST)
      CLOSE ( IPH2)
      CLOSE ( IMH2)
      CLOSE ( IDATA1)
      CLOSE ( IDATA2)
      CLOSE ( IDATA3)
      CLOSE ( IPCOMP)
      CLOSE ( IDELTP)
C
C     That's all folks!
      END
C
C*************************************************************************
C
C
C*************************************************************************
C
      SUBROUTINE PSAT  ( T,P  )
C
C     This subroutine evaluates the the saturation pressure of water,
C  in Bar, given the water temperature in Kelvin.  This subroutine uses
C  a formula for the saturation line given in the ASME steam tables.
C
      IMPLICIT  DOUBLE PRECISION  ( A-H, M-Z )
      IMPLICIT  INTEGER  ( I-L )
C
      COMMON  / FACTOR /  C(9)
C
C*****  REDUCED TEMPERATURE  *****
      THETA = T / 647.3
C*****  FORMULA FACTORS  *****
      THETA1 = 1. - THETA
C
      NUMER1 = 0.
      DO 100  I = 1, 5
      NUMER1 = C(I) * ( THETA1 ** DBLE(I) )  +  NUMER1
  100 CONTINUE
C
      DENOM1 = 1.  +  C(6) * THETA1  +  C(7) * THETA1 * THETA1
C
      DENOM2 = C(8) * THETA1 * THETA1  +  C(9)
C*****  REDUCED PRESSURE  *****
      BETA = DEXP( NUMER1 / ( DENOM1 * THETA )  -  THETA1 / DENOM2 )
```

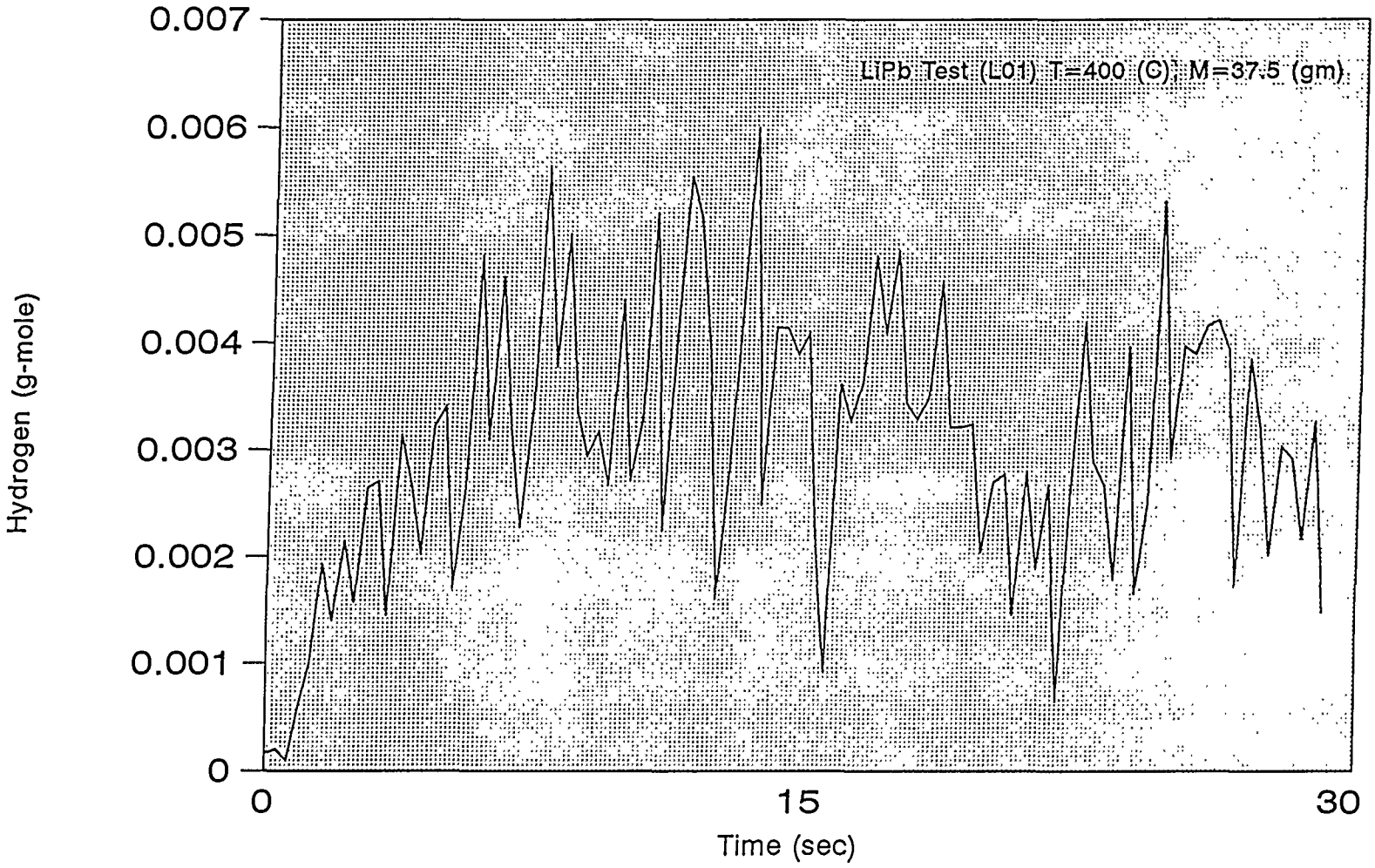
```
C*****  SATURATION PRESSURE  *****
      P = 221.2 * BETA
C
C     That's all folks!
      RETURN
      END
```

APPENDIX D

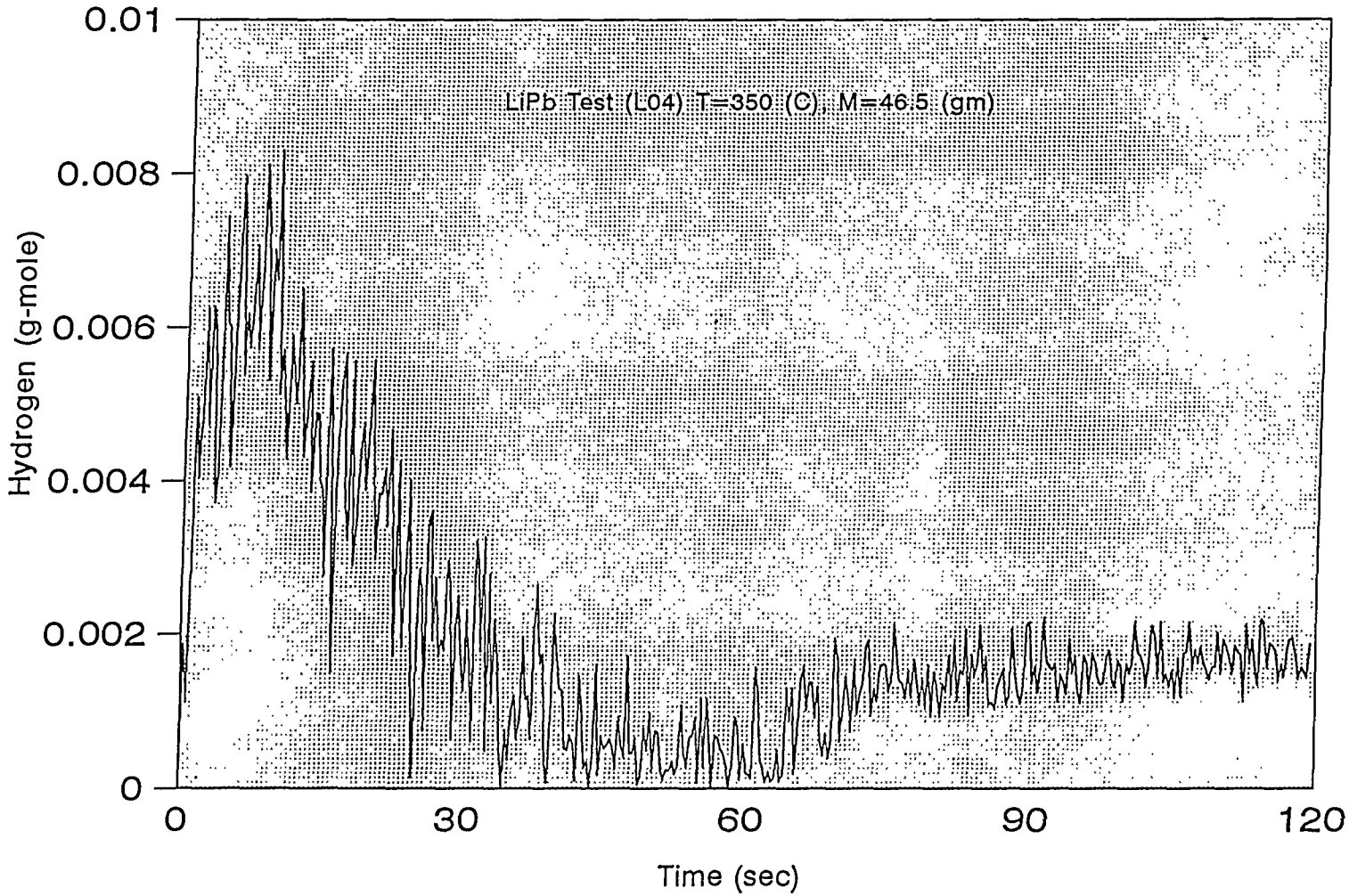
HYDROGEN GENERATED FROM TESTS

The following 14 graphs contain a complete representation of the hydrogen generation drawn from 14 lithium-lead tests . The graphs are listed in the following table. The table gives the test and page numbers.

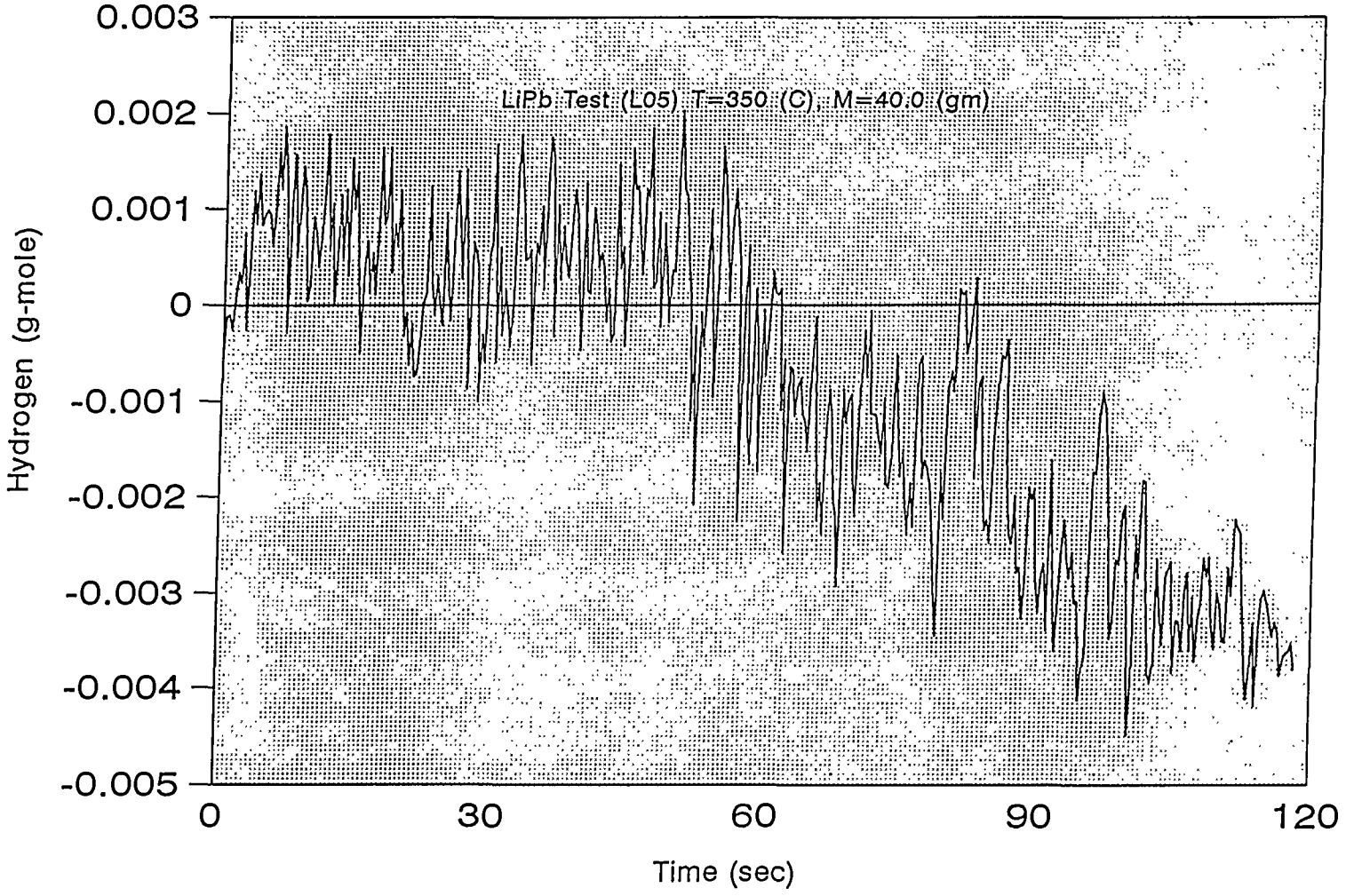
Experiment Number — Page Number



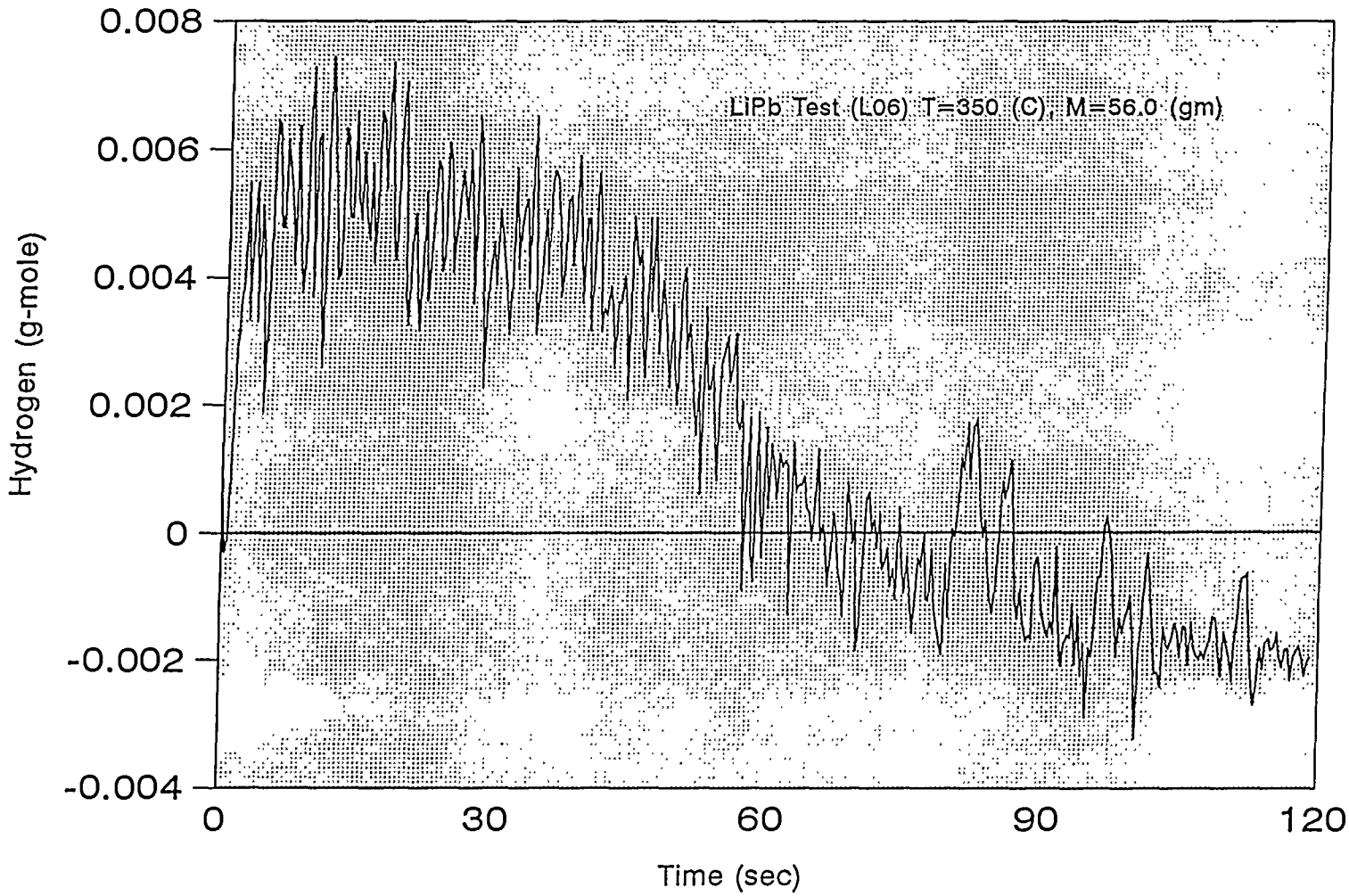
Appendix E Figure 1 Corrected Hydrogen Generation as a Function of Time (L01)



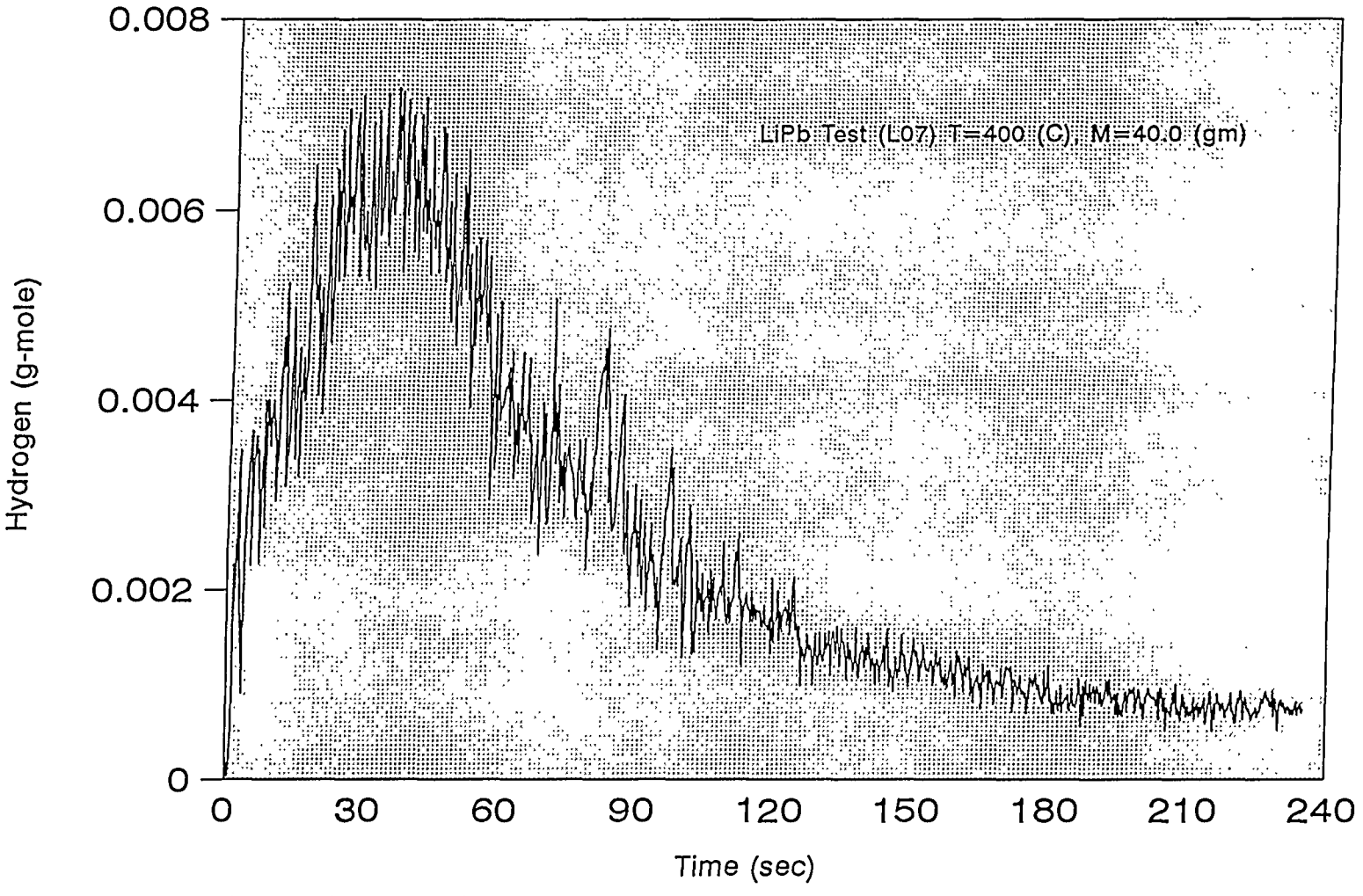
Appendix E Figure 2 Corrected Hydrogen Generation as a Function of Time (L04)



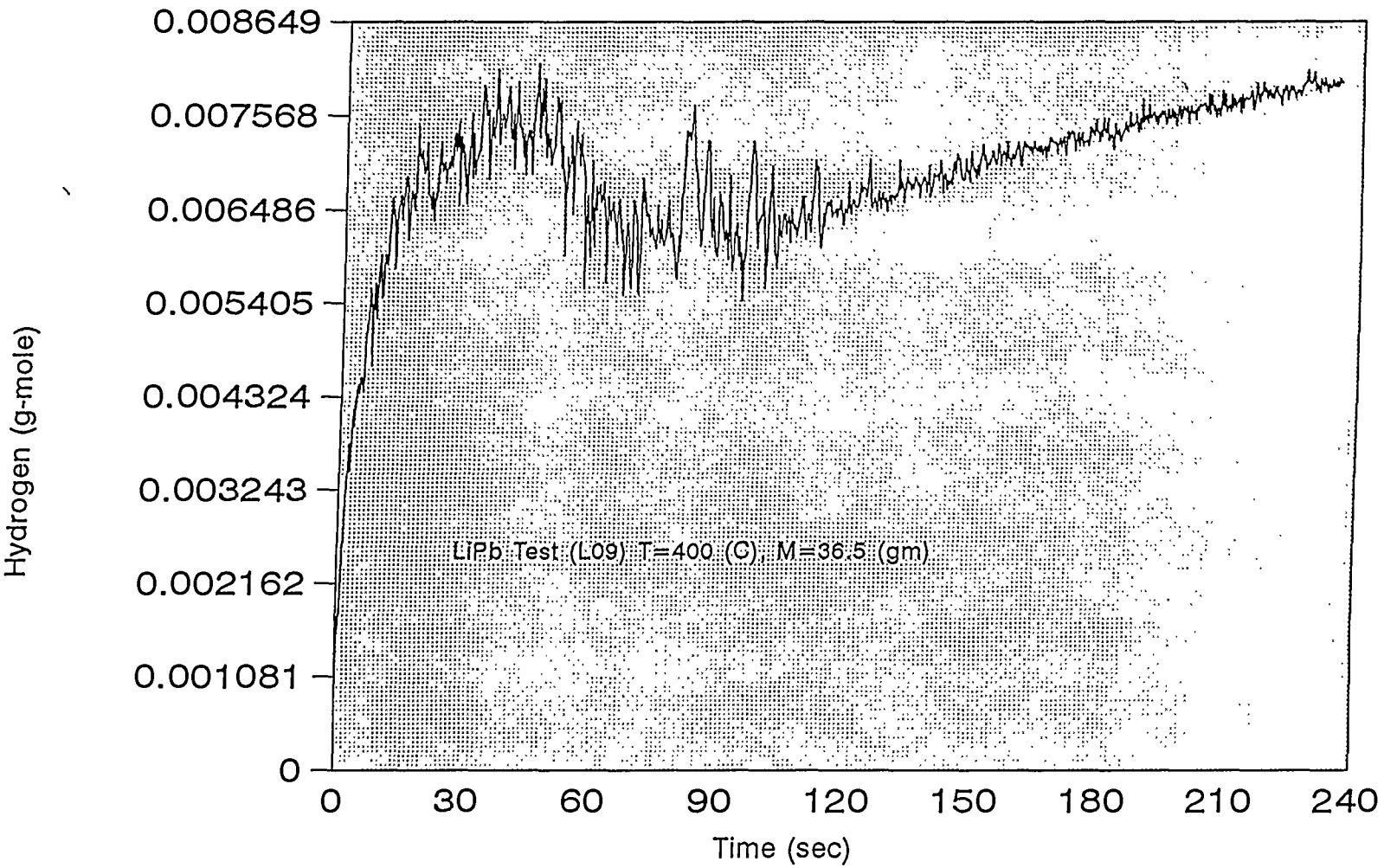
Appendix E Figure 3 Corrected Hydrogen Generation as a Function of Time (L05)



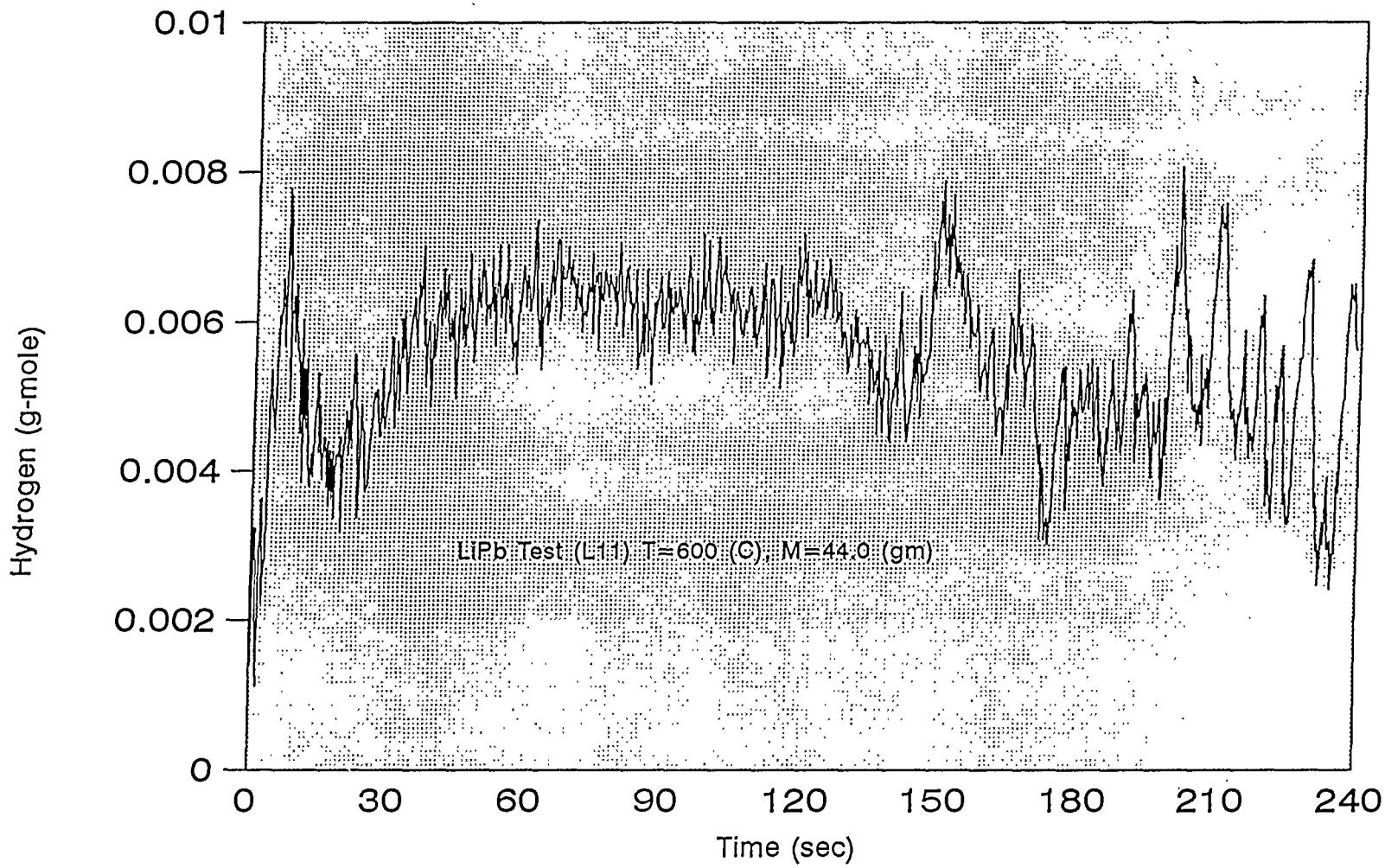
Appendix E Figure 4 Corrected Hydrogen Generation as a Function of Time (L06)



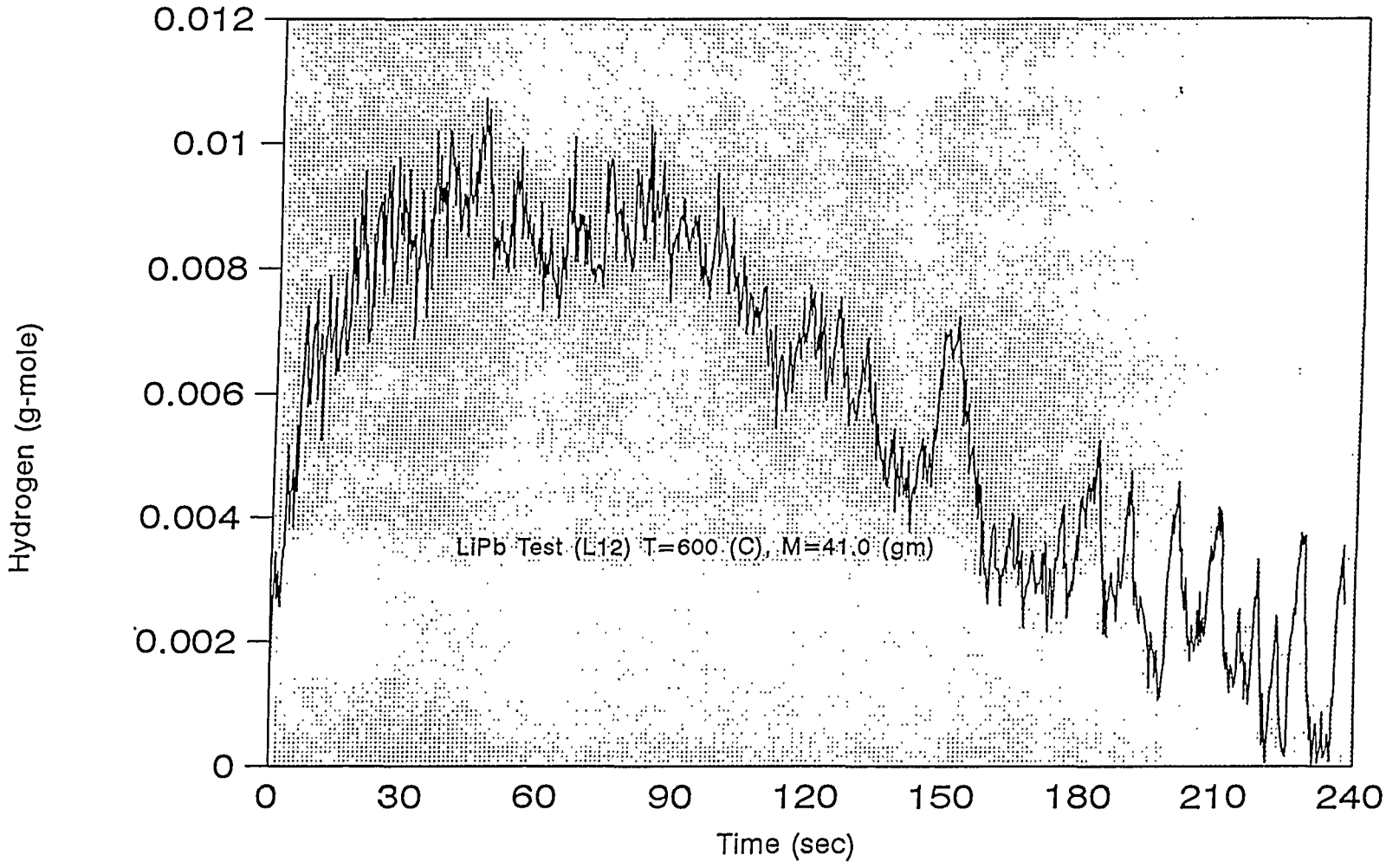
Appendix E Figure 5 Corrected Hydrogen Generation as a Function of Time (L07)



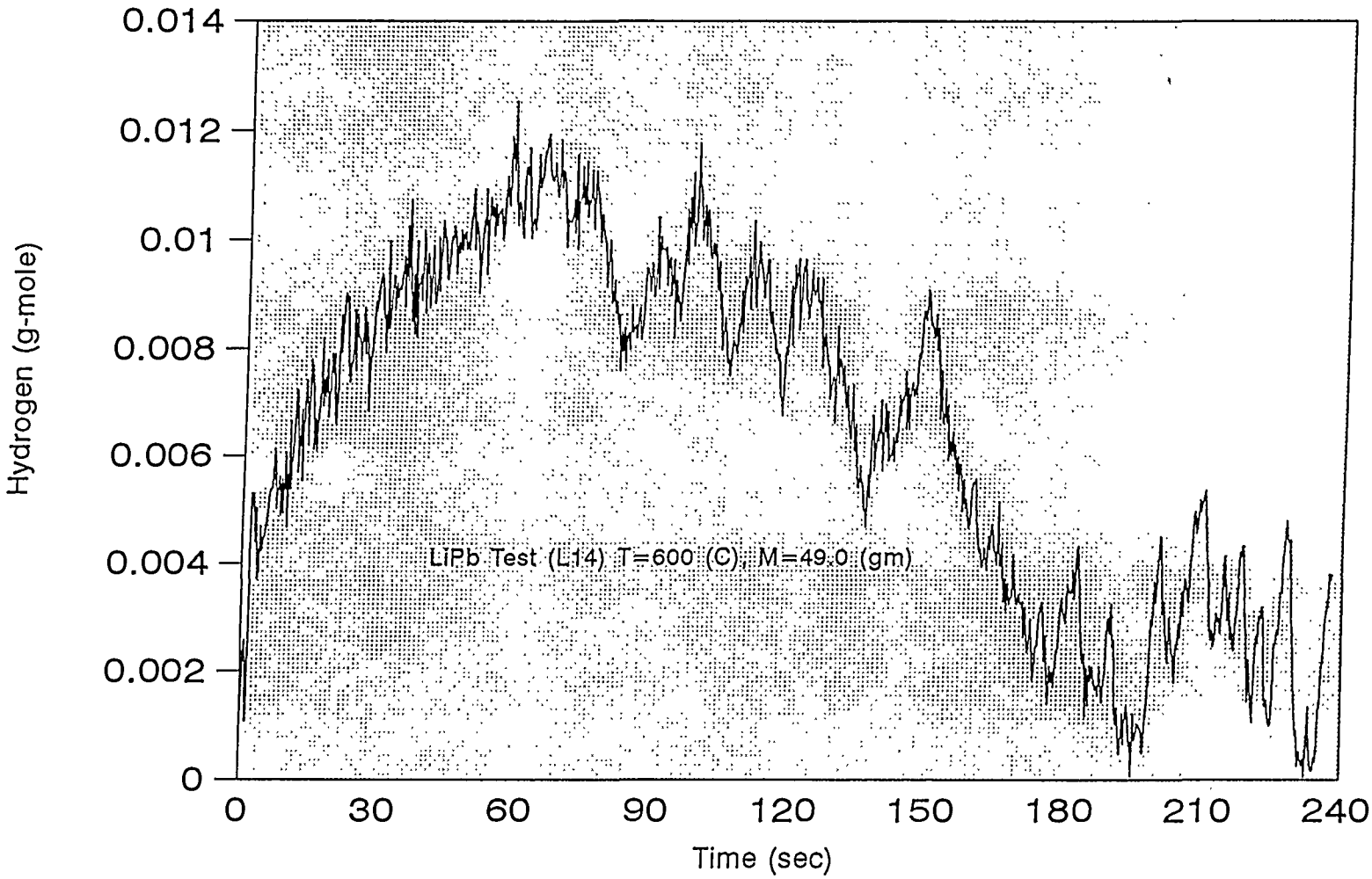
Appendix E Figure 6 Corrected Hydrogen Generation as a Function of Time (L09)



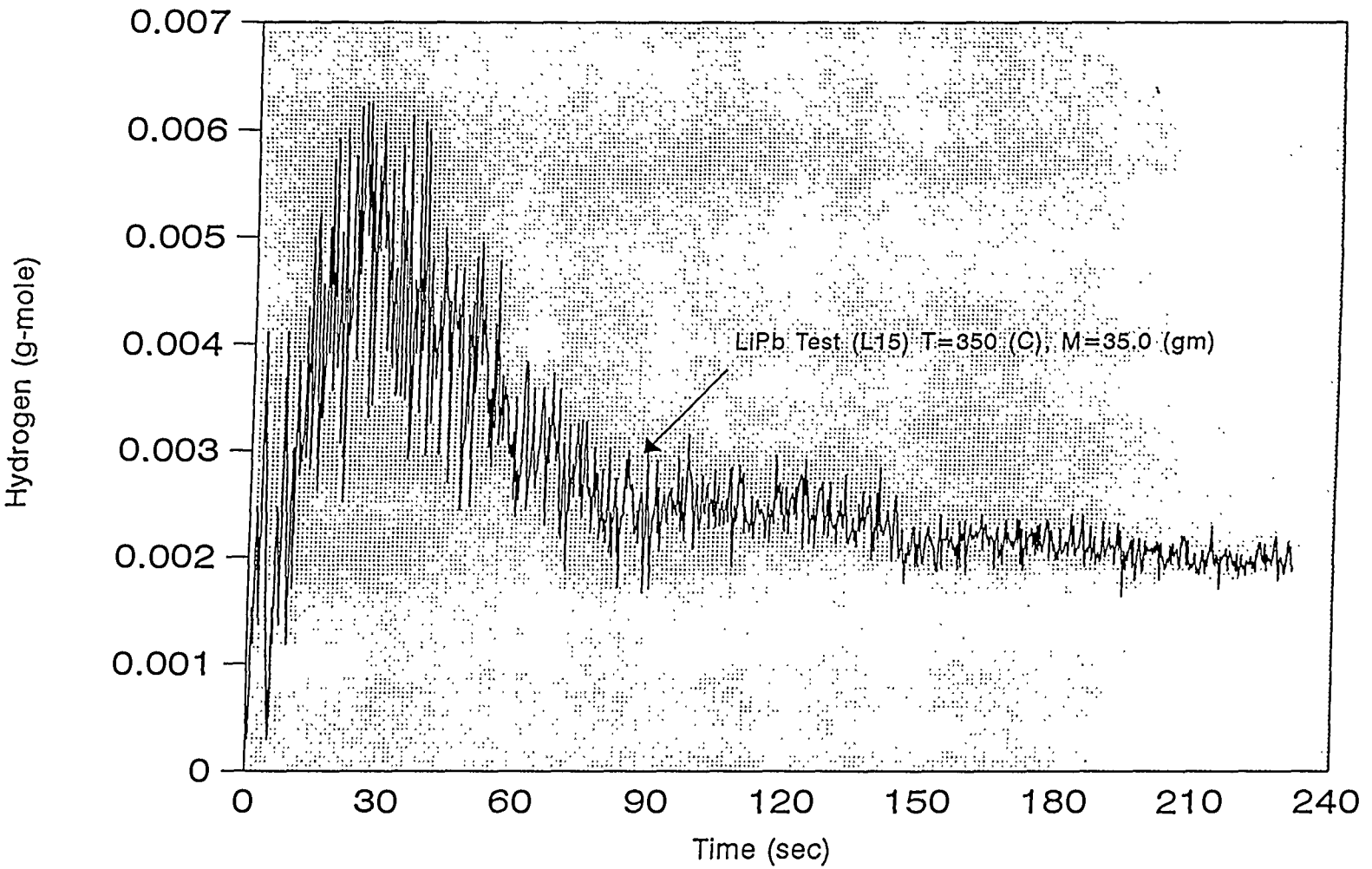
Appendix E Figure 7 Corrected Hydrogen Generation as a Function of Time (L11)



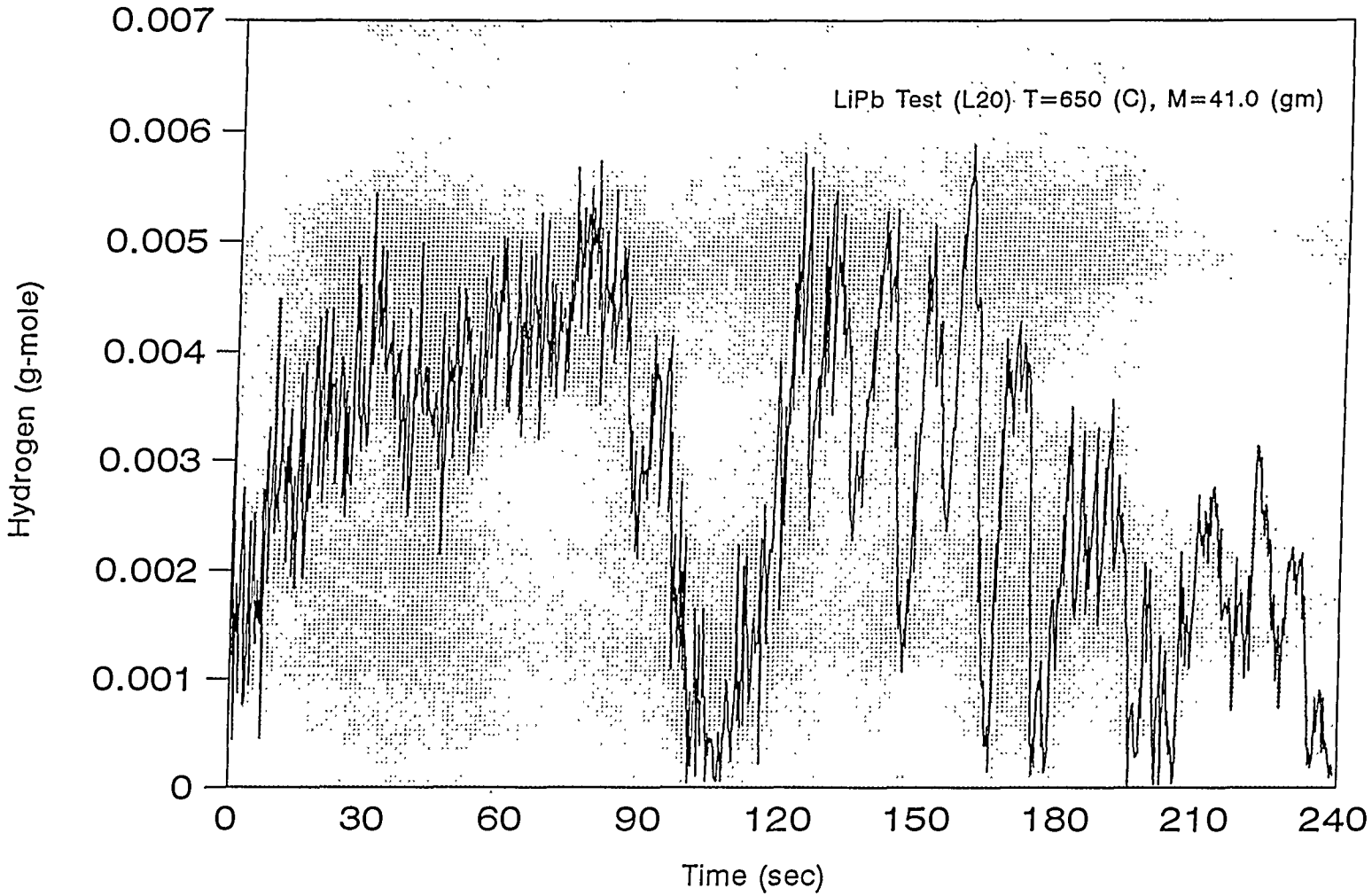
Appendix E Figure 8 Corrected Hydrogen Generation as a Function of Time (L12)



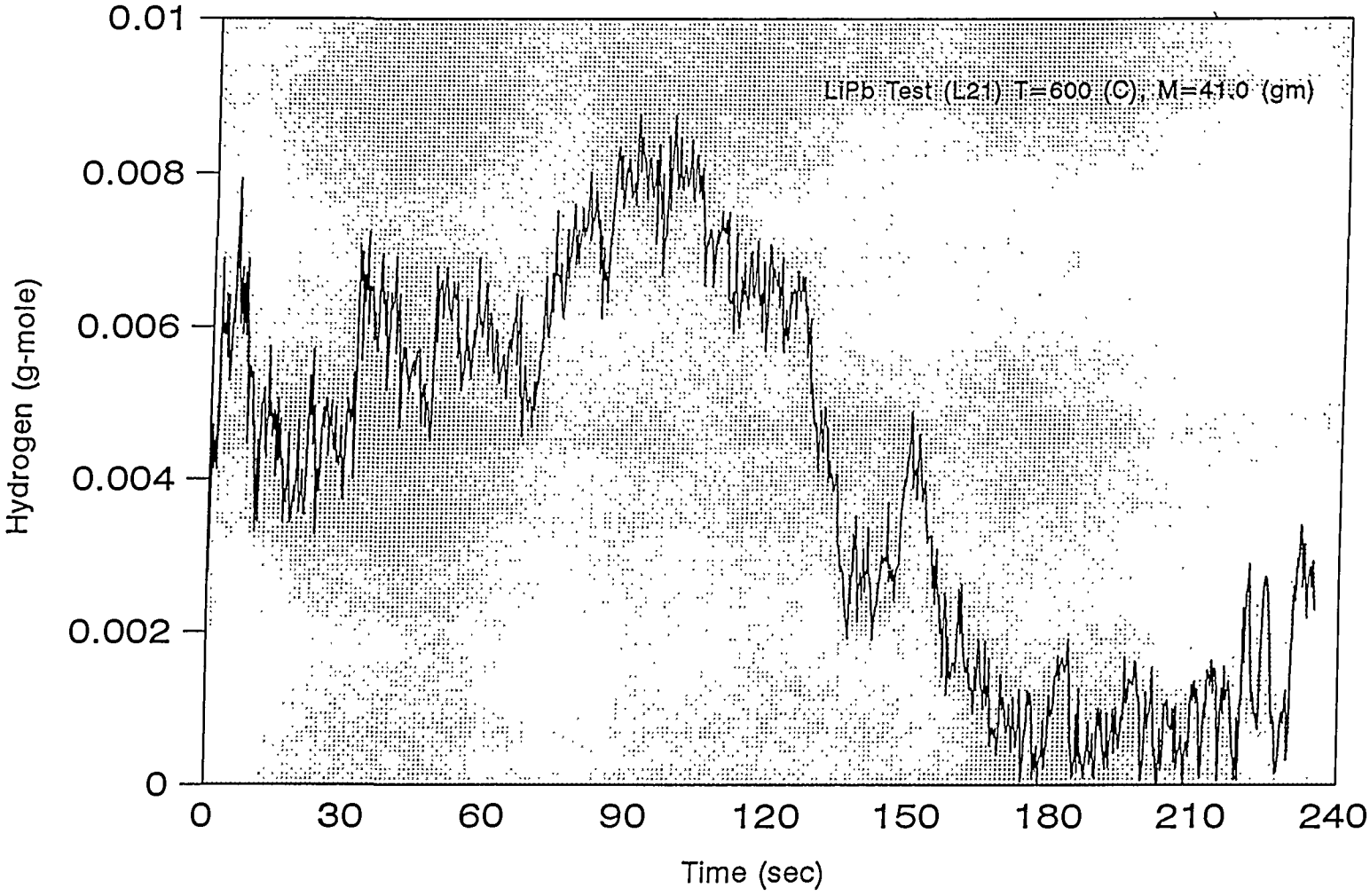
Appendix E Figure 9 Corrected Hydrogen Generation as a Function of Time (L14)



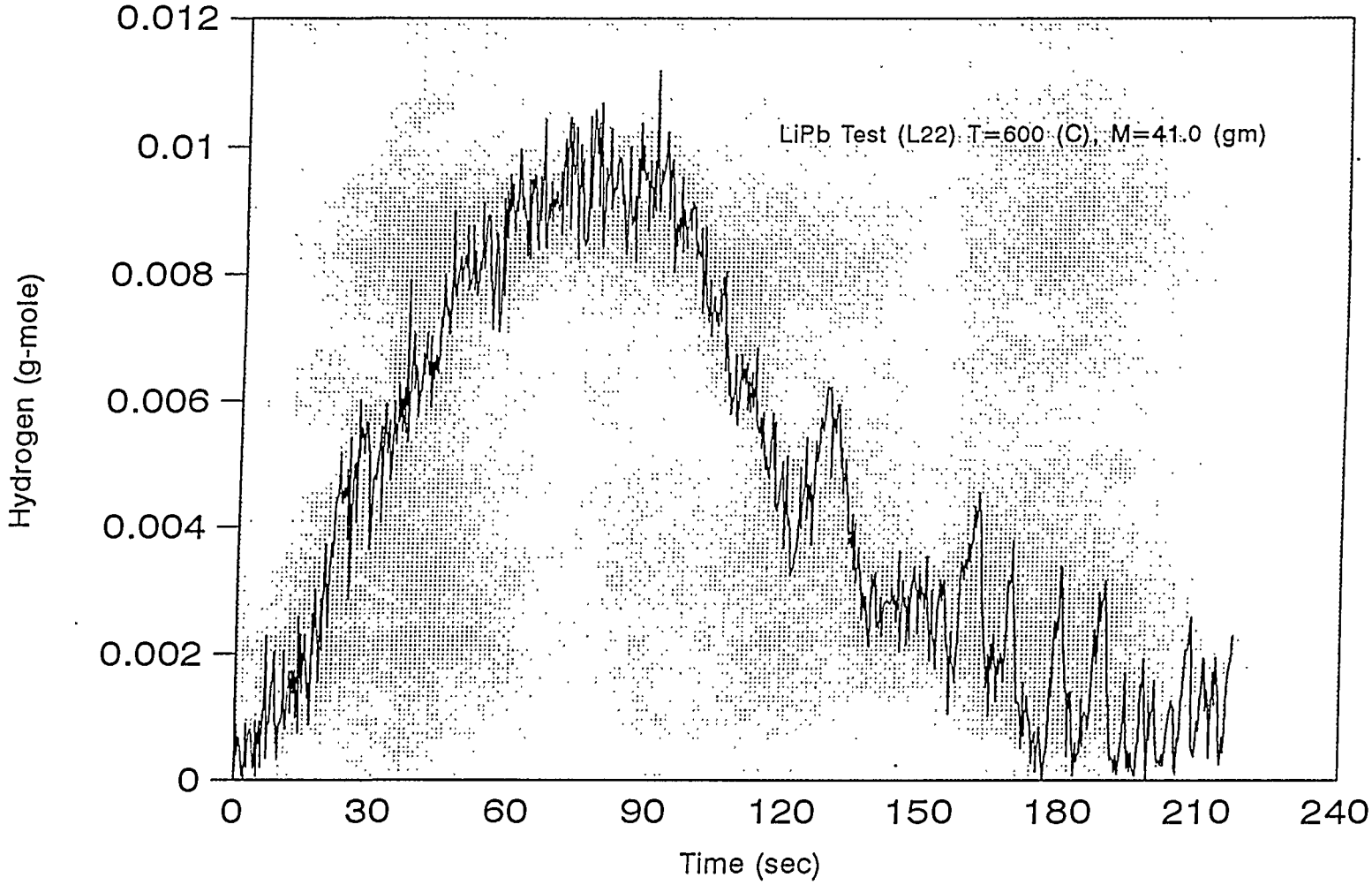
Appendix E Figure 10 Corrected Hydrogen Generation as a Function of Time (L15)



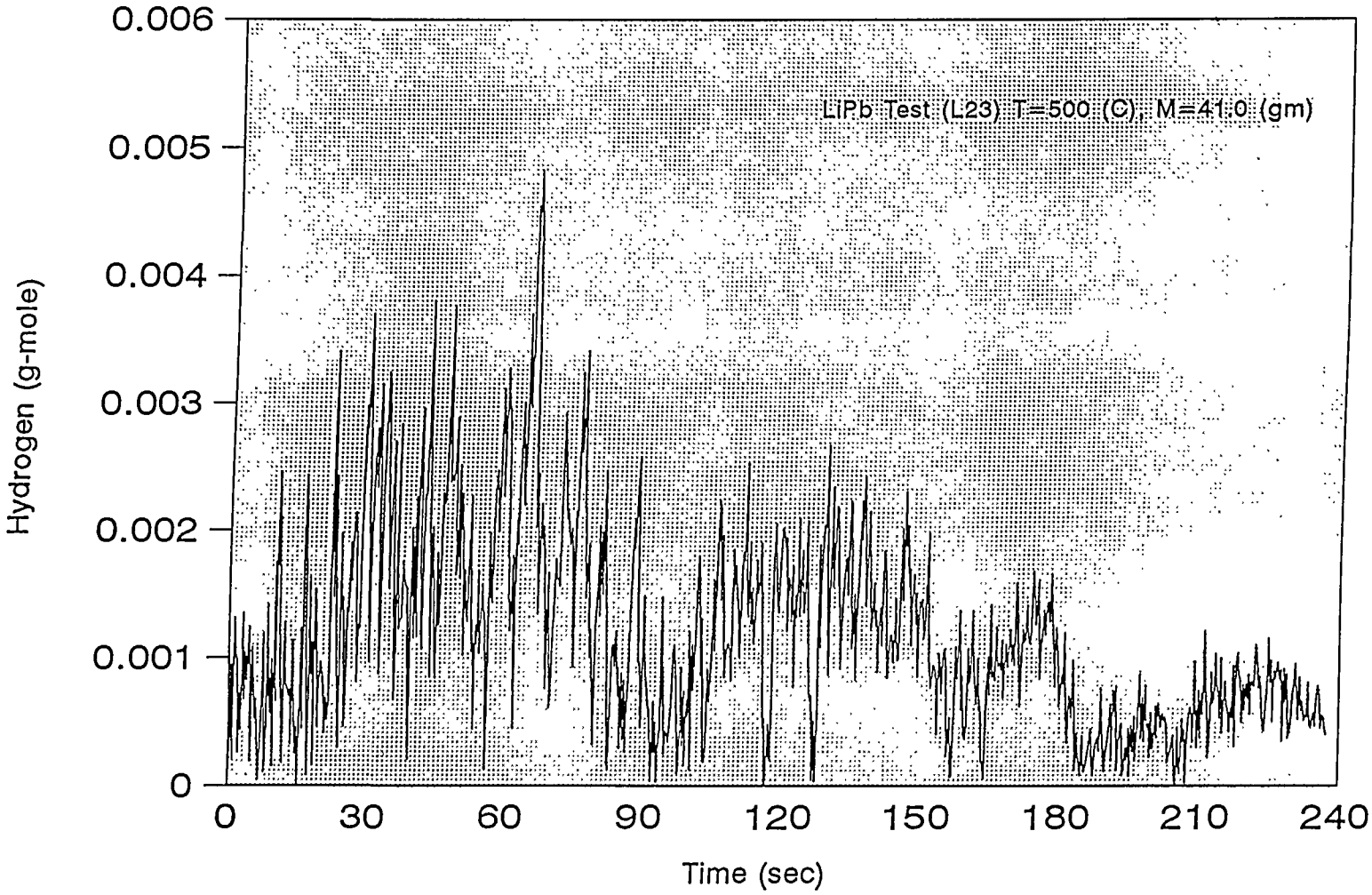
Appendix E Figure 11 Corrected Hydrogen Generation as a Function of Time (L20)



Appendix E Figure 12 Corrected Hydrogen Generation as a Function of Time (L21)



Appendix E Figure 13 Corrected Hydrogen Generation as a Function of Time (L22)

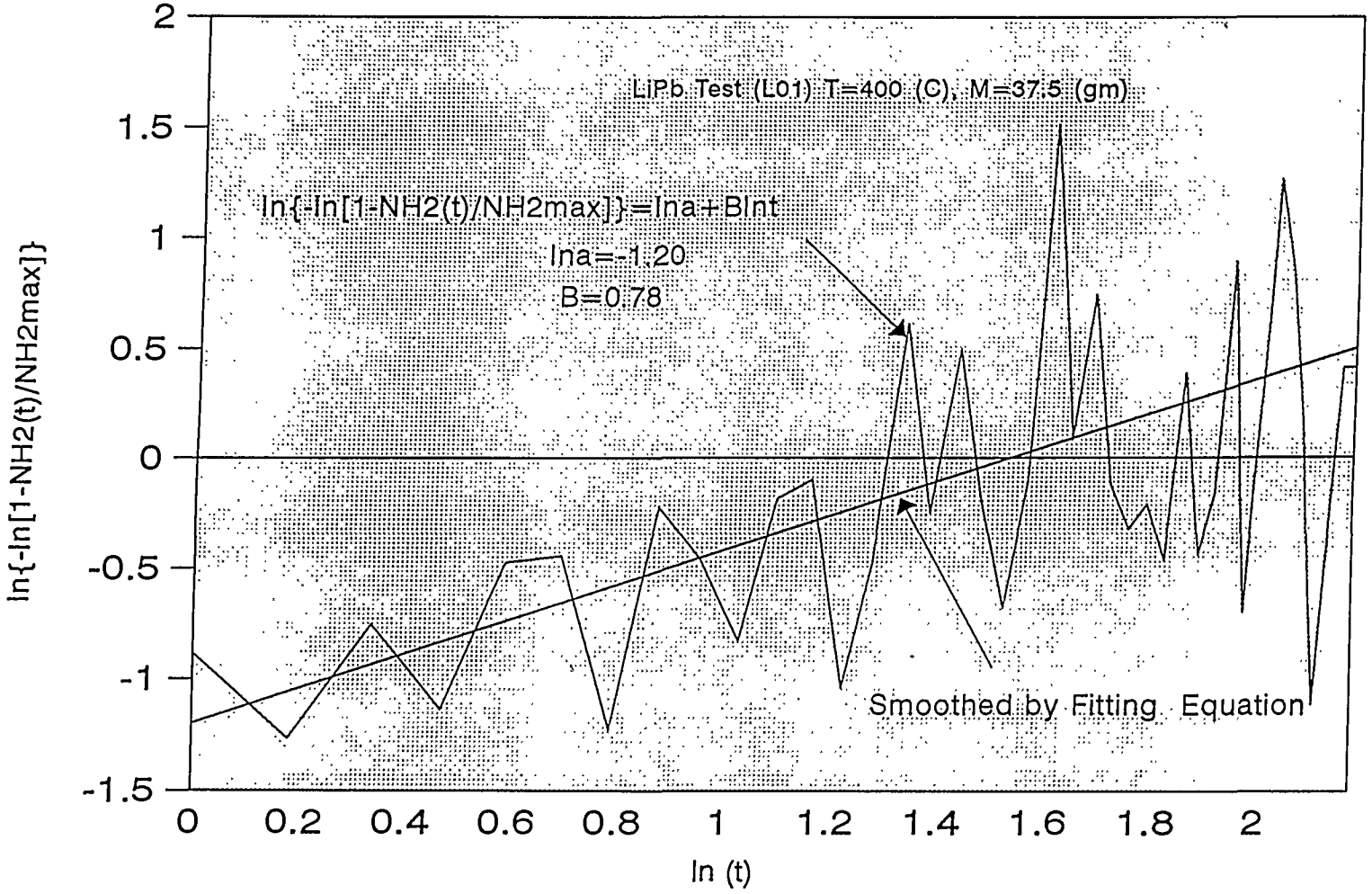


Appendix E Figure 14 Corrected Hydrogen Generation as a Function of Time (L23)

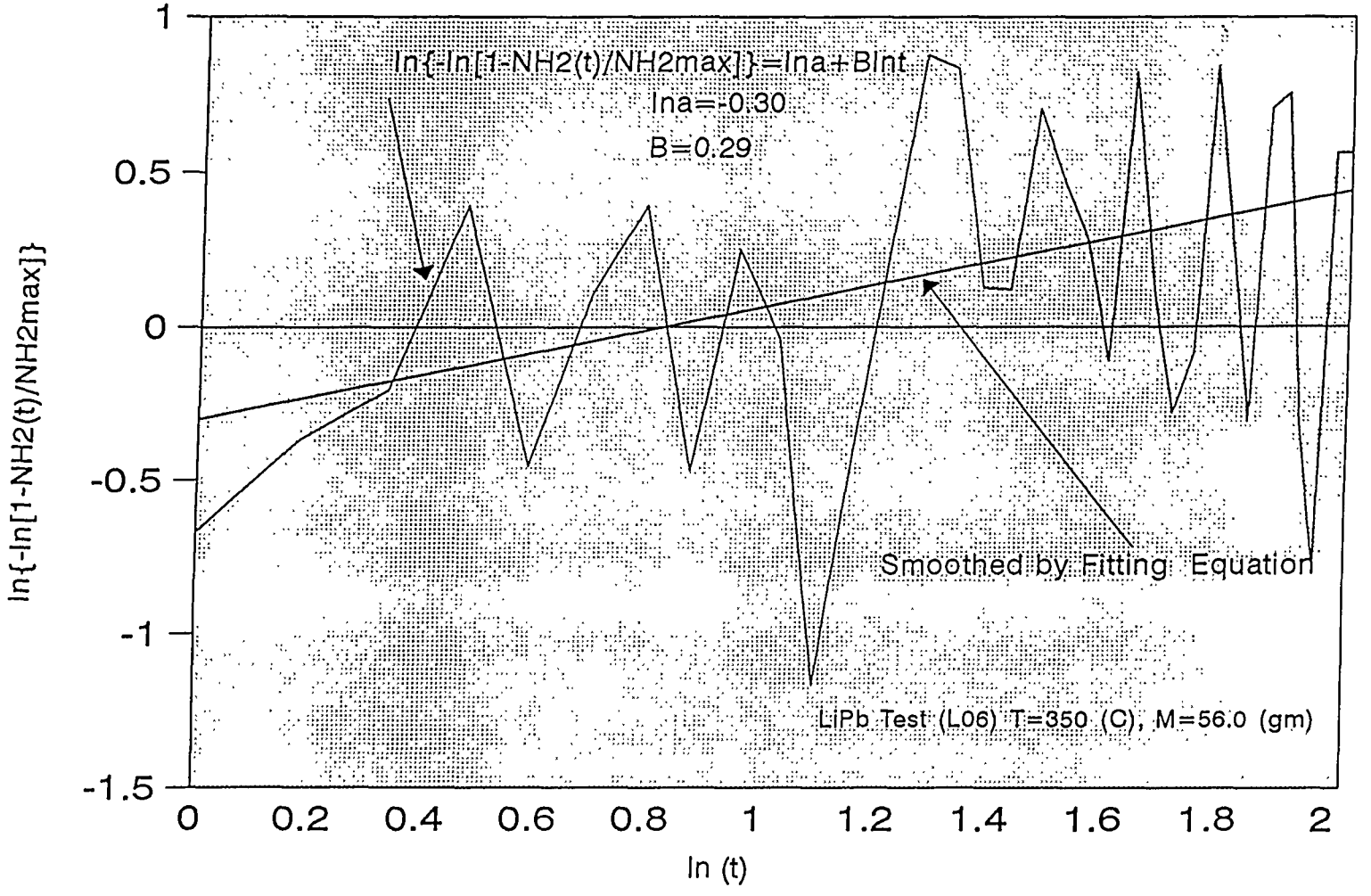
APPENDIX E

RESULTS OF LINEARIZATION FROM TESTS

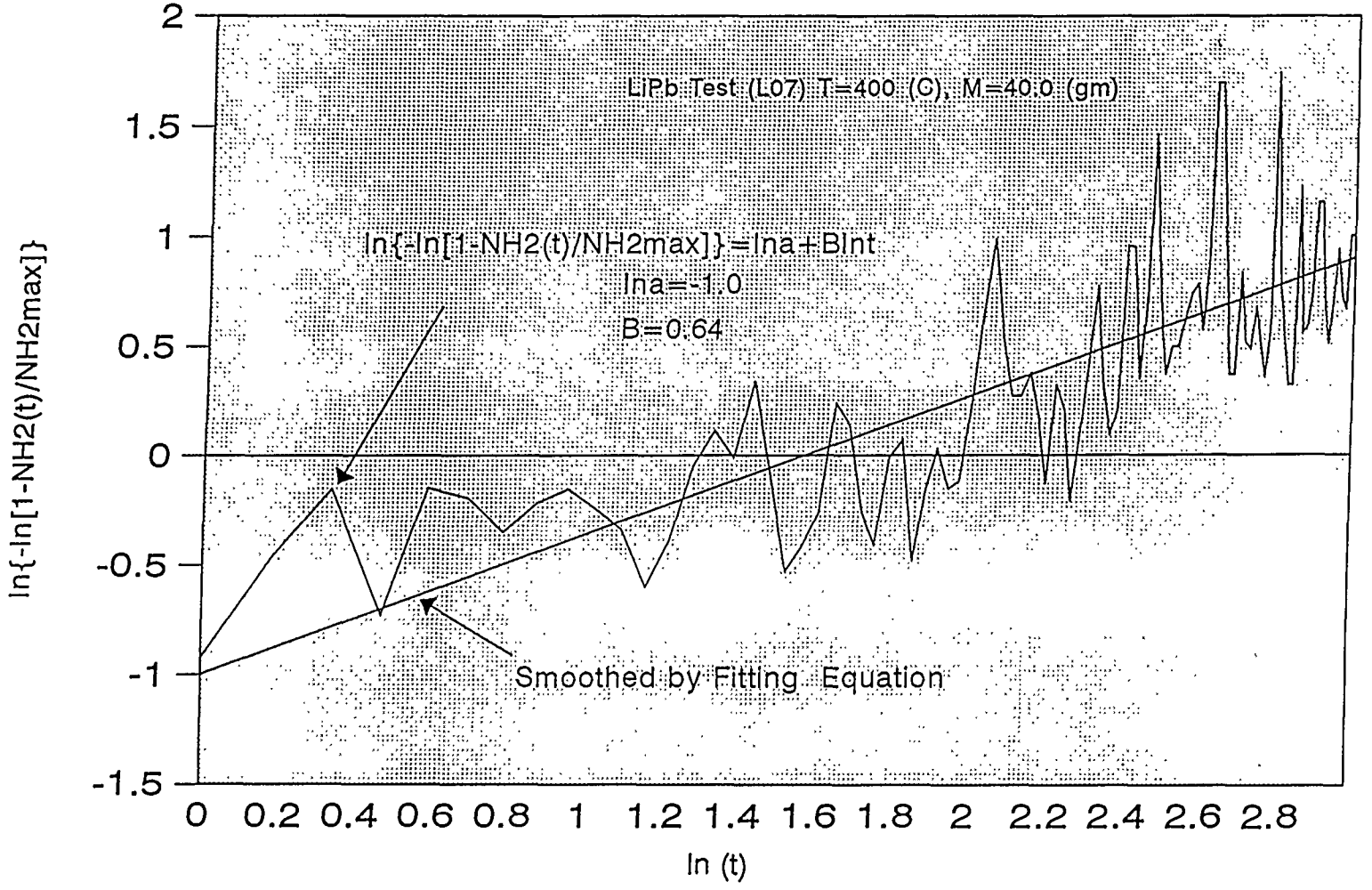
The following 9 graphs contain a complete representation of the results of linearization drawn from 9 lithium-lead tests . The graphs are listed in the following table. The table gives the test and page numbers.



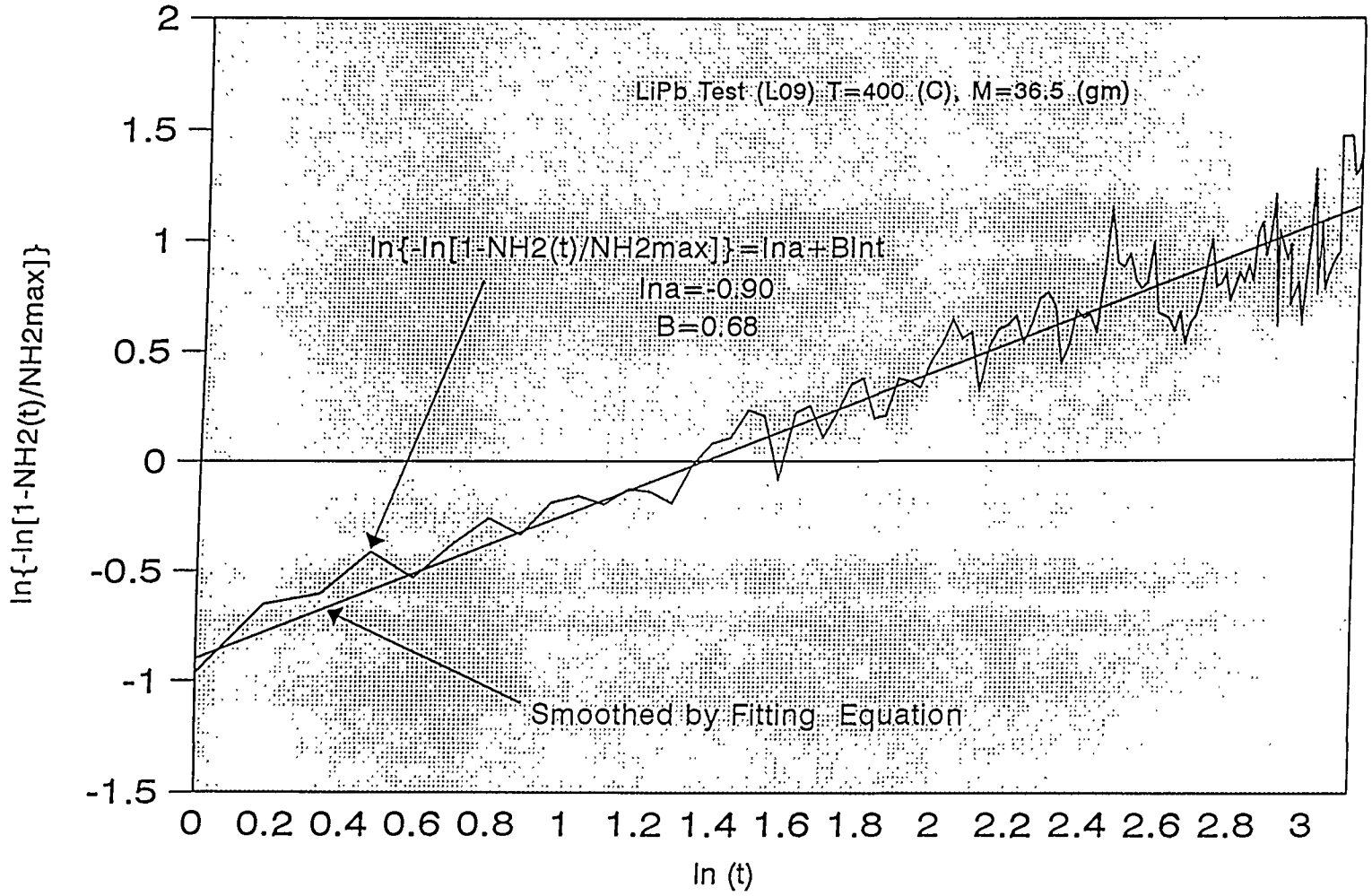
Appendix E Figure 1 Hydrogen Generation Linearized by Equation (78) for Test (L01)



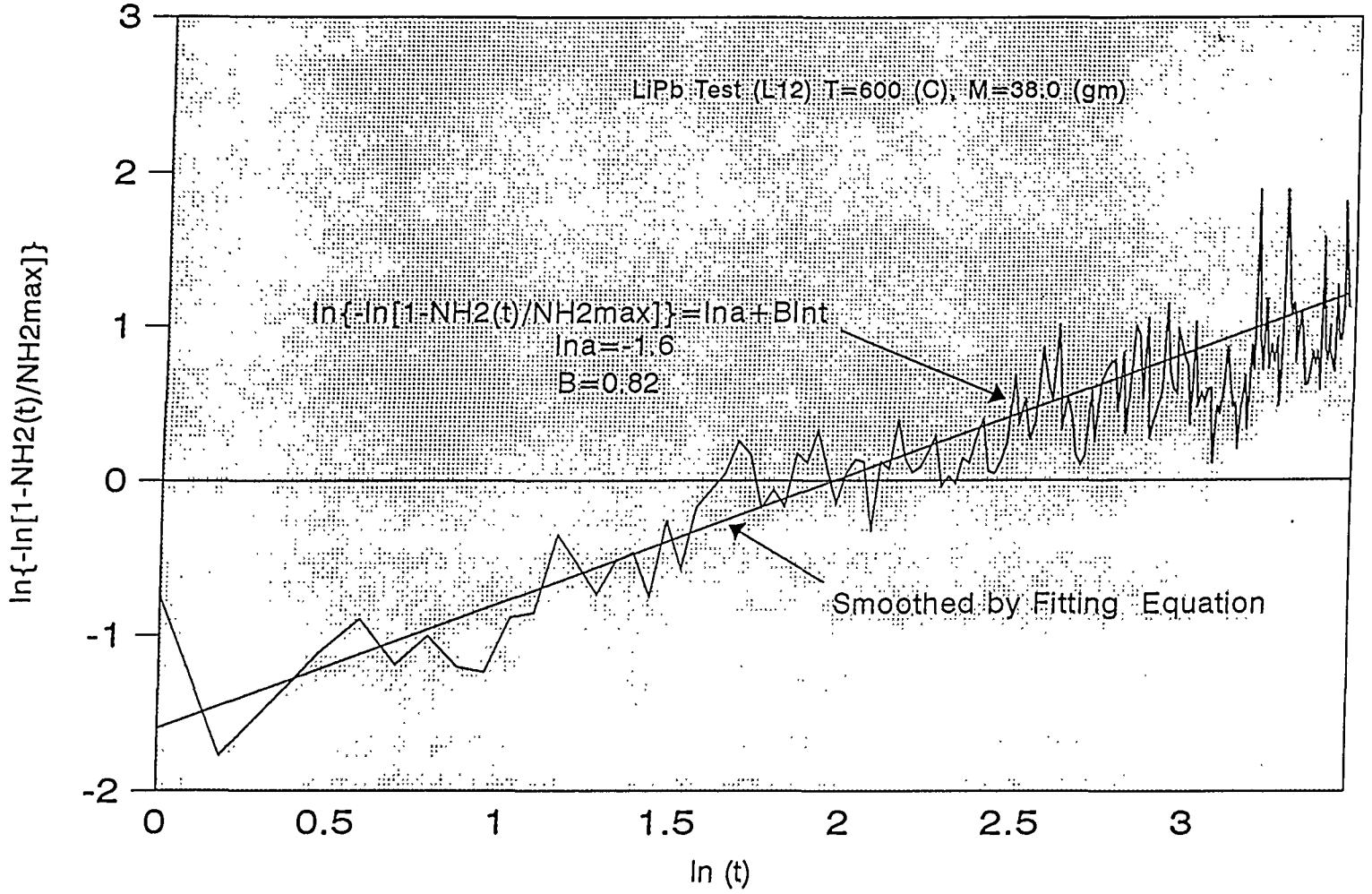
Appendix E Figure 2 Hydrogen Generation Linearized by Equation (78) for Test (L06)



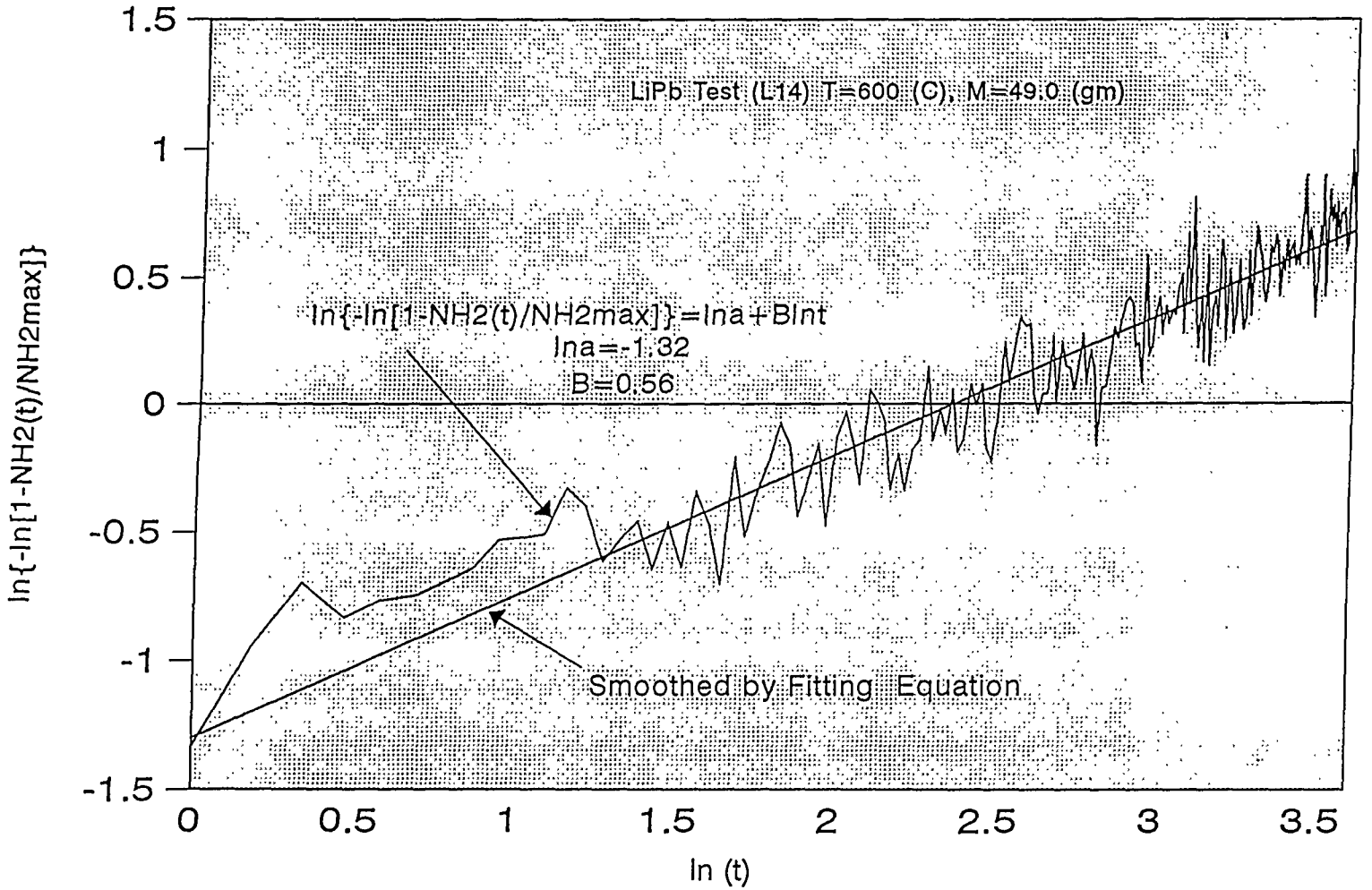
Appendix E Figure 3 Hydrogen Generation Linearized by Equation (78) for Test (L07)



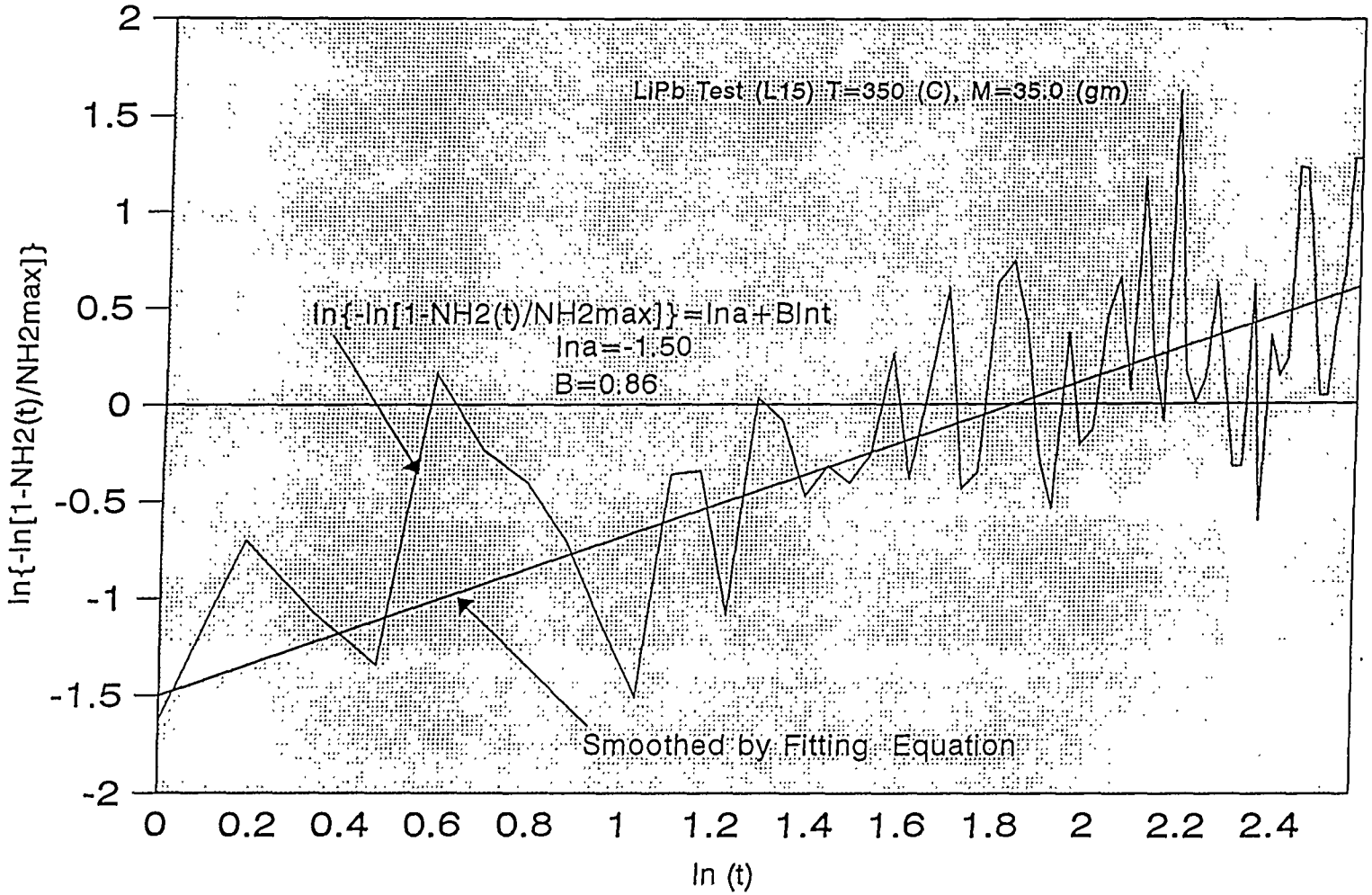
Appendix E Figure 4 Hydrogen Generation Linearized by Equation (78) for Test (L09)



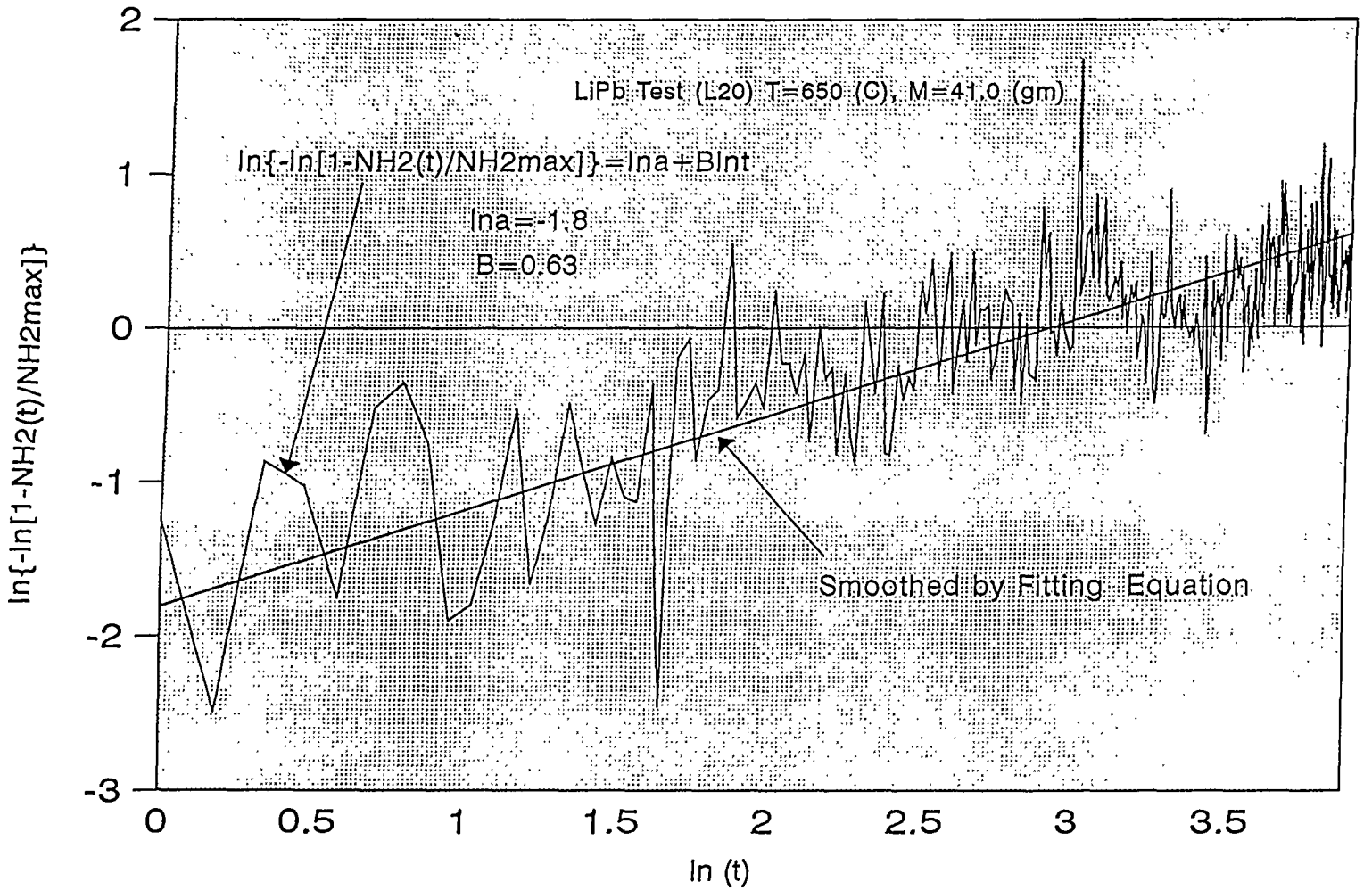
Appendix E Figure 5 Hydrogen Generation Linearized by Equation (78) for Test (L12)



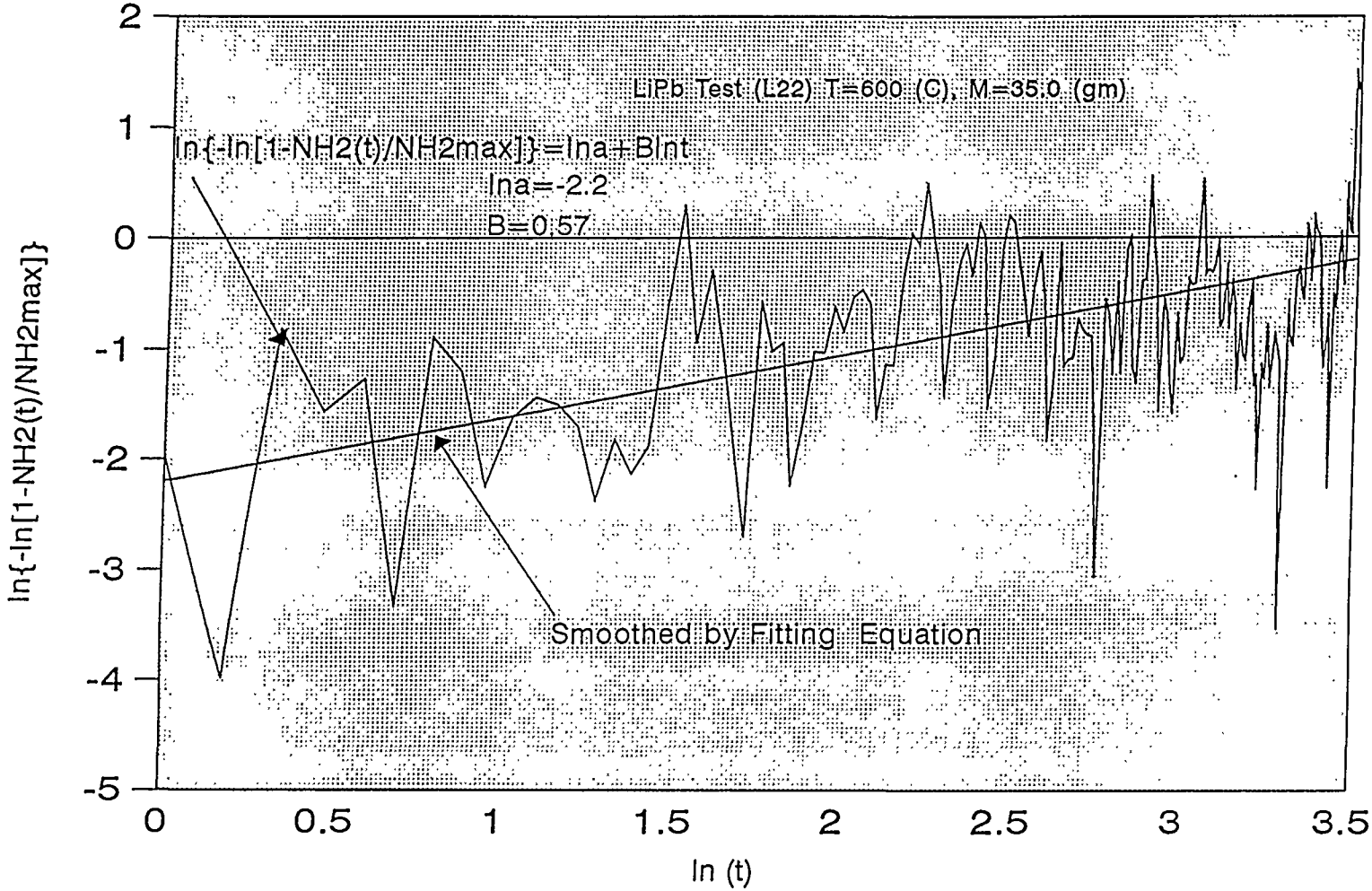
Appendix E Figure 6 Hydrogen Generation Linearized by Equation (78) for Test (L14)



Appendix E Figure 7 Hydrogen Generation Linearized by Equation (78) for Test (L15)



Appendix E Figure 8 Hydrogen Generation Linearized by Equation (78) for Test (L20)



Appendix E Figure 9 Hydrogen Generation Linearized by Equation (78) for Test (L22)

APPENDIX F

DETERMINATION OF THEORETICAL HYDROGEN PRESSURE

The chemical reaction equation is given by

$$Li_{17}Pb_{83} + .17H_2O \rightarrow .17LiOH + .085H_2 + .83Pb$$

Here we have assumed there is enough water for the reaction to form lithium hydroxide. Assuming the lithium-lead in the lower chamber has a depth of 1 cm, then the valveof the metal is

$$V = \pi * D^2 * L / 4$$

$$= \pi * (2.54)^2 (1) / 4$$

$$= 5.07cm^3 = 5.07 * 10^{-6} m^3$$

The molecular weight of lithium lead is calculated using

$$M_{Li_{17}Pb_{83}} = 0.17 * m.wt_{Li} + 0.83 * m.wt_{Pb}$$

$$=0,17(7)+0.83(207)=173 \text{ kg}$$

The density of lithium lead is then given by

$$\rho_{Li_{17}Pb_{83}} = 10375.8kg / m^3$$

The mass of lithium lead is then given by

$$m_{Li_{17}Pb_{83}} = \rho_{Li_{17}Pb_{83}} * V$$

$$= (10375.8kg / m^3) * (5.07) * (10^{-6} m^3)$$

$$= 0.0526kg$$

Mass of H_2 Produced by reaction of ..0526 kg of $Li_{17}Pb_{83}$ is given by

$$m = 0.17 * m_{Li_{17}Pb_{83}} / M_{Li_{17}Pb_{83}}$$

$$=0.17(0.0526)/173$$

$$= 5.17 * 10^{-5} kg$$

The hydrogen produced is assumed to behave as an ideal gas with gas constant

$$R_{H_2} = R / M_{H_2}$$
$$= 8.3243 / 2$$
$$= 4.1572 kJ / kg \cdot K$$

The hydrogen produced bubbles into the gas space in the upper chamber of inside diameter (1.5"). The height of the gas space above the water level in the upper chamber is varied for 5 cm to 25 cm. The volume of H_2 per centimeter height is given by

$$V_1 = \pi * D^2 * (1) / 4$$
$$= \pi * (1.5 * 2.54)^2 * (1) / 4 = 11.401 cc$$
$$= 11.4011 * 10^{-6} m^3$$

The pressure of hydrogen is then given by

$$P_{H_2} = M_{H_2} RT / V$$

The maximum planned gas temperature is 100°C

Thus

$$P_{H_2} = (0.0526) * (4.1572) * (373.15) / (11.401 * 10^{-6})$$
$$= 19553 kPa$$

This calculation was only used to estimate the maximum system pressure as a function of water level as asummarized in Table 2.2. In the experiment, the gas volume is 193 cm^3. This volume is larger than the volume (11.401 cm^3) used in this calculation above.