

To the Graduate Council:

I am submitting herewith a dissertation written by John Paul Foote entitled "A Theoretical and Experimental Investigation of Heat Transfer Involving Melting and Freezing in Encapsulated Lithium Hydride Salt." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mechanical Engineering.

Roy J. Schulz

Roy J. Schulz, Major Professor

We have read this dissertation
and recommend its acceptance:

Ray M. Conrad

R. L. Young

Frank S. Collins

Accepted for the Council:

C. W. Mink

Vice Provost

and Dean of the Graduate School

**A THEORETICAL AND EXPERIMENTAL INVESTIGATION OF
HEAT TRANSFER INVOLVING MELTING AND FREEZING
IN ENCAPSULATED LITHIUM HYDRIDE SALT**

A Dissertation
Presented for the
Doctor of Philosophy
Degree
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ABSTRACT

Thermal energy storage may be used in space-based power generation systems to store waste heat. In systems where the power generation cycle is active only during brief periods, a system employing thermal energy storage can be lighter and more compact than a system that has enough radiator surface to dissipate all of the waste heat as it is generated. Lithium hydride (LiH) salt is well suited for this application, because it has the highest heat of fusion of any ionic salt and melts at a temperature compatible with high-temperature power generation cycles. In one proposed concept for an energy storage system, LiH would be stored in spherical containers arranged in a packed bed, with an externally circulating liquid metal used as the heat transfer fluid.

The purpose of the present study was to investigate, both theoretically and experimentally, the heat transfer characteristics of the individual spherical LiH capsules, including effects due to the solid-liquid phase change. A numerical heat transfer model was developed to simulate the heat transfer performance of spherically encapsulated LiH under both zero-gravity and normal-gravity conditions. The model employs a finite difference formulation and uses an enthalpy-based method to account for phase change. The model also predicts the void that forms as the salt freezes, as well as the effect of natural convection flow in the melted salt.

Experiments were carried out in which instrumented spherical containers filled with LiH were heated rapidly in a high-flux induction furnace to simulate as closely as possible a typical heating cycle in a real thermal energy storage system. The data obtained during these experiments was used to determine the physical behavior of the capsules during melting and solidification, and thus to validate the numerical model. The performance of the numerical model in predicting

temperature-time histories of thermocouples embedded in the salt was generally satisfactory, but the model underpredicted the total time required for melting by ten to fifteen percent. Numerical results for zero-gravity and normal-gravity cases were also compared, and conclusions were drawn about the effects of gravity on the thermal behavior of these systems.

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LIST OF SYMBOLS

a	Acceleration
A_e, B_e, C_e, D_e	Coefficients of energy equation in tridiagonal form
A_P, B_P, C_P, D_P	Coefficients of pressure equation in tridiagonal form
A_e, A_r, A_θ	Control volume surface areas for energy, r -momentum, and θ -momentum calculations
c	Specific heat
C_e	Coefficient in energy equation
div	Velocity divergence
e	Specific energy content
$\mathbf{F}$	Body force
F_e, F_r, F_θ	Convective fluxes of heat, r -momentum, and θ -momentum across control surface
g	Acceleration due to gravity
h	Convection coefficient
h_{sl}	Heat of fusion
k	Thermal conductivity
L	Distance measured along liquid-vapor interface
M_e, M_r, M_θ	Mass fluxes across control surface for energy, r -momentum, and θ -momentum calculations
P	Pressure
P'	Pressure correction
q	Conduction heat flux
r	Radial coordinate in cylindrical or spherical coordinate system

R_c	Inside radius of spherical container
R_o	Radius of curvature at axis of symmetry
R_1, R_2	Principal radii of curvature
s	Velocity source term
t	Time
T	Temperature
T_{mp}	Melting Temperature
u	Liquid velocity
V_e, V_r, V_θ	Volume of control volumes for energy, r -momentum, and θ -momentum calculations
z	Axial coordinate in cylindrical coordinate system

Greek Symbols

α	Contact angle between liquid-vapor interface and solid surface
θ	Polar angle in spherical coordinate system
μ	Liquid viscosity
ρ	Density
$\sigma_{lv}, \sigma_{sl}, \sigma_{sv}$	Surface tensions between liquid and vapor, solid and liquid, and solid and vapor
$\sigma_{rr}, \sigma_{\theta\theta}$	Radial and tangential normal stresses
$\tau_{r\theta}$	Viscous shear stress
ϕ	Longitude angle in spherical coordinate system
ΔM	Net mass source exiting energy control volume
Δr	Finite difference grid spacing in radial direction
Δt	Time step for heat transfer calculations

Δt_c	Time step for fluid flow calculations
Δt_{max}	Maximum time step for stable calculations
ΔV	Volume contained between original and displaced positions of liquid-vapor interface
$\Delta \theta$	Polar angle increment in finite difference grid
$\Delta \phi$	Longitude angle increment in finite difference grid

Subscripts

c	Denotes property of container material
l	Denotes property of liquid salt
o	Denotes reference position or origin
r	Denotes radial direction
s	Denotes property of solid salt
v	Denotes vapor
θ	Denotes tangential direction

Superscripts

t	Denotes value at current time step
$t + \Delta t$	Denotes value at next time step
$*$	Denotes intermediate (unconverged) value

CHAPTER I

INTRODUCTION

Discussion of the Research Program

Thermal energy storage is of interest in systems where heat is developed at a rate different from the rate at which it is used or dissipated. In systems where weight and space limitations are not important, common materials such as bricks are usually the most cost effective energy storage media. However, in applications where weight or space considerations are important, materials with higher energy storage density (per unit weight or unit volume) are considered. One class of materials which is of interest for space power applications is ionic salts. Many of these salts melt at temperatures that are compatible with the high temperature power generation cycles used in space applications, and utilizing the heat of fusion of the salt along with the sensible heat capacity significantly increases the energy storage density that can be attained.

The focus of the present study was to begin to develop an understanding of the heat transfer characteristics of lithium hydride (LiH) salt encapsulated in thin-walled metal containers which are arranged in a packed bed. In the system being considered, encapsulated lithium hydride is used to absorb waste heat generated during the power generation cycle of a satellite-based power system. As shown in Figure 1, heat generated by the power generation cycle is transferred by a circulating liquid metal heat transport medium to the packed bed of LiH spheres. The heat transport fluid also passes through a system of radiators which dissipate heat to space. During power generation the LiH melts, and when the power generation cycle is turned off it refreezes. For systems where the power generation cycle is active for only a short period during each satellite orbit, a

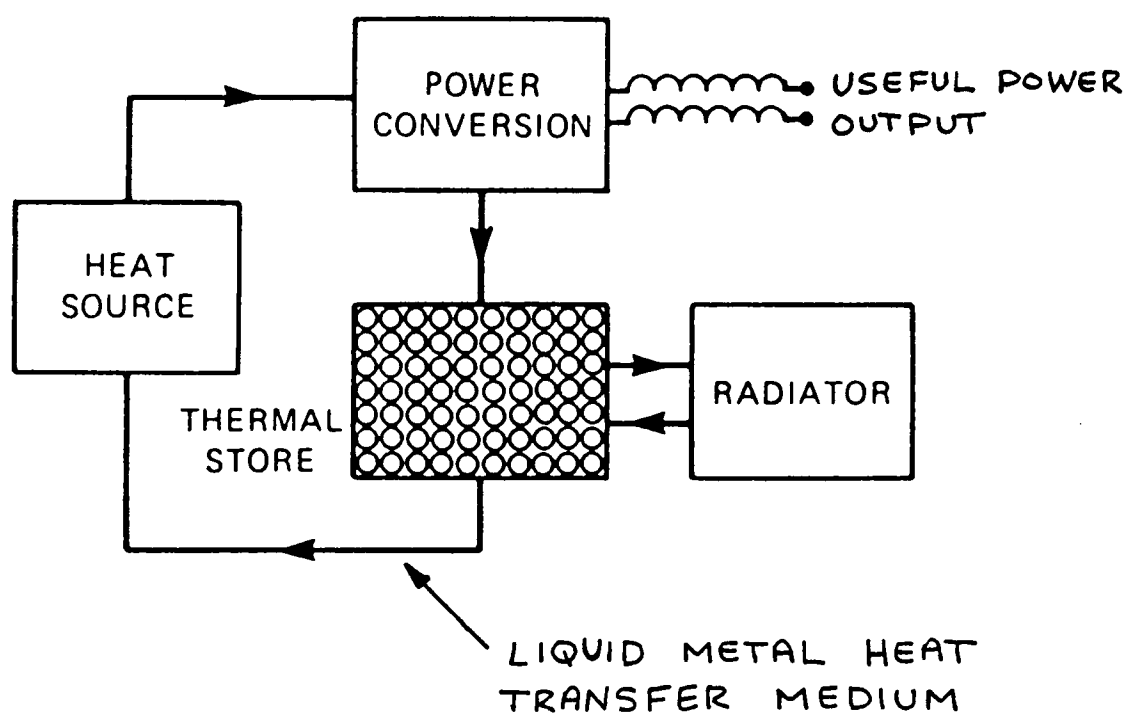


Figure 1. Schematic of a Power System Employing Thermal Energy Storage.

system employing thermal energy storage can be lighter and more compact than a system with enough radiator surface to dissipate the heat as it generated. Lithium hydride was chosen as the energy storage medium because it has a high melting point, about $1260^{\circ}F$ (956 K), and has the highest specific heat of fusion of any ionic salt, about 1224 Btu/lb (2.846 MJ/kg). A complete discussion of the factors influencing the design of an encapsulated LiH energy storage system is given in Ref. [1].

The present study focused on the heat transfer characteristics of an individual spherical LiH capsule. Spherical containers were chosen because they minimize the container surface to volume ratio, and thus the weight of the container material. In addition, spherical containers simplify the design of the packed bed, since they naturally leave external flow passages between them. Spherical containers are also superior to other shapes in terms of resistance to internal pressure that may develop in the capsules. The heat transfer behavior of LiH involving melting and freezing is complicated by a large increase in density when the salt freezes. The density of liquid LiH at its melting point is about 34.3 lb/ft^3 (550 kg/m^3), while the density of solid LiH is about 43.1 lb/ft^3 (690 kg/m^3). A large void develops as the salt freezes which strongly influences the distribution of material in the container, and thus the heat transfer performance. Void shape and location are expected to be quite different under the influence of normal gravity when compared to zero-gravity conditions, as is the extent of natural convection in the melted salt.

In this study, a numerical heat transfer model was developed to predict the heat transfer performance of spherically encapsulated LiH under conditions varying from zero-gravity to normal gravity. The model predicts both void effects and the effects of natural convection in the melted salt. Experiments were also

carried out in which instrumented spherical containers filled with LiH were heated rapidly in a high-flux induction furnace to simulate as closely as possible a typical heating cycle in a real thermal energy storage system. The data obtained during these experiments was used to determine the physical behavior of the capsules during melting and solidification, and thus to validate the numerical model.

Review of Methods for Calculating Heat Transfer Involving Melting and Freezing

The general class of heat transfer problems involving melting and freezing are often referred to as Stefan problems. Because there is a moving phase boundary between the solid and liquid material, analytical solutions for this type of problem can be obtained only for a few one-dimensional cases [2 – 6]. A number of numerical techniques have been developed for solving heat transfer problems involving melting and freezing [3, 4, 7]. The simplest of these is referred to as the “enthalpy method”. The enthalpy method uses a fixed finite difference grid, and does not solve specifically for the location of the moving phase boundary. The phase-change-front location is inferred from the enthalpy level of the material. The main objection to the enthalpy method is that the phase front is located only to within one grid block, thus requiring fine grids in order to calculate accurate interface shapes for complicated problems. An alternate numerical technique for locating the interface is to transform the problem so the solid and liquid regions have a common fixed boundary at the phase front location. This method involves alternately solving for the field variables for a given interface location, and then solving for an updated interface location, with a new grid being generated for each iteration. Finite element formulations are often used for this type of solution method [7].

The enthalpy, or fixed grid, method has commonly been used at Oak Ridge National Laboratory (ORNL) in studies of latent heat energy storage systems [8,9], and was adopted for the present study. The simplicity of the formulation makes it easy to physically interpret the results of calculations as they progress and to make changes in the model as needed. In addition, it seemed adequate for the problem being considered to locate the phase boundary to within one grid spacing, and refine the mesh as necessary for resolution. The accuracy of the predicted phase front location obtained using the enthalpy method can be judged by comparing results of a finite difference calculation (details of the computer model are given in Chapter II) with an analytical solution for a one-dimensional Stefan problem for a sphere. In the problem considered, a 3 in (76.2 mm) diameter sphere of LiH was initially liquid at its fusion temperature. At time $t = 0$, a temperature $100^{\circ}F$ ($55.6\ K$) below the fusion temperature was applied at the outer surface and was maintained thereafter. Density, specific heat, and thermal conductivity were held constant. An asymptotic solution for this problem is given in Ref. [2]. In Figure 2, the phase-front-location predicted by the finite difference calculation is compared to the analytical solution. The sphere radius was subdivided into 20 equally-spaced nodes for the finite difference calculation. Agreement between the two solutions was considered satisfactory, particularly since the analytical, asymptotic solution breaks down in a small region near the center of the sphere (the origin).

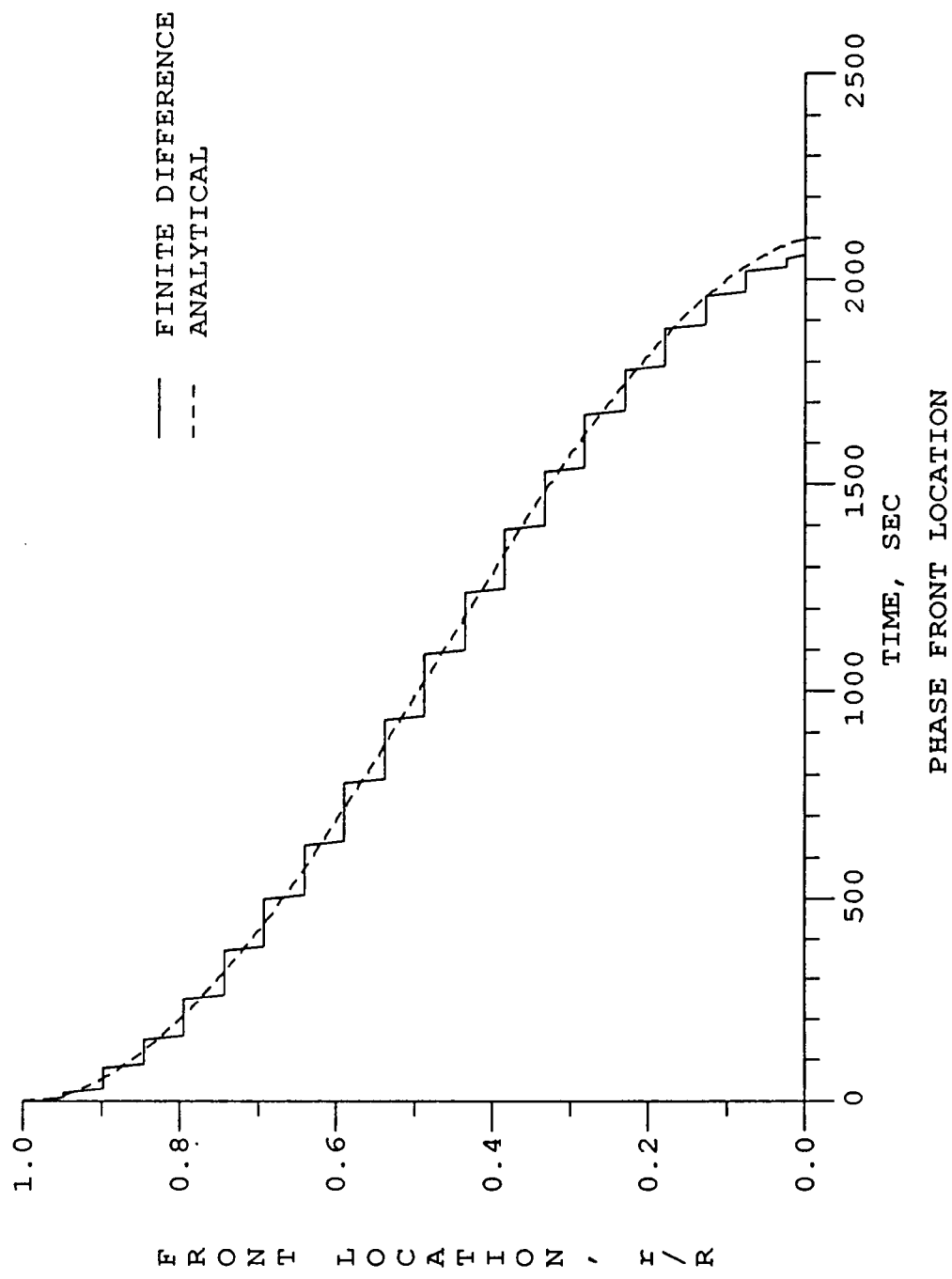


Figure 2. Comparison of Phase Front Location Predicted by Analytical Solution and Finite Difference Calculation for One-Dimensional Stefan Problem.

CHAPTER II

FORMULATION OF THE FINITE DIFFERENCE HEAT TRANSFER MODEL

Governing Differential Equations for the Problem

Since the LiH container is spherical in shape, the governing differential equations are written in spherical coordinates. The three spherical coordinates are the radius, r , the polar angle, θ , and the longitude angle, ϕ . The problem is assumed to be symmetrical about the polar axis, so the ϕ -dependent terms in the differential equations are neglected. The differential equation for energy conservation is [10]

$$\rho \left[u_r \frac{\partial e}{\partial r} + \frac{u_\theta}{r} \frac{\partial e}{\partial \theta} + \frac{\partial e}{\partial t} \right] = -\frac{1}{r^2} \frac{\partial}{\partial r} [r^2 q_r] - \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} [q_\theta \sin \theta], \quad (1)$$

where ρ is the density, e is the specific energy content or enthalpy, and q_r and q_θ are the conduction heat fluxes in the radial and tangential directions. The conduction heat fluxes are given by

$$q_r = -k \frac{\partial T}{\partial r}, \quad (2)$$

$$q_\theta = -k \frac{1}{r} \frac{\partial T}{\partial \theta}, \quad (3)$$

where k is the thermal conductivity and T is temperature.

Assuming the density is constant, the continuity equation in spherical coordinates is

$$\frac{1}{r^2} \frac{\partial}{\partial r} [r^2 u_r] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} [u_\theta \sin \theta] = 0, \quad (4)$$

where u_r and u_θ are the liquid velocities in the r and θ directions. The differential equation for conservation of momentum in the radial direction is

$$\begin{aligned} \rho \left[u_r \frac{\partial u_r}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta^2}{r} + \frac{\partial u_r}{\partial t} \right] \\ = \rho g_r + \left[\frac{1}{r^2} \frac{\partial}{\partial r} [r^2 \sigma_{rr}] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} [\tau_{r\theta} \sin \theta] + \frac{\sigma_{\theta\theta}}{r} \right] - \frac{\partial P}{\partial r}, \end{aligned} \quad (5)$$

where $\tau_{r\theta}$ is the viscous shear stress, σ_{rr} and $\sigma_{\theta\theta}$ are the normal stresses in the radial and tangential directions, g_r is the component of the body force acting in the radial direction, and P is pressure. The equation for momentum conservation in the tangential direction is

$$\begin{aligned} \rho \left[u_r \frac{\partial u_\theta}{\partial r} + \frac{u_\theta}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r u_\theta}{r} + \frac{\partial u_\theta}{\partial t} \right] \\ = \rho g_\theta + \left[\frac{1}{r^2} \frac{\partial}{\partial r} [r^2 \tau_{r\theta}] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} [\sigma_{\theta\theta} \sin \theta] + \frac{\tau_{r\theta}}{r} \right] - \frac{1}{r} \frac{\partial P}{\partial \theta}. \end{aligned} \quad (6)$$

The viscous shear and normal stresses in spherical coordinates are given by

$$\tau_{r\theta} = \tau_{\theta r} = \mu \left[r \frac{\partial}{\partial r} \left(\frac{u_\theta}{r} \right) + \frac{1}{r} \frac{\partial u_r}{\partial \theta} \right], \quad (7)$$

$$\sigma_{rr} = 2\mu \frac{\partial u_r}{\partial r}, \quad (8)$$

$$\sigma_{\theta\theta} = 2\mu \left[\frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r} \right], \quad (9)$$

where μ is the viscosity.

Finite difference approximations for the above equations were developed by balancing fluxes on the finite difference control volumes, as discussed in the following sections.

Description of the Finite Difference Grid

The finite difference model is carried out on a two-dimensional grid in spherical polar coordinates, as shown in Figure 3. The r -axis is subdivided into m equal segments of length Δr , while the polar angle θ is divided into n equal subangles measuring $\Delta \theta$. The increment Δr is given by

$$\Delta r = \frac{R_c}{m},$$

where R_c is the inside radius of the spherical container. The increment $\Delta \theta$ is given by

$$\Delta \theta = \frac{\pi}{n}.$$

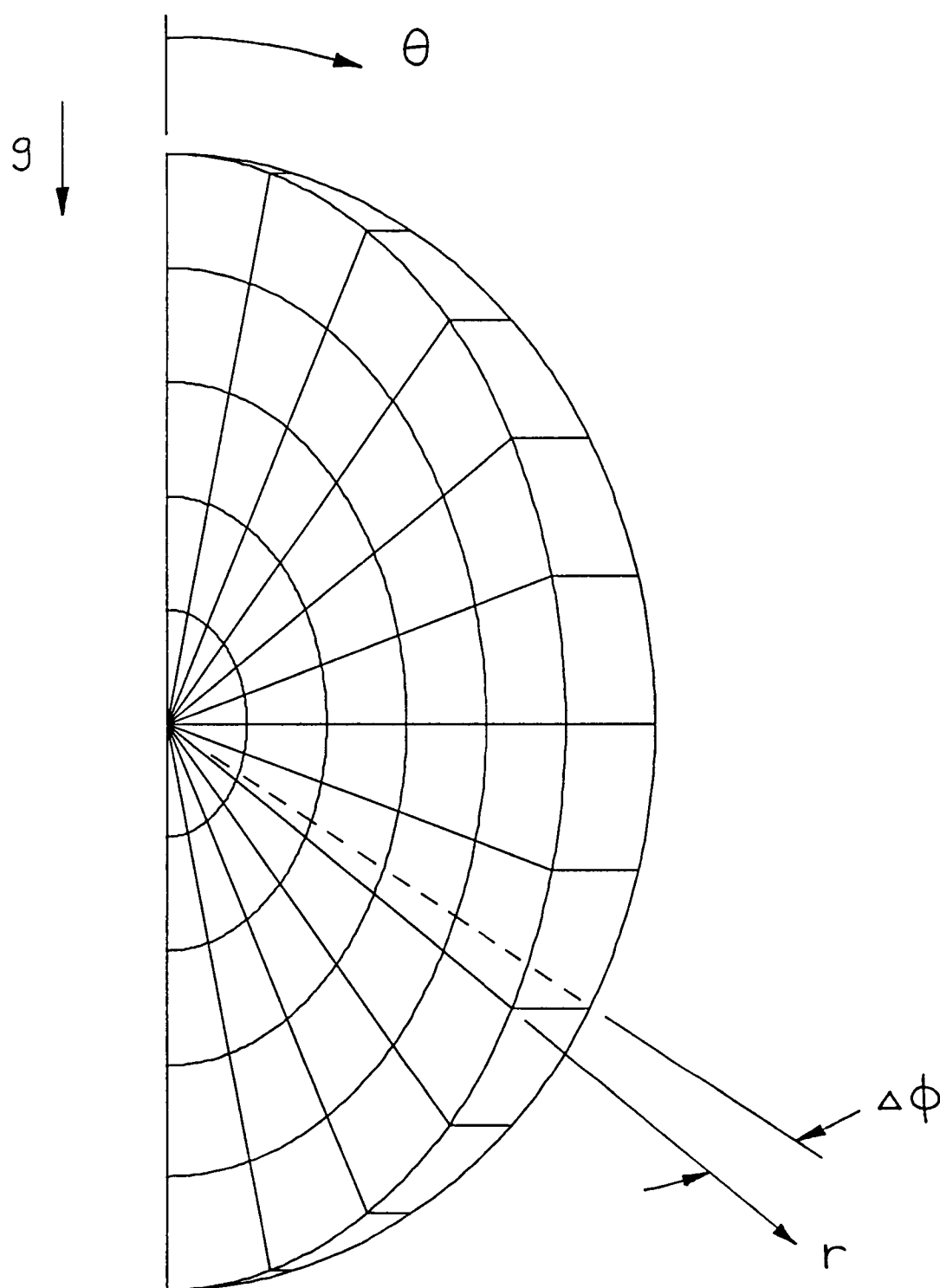


Figure 3. Finite Difference Grid in Spherical Coordinates.

A typical finite difference cell for the heat transfer calculations is shown in Figure 4. The surface area in the radial direction for the cell, $Ae_r(i, j)$, is given by

$$\begin{aligned} Ae_r(i, j) &= [r\Delta\theta] \left[r \sin\left(\theta - \frac{\Delta\theta}{2}\right) \Delta\phi \right] \\ &= r^2 \Delta\theta \sin\left(\theta - \frac{\Delta\theta}{2}\right) \Delta\phi \\ &= (i\Delta r)^2 (\Delta\theta) \sin\left[\left(j - \frac{1}{2}\right)\Delta\theta\right] \Delta\phi. \end{aligned}$$

The surface area in the tangential direction, $Ae_\theta(i, j)$, is given by

$$\begin{aligned} Ae_\theta(i, j) &= \left[\left(r - \frac{\Delta r}{2}\right) \sin\theta \Delta\phi \right] \Delta r \\ &= \left(r - \frac{\Delta r}{2}\right) \Delta r \sin\theta \Delta\phi \\ &= \left(i - \frac{1}{2}\right) \Delta r^2 \sin(j\Delta\theta) \Delta\phi. \end{aligned}$$

The volume of the cell, $Ve(i, j)$, is given by

$$\begin{aligned} Ve(i, j) &= \left[\left(r - \frac{\Delta r}{2}\right) \Delta\theta \right] \left[\left(r - \frac{\Delta r}{2}\right) \sin\left(\theta - \frac{\Delta\theta}{2}\right) \Delta\phi \right] \Delta r \\ &= \left(r - \frac{\Delta r}{2}\right)^2 \Delta r \Delta\theta \sin\left(\theta - \frac{\Delta\theta}{2}\right) \Delta\phi \\ &= \left(i - \frac{1}{2}\right)^2 \Delta r^3 \Delta\theta \sin\left[\left(j - \frac{1}{2}\right)\Delta\theta\right] \Delta\phi. \end{aligned}$$

Cells on the outer boundary of the container are one-half the normal thickness in the r -direction. The temperatures of these cells are calculated at the surface rather than at the center of the cell, which simplifies application of boundary conditions. The radial and tangential surface areas and volume of a surface cell are given by

$$\begin{aligned} Ae_r(k, j) &= \left[\left(k - \frac{1}{2}\right)\Delta r\right]^2 \Delta\theta \sin\left[\left(j - \frac{1}{2}\right)\Delta\theta\right] \Delta\phi, \\ Ae_\theta(k, j) &= \frac{1}{2}\left(k - \frac{3}{4}\right)\Delta r^2 \sin(j\Delta\theta) \Delta\phi, \\ Ve(k, j) &= \frac{1}{2}\left(k - \frac{3}{4}\right)^2 \Delta r^3 \Delta\theta \sin\left[\left(j - \frac{1}{2}\right)\Delta\theta\right] \Delta\phi. \end{aligned}$$

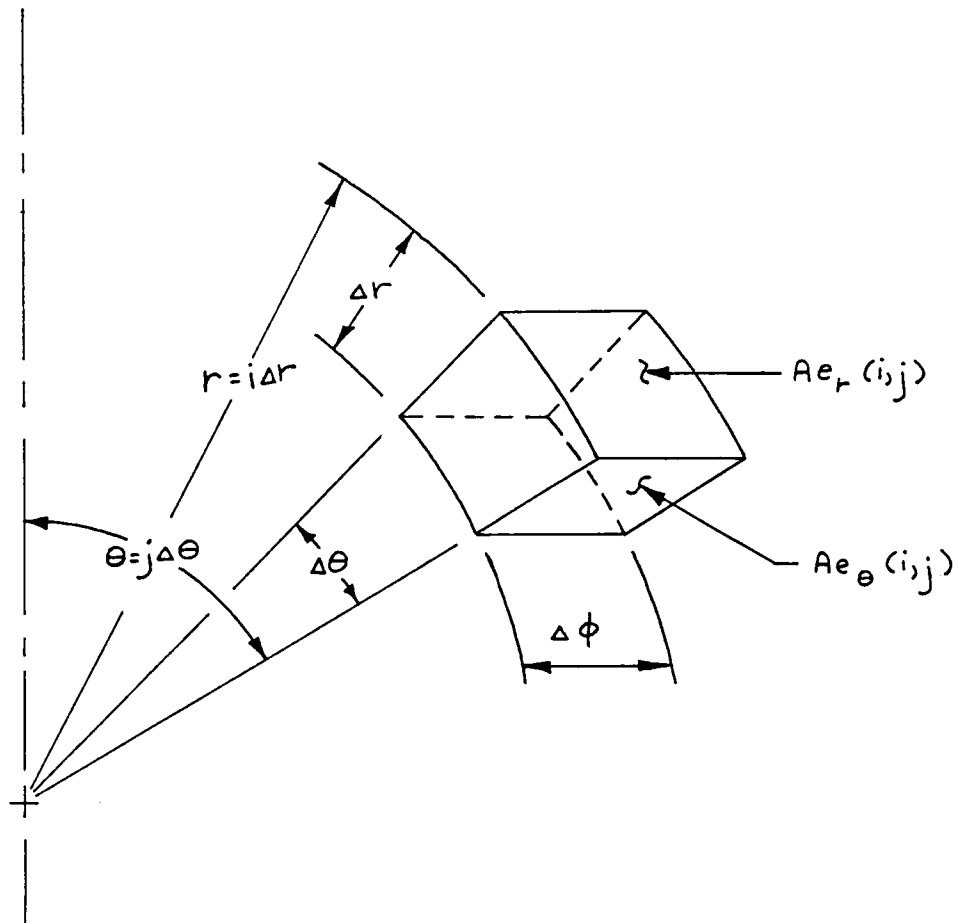


Figure 4. Typical Control Volume for Energy Calculations.

The radial and tangential velocities, u_r and u_θ are calculated using control volumes that are shifted with respect to the main grid, as shown in Figure 5. The control volumes for calculation of u_r are shifted one-half of a cell width in the r -direction, while the volumes for calculation of u_θ are shifted by an angle of $\Delta\theta/2$. The radial and tangential surface areas of the r -velocity cells, $Ar_r(i, j)$ and $Ar_\theta(i, j)$, are given by

$$Ar_r(i, j) = \left[(i + \frac{1}{2})\Delta r\right]^2 \Delta\theta \sin[(j - \frac{1}{2})\Delta\theta] \Delta\phi,$$

$$Ar_\theta(i, j) = i \Delta r^2 \sin(j\Delta\theta) \Delta\phi.$$

The volume of the r -velocity cells, $Vr(i, j)$, is given by

$$Vr(i, j) = i^2 \Delta r^3 \Delta\theta \sin[(j - \frac{1}{2})\Delta\theta] \Delta\phi.$$

The radial and tangential surface areas of the θ -velocity cells, $A\theta_r$ and $A\theta_\theta$, are given by

$$A\theta_r(i, j) = (i\Delta r)^2 \Delta\theta \sin(j\Delta\theta) \Delta\phi,$$

$$A\theta_\theta(i, j) = (i - \frac{1}{2})^2 \Delta\theta \sin(j\Delta\theta) \Delta\phi.$$

The volume of the θ -velocity cells, $V\theta(i, j)$, is given by

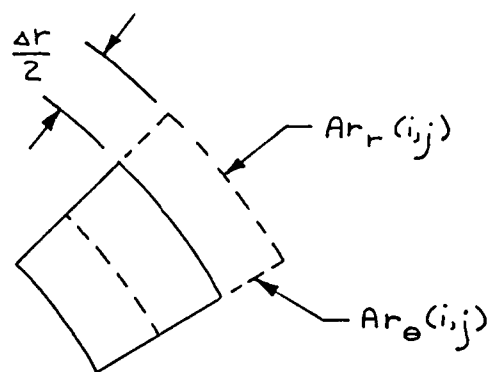
$$V\theta(i, j) = (i - \frac{1}{2})^2 \Delta r^3 \Delta\theta \sin(j\Delta\theta) \Delta\phi.$$

Formulation of the Fully Implicit Heat Equation

The equation for rate of change of energy content for a typical control volume, considering conduction only, can be written

$$\begin{aligned} \rho(i, j)Ve(i, j)[e^{t+\Delta t}(i, j) - e^t(i, j)] \\ = \Delta t[q_r(i, j) - q_r(i - 1, j) + q_\theta(i, j) - q_\theta(i, j - 1)], \end{aligned} \quad (10)$$

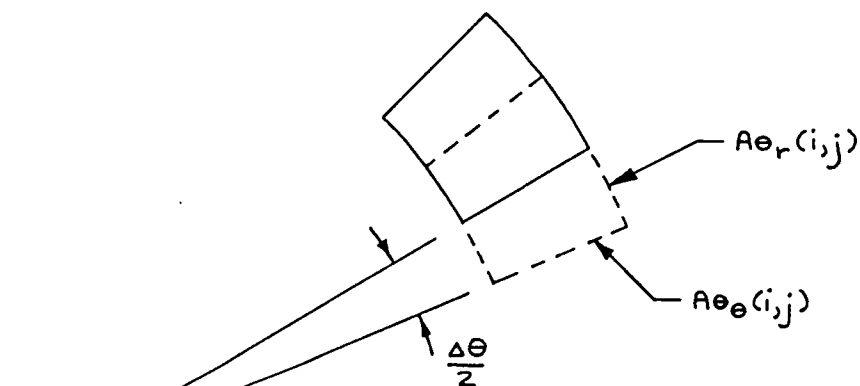
where ρ is the volume-averaged density, e is the volume-averaged specific energy



— VOLUME FOR CALCULATION
OF $e(i,j)$

--- VOLUME FOR CALCULATION
OF $u_r(i,j)$

(A) Staggered Grid for Calculation of u_r .



— VOLUME FOR CALCULATION
OF $e(i,j)$

--- VOLUME FOR CALCULATION
OF $u_\theta(i,j)$

(B) Staggered Grid for Calculation of u_θ .

Figure 5. Grids for Calculation of u_r and u_θ .

content, and q_r and q_θ are the conduction heat fluxes in the r and θ directions, as shown in Figure 6. The conduction heat fluxes are given by

$$\begin{aligned} q_r(i, j) &= k_r(i, j) A e_r(i, j) \frac{T(i+1, j) - T(i, j)}{\Delta r} \\ &= C e_r(i, j) [T(i+1, j) - T(i, j)], \end{aligned} \quad (11)$$

$$\begin{aligned} q_\theta(i, j) &= k_\theta(i, j) A e_\theta(i, j) \frac{T(i, j+1) - T(i, j)}{r \Delta \theta} \\ &= C e_\theta(i, j) [T(i, j+1) - T(i, j)], \end{aligned} \quad (12)$$

where k_r and k_θ are the thermal conductivities, and T is temperature. Eqs. (11) and (12) are first order finite difference approximations for the conduction heat fluxes, as defined by Eqs. (2) and (3). Coefficients $C e_r(i, j)$ and $C e_\theta(i, j)$ are defined by

$$\begin{aligned} C e_r(i, j) &= \frac{k_r(i, j) A e_r(i, j)}{\Delta r}, \\ C e_\theta(i, j) &= \frac{k_\theta(i, j) A e_\theta(i, j)}{(i - \frac{1}{2}) \Delta r \Delta \theta}, \end{aligned}$$

where $r = (i - 1/2) \Delta r$ has been substituted in the expression for $C e_\theta$. The values of k_r and k_θ are determined based on the types of materials contained in volume (i, j) and its neighbors. The thermal conductivities of solid salt, k_s , liquid salt, k_l , and the container material, k_c , are assigned constant values in the heat transfer model. If, for example, volume (i, j) and volume $(i+1, j)$ both contain solid salt, then $k_r(i, j) = k_s$. If the two volumes contain different materials, the conductivity is taken to be the harmonic mean of the individual conductivities [11]. For example, if volume (i, j) contains solid salt and volume $(i+1, j)$ is part of the container wall, the value of $k_r(i, j)$ is

$$k_r(i, j) = \frac{2k_s k_c}{k_s + k_c}.$$

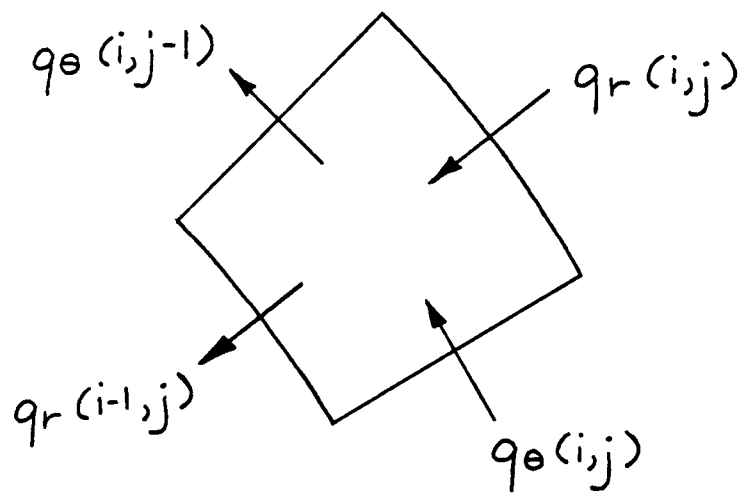


Figure 6. Conduction Heat Fluxes for a Typical Control Volume.

Energy content is scaled so $e(i, j) = 0$ when the salt is solid at the melting temperature, T_{mp} . Temperature is scaled so the scaled temperature is zero at the melting point, i.e., $T = T(^{\circ}F) - T_{mp}$. Energy content of the salt is related to temperature as follows:

$$\begin{aligned} T(i, j) &= \frac{e(i, j)}{c_s} && \text{when } e(i, j) \leq 0, \\ &= 0 && \text{when } 0 < e(i, j) < h_{sl}, \\ &= \frac{e(i, j) - h_{sl}}{c_l} && \text{when } e(i, j) \geq h_{sl}, \end{aligned} \quad (13)$$

where h_{sl} is the heat of fusion, and c_s and c_l are the solid and liquid specific heats. Energy content of shell volumes is related to temperature by $T(i, j) = e(i, j)/c_c$, where c_c is the specific heat of the shell material. The solid, liquid, and shell specific heats are assigned representative constant values in the heat transfer model. The assigned values are averages over the appropriate temperature ranges. The specific heat is indexed to the nodal location (i, j) , with the specific heat for a given node being designated by $c(i, j)$.

Energy equation for shell and solid LiH. Equations (11), (12), and (13) can be substituted into Eq. (10) to give a fully implicit form of the energy equation, i.e., in terms of temperatures at time step $t + \Delta t$. The resulting equation, valid for solid and shell nodes only, is

$$\begin{aligned} \rho(i, j)V e(i, j) [c(i, j)T(i, j) - e^t(i, j)] &= \Delta t \left[C e_r(i, j) [T(i + 1, j) - T(i, j)] \right. \\ &\quad - C e_r(i - 1, j) [T(i, j) - T(i - 1, j)] + C e_{\theta}(i, j) [T(i, j + 1) - T(i, j)] \\ &\quad \left. - C e_{\theta}(i, j - 1) [T(i, j) - T(i, j - 1)] \right]. \end{aligned}$$

The above equation can be rearranged to give

$$\begin{aligned}
 & \left[\Delta t [C_{e_r}(i, j) + C_{e_r}(i - 1, j) + C_{e_\theta}(i, j) + C_{e_\theta}(i, j - 1)] \right. \\
 & \quad \left. + \rho(i, j) V e(i, j) c(i, j) \right] T(i, j) = \Delta t C_{e_r}(i, j) T(i + 1, j) \\
 & \quad + \Delta t C_{e_r}(i - 1, j) T(i - 1, j) + \Delta t C_{e_\theta}(i, j) T(i, j + 1) \\
 & \quad + \Delta t C_{e_\theta}(i, j - 1) T(i, j - 1) + \rho(i, j) V e(i, j) e^t(i, j). \quad (14)
 \end{aligned}$$

Equation (14) can be written in the tridiagonal form for a radial line of nodes:

$$A_e(i, j) T(i, j) = B_e(i, j) T(i + 1, j) + C_e(i, j) T(i - 1, j) + D_e(i, j), \quad (15)$$

where

$$\begin{aligned}
 A_e(i, j) = & \rho(i, j) V e(i, j) c(i, j) + \Delta t [C_{e_r}(i, j) + C_{e_r}(i - 1, j) + C_{e_\theta}(i, j) \\
 & + C_{e_\theta}(i, j - 1)],
 \end{aligned}$$

$$B_e(i, j) = \Delta t C_{e_r}(i, j),$$

$$C_e(i, j) = \Delta t C_{e_r}(i - 1, j),$$

$$\begin{aligned}
 D_e(i, j) = & \Delta t [C_{e_\theta}(i, j) T(i, j + 1) + C_{e_\theta}(i, j - 1) T(i, j - 1)] \\
 & + \rho(i, j) V e(i, j) e^t(i, j).
 \end{aligned}$$

Equations in this form were solved by an iterative line relaxation technique using tridiagonal matrix reduction to solve for each line of nodes along a radius. The calculations were continued by repeating the tridiagonal matrix algorithm (TDMA) successively for $\theta = 1$ to n until the maximum temperature difference at any node after successive iterations was less than some small fixed value. The new temperature field determined by this procedure was the temperature field for time step $t + \Delta t$. The TDMA solution procedure will be explained later.

Energy equation for liquid, melting, and freezing LiH. Equations for liquid and melting/freezing nodes must be modified to account for energy transferred by

convection. The mass fluxes, Me_r and Me_θ , and the convective heat fluxes, Fe_r and Fe_θ , for a typical volume are shown in Figure 7. A pure upwind differencing scheme (UDS) is used for convective fluxes, i.e., the energy entering or exiting a control volume is considered to be at the temperature of the volume it comes from. Therefore,

$$\begin{aligned} Fe_r(i, j) &= -Me_r(i, j)c_l T(i, j) \quad \text{when } u_r(i, j) > 0, \\ &= -Me_r(i, j)c_l T(i + 1, j) \quad \text{when } u_r(i, j) < 0, \end{aligned}$$

$$\begin{aligned} Fe_\theta(i, j) &= -Me_\theta(i, j)c_l T(i, j) \quad \text{when } u_\theta(i, j) > 0, \\ &= -Me_\theta(i, j)c_l T(i, j + 1) \quad \text{when } u_\theta(i, j) < 0, \end{aligned}$$

where the mass fluxes, Me_r and Me_θ , are given by

$$Me_r(i, j) = \rho_l u_r(i, j) A e_r(i, j), \quad (16)$$

$$Me_\theta(i, j) = \rho_l u_\theta(i, j) A e_\theta(i, j). \quad (17)$$

As will be shown later, $u_r(i, j)$ and $u_\theta(i, j)$ are each calculated on their own mesh systems, so that $u_r(i, j)$ and $u_\theta(i, j)$ are shifted spatially with respect to $e(i, j)$ and $T(i, j)$. Values of u_r and u_θ are calculated by solution of the equations of motion, discussed in the next section. The conduction heat Eq. (10), modified to include the convective heat fluxes, becomes

$$\begin{aligned} &[\rho^{t+\Delta t}(i, j)e^{t+\Delta t}(i, j) - \rho^t e^t(i, j)] V e(i, j) \\ &= \Delta t [q_r(i, j) + Fe_r(i, j) - q_r(i - 1, j) - Fe_r(i - 1, j) + q_\theta(i, j) \\ &+ Fe_\theta(i, j) - q_\theta(i, j - 1) - Fe_\theta(i, j - 1)]. \end{aligned} \quad (18)$$

The density may change between time steps due to melting or freezing, or in volumes that contain a liquid-vapor interface. Equation (18) can be written in

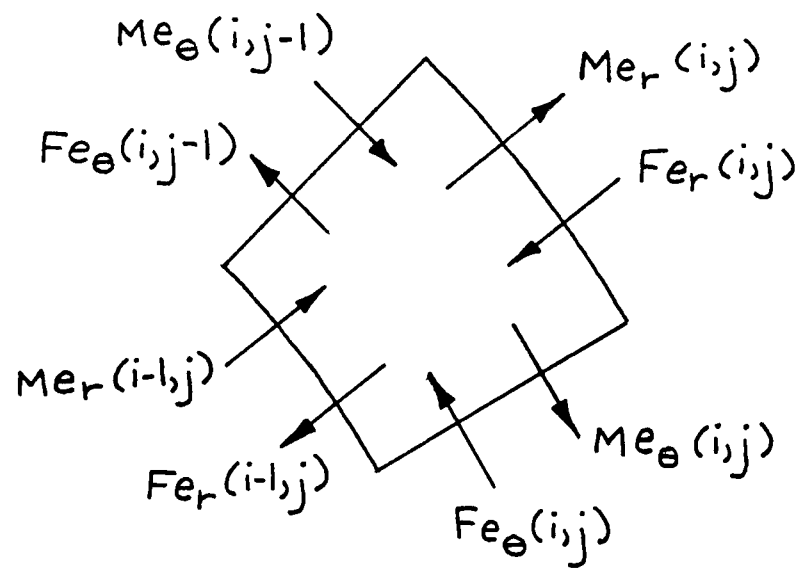


Figure 7. Mass and Convective Heat Fluxes for a Typical Control Volume.

the tridiagonal form given by Eq. (15). The coefficients for the tridiagonal form of the fully implicit heat equation, neglecting convective terms, are

$$\begin{aligned}
 A_e(i, j) &= \rho^{t+\Delta t}(i, j)Ve(i, j)c(i, j) + \Delta t [Ce_r(i, j) + Ce_r(i-1, j) + Ce_\theta(i, j) \\
 &\quad + Ce_\theta(i, j-1)], \\
 B_e(i, j) &= \Delta t Ce_r(i, j), \\
 C_e(i, j) &= \Delta t Ce_r(i-1, j), \\
 D_e(i, j) &= \Delta t [Ce_\theta(i, j)T(i, j+1) + Ce_\theta(i, j-1)T(i, j-1)] \\
 &\quad + \rho^t(i, j)Ve(i, j)[e^t(i, j) - h_{sl}].
 \end{aligned}$$

The above coefficients are modified to include the convection terms using the UDS scheme, based on the values of $u_r(i, j)$, $u_r(i+1, j)$, $u_\theta(i, j)$, and $u_\theta(i, j-1)$, as follows:

$$\begin{aligned}
 A_e(i, j) &= A_e(i, j) + \Delta t Me_r(i, j)c_l && \text{when } u_r(i, j) > 0, \\
 B_e(i, j) &= B_e(i, j) - \Delta t Me_r(i, j)c_l && \text{when } u_r(i, j) < 0, \\
 A_e(i, j) &= A_e(i, j) - \Delta t Me_r(i-1, j)c_l && \text{when } u_r(i-1, j) < 0, \\
 C_e(i, j) &= C_e(i, j) + \Delta t Me_r(i-1, j)c_l && \text{when } u_r(i-1, j) > 0, \\
 A_e(i, j) &= A_e(i, j) + \Delta t Me_\theta(i, j)c_l && \text{when } u_\theta(i, j) > 0, \\
 D_e(i, j) &= D_e(i, j) - \Delta t Me_\theta(i, j)c_l T(i, j+1) && \text{when } u_\theta(i, j) < 0, \\
 A_e(i, j) &= A_e(i, j) - \Delta t Me_\theta(i, j-1)c_l && \text{when } u_\theta(i, j-1) < 0, \\
 D_e(i, j) &= D_e(i, j) + \Delta t Me_\theta(i, j-1)c_l T(i, j-1) && \text{when } u_\theta(i, j-1) > 0.
 \end{aligned}$$

Boundary conditions for the energy equation. Specified temperature boundary conditions are provided by fixing the temperature of the boundary volumes

(k, j) . For volumes $(k-1, j)$, coefficients B_e and D_e in the tridiagonal formulation become

$$B_e(k-1, j) = 0,$$

$$D_e(k-1, j) = \Delta t [C e_r(k-1, j) T(k, j) + C e_\theta(k-1, j) T(k-1, j+1) + C e_\theta(k-1, j-1) T(k-1, j-1)] + \rho(k-1, j) V e(k-1, j) e^t(k-1, j),$$

where $T(k, j)$ is given. For a convection boundary condition, $q_r(k, j)$ in equation (10) is given by

$$q_r(k, j) = h(j) A e_r(k, j) [T_f - T(k, j)],$$

where $h(j)$ is the convection coefficient and T_f is the fluid temperature. For this case, coefficients A_e , B_e , and D_e in the tridiagonal formulation for boundary node (k, j) are

$$A_e(k, j) = \rho(k, j) V e(k, j) c(k, j) + \Delta t [h(j) A e_r(k, j) + C e_r(k-1, j) + C e_\theta(k, j) + C e_\theta(k, j-1)],$$

$$B_e(k, j) = 0,$$

$$D_e(k, j) = \Delta t [h(j) A e_r(k, j) T_f + C e_\theta(k, j) T(k, j+1) + C e_\theta(k, j-1) T(k, j-1)] + \rho(k, j) V e(k, j) e^t(k, j).$$

In all cases the boundary condition is automatically supplied at the origin as $A e_r(0, j) = 0$.

TDMA solution procedure. Equations in tridiagonal form are solved using the Tridiagonal Matrix Algorithm (TDMA) [11]. Equations are written for n nodes in the form

$$A_i T_i = B_i T_{i+1} + C_i T_{i-1} + D_i, \quad (19)$$

where $C_1 = 0$ and $B_n = 0$. Equation (19) can be rewritten

$$T_i = P_i T_{i+1} + Q_i. \quad (20)$$

Therefore,

$$T_{i-1} = P_{i-1}T_i + Q_{i-1}. \quad (21)$$

Substitution of (21) into (19) gives

$$A_i T_i = B_i T_{i+1} + C_i [P_{i-1} T_i + Q_{i-1}] + D_i,$$

which when rearranged gives

$$T_i = \frac{B_i}{A_i - C_i P_{i-1}} T_{i+1} + \frac{C_i Q_{i-1} + D_i}{A_i - C_i P_{i-1}}. \quad (22)$$

Comparison of (20) with (22) shows that

$$P_i = \frac{B_i}{A_i - C_i P_{i-1}}, \quad Q_i = \frac{C_i Q_{i-1} + D_i}{A_i - C_i P_{i-1}}.$$

Since $C_1 = 0$, $P_1 = B_1/A_1$ and $Q_1 = D_1/A_1$, and since $B_n = 0$, $P_n = 0$ and thus $T_n = Q_n$. Values of P_i and Q_i are found by forward substitution, then values of T_i are found by back substitution.

Application of this method to freezing/melting nodes requires special treatment. Equations for these nodes are not solved by the line relaxation scheme. The temperatures of freezing /melting nodes must be held constant at $T_i = 0$ due to the presence of the phase boundary. Thus, for a node i which has a neighboring node $i + 1$ with $T_{i+1} = 0$, Eq. (20) gives

$$T_i = Q_i,$$

and for node i that has a neighboring node $i - 1$ with $T_{i-1} = 0$, Eq. (19) gives

$$A_i T_i = B_i T_{i+1} + D_i,$$

which can be rearranged to give

$$T_i = \frac{B_i}{A_i} T_{i+1} + \frac{D_i}{A_i}.$$

Comparison with (20) shows that $P_i = B_i/A_i$ and $Q_i = D_i/A_i$. Thus, the freezing/melting nodes act as internal boundary conditions.

After all equations with $T_i \neq 0$ are solved by line relaxation, energy equations for the melting/freezing nodes are solved for $e^{t+\Delta t}(i, j)$ by substituting known temperature values into Eq. (18). If, after time step Δt , the value of $e(i, j)$ exceeds h_{sl} , the volume has completely melted and is assigned a new temperature as follows:

$$T(i, j) = \frac{e(i, j) - h_{sl}}{c_l}.$$

Similarly, if the value of $e(i, j)$ is less than zero, the volume has completely frozen, and its new temperature is given by

$$T(i, j) = \frac{e(i, j)}{c_s}.$$

The freezing/melting front naturally progresses as the energy contents of neighboring nodes enter the range $0 < e(i, j) < h_{sl}$, and the temperatures of these nodes are set to zero. However, in cases involving melting with rapid heat addition, the temperatures of adjoining volumes containing solid salt were arbitrarily set to zero as soon as complete melting occurred at a given node. This numerical artifice was required to insure that there was always a well-defined phase-change front, i.e., that the correct internal boundary condition for the TDMA solution procedure was always maintained. Otherwise, the two-phase region tended to become several nodes thick, causing difficulties in the fluid flow calculations.

The density of a melting/freezing node was determined by its energy content as follows:

$$\rho^{t+\Delta t}(i, j) = \rho_s + \frac{e^{t+\Delta t}(i, j)}{h_{sl}}(\rho_l - \rho_s).$$

The solid, liquid, and shell material densities are assigned constant values in the model. Since the density of the material in a given volume changes during melting

or solidification, an effective mass source arises that must be taken into account in the mass conservation (continuity) equation. The mass source or sink for the volume, i.e., the rate at which liquid enters or exits the volume during time step Δt as a result of the phase change, is given by

$$\Delta M(i, j) = \frac{[\rho^t(i, j) - \rho^{t+\Delta t}(i, j)] V e(i, j)}{\Delta t}. \quad (23)$$

The mass source ΔM is incorporated into the mass conservation equation for the liquid phase.

Development of the Fluid Flow Model

The continuity equation for the incompressible liquid phase was written in terms of the main grid control volume used for solution of the energy equation. The continuity equation is given as

$$Me_r(i, j) - Me_r(i - 1, j) + Me_\theta(i, j) - Me_\theta(i, j - 1) = \Delta M(i, j),$$

where the mass fluxes Me_r and Me_θ are defined by (16) and (17), and the mass source ΔM is defined by (23). The continuity equation can be rewritten as

$$\begin{aligned} &u_r(i, j)Ae_r(i, j) - u_r(i - 1, j)Ae_r(i - 1, j) + u_\theta(i, j)Ae_\theta(i, j) \\ &- u_\theta(i, j - 1)Ae_\theta(i, j - 1) = \frac{\Delta M(i, j)}{\rho_l}. \end{aligned} \quad (24)$$

The momentum conservation equation for u_r was solved on a grid which was staggered or shifted with respect to the main grid, as shown in Figure 8. The balance of forces on the control volume in the radial direction is given by

$$\begin{aligned} &Fr_r(i, j) - Fr_r(i - 1, j) + Fr_\theta(i, j) - Fr_\theta(i, j - 1) + \rho_l V r(i, j)a_r(i, j) \\ &= \mathbf{F}_r(i, j), \end{aligned} \quad (25)$$

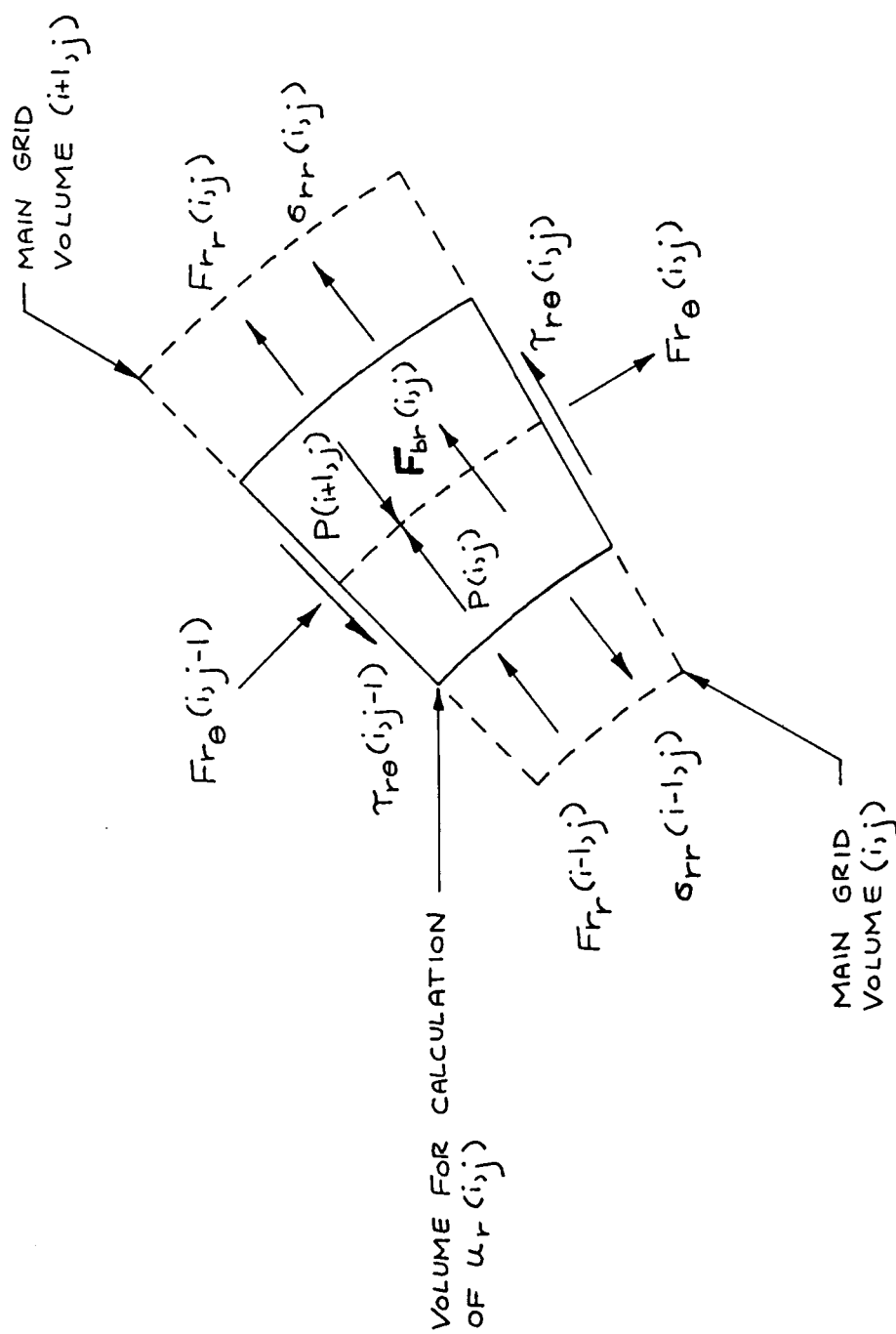


Figure 8. Grid Volume for Calculation of $u_r(i, j)$.

where a_r is the radial acceleration, Fr_r and Fr_θ are the fluxes of radial momentum in the r and θ directions, and $\mathbf{F}_r$ is the sum of body forces, forces due to viscous stresses, and pressure forces acting in the radial direction. The acceleration a_r can be written

$$a_r = \frac{\partial u_r}{\partial t} - \frac{u_\theta^2}{r}.$$

The upwind differencing scheme was used for the convective momentum flux $Fr_r(i, j)$, depending on the sign of the mass flux $Mr_r(i, j)$, where

$$Mr_r(i, j) = \rho_l A r_r(i, j) \frac{u_r(i+1, j) + u_r(i, j)}{2}.$$

The average of $u_r(i+1, j)$ and $u_r(i, j)$ was used for u_r because of the staggered grid arrangement. The momentum flux Fr_r was given by

$$\begin{aligned} Fr_r(i, j) &= Mr_r(i, j) u_r(i, j) \quad \text{when } Mr_r(i, j) > 0, \\ &= Mr_r(i, j) u_r(i+1, j) \quad \text{when } Mr_r(i, j) < 0. \end{aligned}$$

The mass flux in the tangential direction was given by

$$Mr_\theta(i, j) = \rho_l A r_\theta(i, j) \frac{u_\theta(i+1, j) + u_\theta(i, j)}{2},$$

and the flux of radial momentum in the tangential direction, $Fr_\theta(i, j)$ was given by

$$\begin{aligned} Fr_\theta(i, j) &= Mr_\theta(i, j) u_r(i, j) \quad \text{when } Mr_\theta(i, j) > 0, \\ &= Mr_\theta(i, j) u_r(i, j+1) \quad \text{when } Mr_\theta(i, j) < 0. \end{aligned}$$

The forces on the control volume include a body force, $\mathbf{F}_{br}$, given by

$$\mathbf{F}_{br}(i, j) = -\rho_l(T) V r(i, j) g \cos\left[\left(j - \frac{1}{2}\right) \Delta\theta\right],$$

where $\rho_l(T)$ is a special temperature-dependent value of the liquid density calculated at the average of $T(i, j)$ and $T(i+1, j)$, and g is the acceleration due to

gravity. This formulation for the body force is equivalent to the Boussinesq approximation. To model buoyancy-driven flow, it is necessary have a temperature-dependent density in the body force term. Liquid density is held constant everywhere else.

Forces due to viscous stresses act on the control surfaces. The finite difference approximations for the viscous shear stress, $\tau_{r\theta}$, and the viscous normal stresses, σ_{rr} and $\sigma_{\theta\theta}$, defined by Eqs. (7)-(9), are

$$\begin{aligned}\tau_{r\theta}(i, j) &= \mu \left[i \left[\frac{u_{\theta}(i+1, j)}{(i + \frac{1}{2})\Delta r} - \frac{u_{\theta}(i, j)}{(i - \frac{1}{2})\Delta r} \right] + \frac{1}{i\Delta r} \left[\frac{u_r(i, j+1) - u_r(i, j)}{\Delta \theta} \right] \right], \\ \sigma_{rr}(i, j) &= 2\mu \left[\frac{u_r(i+1, j) - u_r(i, j)}{\Delta r} \right], \\ \sigma_{\theta\theta}(i, j) &= \frac{2\mu}{(i - \frac{1}{2})\Delta r} \left[\frac{u_{\theta}(i, j+1) - u_{\theta}(i, j)}{\Delta \theta} + \frac{u_r(i, j+1) + u_r(i-1, j+1)}{2} \right].\end{aligned}$$

Note that the finite difference approximations given above are valid only for a grid using uniform increments of Δr and $\Delta \theta$. Neglecting the u_{θ}^2/r term in the radial acceleration, which is expected to be small, the radial force balance equation, (25), can be written

$$\begin{aligned}& Fr_r(i, j) - Fr_r(i-1, j) + Fr_{\theta}(i, j) - Fr_{\theta}(i, j-1) \\ & + \rho_l V r(i, j) \frac{u_r^{t+\Delta t}(i, j) - u_r^t(i, j)}{\Delta t_c} = -\rho_l(T) V r(i, j) g \cos[(j - \frac{1}{2})\Delta \theta] \\ & + Ar_r(i, j)\sigma_{rr}(i, j) - Ar_r(i-1, j)\sigma_{rr}(i-1, j) + Ar_{\theta}(i, j)\tau_{r\theta}(i, j) \\ & - Ar_{\theta}(i, j-1)\tau_{r\theta}(i, j-1) - Ae_r(i, j)[P(i+1, j) - P(i, j)].\end{aligned}$$

In this formulation, a small term accounting for the radial force due to the tangential normal stress, $\sigma_{\theta\theta}$, acting on the angled surfaces of the control volume is neglected. Except for this term and the u_{θ}^2/r term in the radial acceleration, it can be shown that in the limit as the volume and time step approach zero, the above equation reduces to the equation of motion for u_r given by Eq. (5). It should be noted that the pressures $P(i+1, j)$ and $P(i, j)$ act on the same area, but in opposite directions, as shown in Figure 8.

The above equation can be rewritten

$$\begin{aligned}
 u_r^{t+\Delta t}(i, j) = & u_r^t(i, j) + \frac{\Delta t_c}{\rho_l V r(i, j)} \left[-Fr_r(i, j) + Fr_r(i-1, j) - Fr_\theta(i, j) \right. \\
 & + Fr_\theta(i, j-1) - \rho_l(T) V r(i, j) g \cos\left[\left(j - \frac{1}{2}\right)\Delta\theta\right] + Ar_r(i, j)\sigma_{rr}(i, j) \\
 & - Ar_r(i-1, j)\sigma_{rr}(i-1, j) + Ar_\theta(i, j)\tau_{r\theta}(i, j) - Ar_\theta(i, j-1)\tau_{r\theta}(i, j-1) \\
 & \left. - A\epsilon_r(i, j)[P(i+1, j) - P(i, j)] \right]. \quad (26)
 \end{aligned}$$

All of the terms on the righthand side of the above equation except for the pressure term may be combined into a velocity source term, $s_r(i, j)$, defined as

$$\begin{aligned}
 s_r(i, j) = & u_r^t(i, j) + \frac{\Delta t_c}{\rho_l V r(i, j)} \left[-Fr_r(i, j) + Fr_r(i-1, j) - Fr_\theta(i, j) \right. \\
 & + Fr_\theta(i, j-1) - \rho_l(T) V r(i, j) g \cos\left[\left(j - \frac{1}{2}\right)\Delta\theta\right] \\
 & + Ar_r(i, j)\sigma_{rr}(i, j) - Ar_r(i-1, j)\sigma_{rr}(i-1, j) \\
 & \left. + Ar_\theta(i, j)\tau_{r\theta}(i, j) - Ar_\theta(i, j-1)\tau_{r\theta}(i, j-1) \right]. \quad (27)
 \end{aligned}$$

The equation for $u_r^{t+\Delta t}(i, j)$ thus becomes

$$u_r^{t+\Delta t}(i, j) = s_r(i, j) - \frac{\Delta t_c A \epsilon_r(i, j)}{\rho_l V r(i, j)} [P(i+1, j) - P(i, j)]. \quad (28)$$

The source term is calculated using values for u_r , u_θ , and temperature at the previous time step.

Momentum equations for u_θ are also solved on a staggered grid, as shown in Figure 9. The balance of tangential forces on the control volume is given by

$$\begin{aligned}
 & F\theta_\theta(i, j) - F\theta_\theta(i, j-1) + F\theta_r(i, j) - F\theta_r(i-1, j) + \rho_l V \theta(i, j) a_\theta(i, j) \\
 & = \mathbf{F}_\theta(i, j), \quad (29)
 \end{aligned}$$

where a_θ is the tangential acceleration, $F\theta_\theta$ and $F\theta_r$ are the fluxes of tangential momentum in the θ and r directions, and $\mathbf{F}_\theta$ is the sum of body forces, forces due

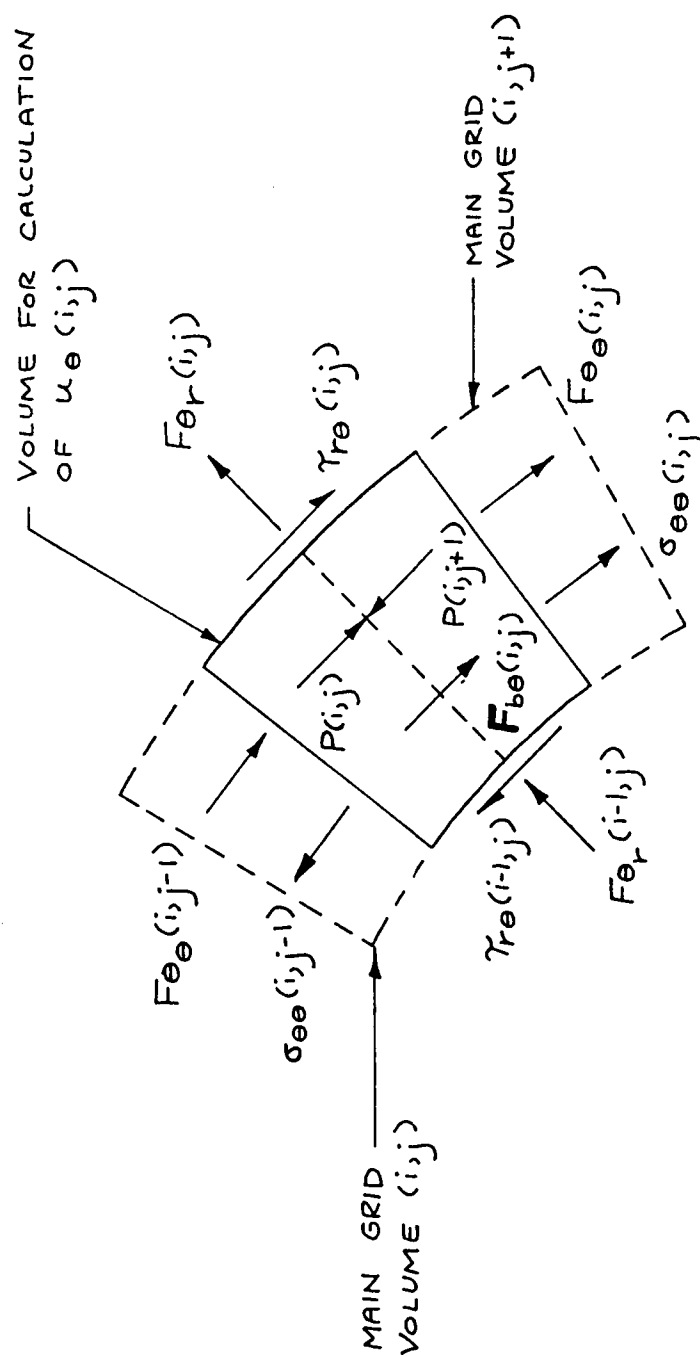


Figure 9. Grid Volume for Calculation of $u_\theta(i,j)$.

to viscous stresses, and pressure forces acting in the tangential direction. The acceleration a_θ can be written as

$$a_\theta = \frac{\partial u_\theta}{\partial t} + \frac{u_\theta u_r}{r}.$$

The upwind differencing scheme was used for the convective momentum flux $F\theta_\theta(i, j)$, depending on the sign of the mass flux $M\theta_\theta(i, j)$, where

$$M\theta_\theta(i, j) = \rho_l A \theta_\theta(i, j) \frac{u_\theta(i, j+1) + u_\theta(i, j)}{2}.$$

Values of $F\theta_\theta(i, j)$ were determined as follows:

$$F\theta_\theta(i, j) = M\theta_\theta(i, j)u_\theta(i, j) \quad \text{when } M\theta_\theta(i, j) > 0,$$

$$F\theta_\theta(i, j) = M\theta_\theta(i, j)u_\theta(i, j+1) \quad \text{when } M\theta_\theta(i, j) < 0.$$

The mass flux in the radial direction, $M\theta_r$, was given by

$$M\theta_r(i, j) = \rho_l A \theta_r(i, j) \frac{u_r(i, j+1) + u_r(i, j)}{2}.$$

and the flux of tangential momentum in the radial direction, $F\theta_r(i, j)$, was given by

$$F\theta_r(i, j) = M\theta_r(i, j)u_\theta(i, j) \quad \text{when } M\theta_r(i, j) > 0,$$

$$F\theta_r(i, j) = M\theta_r(i, j)u_\theta(i+1, j) \quad \text{when } M\theta_r(i, j) < 0.$$

The forces on the control volume include the body force, $\mathbf{F}_{b\theta}$, given by

$$\mathbf{F}_{b\theta}(i, j) = \rho_l(T)V\theta(i, j)g \sin(j\Delta\theta),$$

where $\rho_l(T)$ is the temperature-dependent density calculated at the average of $T(i, j)$ and $T(i, j+1)$. Neglecting the $u_\theta u_r/r$ term in the radial acceleration, which is expected to be small, the tangential force balance equation, (29), can be written

$$\begin{aligned} & F\theta_\theta(i, j) - F\theta_\theta(i, j-1) + F\theta_r(i, j) - F\theta_r(i-1, j) \\ & + \rho_l V \theta(i, j) \frac{u_\theta^{t+\Delta t}(i, j) - u_\theta^t(i, j)}{\Delta t_c} = \rho_l(T) V \theta(i, j) g \sin(j\Delta\theta) \\ & + A \theta_r(i, j) \tau_{r\theta}(i, j) - A \theta_r(i-1, j) \tau_{r\theta}(i-1, j) + A \theta_\theta(i, j) \sigma_{\theta\theta}(i, j) \\ & - A \theta_\theta(i, j-1) \sigma_{\theta\theta}(i, j-1) - A e_\theta(i, j) [P(i, j+1) - P(i, j)]. \end{aligned}$$

A small term accounting for the tangential force due to the viscous stress $\tau_{r\theta}$ acting on the angled surfaces of the control volume is neglected in this formulation. It can be shown that, excepting this term and the $u_\theta u_r/r$ term in the tangential acceleration, the above equation reduces in the limit as the volume and time step approach zero, to the equation of motion for u_θ given by Eq. (6).

The above equation can be rewritten

$$\begin{aligned} u_\theta^{t+\Delta t}(i, j) = & u_\theta^t(i, j) + \frac{\Delta t_c}{\rho_l V \theta(i, j)} \left[-F\theta_\theta(i, j) + F\theta_\theta(i, j-1) - F\theta_r(i, j) \right. \\ & + F\theta_r(i-1, j) + \rho_l(T)V\theta(i, j)g \sin(j\Delta\theta) + A\theta_r(i, j)\tau_{r\theta}(i, j) \\ & - A\theta_r(i-1, j)\tau_{r\theta}(i-1, j) + A\theta_\theta(i, j)\sigma_{\theta\theta}(i, j) - A\theta_\theta(i, j-1)\sigma_{\theta\theta}(i, j-1) \\ & \left. - Ae_\theta(i, j)[P(i, j+1) - P(i, j)] \right]. \end{aligned} \quad (30)$$

All of the terms on the righthand side of the above equation except for the pressure term may be combined into a velocity source term, $s_\theta(i, j)$, defined as

$$\begin{aligned} s_\theta(i, j) = & u_\theta^t(i, j) + \frac{\Delta t_c}{\rho_l V \theta(i, j)} \left[-F\theta_\theta(i, j) + F\theta_\theta(i, j-1) - F\theta_r(i, j) \right. \\ & + F\theta_r(i-1, j) + \rho_l(T)V\theta(i, j)g \sin(j\Delta\theta) \\ & + A\theta_r(i, j)\tau_{r\theta}(i, j) - A\theta_r(i-1, j)\tau_{r\theta}(i-1, j) + A\theta_\theta(i, j)\sigma_{\theta\theta}(i, j) \\ & \left. - A\theta_\theta(i, j-1)\sigma_{\theta\theta}(i, j-1) \right]. \end{aligned} \quad (31)$$

The equation for $u_\theta^{t+\Delta t}(i, j)$ thus becomes

$$u_\theta^{t+\Delta t}(i, j) = s_\theta(i, j) - \frac{\Delta t_c Ae_\theta(i, j)}{\rho_l V \theta(i, j)} [P(i, j+1) - P(i, j)]. \quad (32)$$

A slight modification to the term $Ae_\theta(i, j)/V\theta(i, j)$ is required to maintain the correct balance between the body force and the pressure field. The term $Ae_\theta(i, j)/V\theta(i, j)$ can be reduced to

$$\frac{Ae_\theta(i, j)}{V\theta(i, j)} = \frac{(i - \frac{1}{2})\Delta r^2 \sin(j\Delta\theta)}{(i - \frac{1}{2})^2 \Delta r^3 \Delta\theta \sin(j\Delta\theta)} = \frac{1}{(i - \frac{1}{2})\Delta r \Delta\theta}. \quad (33)$$

However, this value for $Ae_\theta(i, j)/V\theta(i, j)$ does not quite maintain the force balance in a hydrostatic pressure field. For the hydrostatic case, $s_\theta(i, j)$ is given by

$$s_\theta(i, j) = \Delta t_c g \sin(j\Delta\theta). \quad (34)$$

The hydrostatic pressure field is given by

$$P = P_o - \rho_l g h,$$

where h is the vertical distance from a reference plane where the pressure is P_o .

Therefore, for static conditions $P(i, j)$ is given by

$$P(i, j) = P_o - \rho_l g (i - \frac{1}{2}) \Delta r \cos[(j - \frac{1}{2})\Delta\theta]. \quad (35)$$

Substitution of (34) and (35) into (32) gives

$$\begin{aligned} u_\theta^{t+\Delta t}(i, j) = & \Delta t_c g \sin(j\Delta\theta) - \frac{\Delta t_c Ae_\theta(i, j)}{\rho_l V\theta(i, j)} \left[\left[P_o - \rho_l g (i - \frac{1}{2}) \Delta r \cos[(j + \frac{1}{2})\Delta\theta] \right] \right. \\ & \left. - \left[P_o - \rho_l g (i - \frac{1}{2}) \Delta r \cos[(j - \frac{1}{2})\Delta\theta] \right] \right]. \end{aligned}$$

Reducing and setting $\theta = j\Delta\theta$ gives

$$u_\theta^{t+\Delta t}(i, j) = \Delta t_c g \left[\sin\theta - \frac{Ae_\theta(i, j) (i - \frac{1}{2}) \Delta r}{V\theta(i, j)} \left[\cos(\theta - \frac{\Delta\theta}{2}) - \cos(\theta + \frac{\Delta\theta}{2}) \right] \right].$$

For the hydrostatic case, $u_\theta(i, j)$ must be zero, so

$$\sin\theta = \frac{Ae_\theta(i, j) (i - \frac{1}{2}) \Delta r}{V\theta(i, j)} \left[\cos(\theta - \frac{\Delta\theta}{2}) - \cos(\theta + \frac{\Delta\theta}{2}) \right].$$

Comparison with the trigonometric identity

$$2 \sin A \sin B = \cos(A - B) - \cos(A + B)$$

shows that to maintain the hydrostatic balance

$$\frac{Ae_\theta(i, j)}{V\theta(i, j)} = \frac{1}{2 \sin \frac{\Delta\theta}{2} (i - \frac{1}{2}) \Delta r}. \quad (36)$$

Comparison of (36) and (33) shows that the difference in the expressions for the term $Ae_\theta(i,j)/V\theta(i,j)$ is the difference between the linear distance between the centers of volumes (i,j) and $(i,j+1)$ and the distance approximated by a circular arc. The difficulty arises because of the geometrical approximations used in defining the control volumes. No similar difficulty arises in the equation for u_r . The expression for $Ae_\theta(i,j)/V\theta(i,j)$ given by Eq. (36) was used in Eq. (32) when solving for $u_\theta(i,j)$.

Boundary Conditions for the Fluid Flow Model

Boundary conditions for u_r and u_θ are provided at solid boundaries by setting velocities to zero at all points in the solid. Velocities between two melting/freezing volumes are also set to zero. Boundary conditions for cells on the liquid-vapor interface are based on satisfying mass conservation (continuity) for the surface cells [12]. For a cell with one surface outside the liquid, the required velocity for calculating stresses in the liquid is obtained from solution of the continuity equation, [12],

$$u_r(i,j)Ae_r(i,j) - u_r(i-1,j)Ae_r(i-1,j) + u_\theta(i,j)Ae_\theta(i,j) - u_\theta(i,j-1)Ae_\theta(i,j-1) = 0.$$

The above calculation yields the unknown velocity in terms of the three other known velocities. For cells having two adjacent sides outside the liquid, the velocities are determined so

$$Ae_r(i,j)u_r(i,j) = Ae_r(i-1,j)u_r(i-1,j),$$

$$Ae_\theta(i,j)u_\theta(i,j) = Ae_\theta(i,j-1)u_\theta(i,j-1).$$

This formulation also approximates the condition that there should be no tangential stress at the free surface [13].

Boundary conditions are also required when the liquid is divided into two regions separated by solid. This situation occurs in the model when the layer of

salt near the outer container wall starts to melt, and the excess liquid generated by the melting density change makes its way up along the wall and flows into the void, forming a separate liquid volume. In this case, velocity outflow and inflow boundary conditions are applied so mass is conserved for the total liquid, as shown in Figure 10. The difficulties associated with establishing boundary conditions at the origin are avoided by not calculating velocities in the volumes surrounding the origin ($i = 1$). For a grid having 20 nodes in the r direction, $(1/20)^3$, or about 0.01 percent of the total volume is contained in these volumes, so the effect on the overall calculation should be very small. By not making velocity calculations in the volumes surrounding the origin, the time step size allowed for stable calculations is greatly increased.

The Pressure/Pressure Correction Equation

In order to satisfy the continuity equation in each grid volume, the continuity equation is converted into both a pressure-field equation and a pressure-correction equation, which are required to solve the momentum equations [11]. The equation for determining the pressure field can be derived by substituting the right-hand sides of (28) and (32), for u_r and u_θ , respectively, into the continuity equation (24). The result is

$$\begin{aligned}
 & Ae_r(i, j) \left[s_r(i, j) - \frac{\Delta t_c Ae_r(i, j)}{\rho_l V r(i, j)} [P(i+1, j) - P(i, j)] \right] \\
 & - Ae_r(i-1, j) \left[s_r(i-1, j) - \frac{\Delta t_c Ae_r(i-1, j)}{\rho_l V r(i-1, j)} [P(i, j) - P(i-1, j)] \right] \\
 & + Ae_\theta(i, j) \left[s_\theta(i, j) - \frac{\Delta t_c Ae_\theta(i, j)}{\rho_l V \theta(i, j)} [P(i, j+1) - P(i, j)] \right] \\
 & - Ae_\theta(i, j-1) \left[s_\theta(i, j-1) - \frac{\Delta t_c Ae_\theta(i, j-1)}{\rho_l V \theta(i, j-1)} [P(i, j) - P(i, j-1)] \right] \\
 & = \frac{\Delta M(i, j)}{\rho_l}.
 \end{aligned}$$

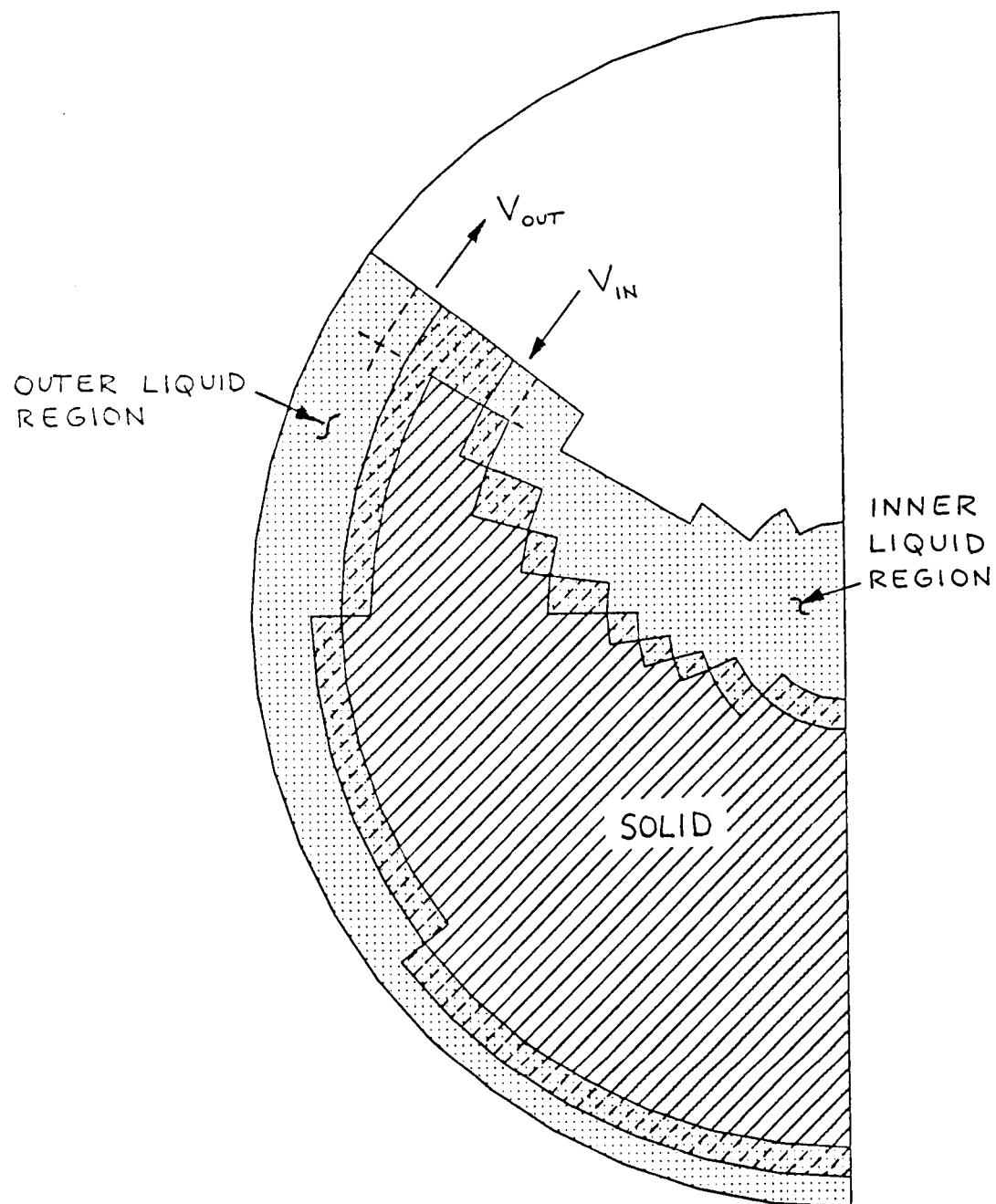


Figure 10. Velocity Boundary Conditions for Separated Liquid Regions.

Rearrangement gives

$$\begin{aligned}
 & s_r(i, j)A\epsilon_r(i, j) - s_r(i-1, j)A\epsilon_r(i-1, j) + s_\theta(i, j)A\epsilon_\theta(i, j) \\
 & - s_\theta(i, j-1)A\epsilon_\theta(i, j-1) - \frac{\Delta M(i, j)}{\rho_l} = \frac{\Delta t_c A\epsilon_r(i, j)^2}{\rho_l V r(i, j)} [P(i+1, j) - P(i, j)] \\
 & - \frac{\Delta t_c A\epsilon_r(i-1, j)^2}{\rho_l V r(i-1, j)} [P(i, j) - P(i-1, j)] + \frac{\Delta t_c A\epsilon_\theta(i, j)^2}{\rho_l V \theta(i, j)} [P(i, j+1) - P(i, j)] \\
 & - \frac{\Delta t_c A\epsilon_\theta(i, j-1)^2}{\rho_l V \theta(i, j-1)} [P(i, j) - P(i, j-1)]. \quad (37)
 \end{aligned}$$

Terms on the lefthand side of Eq. (37) were next grouped together as a velocity divergence, $div_s(i, j)$, where

$$\begin{aligned}
 div_s(i, j) = & s_r(i, j)A\epsilon_r(i, j) - s_r(i-1, j)A\epsilon_r(i-1, j) + s_\theta(i, j)A\epsilon_\theta(i, j) \\
 & - s_\theta(i, j-1)A\epsilon_\theta(i, j-1) - \frac{\Delta M(i, j)}{\rho_l}.
 \end{aligned}$$

The equation was then written in tridiagonal form for solution by line relaxation using the tridiagonal matrix algorithm. The tridiagonal form of the equation is

$$A_P(i, j)P(i, j) = B_P(i, j)P(i+1, j) + C_P(i, j)P(i-1, j) + D_P(i, j),$$

where

$$A_P(i, j) = \frac{\Delta t_c A\epsilon_r(i, j)^2}{\rho_l V r(i, j)} + \frac{A\epsilon_r(i-1, j)^2}{V r(i-1, j)} + \frac{A\epsilon_\theta(i, j)^2}{V \theta(i, j)} + \frac{A\epsilon_\theta(i, j-1)^2}{V \theta(i, j-1)} \quad (38)$$

$$B_P(i, j) = \frac{\Delta t_c A\epsilon_r(i, j)^2}{\rho_l V r(i, j)}, \quad (39)$$

$$C_P(i, j) = \frac{\Delta t_c A\epsilon_r(i-1, j)^2}{\rho_l V r(i-1, j)}, \quad (40)$$

$$\begin{aligned}
 D_P(i, j) = & \frac{\Delta t_c A\epsilon_\theta(i, j)^2}{\rho_l V \theta(i, j)} P(i, j+1) + \frac{\Delta t_c A\epsilon_\theta(i, j-1)^2}{\rho_l V \theta(i, j-1)} P(i, j-1) \\
 & - div_s(i, j). \quad (41)
 \end{aligned}$$

Boundary conditions for the pressure equation follow automatically when velocity values at the boundaries are specified. For example, if the value of

$u_r^{t+\Delta t}(i, j)$ is given. the known value is used directly in the pressure equation and the pressure equation can be written

$$\begin{aligned} & u_r^{t+\Delta t}(i, j)A\epsilon_r(i, j) - s_r(i-1, j)A\epsilon_r(i-1, j) + s_\theta(i, j)A\epsilon_\theta(i, j) \\ & - s_\theta(i, j-1)A\epsilon_\theta(i, j-1) - \frac{\Delta M(i, j)}{\rho_l} = -\frac{\Delta t_c A\epsilon_r(i-1, j)^2}{\rho_l V r(i-1, j)} [P(i, j) - P(i-1, j)] \\ & + \frac{\Delta t_c A\epsilon_\theta(i, j)^2}{\rho_l V \theta(i, j)} [P(i, j+1) - P(i, j)] - \frac{\Delta t_c A\epsilon_\theta(i, j-1)^2}{\rho_l V \theta(i, j-1)} [P(i, j) - P(i, j-1)]. \end{aligned}$$

The pressure outside the boundary, $P(i+1, j)$, does not appear in the equation and so does not need to be specified. The derivation of the boundary condition equation is the same when $u_r(i-1, j)$, $u_\theta(i, j)$, or $u_\theta(i, j-1)$ is given.

Iteration of the pressure equations was continued until the maximum change in any of the pressure values from one iteration to the next was less than some small fraction of the maximum pressure. The new pressure field determined by this procedure was the pressure field for time step $t + \Delta t_c$. When the pressure field was converged, estimated values of $u_r^{t+\Delta t}$ and $u_\theta^{t+\Delta t}$, designated u_r^* and u_θ^* were calculated using

$$u_r^*(i, j) = s_r(i, j) - \frac{\Delta t_c A\epsilon_r(i, j)}{\rho_l V r(i, j)} [P(i+1, j) - P(i, j)],$$

$$u_\theta^*(i, j) = s_\theta(i, j) - \frac{\Delta t_c A\epsilon_\theta(i, j)}{\rho_l V \theta(i, j)} [P(i, j+1) - P(i, j)].$$

The estimated velocity values in general do not satisfy the continuity equation.

The actual values of $u_r^{t+\Delta t}$ and $u_\theta^{t+\Delta t}$ are given by

$$u_r^{t+\Delta t}(i, j) = u_r^*(i, j) - \frac{\Delta t_c A\epsilon_r(i, j)}{\rho_l V r(i, j)} [P'(i+1, j) - P'(i, j)], \quad (42)$$

$$u_\theta^{t+\Delta t}(i, j) = u_\theta^*(i, j) - \frac{\Delta t_c A\epsilon_\theta(i, j)}{\rho_l V \theta(i, j)} [P'(i, j+1) - P'(i, j)], \quad (43)$$

where $P'(i, j)$ is the correction to the pressure field required required to satisfy

continuity. Substitution of (42) and (43) into the continuity equation, (24), gives after rearrangement

$$\begin{aligned}
 & u_r^*(i, j)A\epsilon_r(i, j) - u_r^*(i-1, j)A\epsilon_r(i-1, j) + u_\theta^*(i, j)A\epsilon_\theta(i, j) \\
 & - u_\theta^*(i, j-1)A\epsilon_\theta(i, j-1) - \frac{\Delta M(i, j)}{\rho l} = \frac{\Delta t_c A\epsilon_r(i, j)^2}{\rho l V r(i, j)} [P'(i+1, j) - P'(i, j)] \\
 & - \frac{\Delta t_c A\epsilon_r(i-1, j)^2}{\rho l V r(i-1, j)} [P'(i, j) - P'(i-1, j)] + \frac{\Delta t_c A\epsilon_\theta(i, j)^2}{\rho l V \theta(i, j)} [P'(i, j+1) - P'(i, j)] \\
 & - \frac{\Delta t_c A\epsilon_\theta(i, j-1)^2}{\rho l V \theta(i, j-1)} [P'(i, j) - P'(i, j-1)]. \quad (44)
 \end{aligned}$$

Terms on the lefthand side of Eq. (44) are grouped together as a velocity divergence, $div^*(i, j)$, where

$$\begin{aligned}
 div^*(i, j) &= u_r^*(i, j)A\epsilon_r(i, j) - u_r^*(i-1, j)A\epsilon_r(i-1, j) + u_\theta^*(i, j)A\epsilon_\theta(i, j) \\
 & - u_\theta^*(i, j-1)A\epsilon_\theta(i, j-1) - \frac{\Delta M(i, j)}{\rho l}.
 \end{aligned}$$

The pressure correction equation can be written in tridiagonal form, becoming

$$A_P(i, j)P'(i, j) = B_P(i, j)P'(i+1, j) + C_P(i, j)P'(i-1, j) + D'_P(i, j).$$

Coefficients A_P , B_P , and C_P are the same coefficients used for the pressure equation, given by (38), (39), and (40). Coefficient D'_P differs from D_P , given by Eq. (41), in that $div_s(i, j)$ is replaced by $div^*(i, j)$. Boundary conditions for the pressure correction equation are derived in exactly the same way as for the pressure equation. The pressure correction equation is solved by line relaxation using the TDMA. After each iteration, tentative values of $u_r^{t+\Delta t}$ and $u_\theta^{t+\Delta t}$ are calculated using (42) and (43), and a divergence $div(i, j)$ is calculated, where

$$\begin{aligned}
 div(i, j) &= u_r(i, j)A\epsilon_r(i, j) - u_r(i-1, j)A\epsilon_r(i-1, j) + u_\theta(i, j)A\epsilon_\theta(i, j) \\
 & - u_\theta(i, j-1)A\epsilon_\theta(i, j-1) - \frac{\Delta M(i, j)}{\rho l}.
 \end{aligned}$$

Iterations are continued until the maximum divergence is less than some small fraction of the cell volume, i.e.,

$$\left| \frac{div(i,j)}{V\epsilon(i,j)} \right| < div_{max}$$

for all cells. It has been found that the maximum divergence can be driven to less than 10^{-6} (1 part in 10^6 of the cell volume gained or lost per second) using double precision calculations. Roundoff error usually causes the equations to converge with a maximum divergence in the range of 10^{-4} to 10^{-5} when single precision is used.

Stability Requirements

The time step for solution of the energy equations, Δt , is not limited by stability requirements, since the fully implicit form of the equations is used. The time step size is set to keep the energy gain or loss during each time step reasonably small. The time step used for calculation of u_r and u_θ , Δt_c , must be small enough to satisfy two types of stability criteria. It can be shown that, neglecting the convective flux terms, the coefficient of $u_r^t(i,j)$ in the radial momentum equation, Eq. (26), is

$$\rho_l V r(i,j) - \Delta t_c \left[\frac{2\mu}{\Delta r} [Ar_r(i,j) + Ar_r(i-1,j)] + \frac{\mu}{i\Delta r\Delta\theta} [Ar_\theta(i,j) + Ar_\theta(i,j-1)] \right].$$

Similarly, the coefficient of $u_\theta^t(i,j)$ in the tangential momentum equation, Eq. (30), is

$$\begin{aligned} \rho_l V \theta(i,j) - \Delta t_c \left[\frac{i\mu}{(i-\frac{1}{2})\Delta r} [A\theta_r(i,j) + A\theta_r(i-1,j)] \right. \\ \left. + \frac{2\mu}{(i-\frac{1}{2})\Delta r\Delta\theta} [A\theta_\theta(i,j) + A\theta_\theta(i,j-1)] \right]. \end{aligned}$$

To insure stable calculations, these coefficients must be positive. Otherwise, a positive value of u_r or u_θ at time t would cause a negative value of u_r or u_θ at

time $t + \Delta t_c$, and an oscillating solution would result. Thus, to avoid oscillating solutions, the maximum allowable step size is approximately given by

$$\Delta t_{max} < \frac{\rho_l V r(i, j)}{\frac{2\mu}{\Delta r} [Ar_r(i, j) + Ar_r(i-1, j)] + \frac{\mu}{i\Delta r\Delta\theta} [Ar_\theta(i, j) + Ar_\theta(i, j-1)]},$$

or

$$\Delta t_{max} < \frac{\rho_l V \theta(i, j)}{\frac{i\mu}{(i-\frac{1}{2})\Delta r} [A\theta_r(i, j) + A\theta_r(i-1, j)] + \frac{2\mu}{(i-\frac{1}{2})\Delta r\Delta\theta} [A\theta_\theta(i, j) + A\theta_\theta(i, j-1)]}.$$

The allowable time step is the minimum given by either equation over the whole grid. The above equations are not exact because the convective terms were neglected, but based on experience they appear to give reasonable values for Δt_{max} .

A second stability requirement is that the fluid must not cross more than one grid volume in a single time step. Under this condition, the maximum allowable time step is the minimum given by

$$\Delta t_{max} < \frac{\Delta r}{|u_r(i, j)|},$$

or

$$\Delta t_{max} < \frac{(i-\frac{1}{2})\Delta r\Delta\theta}{|u_\theta(i, j)|}$$

over the whole grid. The allowable time step is the smallest Δt_{max} given by either constraint. The time step for convection calculations was chosen to be some fraction of the time step for the energy calculations, i.e., $\Delta t_c = \Delta t/n$. The value of Δt_c was adjusted as the calculations progressed to minimize computation times. The calculation cycle is shown in Figure 11.

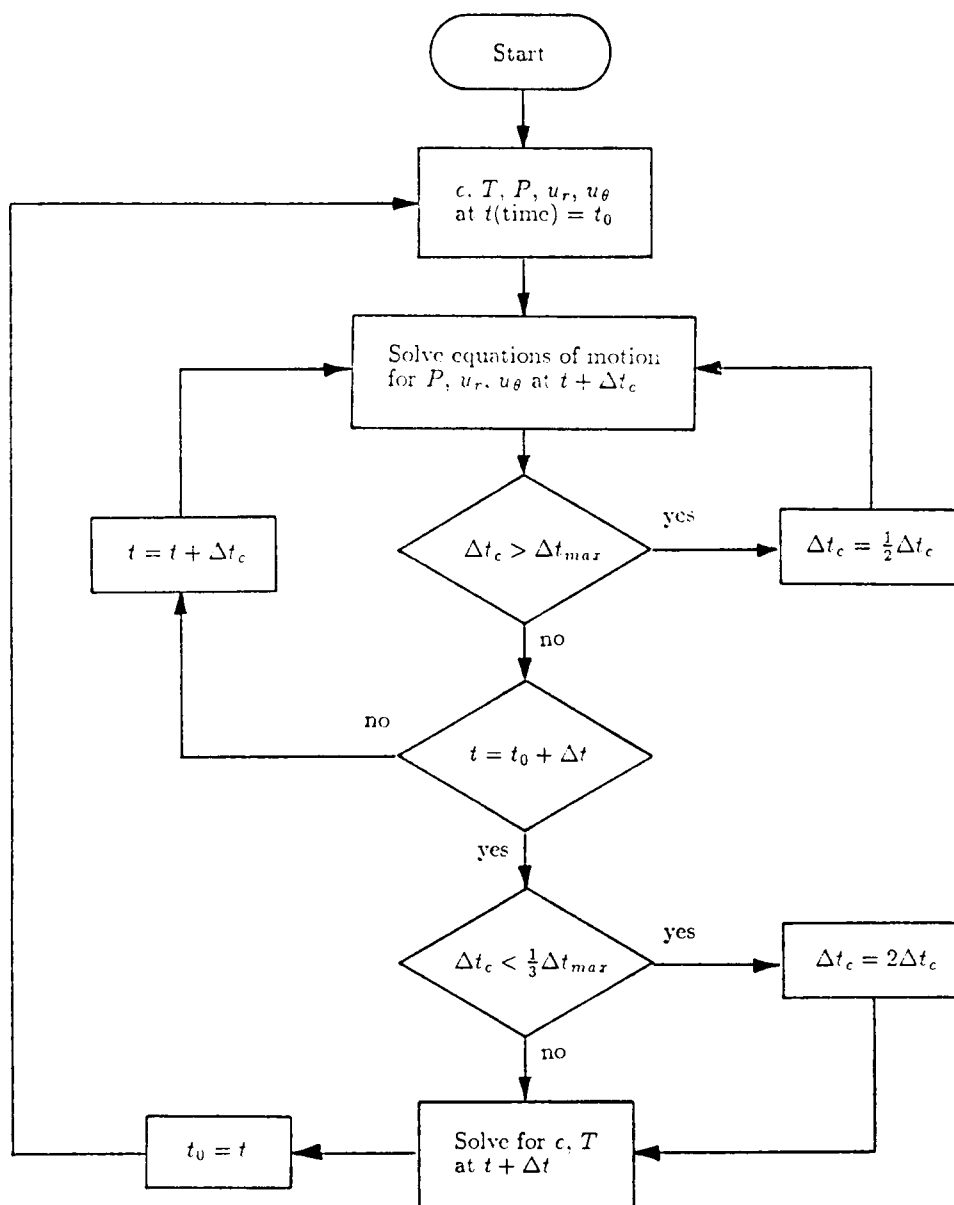


Figure 11. Calculation Cycle for Solution of Energy and Momentum Equations.

CHAPTER III

FORMULATION OF THE LIQUID-VAPOR INTERFACE MODEL

Physics of Solid-Liquid-Vapor Systems

Determination of liquid-vapor interface shapes is a class of problems which has received a great deal of study. However, with the exception of some relatively simple geometries, no straightforward method of solving for interface shapes is available. Surface tension arises because molecules at the surface of a liquid are not attracted equally from all sides as are those in the bulk liquid. Thus, these molecules have some excess energy compared to molecules in the bulk liquid. The unequal attraction experienced by the surface molecules results in a force acting along the liquid surface. This force can be represented as a uniform tension acting on a hypothetical membrane stretched over the surface and is referred to as surface tension, σ . The surface tension also represents the free energy per unit area required to maintain the interface. The relationship of the surface tensions between the liquid and vapor, σ_{lv} , the solid and vapor, σ_{sv} , and the solid and liquid, σ_{sl} , is expressed by the equation

$$\sigma_{lv} \cos \alpha = \sigma_{sv} - \sigma_{sl},$$

where α is the angle of contact between the solid and liquid. This relationship, known as Young's equation, is usually represented as a force balance as shown in Figure 12. However, it is questionable if it can be justified on that basis since the force normal to the solid surface is not balanced. Alternately, Young's equation can be derived based on thermodynamic considerations [14].

Although the surface tension and contact angle are manifestations of microscopic forces, together they have been found to provide an adequate representation of the macroscopic behavior of capillary systems. The main disadvantage of

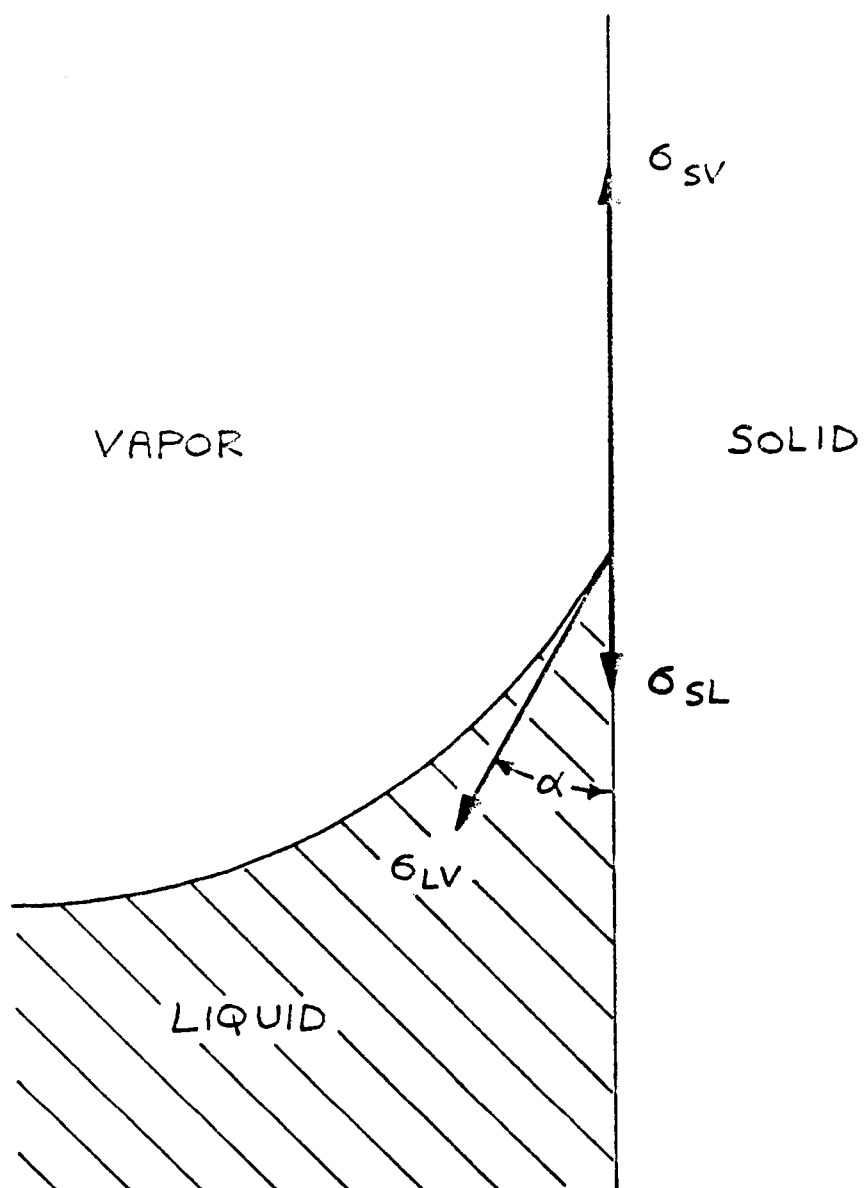


Figure 12. Young's Equation-Contact Angle.

the surface tension-contact angle representation is that the contact angle can be strongly influenced by the condition of the surface and is subject to hysteresis when the liquid advances or recedes, thus causing some uncertainty in calculations.

There are two basic approaches that can be used to calculate interface shapes. The first involves minimizing the free energy, F , of the system, which for an isothermal capillary system of mass, m , is the sum of the surface energy and potential energy, and can be expressed as

$$F = \int_{A_c} \sigma dA + \int_V \rho gh dV,$$

where A_c is the capillary area, V is the total system volume, and h is the elevation relative to a fixed reference. The equation for the minimum free energy can be determined by applying the calculus of variations with the constraint that the liquid volume is constant. This method has been applied successfully to determine equilibrium interface shapes in axisymmetric containers [15].

A second method that can be used to calculate interface shapes involves balancing forces on the interface. Consider a small surface area dA of the liquid-vapor interface, as shown in Figure 13. Element dA has maximum and minimum radii of curvature R_1 and R_2 with origins along the normal to dA . Since they represent principle curvatures, the planes of R_1 and R_2 are perpendicular to each other. The length L_1 of dA in the plane of R_1 is approximated by $R_1 \Delta\theta_1$, where $\Delta\theta_1$ is assumed to be very small. Similarly, the length L_2 of dA in the plane of R_2 is $R_2 \Delta\theta_2$. In order for forces directed along the normal to be balanced, the normal component of the surface tension forces acting on the edges of dA must equal the pressure force on dA . The equation expressing the force balance is

$$(P_1 - P_2)L_1L_2 = 2L_1\sigma_{lv} \sin \frac{\Delta\theta_2}{2} + 2L_2\sigma_{lv} \sin \frac{\Delta\theta_1}{2}.$$

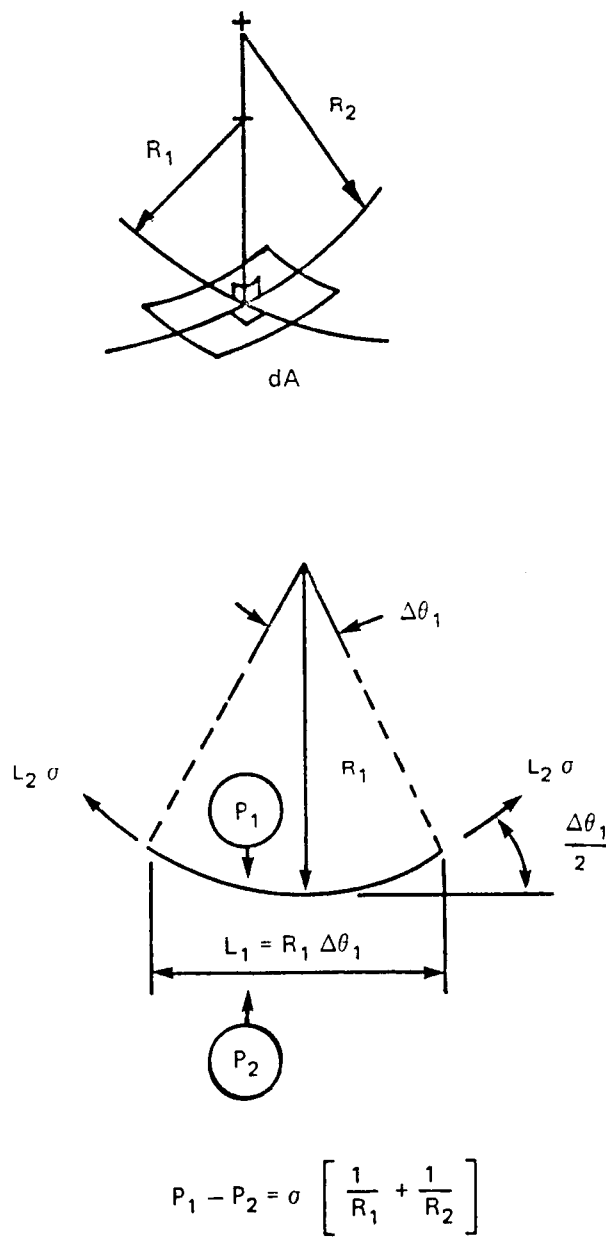


Figure 13. Surface Element for Derivation of Laplace Equation.

Substituting for L_1 and L_2 in terms of R and θ , and assuming that $\sin \Delta\theta \approx \Delta\theta$, the above equation becomes

$$(P_1 - P_2)(R_1\Delta\theta_1)(R_2\Delta\theta_2) = 2(R_1\Delta\theta_1)\sigma_{lv}\frac{\Delta\theta_2}{2} + 2(R_2\Delta\theta_2)\sigma_{lv}\frac{\Delta\theta_1}{2},$$

which reduces to

$$P_1 - P_2 = \sigma_{lv} \left[\frac{1}{R_1} + \frac{1}{R_2} \right]. \quad (45)$$

Equation (45) is called the Laplace equation and is the classical expression for equilibrium of a liquid-vapor interface. It should be noted that the Laplace equation can also be derived from minimum energy considerations [16]. Both the minimum energy method and the force balance method for finding interface shapes give the same result, so the choice of method depends on the particular problem being considered. Most references indicate that the minimum energy formulation is more straightforward for most situations, with the exception of a few simple cases. However, the number of cases for which a closed form solution can be obtained is very limited.

Determination of Interface Shape for an Axisymmetric Container

Fortunately, for an axisymmetric case a vertical force balance can be used to find the interface shape [17]. Consider an element of the interface with length dL , as shown in Figure 14. This element forms an annular ring about the axis of symmetry. The pressure difference across the interface is $P_v - P_l$, where P_v and P_l are the vapor and liquid pressures. P_l can be expressed in terms of the liquid pressure at the origin, P_{lo} , and the hydrostatic head, as follows:

$$P_v - P_l = P_v - P_{lo} + \rho g z.$$

The projected area that the pressure difference acts over is $2\pi r \Delta r$. Therefore, the pressure force acting in the $-z$ direction is

$$(P_v - P_{lo} + \rho g z)2\pi r \Delta r.$$

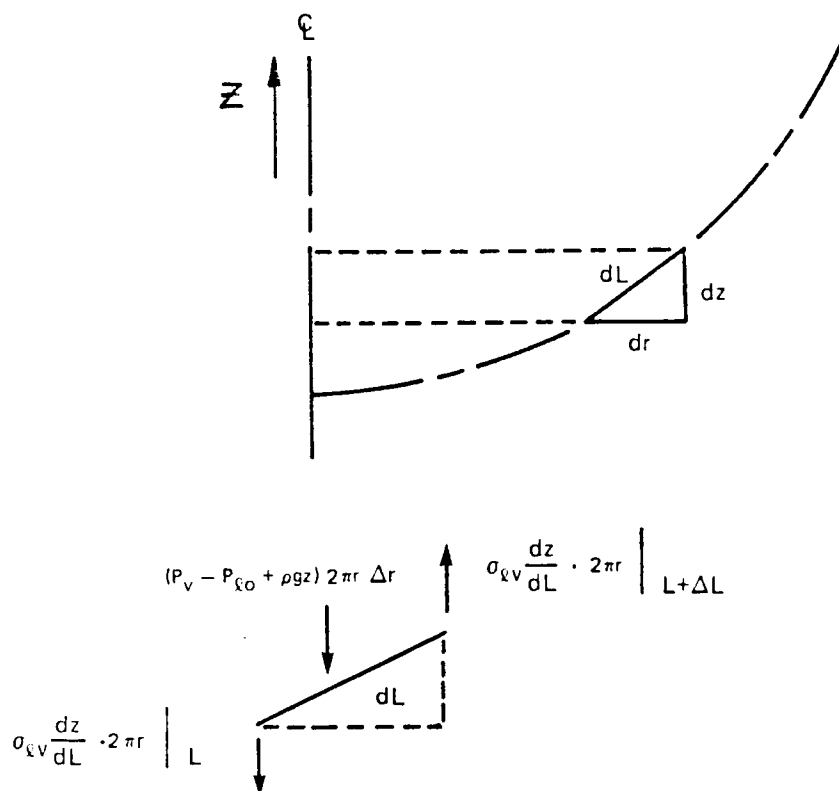


Figure 14. Vertical Force Balance for an Axisymmetric Interface.

Surface tension forces act along the edges of the element at L and $L + \Delta L$. The surface tension force at each edge is given by $\sigma_{lv}(2\pi r)$, and the vertical component is

$$\sigma_{lv}(2\pi r) \frac{\Delta z}{\Delta L}.$$

The expression for the force balance is therefore

$$(P_v - P_{lo} + \rho g z) 2\pi r \Delta r = \sigma_{lv}(2\pi r) \frac{\Delta z}{\Delta L} \Big|_{L+\Delta L} - \sigma_{lv}(2\pi r) \frac{\Delta z}{\Delta L} \Big|_L,$$

which can be rewritten

$$(P_v - P_{lo} + \rho g z) r \frac{\Delta r}{\Delta L} = \frac{\sigma_{lv} r \frac{\Delta z}{\Delta L} \Big|_{L+\Delta L} - \sigma_{lv} r \frac{\Delta z}{\Delta L} \Big|_L}{\Delta L}.$$

Taking the limit as $\Delta L \rightarrow 0$, the resulting differential equation is

$$(P_v - P_{lo} + \rho g z) r \frac{dr}{dL} = \frac{d}{dL} \left[\sigma_{lv} r \frac{dz}{dL} \right].$$

Assuming the surface tension is constant, the righthand side of the above equation can be differentiated to give

$$(P_v - P_{lo} + \rho g z) r \frac{dr}{dL} = \sigma_{lv} \left[\frac{dr}{dL} \frac{dz}{dL} + r \frac{d^2 z}{dL^2} \right],$$

which can be rearranged yielding

$$\frac{d^2 z}{dL^2} = \left[\frac{P_v - P_{lo}}{\sigma_{lv}} + \frac{\rho g z}{\sigma_{lv}} - \frac{1}{r} \frac{dz}{dL} \right] \frac{dr}{dL}. \quad (46)$$

At this point, two simplifications can be introduced. Using Eq. (45), the pressure

difference at the origin can be expressed in terms of the radius of curvature at the origin, where $R_1 = R_2 = R_o$, giving

$$P_v - P_{lo} = \frac{2\sigma_{lv}}{R_o},$$

or

$$\frac{P_v - P_{lo}}{\sigma_{lv}} = \frac{2}{R_o}. \quad (47)$$

The relationship between dr/dL and dz/dL is

$$\left[\frac{dr}{dL}\right]^2 + \left[\frac{dz}{dL}\right]^2 = 1,$$

or

$$\frac{dr}{dL} = \sqrt{1 - \left[\frac{dz}{dL}\right]^2}. \quad (48)$$

Substituting Eqs. (47) and (48) into Eq. (46) yields

$$\frac{d^2z}{dL^2} = \left[\frac{2}{R_o} + \frac{\rho g z}{\sigma_{lv}} - \frac{1}{r} \frac{dz}{dL}\right] \sqrt{1 - \left[\frac{dz}{dL}\right]^2}. \quad (49)$$

Eqs. (48) and (49) can be solved by the Runge-Kutta method to yield interface shapes for given values of σ_{lv} , ρ , and g . The solution is iterative, with values of R_o being guessed to provide the required vapor volume. Eqs. (48) and (49) are valid as long as $dz/dL < 1$. At the point where $dz/dL = 1$, the direction of curvature changes sign and the correct form of the equations becomes

$$\frac{dr}{dL} = -\sqrt{1 - \left[\frac{dz}{dL}\right]^2}, \quad (50)$$

$$\frac{d^2z}{dL^2} = -\left[\frac{2}{R_o} + \frac{\rho g z}{\sigma_{lv}} - \frac{1}{r} \frac{dz}{dL}\right] \sqrt{1 - \left[\frac{dz}{dL}\right]^2}. \quad (51)$$

The positive value of the square root is assumed in Eqs. (50) and (51).

The Runge-Kutta approximation gives the interface shape as a series of r and z values, (r_0, z_0) , (r_1, z_1) , $\dots$, (r_n, z_n) . The end condition for the calculation

is given by the requirement for the liquid-vapor interface to meet the container wall at the correct contact angle, α . For a spherical container, as shown in Figure 15, the angle of a line tangent to the container wall measured from the horizontal, ϕ , is given by

$$\phi = \sin^{-1} \frac{r}{R_c},$$

where R_c is the radius of the container wall. The angle of a line tangent to the liquid-vapor interface measured from the horizontal, β , is given by

$$\beta = \sin^{-1} \frac{\Delta z}{\Delta L}.$$

The contact angle is the difference between ϕ and β . In the upper hemisphere $\alpha = \beta - \phi$, while in the lower hemisphere $\alpha = \phi - \beta$. A given interface shape may meet the container wall at the correct angle either (a) in the lower hemisphere only, (b) in the upper hemisphere only, (c) in both the upper and lower hemispheres, or (d) not at all, depending on whether or not the vapor bubble will "fit" inside the container. The volume of vapor up to the point where the interface contacts the wall, designated V_1 , is found by numerical integration using the trapezoidal rule, as follows:

$$V_1 = \sum_{i=0}^{n-1} \pi \left[\frac{r_{i+1}^2 + r_i^2}{2} \right] (z_{i+1} - z_i).$$

The vertical distance along the container axis from the origin to the point where the interface contacts the wall, z_c , is given by

$$z_c = \pm \sqrt{R_c^2 - r_n^2}.$$

If the point of contact is in the upper hemisphere, z_c is positive. If the point of contact is in the lower hemisphere, z_c is negative. The container volume above the point of contact, V_2 , is

$$V_2 = \pi \left[\frac{2}{3} R_c^3 - R_c^2 z_c + \frac{1}{3} z_c^3 \right].$$

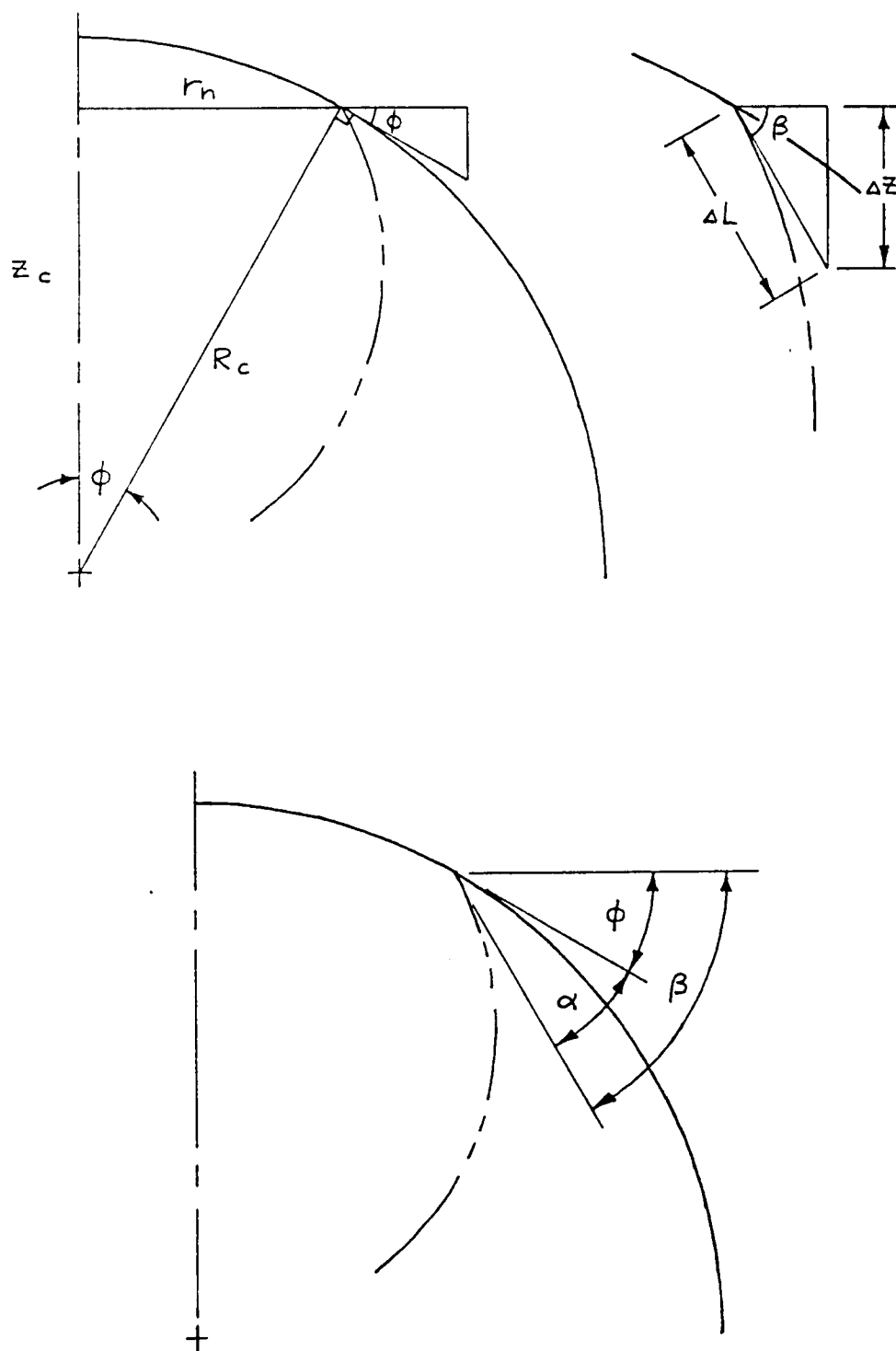


Figure 15. Determination of Contact Angle in a Spherical Container.

The total vapor volume is the sum of the volumes above and below the contact point, $V_1 + V_2$. Values of the vertical distance z are scaled so the scaled value, z' , is zero at the container origin. The relationship between z' and z is

$$z'_i = z_c - z_n + z_i.$$

Some typical examples of liquid-vapor interface shapes calculated by the model are shown in Figure 16.

Application to the Heat Transfer Model

The liquid-vapor interface model is used in the heat transfer model to specify the distribution of liquid in the container. The model is also used to calculate mass sources (freezing case), or mass sinks (melting case), for grid volumes along the liquid-vapor interface. In the heat transfer model, the solid boundary for the liquid-vapor interface calculation is formed by the container wall, frozen salt, or both. The interior boundary of the solid material is modeled as a series of concentric spherical shell segments. Each shell contains salt only in the volume where $\theta > \theta_i$, where θ_i is measured from the container axis as shown in Figure 17. The solid boundary is thus defined by a series of r and θ values (r_0, θ_0) , (r_1, θ_1) , $\dots$, (r_n, θ_n) . The contact angle is always assumed to be zero for liquid lithium hydride, due to the tendency of liquid LiH to wet (and even crawl out of) containers [22].

The proper vapor volume at a given time can be found by subtracting the volume occupied by solid and liquid salt from the total container volume. Once an acceptable interface shape has been calculated, the interface shape is mapped onto the finite difference grid by locating the points where the interface crosses r and θ grid lines, as shown in Figure 18. With this information, the required liquid volume in the grid volumes the interface passes through can be estimated.

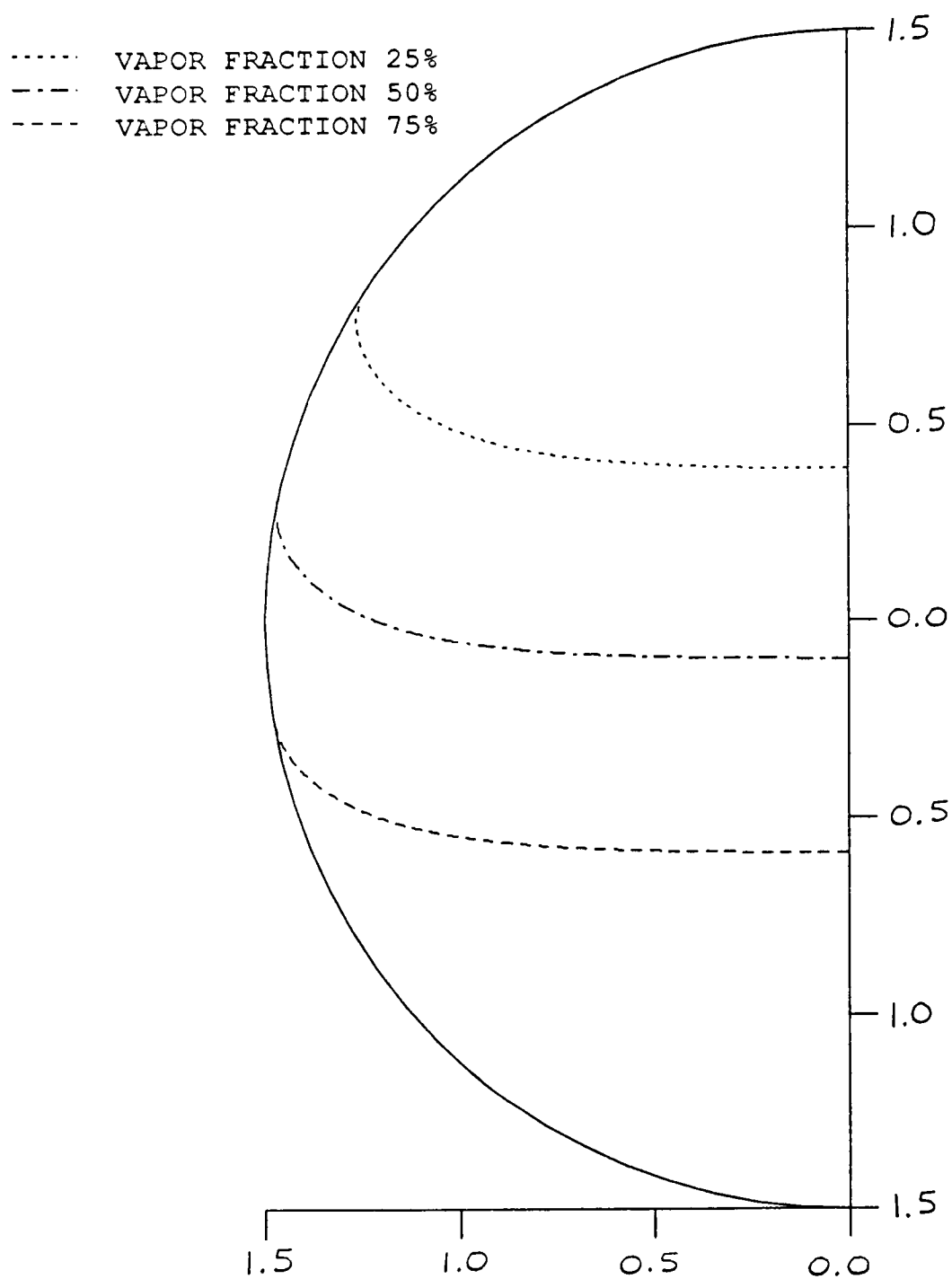


Figure 16. Predicted Liquid-Vapor Interface Shapes for LiH Under Normal Gravity, $\alpha = 0^\circ$.

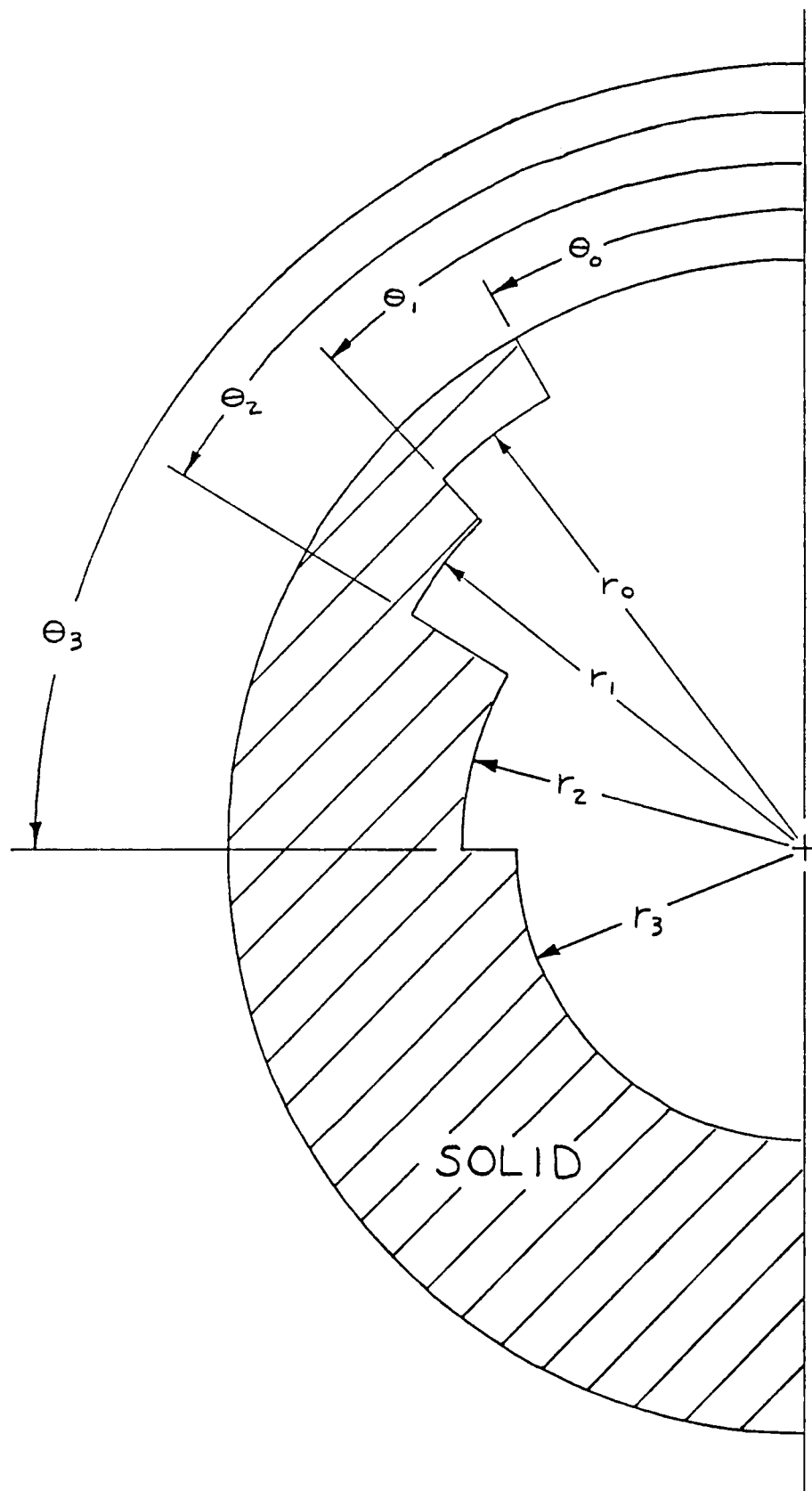


Figure 17. Solid Boundary for Liquid-Vapor Interface Calculation.

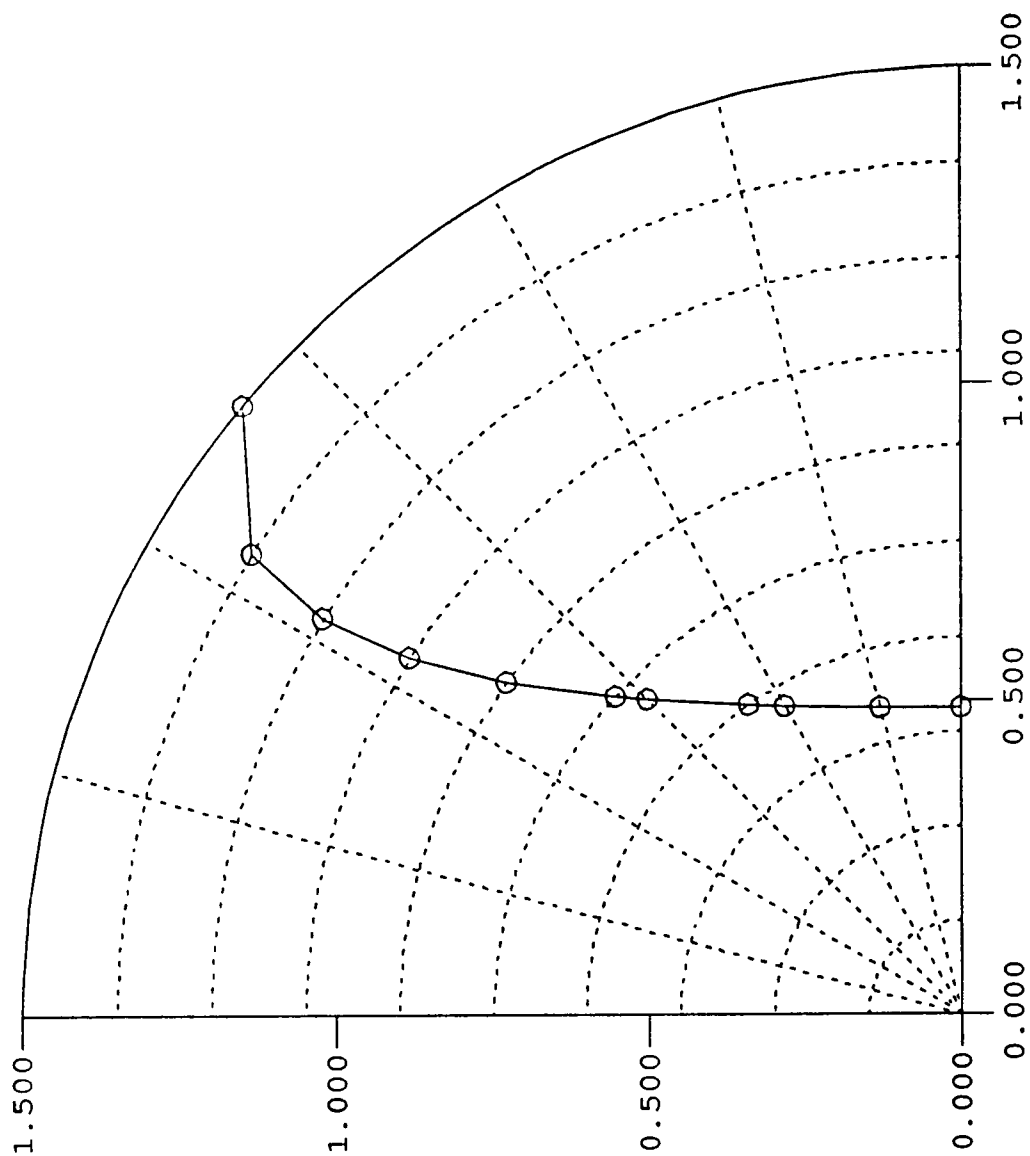


Figure 18. Liquid-Vapor Interface Shape Mapped onto Finite Difference Grid.

Mass sources or sinks are determined by expanding or contracting the vapor volume slightly, which causes a small displacement of the liquid-vapor interface. The change in liquid volume in a given grid volume due to shifting the interface from the original position to the new position, $\Delta V(i, j)$, is given by

$$\Delta V(i, j) = V'_{liq} - \frac{\rho(i, j)}{\rho_l} V(i, j),$$

where $V'_{liq}(i, j)$ is the liquid volume at the new interface location. The total volume contained between the original and new interface positions, ΔV_{total} , is the sum of $\Delta V(i, j)$ for all cells. Mass sources or sinks are required to balance the sources or sinks due to melting or freezing, given by Eq. (23). The total mass source/sink required in time step Δt , ΔM_{reqd} , is the sum of $\Delta M(i, j)$ for all of the melting/freezing cells. The mass source/sink for a given volume on the liquid-vapor interface in time step Δt is given by

$$\Delta M(i, j) = -\Delta M_{reqd} \frac{\Delta V(i, j)}{\Delta V_{total}}.$$

When the volume between the original and displaced interface positions is completely filled with liquid (melting case), or completely empty (freezing case), a new displaced interface shape is calculated.

CHAPTER IV

EXPERIMENTAL EVALUATION OF ENCAPSULATED LiH HEAT TRANSFER

In order to characterize the thermal behavior of encapsulated LiH and provide data for validation of the heat transfer model, a series of experiments were carried out in which spherical containers filled with LiH were rapidly heated above the LiH melting point in a 60 kW induction furnace. The experimental setup is shown in Figure 19. A 3 in (76.2 mm) diameter spherical capsule containing enough lithium hydride to be 90 percent full when the LiH was completely melted was placed inside the graphite susceptor of the furnace. The container was supported by a stand constructed from stainless steel wire. A 0.25 in (6.4 mm) diameter tube welded into the top of the container passed through the top of the furnace, providing access for thermocouples and a vent for any hydrogen evolved during heating. A total of 21 Type K thermocouples were attached at various locations inside the container and on its outside surface. One thermocouple was left hanging inside the furnace to provide a control temperature, and an additional thermocouple was located inside the access tube as a safety measure to detect the presence of liquid LiH.

The thermocouples used were ungrounded and were encased in 0.020 in (0.5 mm) diameter stainless steel sheaths. Temperature data was recorded by an IBM PC-XT computer. The necessary expansion boards were installed in the computer to amplify the thermocouple signals and provide analog to digital conversion. Thermocouples were suspended inside the container by means of 0.020 in (0.5 mm) diameter stainless steel wires which were attached to the container walls. The container construction and wire installation are shown in

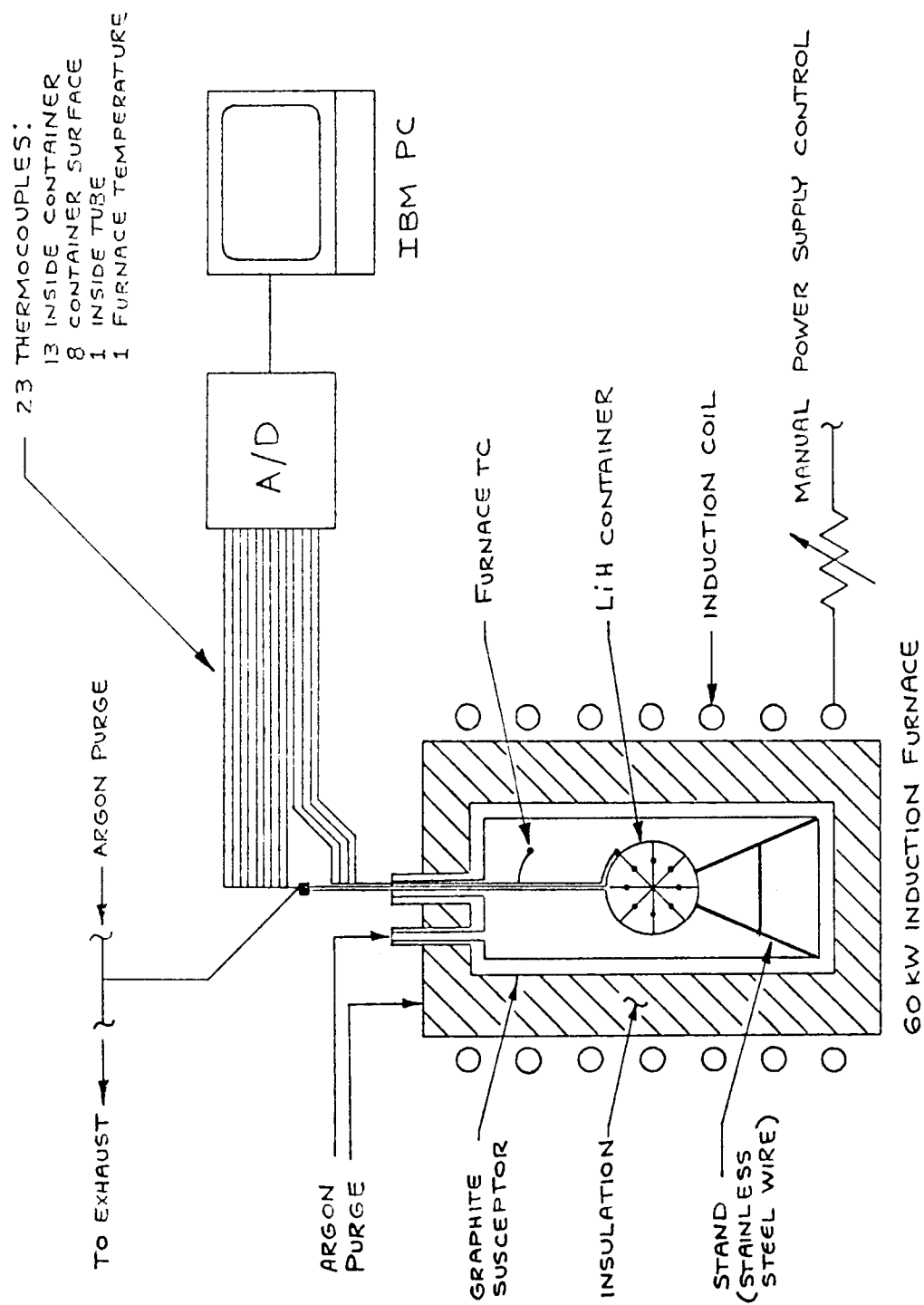


Figure 19. Experimental Setup for Thermal Characterization Test.

Figure 20. Probably the greatest uncertainty as to the reliability of the temperatures measured inside the container is due to the conduction effect of the support wires. Conduction along the wires is not believed to be great enough to cause a significant error as long as the wire and the thermocouple junction have good thermal contact with the salt, since the thermal diffusivity of stainless steel is reasonably low—about $0.190 \text{ ft}^2/\text{hr}$ ($4.90 \times 10^{-6} \text{ m}^2/\text{s}$) for stainless steel vs. about $0.038 \text{ ft}^2/\text{hr}$ ($9.80 \times 10^{-7} \text{ m}^2/\text{s}$) for solid LiH—and the wires are thin. In any case, the uncertainty caused by the wires is unavoidable, since no better way to keep the thermocouple junctions in the proper locations could be devised.

Thirteen thermocouples were installed inside the container, while eight thermocouples were attached to the outside of the shell. The locations and numbering scheme used for the thermocouples is shown in Figure 21. Thermocouples were placed in corresponding locations on opposite sides of the container axis in order to determine if the thermal behavior was reasonably axisymmetric.

A total of three thermal characterization tests were carried out. The first test was a shakedown to determine the feasibility of the experiment, and did not provide any useful data. The second and third tests were both successful, providing repeatable thermal data over several heating cycles. In both tests, several of the thermocouples inside the container appeared to read incorrectly; however, enough of the readings were usable to provide an adequate characterization of the heat transfer performance. Other than obvious malfunctions such as open circuit readings, the main way inaccurate thermocouple readings were detected was by comparison with the shell thermocouples. The suspected thermocouples would usually read higher than any of the shell thermocouples during the heatup and cooler than any of the shell thermocouples during the cooldown. A possible explanation for this behavior is liquid LiH getting inside the thermocouple

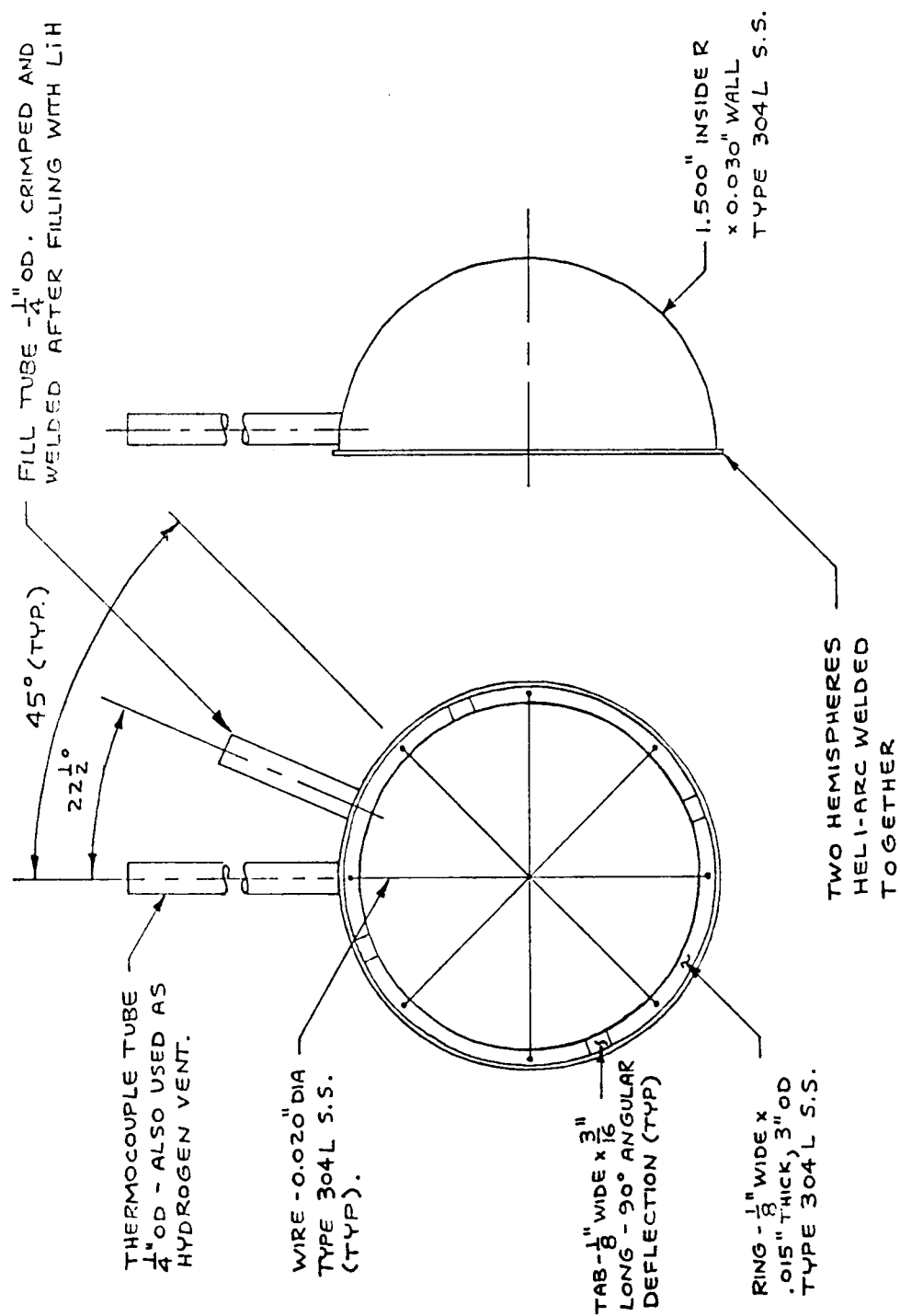
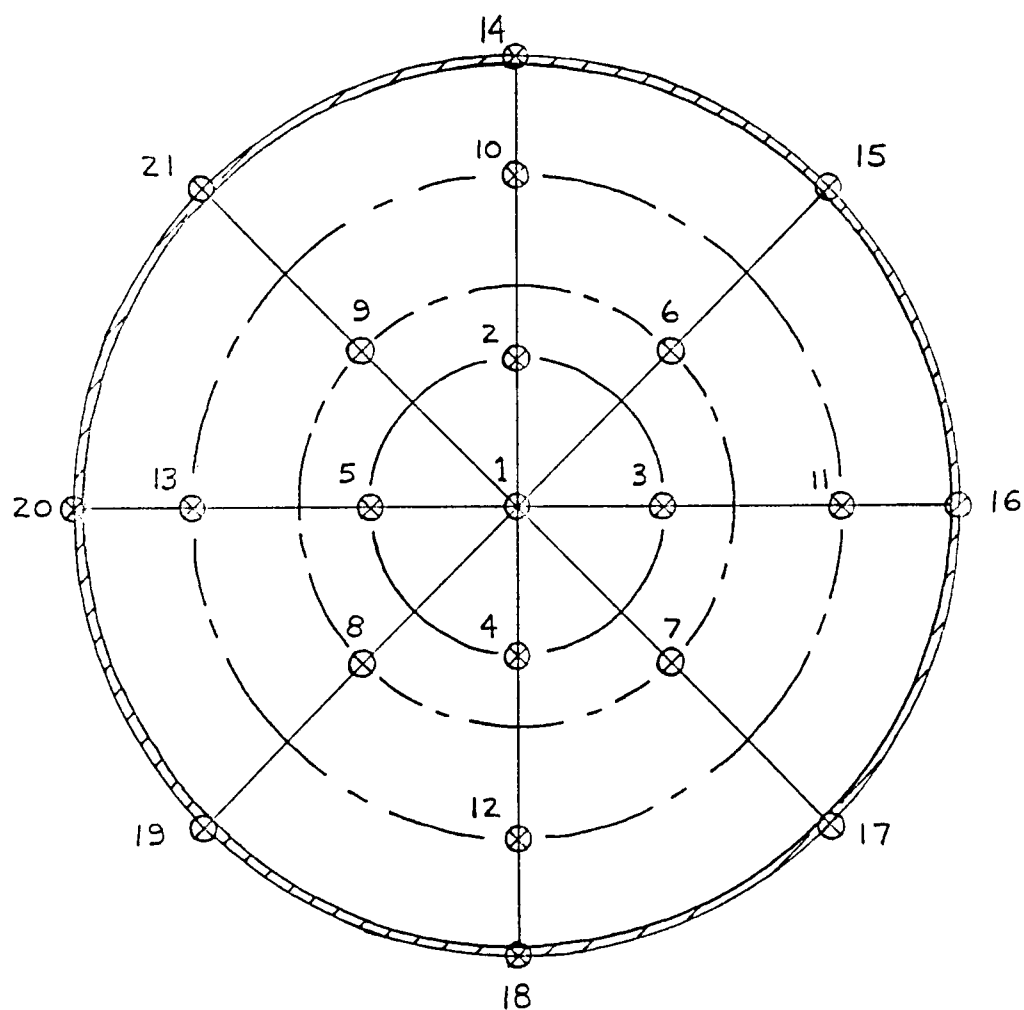


Figure 20. Container Construction.



RADIUS	THERMOCOUPLE NUMBERS
0.000"	1
0.500"	2, 3, 4, 5
0.750"	6, 7, 8, 9
1.125"	10, 11, 12, 13
1.530"	14, 15, 16, 17, 18, 19, 20, 21

Figure 21. Thermocouple Locations.

sheaths, which would result in the thermocouple wires being shorted together up to wherever the LiH reached and thus cause the temperature to be measured at that point rather than at the normal junction.

In order to provide repeatable data, an effort was made to operate the furnace so the heating and cooling rates were as constant as possible from cycle to cycle. The container was initially heated slowly above the melt point to melt the LiH, which was loaded into the capsules in powdered form. A slow initial heatup was employed to allow outgassing of hydrogen as required to establish an equilibrium mixture of Li and LiH. Lithium hydride tends to dissociate into lithium and hydrogen gas as it is heated (a common feature of metal hydrides), and an overpressure of hydrogen is required to prevent dissociation. Roughly 98 percent of a liquid Li-LiH mixture can be maintained as LiH by a hydrogen partial pressure of less than 1 atm, so significant outgassing will occur if the initial mixture contains more than about 98 percent LiH. After the initial slow heatup, the container was allowed to cool to about 700°F (644 K). At that point, full power was applied to the furnace and maintained until the furnace temperature reached about 1550°F (1117 K). The furnace power was then reduced to maintain the furnace temperature at around 1550°F (1117 K) until all of the interior thermocouples read well above the melting temperature. The furnace was then turned off and the container was once again allowed to cool to around 700°F (644 K), at which point the process was repeated. A typical heating cycle lasted about 1000 seconds, while the total cycle time including cooldown was about 1.5 hours long.

The second test consisted of 7 cycles, including the initial heat from powder, while the third test consisted of 6 cycles. Both tests had to be terminated when small hydrogen leaks occurred in the containers. The excellent repeatability of the

temperature data is demonstrated in Figure 22, which shows average, minimum, and maximum temperatures for the thermocouple located at the container origin for three cycles during the third test. The thermal behavior observed during the second and third tests was very similar, despite a difference in the heating and cooling rates caused by improving the insulation in the furnace prior to the third test. The test results will be discussed in detail in the Chapter V.

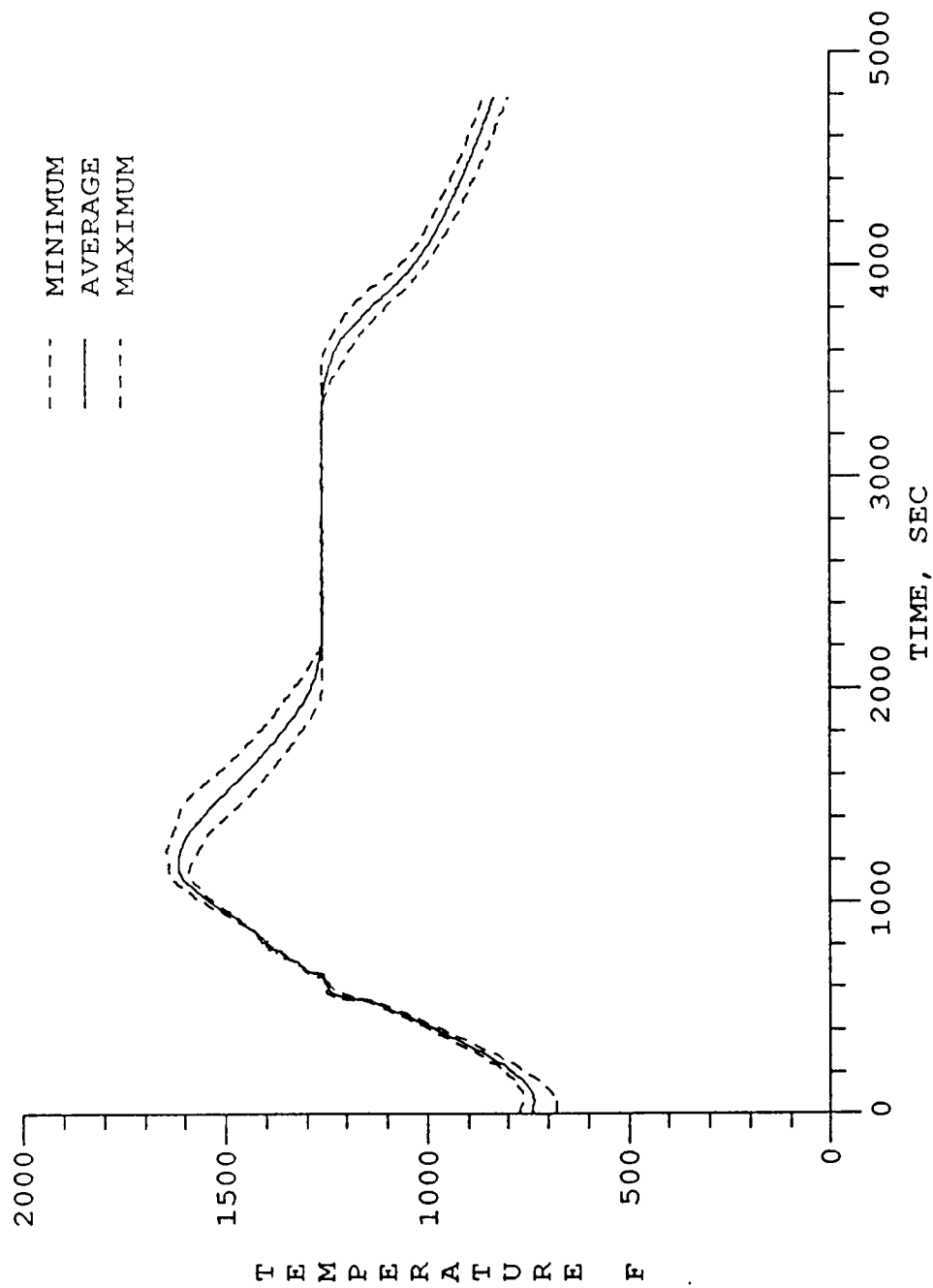


Figure 22. Thermocouple No. 1 Measured Temperature Data (Average for Three Cycles).

CHAPTER V

DISCUSSION OF RESULTS

Numerical Study of the Effect of Radiation Across the Void

It was initially thought that radiation across the void might be a significant heat transfer mechanism during the heating cycle. In an effort to determine the approximate effect of radiation, a simplified version of the heat transfer model was developed in which radiation across the void was calculated. In this version of the model, the density of the salt was assumed to be the same for the solid and liquid phases, and the void shape predicted by the freezing model for a completely frozen situation was assumed. The void size and shape were assumed to be constant, and the effect of natural convection in the liquid was neglected. For an axisymmetric, concave void shape, view factors for each volume bordering the void can be developed from the view factor for two circular disks with a common normal through their centers, given in Ref. [18]. Once the view factors are known, the equations for radiation heat transfer in an enclosure with diffuse-gray surfaces can be used to solve for the radiation across the void [19]. It was assumed that the gas in the void was transparent to radiation, and an emissivity of 0.9 was assumed for the salt and shell material.

For the test case, it was assumed that a three-inch diameter stainless steel container with 0.030 *in* (0.76 *mm*) thick walls was filled with enough LiH to be 90 percent full at the normal liquid density. The initial temperature of the container was 800°F (700 *K*). The container was surrounded by a liquid metal heat transfer medium, which at time zero underwent a step change in temperature from 800°F (700 *K*) to 1520°F (1100 *K*). A uniform convection coefficient of 3000 *Btu/hr · ft² · °F* (17 *kW/m² · K*) was assumed, based on an empirical

correlation given in Ref. [20]. The local convection coefficient for a single sphere in crossflow is predicted to vary strongly, with a maximum at the forward stagnation point and a minimum at the rear stagnation point [21]. However, this effect would be much less pronounced in a packed bed, and in any case, the convection coefficient is so large that the situation approximates a constant temperature boundary condition.

Calculations for the above case were carried out both with and without radiation included. It was found that at any instant the maximum heat transfer due to radiation was less than one percent of the total heat transfer. Therefore, it was determined that radiation across the void can be neglected, and no radiation calculations are included in the results presented.

Physical Properties of LiH Used in the Model

There is much uncertainty in the values of the physical properties of lithium hydride, because LiH is a difficult material to work with (especially in liquid form), and the properties vary depending on the equilibrium concentration of Li and LiH in the mixture, as there must always be a certain amount of Li present to maintain a given partial pressure of hydrogen over the mixture. In addition, the thermal conductivity of solid LiH is dependent on how the material is prepared, i.e., its crystalline structure. Several tabulations of LiH properties exist [22 – 24]. The property values used in the numerical heat transfer model are given in Table I, along with the sources for the property values.

The value of 1260°F (956 K) for the fusion temperature was determined from the temperature data obtained during the experiments. This value is $5 - 10^{\circ}\text{F}$ ($3 - 6\text{ K}$) lower than the values given in the literature [22, 24]. As discussed in Chapter II, constant values for the solid and liquid density were used in the

Table I. LiH Property Values Used in the Heat Transfer Model.

Property	Symbol	Value (English Units)	Value (SI Units)	Source
Fusion Temperature	T_{mp}	1260° <i>F</i>	956 <i>K</i>	See Text
Heat of Fusion	h_{st}	1223.7 <i>Btu/lb</i>	2.846 <i>MJ/kg</i>	[23]
Solid Density	ρ_s	43.1 <i>lb/ft</i> ³	690 <i>kg/m</i> ³	[22]
Liquid Density	ρ_l	34.3 <i>lb/ft</i> ³	550 <i>kg/m</i> ³	[22]
Liquid Thermal Expansion Coeff.	$\Delta\rho/\Delta T$	-2.77×10^{-3} <i>lb/ft</i> ³ · ° <i>F</i>	-8×10^{-2} <i>kg/m</i> ³ · <i>K</i>	[22]
Solid Specific Heat	c_s	1.50 <i>Btu/lb</i> · ° <i>F</i>	6.28 <i>kJ/kg</i> · <i>K</i>	See Text
Liquid Specific Heat	c_l	1.76 <i>Btu/lb</i> · ° <i>F</i>	7.36 <i>kJ/kg</i> · <i>K</i>	[23]
Solid Thermal Conductivity	k_s	0.81 – 2.42 <i>Btu/hr</i> · <i>ft</i> · ° <i>F</i>	1.40 – 4.19 <i>W/m</i> · <i>K</i>	See Text
Liquid Thermal Conductivity	k_l	1.45 <i>Btu/hr</i> · <i>ft</i> · ° <i>F</i>	2.51 <i>W/m</i> · <i>K</i>	[22, 24]
Liquid Viscosity	μ	2.56×10^{-4} <i>lbm/s</i> · <i>ft</i>	3.8×10^{-4} <i>Pa</i> · <i>s</i>	[22]
Liquid-Vapor Surface Tension	σ_{lv}	0.015 <i>lbf/ft</i>	0.219 <i>N/m</i>	[25]

model, except for the liquid density in the body force term in the momentum equations. The solid and liquid densities are taken to be the values at the melting point.

The value used for the solid specific heat is an average value for the range from about $400^{\circ}F$ ($478\ K$) to the melting point, based on data given in Ref. [22]. Initial parametric studies in which temperature-dependent values of the solid specific heat and thermal conductivity were used in the heat transfer model showed that the results did not change much when average values were used for these properties rather than the temperature-dependent values. However, the solid specific heat increases with increasing temperature, and the starting temperature thus affects the average value. The value that was used in the computer model is probably too low, since the calculations usually started at a higher initial temperature. For an initial temperature of $700^{\circ}F$ ($644\ K$), the correct average specific heat would be about $1.7\ Btu/lb \cdot ^{\circ}F$ ($7.11\ kJ/kg \cdot K$). After comparing the model results with the experimental data, it appears that using the lower average value for the solid specific heat could be one reason why the heat transfer model predicted a higher melting rate than observed in the experiments. The author recommends that a temperature-dependent value for the solid specific heat be used in future calculations in order to avoid this difficulty.

The solid thermal conductivity is the property for which the correct value is most uncertain, since the thermal conductivity is strongly affected by the condition of the material. A wide range of values is reported in the literature, so for the present study the heat transfer model was run with a series of values for k_s and the values that agreed best with the experimental data during heating and cooling were adopted. A nominal value for k_s of $2.42\ Btu/hr \cdot ft \cdot ^{\circ}F$ ($4.19\ W/m \cdot K$) was chosen based on data given in Ref. [22]. This value is an average for the range

from about 400°F (478 K) to the melting point. Comparison of results from the computer model with the experimental data showed that the nominal value provided the best agreement during the cooling cycle. However, during the heatup, lower values for k_s were found to provide better agreement. For the averaged data from the second test, a value of $0.81\text{ Btu/hr} \cdot \text{ft} \cdot ^{\circ}\text{F}$ ($1.40\text{ W/m} \cdot \text{K}$), or one-third of the nominal value, provided the best agreement, while for the third test, a value of $1.21\text{ Btu/hr} \cdot \text{ft} \cdot ^{\circ}\text{F}$ ($2.80\text{ W/m} \cdot \text{K}$), or 50 percent of the nominal value, provided the best agreement. These values for k_s appear to be lower than most, but perhaps not all, of the values reported in the literature. Most of the data given in the literature is for temperatures lower than 950°F (783 K), which makes it difficult to make a comparison. The reported values for k_s are generally lower for material in crystalline form than for hot pressed material. Solid LiH is known to crack extensively on cooling due to differential thermal expansion. Extensive cracking has been noted in radiographs of the containers tested during the present study which were made after the material had been heated above the melting point and cooled to room temperature, and an acoustic emission test performed on an encapsulated LiH specimen during cooling indicated that cracking is initiated at about 1180°F (911 K) and continues at an approximately constant rate down to room temperature [26]. This behavior offers a possible explanation for the apparently lower thermal conductivity observed during heating. The material would be much more extensively cracked during heating, and the cracks would be expected to interfere with the flow of heat, causing the observed reduction in thermal conductivity.

Comparison of Model Results With Test Data

Comparisons of computer model results with the test data from the second and third thermal characterization tests were made during both the heating and

cooling portions of the thermal cycle. The averaged temperature data recorded by the thermocouples attached to the outside of the container was used as the boundary condition for the model, and the averaged temperature data measured by the thermocouples inside the container was compared with the temperatures predicted by the model for the corresponding locations.

Predicted thermal behavior and void formation during cooling and freezing.

Numerical calculations for the cooling part of the thermal cycle were started at 1600 seconds, with a uniform initial temperature imposed on the shell and the liquid LiH. The measured data showed that the temperature of the shell and the liquid LiH became very uniform during the period between the completion of melting and the initiation of freezing, so it was not considered worthwhile to continue the calculations through this period. A 20 x 24 finite difference grid was used for the calculations. The r -axis was divided into 20 equal increments, while the polar angle was divided into 24 equal increments. Comparisons of temperatures predicted by the model with temperature data measured by thermocouples 7, 11, and 12 during the cooldown in the third test are shown in Figures 23 through 25. Thermocouples 7, 11, 12, and 13 were the only thermocouples that the model predicted would remain embedded in the solid salt when the capsule was completely frozen. Thermocouples 11 and 13 were located in corresponding positions on opposite sides of the container axis and gave similar readings. Calculations for the nominal value of k_s and for 50 percent of the nominal value are plotted for comparison. Both the measured temperature data and the numerical results were very similar for the second and third tests.

Comparison of numerical results with the experimental data showed that a lumped mass approximation for the liquid thermal behavior provided reasonable agreement with the data during cooling, presumably because the liquid was well

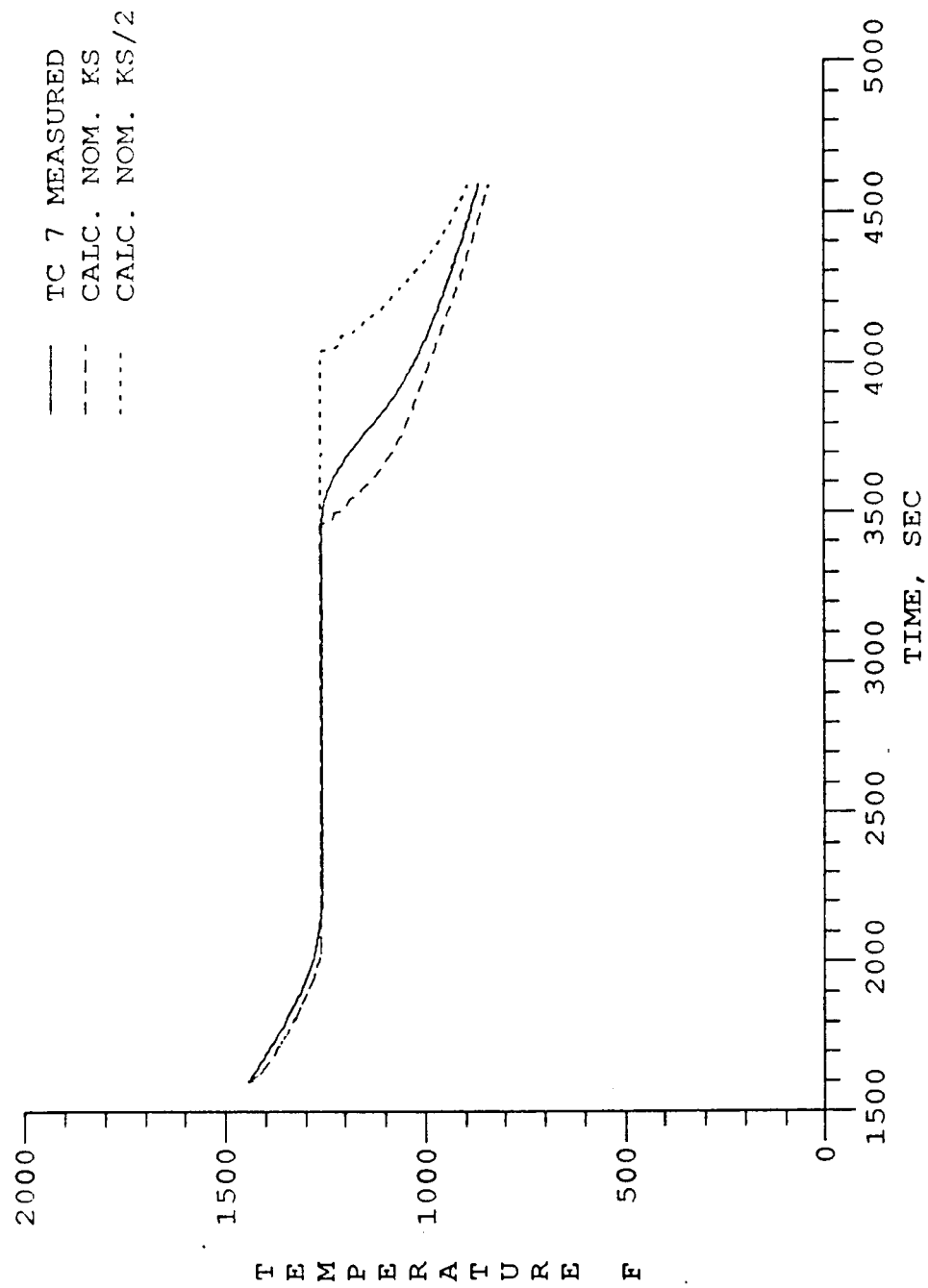


Figure 23. Thermocouple No. 7 Measured vs. Predicted Temperature During Cooling.

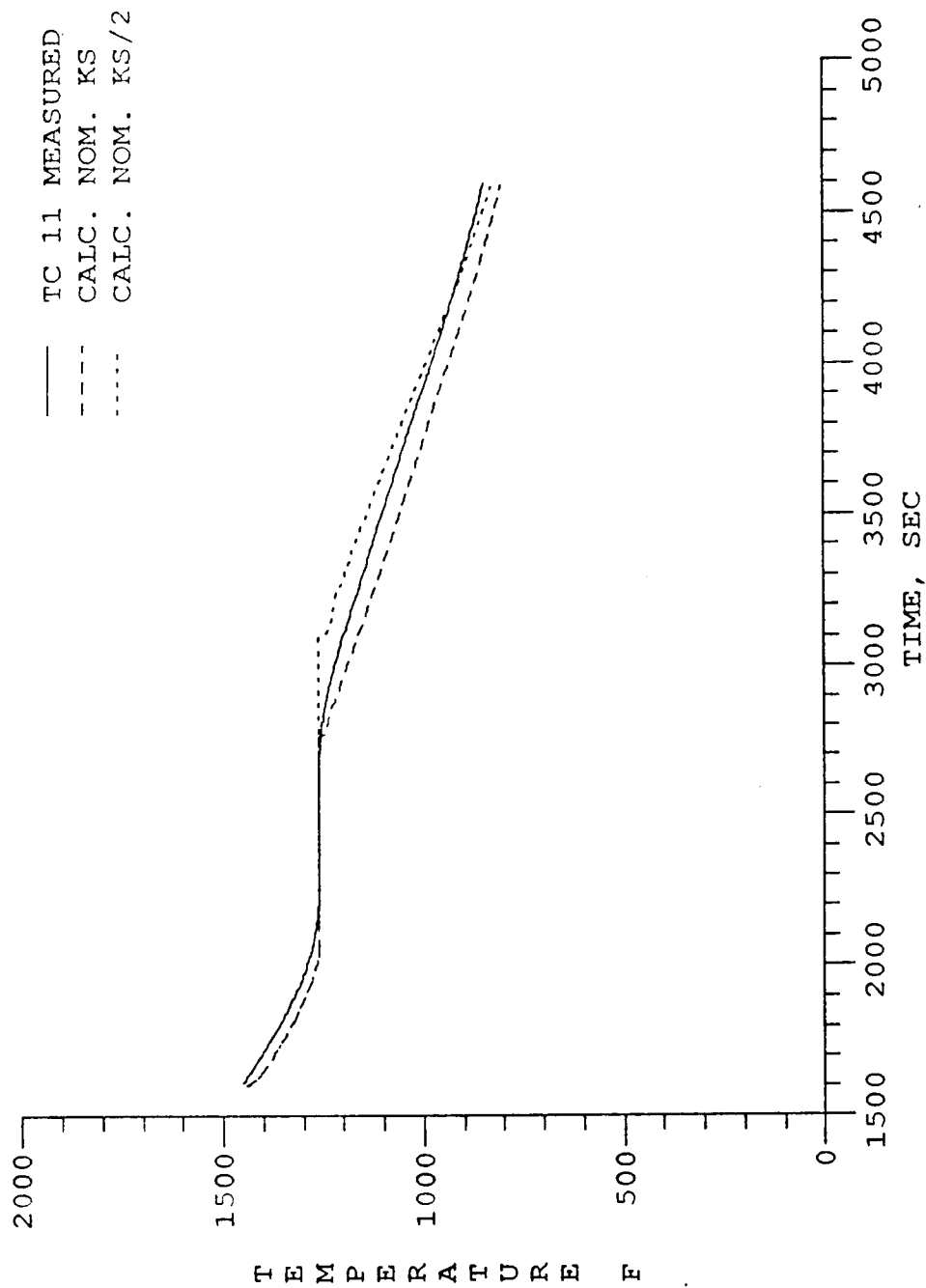


Figure 24. Thermocouple No. 11 Measured vs. Predicted Temperature During Cooling.

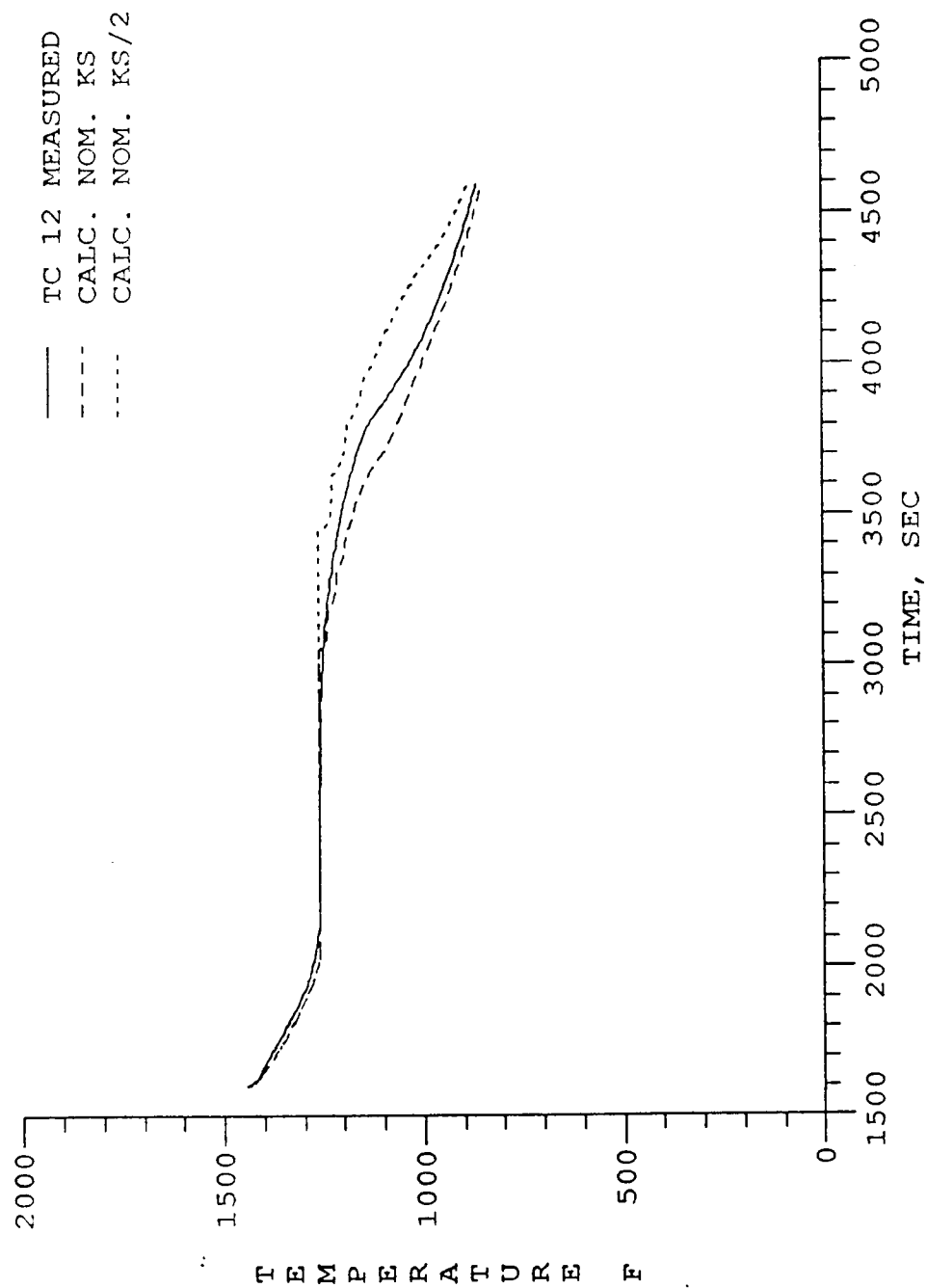
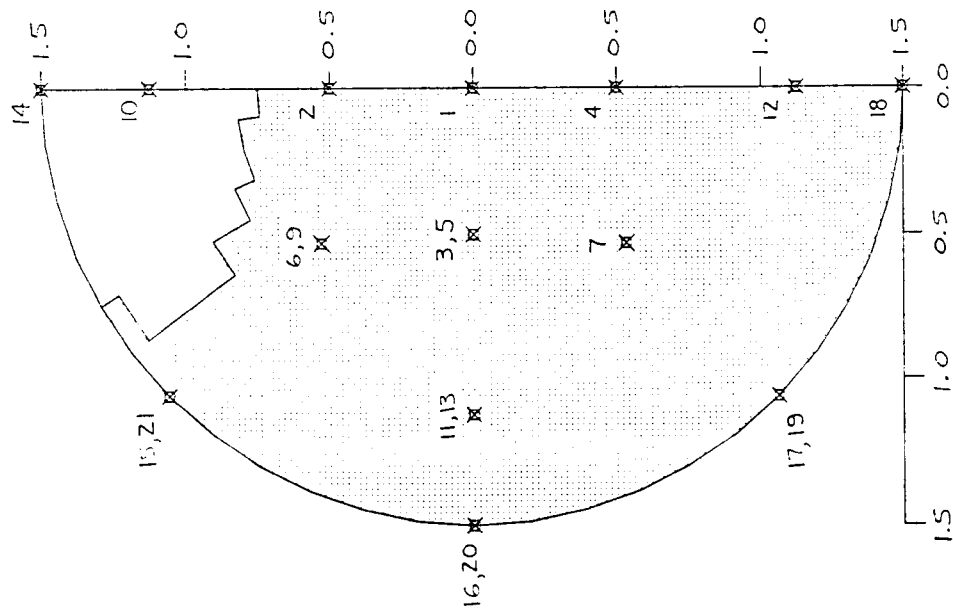


Figure 25. Thermocouple No. 12 Measured vs. Predicted Temperature During Cooling.

mixed by natural convection and the cooling rate was relatively slow. The lumped mass approximation was therefore adopted for the liquid to save computer time. The lumped mass approximation was implemented by finding the total energy contained in the liquid after each time step, and then assigning an average specific energy and temperature to all of the grid volumes containing liquid.

Figure 26 shows the distribution of solid and liquid salt in the container during cooling predicted by the model for selected times during the third thermal characterization test. The solid LiH is indicated by cross-hatching, while the liquid LiH is shaded. The two-phase region is indicated by dashed cross-hatching and shading. Thermocouple locations are indicated by X's. Also listed in Figure 26 are the measured and predicted temperatures for the interior thermocouple locations. The measured data for thermocouples 3, 5, 6, and 9 are very questionable, since these thermocouples usually read lower than any of the surface thermocouples. As discussed in Chapter IV, it is suspected that these thermocouples were shorted by LiH and were reading the furnace temperature. The data from these thermocouples was not disregarded because the readings were consistent, i.e., thermocouple 3 showed reasonable agreement with thermocouple 5 and thermocouple 6 showed reasonable agreement with thermocouple 9.

Figure 27 shows the distribution of salt in the container predicted by the model when the salt is completely frozen overlayed on a radiograph of the container used in the second test. The agreement between the predicted and actual shapes was considered satisfactory, particularly considering that the salt shrinks by about ten percent when cooling from the melting point to room temperature. Radiographs of capsules containing frozen LiH often show several interconnected voids rather than one large void. This may be due to cooling of the liquid surface by radiation or some sort of crystal growth phenomenon. However, the overall

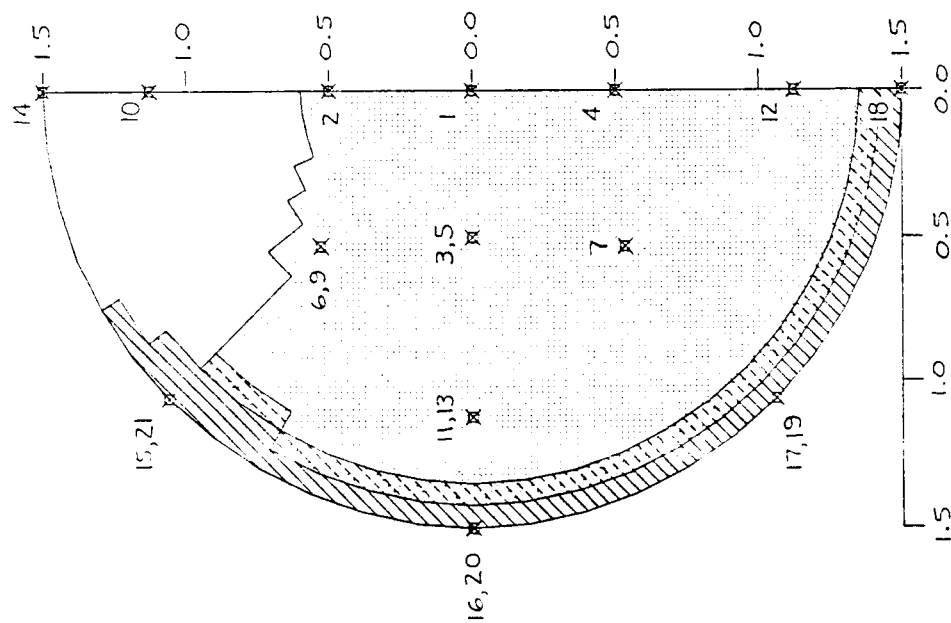


(A) Time = 1800 s. (Completely liquid.)

Figure 26. Predicted Freezing Pattern.

Thermocouple Number(s)	Measured Temperature (°F)	Calculated Temperature (°F)	Calculated - Average Measured
1	1302.8	1333.1	29.7
2	1329.9	1333.1	26.8
3,5	1298.4, 1295.7	1333.1	4127.6
4	1333.3	1333.1	20.2
6,9	1195.0, 1198.1	1333.1	4136.6
7	1351.3	1333.1	-18.2
10	1340.6	†	†
11,13	1363.2, 1360.8	1333.1	-28.9
12	1347.0	1333.1	-13.9
14	1288.4	1288.4	*
15,21	1337.9, 1306.7	1322.3	*
16,20	1329.6, 1322.5	1326.1	*
17,19	1322.4, 1327.6	1325.0	*
18	1316.1	1316.1	*

* Boundary Condition
† Temperatures not calculated in void.



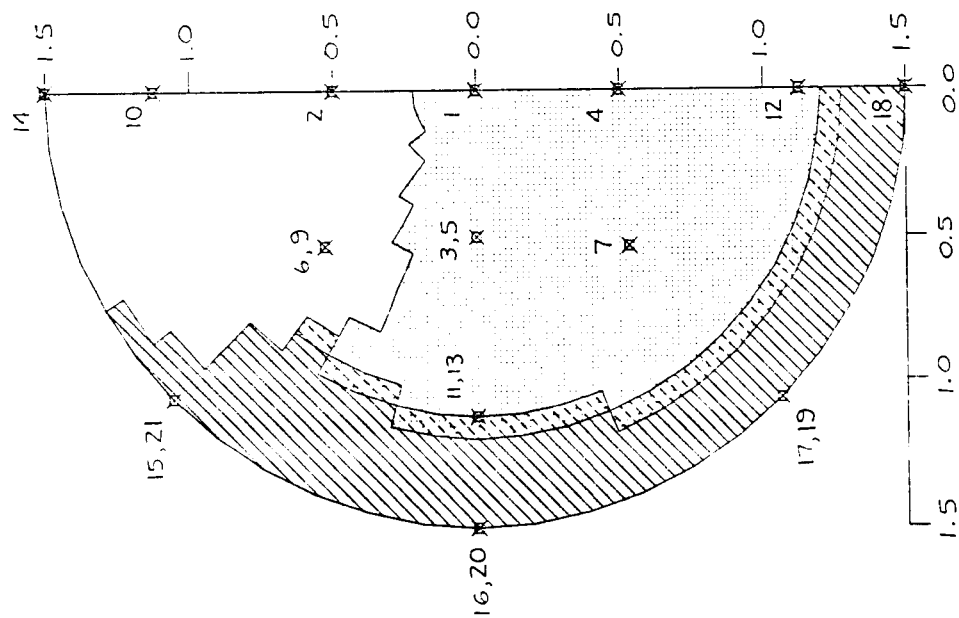
(B) Time = 2200 s.

Figure 26 (continued)

Thermocouple Number(s)	Measured Temperature(s) ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	1261.2	1260.0	-2.4
2	1258.7	1260.0	+1.3
3,5	1166.0, 1187.4	1260.0	+83.3
4	1256.6	1260.0	+3.4
6,9	1117.6, 1157.9	1260.0	+122.3
7	1258.2	1260.0	+1.8
10	1226.1	†	†
11,13	1262.4, 1262.4	1260.0	-2.4
12	1260.8	1260.0	-0.8
14	1140.1	1138.3	*
15,21	1225.9, 1171.2	1196.7	*
16,20	1225.1, 1227.6	1225.3	*
17,19	1244.3, 1239.5	1241.9	*
18	1240.4	1240.2	*

* Boundary Condition

† Temperatures not calculated in void.



(C) Time = 2600 s.

Figure 26 (continued)

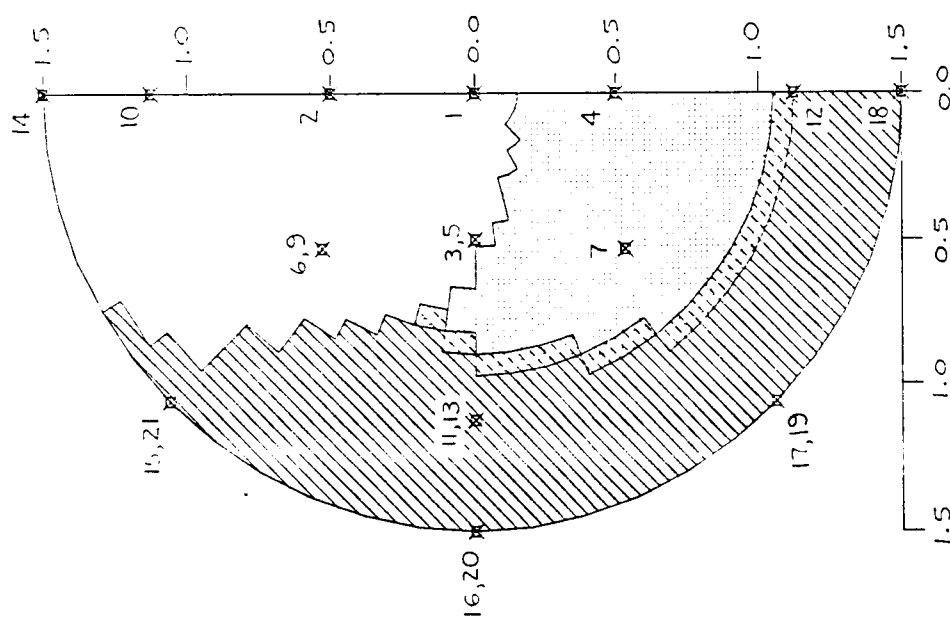
Thermocouple Number(s)	Measured Temperature ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	1261.3	1259.6	-1.7
2	1248.9	†	†
3,5	1145.0, 1155.8	1259.6	+109.2
4	1257.1	1259.6	+2.5
6,9	1044.5, 1122.5	†	†
7	1257.4	1259.6	+2.2
10	1188.4	†	†
11,13	1260.8, 1261.5	1259.6	-1.6
12	1258.9	1259.6	+0.7
14	1072.0	1071.5	*
15,21	1158.0, 1092.5	1124.3	*
16,20	1176.6, 1174.9	1175.4	*
17,19	1216.0, 1212.2	1214.1	*
18	1213.5	1213.3	*

* Boundary Condition

† Temperatures not calculated in void.

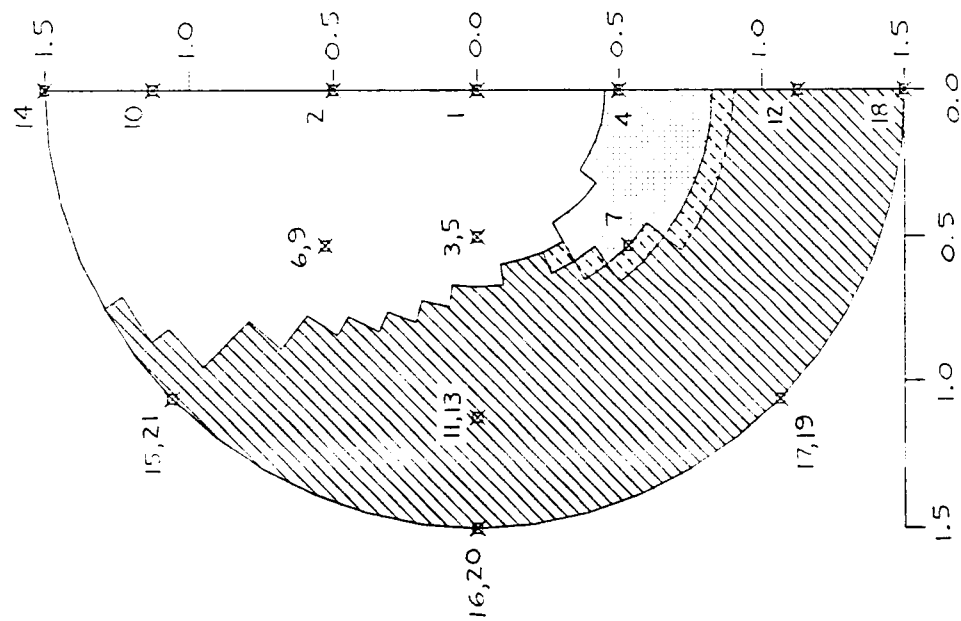
Thermocouple Number(s)	Measured Temperature(s) (°F)	Calculated Temperature (°F)	Calculated -Average Measured
1	1260.9	†	†
2	1236.2	†	†
3,5	1118.0, 1103.9	†	†
4	1256.4	1259.3	+2.9
6,9	980.1, 1068.7	†	†
7	1257.5	1259.3	+1.8
10	1141.7	†	†
11,13	1221.6, 1251.7	1189.8	-46.9
12	1251.3	1260.0	+8.7
14	1010.8	1010.8	•
15,21	1085.9, 1021.2	1055.1	•
16,20	1120.3, 1113.1	1116.7	•
17,19	1171.4, 1171.3	1171.3	•
18	1174.2	1174.2	•

• Boundary Condition
† Temperatures not calculated in void.



(D) Time = 3000 s.

Figure 26 (continued)

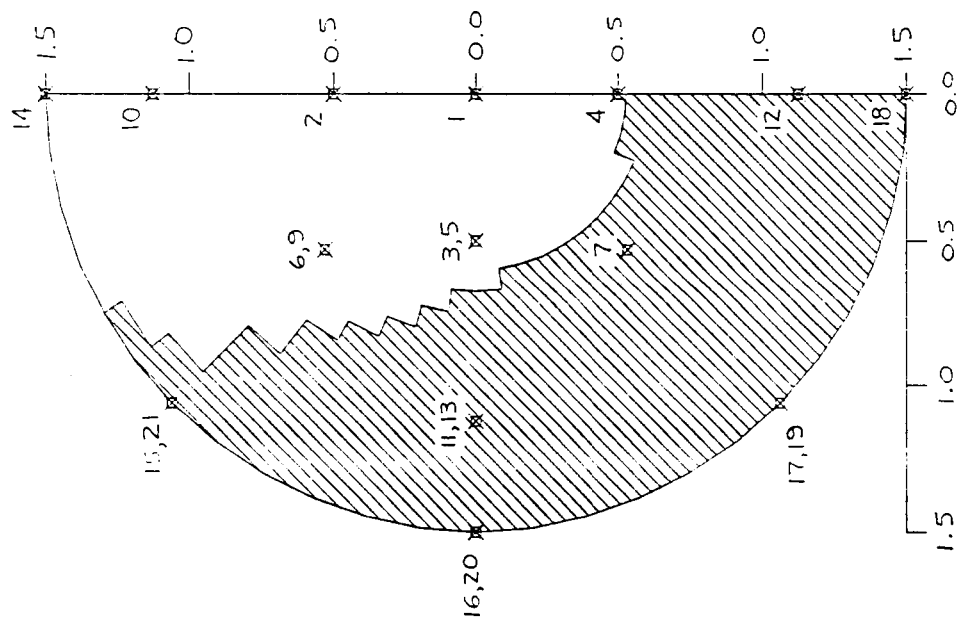


(E) Time = 3400 s.

Figure 26 (continued)

Thermocouple Number(s)	Measured Temperature ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	1256.6	†	†
2	1169.6	†	†
3,5	1062.5, 1031.9	†	†
4	1255.3	1260.0	-44.7
6,9	917.2, 1003.8	†	†
7	1257.5	1258.2	-40.7
10	1073.2	†	†
11,13	1136.0, 1163.9	1082.9	-62.1
12	1216.8	1194.5	-22.3
14	916.8	945.4	†
15,21	1016.9, 958.5	985.9	†
16,20	1048.6, 1033.7	1010.1	†
17,19	1120.5, 1110.1	1113.8	†
18	1123.1	1123.7	†

† Boundary Condition
 † Temperatures not calculated in void.



(F) Time = 3800 s. (Completely frozen.)

Figure 26 (continued)

Thermocouple Number(s)	Measured Temperature ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	1143.4	†	†
2	1061.2	†	†
3,5	975.9, 954.9	†	†
4	1230.0	†	†
6,9	849.1, 936.2	†	†
7	1198.9	1044.0	-84.9
10	985.3	†	†
11,13	1028.7, 1055.3	985.1	-56.9
12	1134.9	1062.0	-72.9
14	876.0	875.4	*
15,21	935.8, 886.3	910.2	*
16,20	966.5, 952.5	958.3	*
17,19	1043.9, 1024.4	1033.2	*
18	1053.7	1053.3	*

* Boundary Condition
† Temperatures not calculated in void.

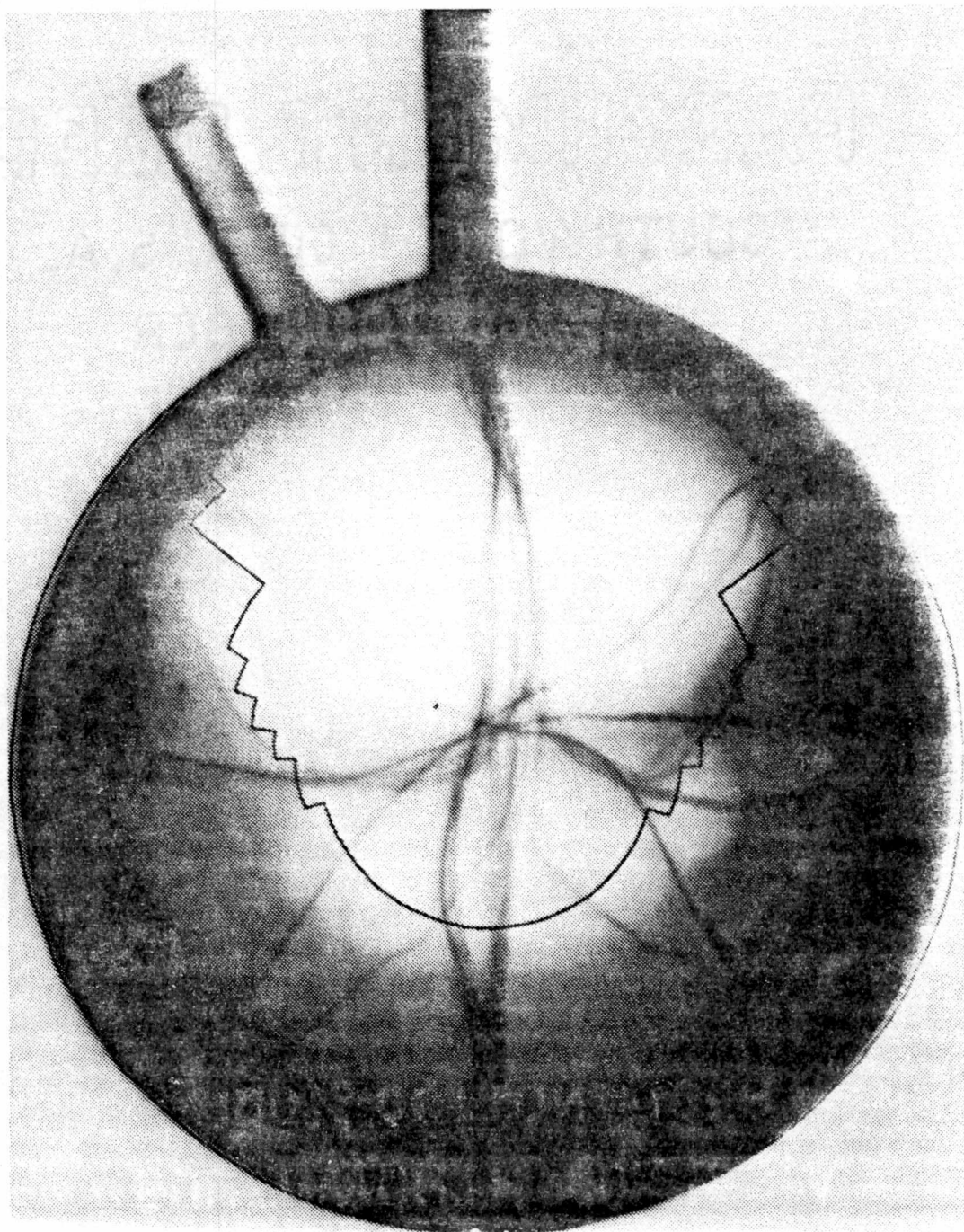


Figure 27. Predicted Frozen Solid Distribution Overlayed on Radiograph.

distribution of salt in the container is generally similar to that shown in Figure 27.

Predicted thermal and void behavior during heating and melting. Heat transfer calculations for the heating part of the thermal cycle were carried out using the full natural convection model described in Chapter II. Predicted temperatures during the heatup for thermocouples 7, 11, and 12, together with the average measured data from the third test, are plotted in Figures 28 through 30. Agreement between the model prediction and the measured data appears to be reasonable during the initial part of the heatup. However, the model gains energy too rapidly; for example, for thermocouple 12, final melting occurs about 150 seconds too soon. The predicted time for complete melting during the second test was also about 150 seconds too short, even though the heating rates were somewhat different.

Due to the complexity of the problem, there are many possible reasons for the discrepancy between the model and the measured data. Some of the most obvious are:

1. Uncertainty in property value information;
2. The natural convection model predicting more circulation than actually occurs;
3. Incorrect assumption about how the liquid gets into the void, or effects due to the void not really being axisymmetric or being composed of multiple voids;
4. Bad thermocouple readings, thermocouples not located where we thought they were, or effects due to the presence of the thermocouples and support wires.

There are probably several other potential sources of error. It should be noted that the assumption was made that the support wires hold the solid in a

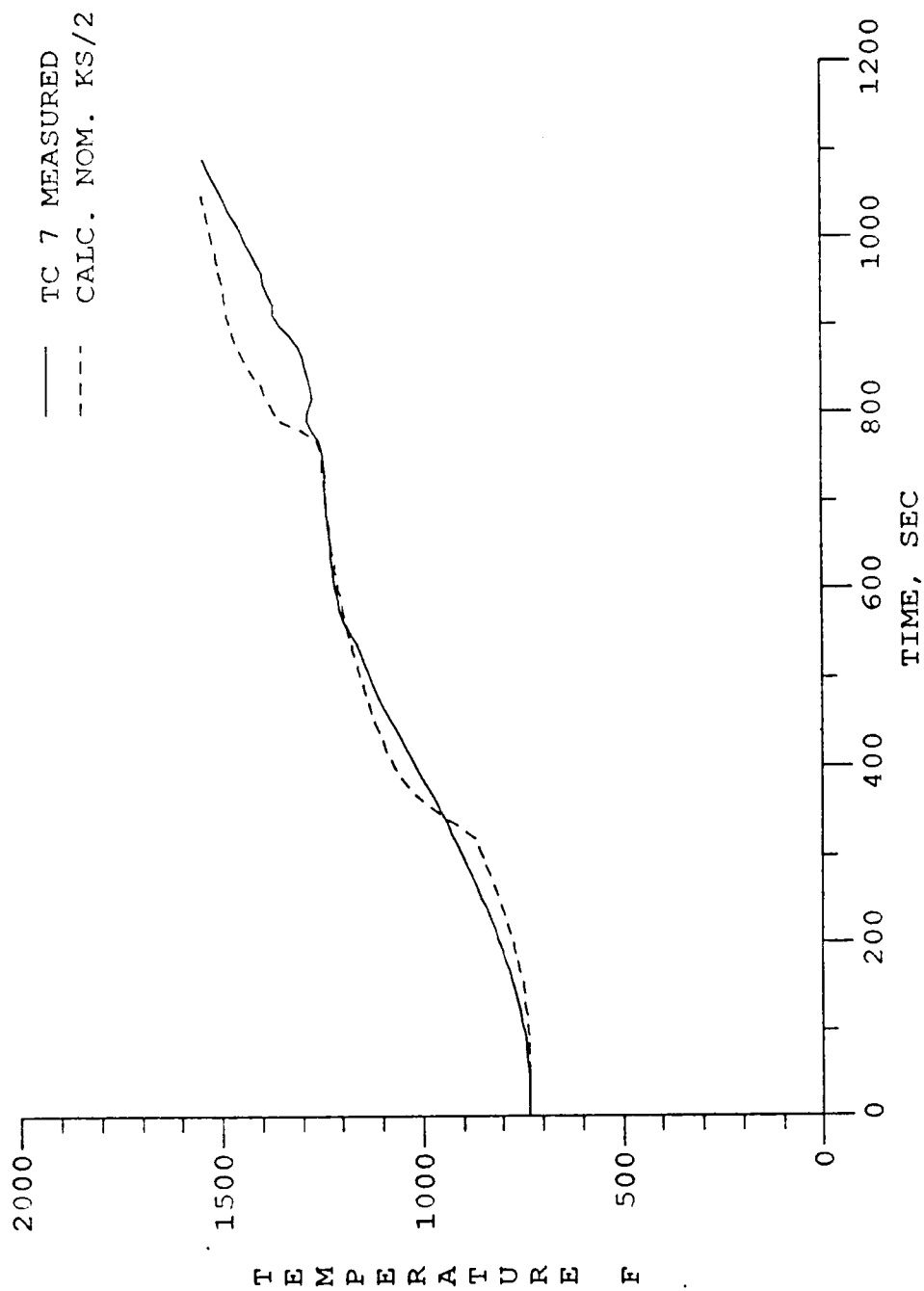


Figure 28. Thermocouple No. 7 Measured vs. Predicted Temperature During Heating.

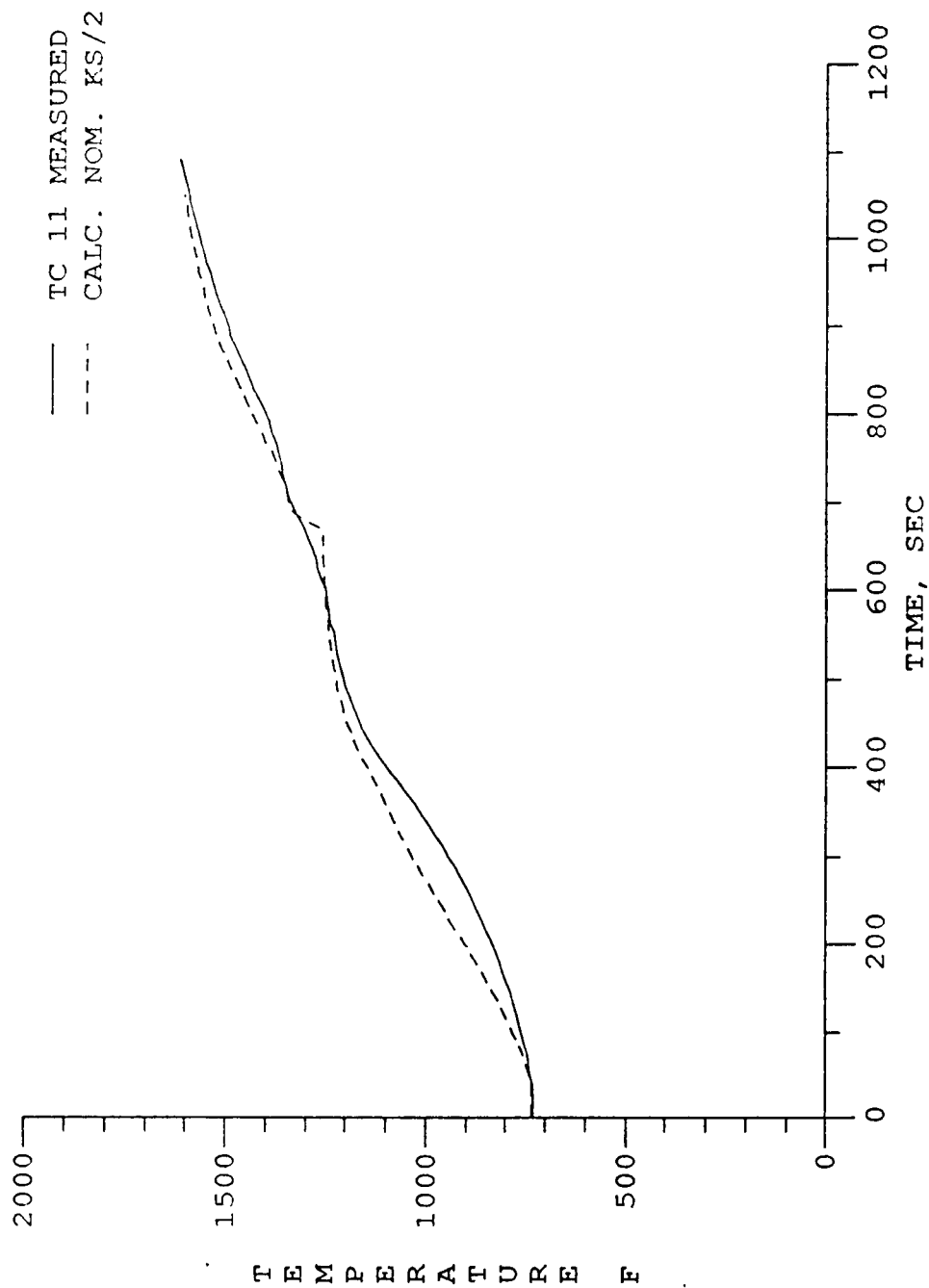


Figure 29. Thermocouple No. 11 Measured vs. Predicted Temperature During Heating.

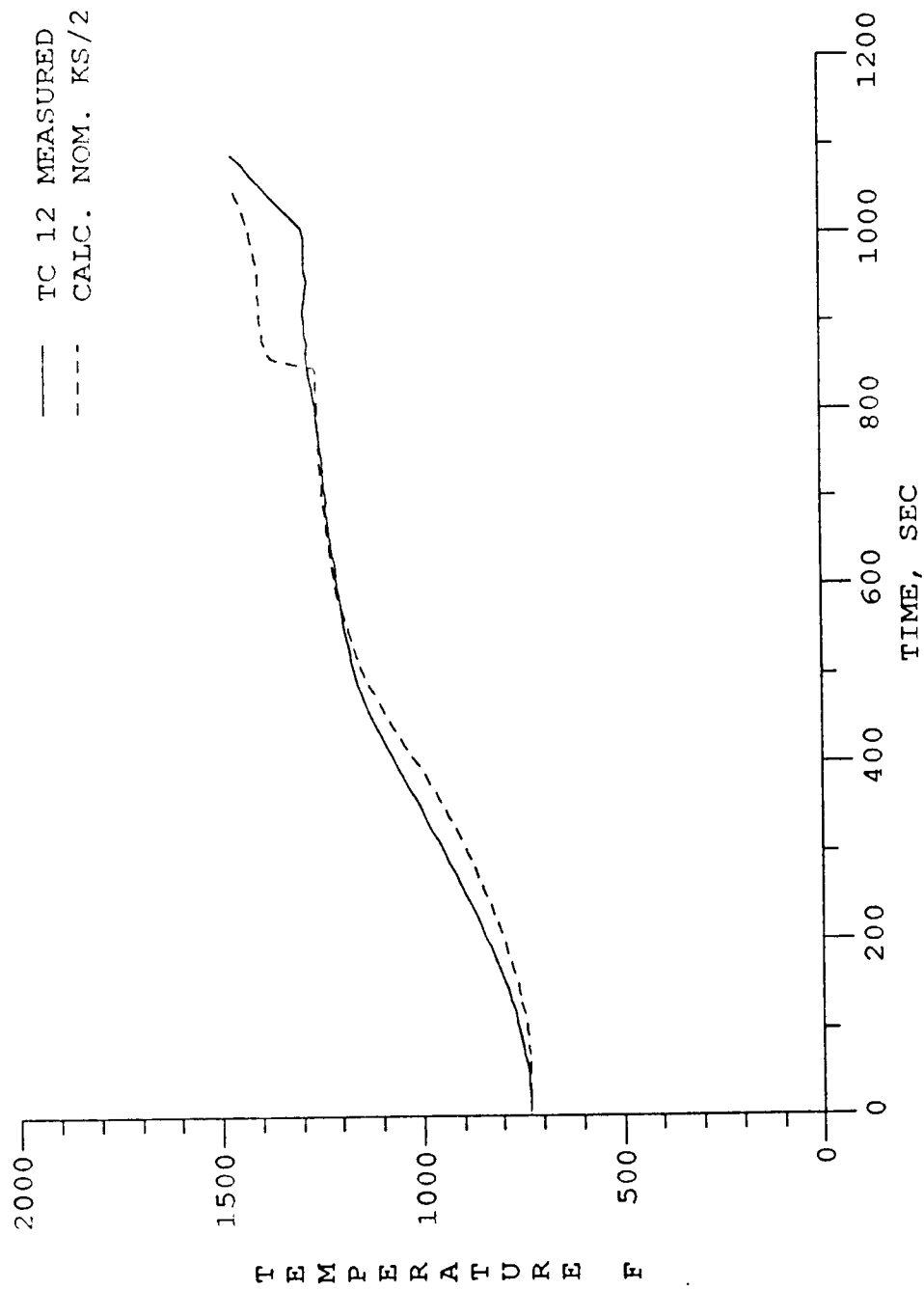


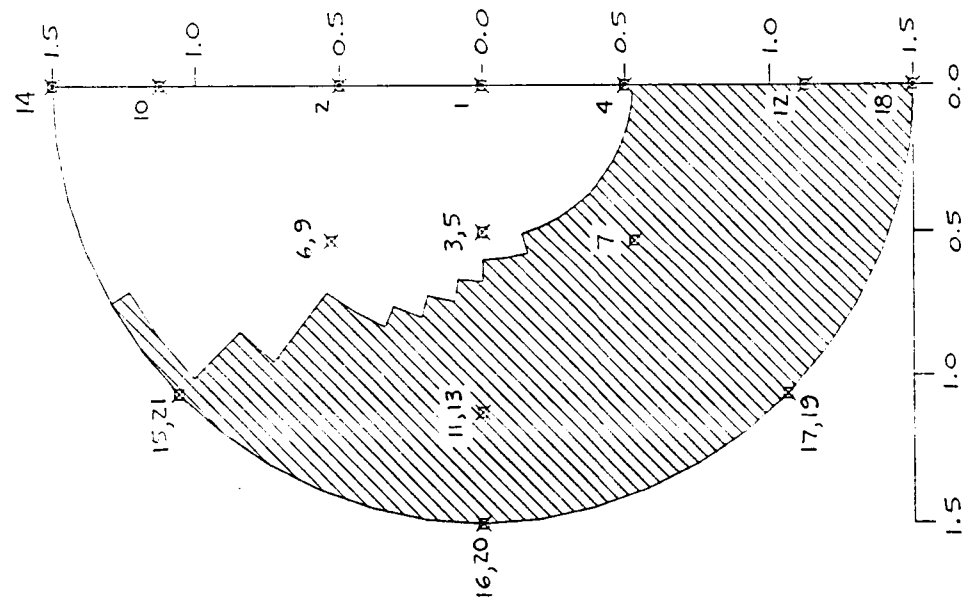
Figure 30. Thermocouple No. 12 Measured vs. Predicted Temperature During Heating.

fixed position in the container during melting, preventing the solid mass from settling to the bottom of the container as would occur if the wires were not present. If the wires did not actually hold the solid in position, there would probably be a substantial effect on the heat transfer performance.

Figure 31 shows the distribution of solid and liquid salt in the container predicted by the model at selected times during the heatup in the third thermal characterization test. The solid LiH is indicated by cross-hatching, while the liquid LiH is shaded. The two-phase region is indicated by dashed cross-hatching and shading. Thermocouple locations are indicated by X's. Also listed in Figure 31 are the measured and predicted temperatures for the interior thermocouple locations.

Comparison of Model Results for Zero-Gravity and Normal Gravity Conditions

In an effort to determine how the heat transfer performance of encapsulated LiH would differ under zero-g conditions when compared to normal gravity results, the computer model was run to simulate the heat-up part of the cycle using the same boundary condition for both cases. For the test case, it was assumed that a three-inch diameter stainless steel container with 0.030 *in* (0.76 *mm*) thick walls was filled with enough LiH to be 90 percent full when completely melted. The initial temperature of the container was 620°F (600 K). The container was surrounded by a liquid metal heat transfer medium, which at time zero underwent a step change in temperature from 620°F (600 K) to 1520°F (1100 K). A uniform convection coefficient of 3000 *Btu/hr · ft² · °F* (17 *kW/m² · K*) was assumed. This boundary condition approximates the operation of the proposed heat storage system for a satellite-based power system, in which a nuclear reactor would be powered-up very rapidly when heat was needed for the power generation cycle.



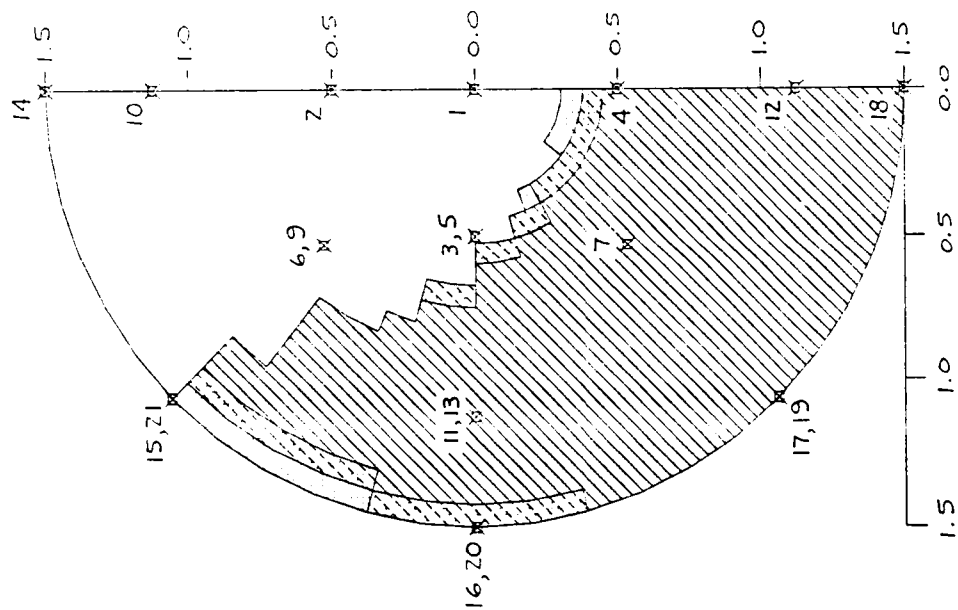
(A) Time = 300 s. (Completely solid.)

Figure 31. Predicted Melting Pattern.

Thermocouple Number(s)	Measured Temperature(s) ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	868.6	†	†
2	912.6	†	†
3,5	1192.2, 1197.7	†	†
4	876.1	†	†
6,9	1169.0, 1186.8	†	†
7	900.2	851.6	-48.6
10	1078.7	†	†
11,13	944.2, 960.5	1034.9	+82.6
12	945.4	889.9	-55.5
14	1212.7	1212.7	*
15,21	1272.5, 1238.6	1255.6	*
16,20	1267.0, 1292.4	1279.7	*
17,19	1085.7, 1150.6	1118.2	*
18	1063.6	1063.6	*

* Boundary Condition

† Temperatures not calculated in void.

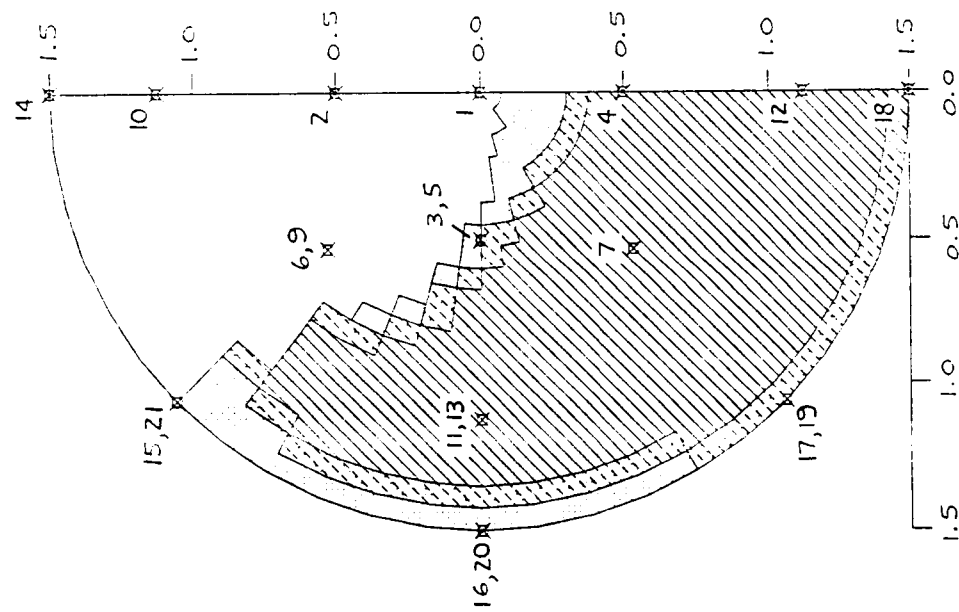


(B) Time = 400 s.

Figure 31 (continued)

Thermocouple Number(s)	Measured Temperature ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	975.1	†	†
2	1023.5	†	†
3,5	1222.3, 1235.7	†	†
4	980.9	1175.4	+194.5
6,9	1239.4, 1235.7	†	†
7	1014.2	1069.2	+55.0
10	1167.3	†	†
11,13	1097.2, 1100.2	1147.7	+49.0
12	1063.3	1011.7	-51.6
14	1294.6	1294.6	*
15,21	1390.7, 1353.6	1372.2	*
16,20	1286.1, 1300.0	1293.1	*
17,19	1220.1, 1258.5	1239.3	*
18	1201.5	1204.5	*

* Boundary Condition
† Temperatures not calculated in void.



(C) Time = 500 s.

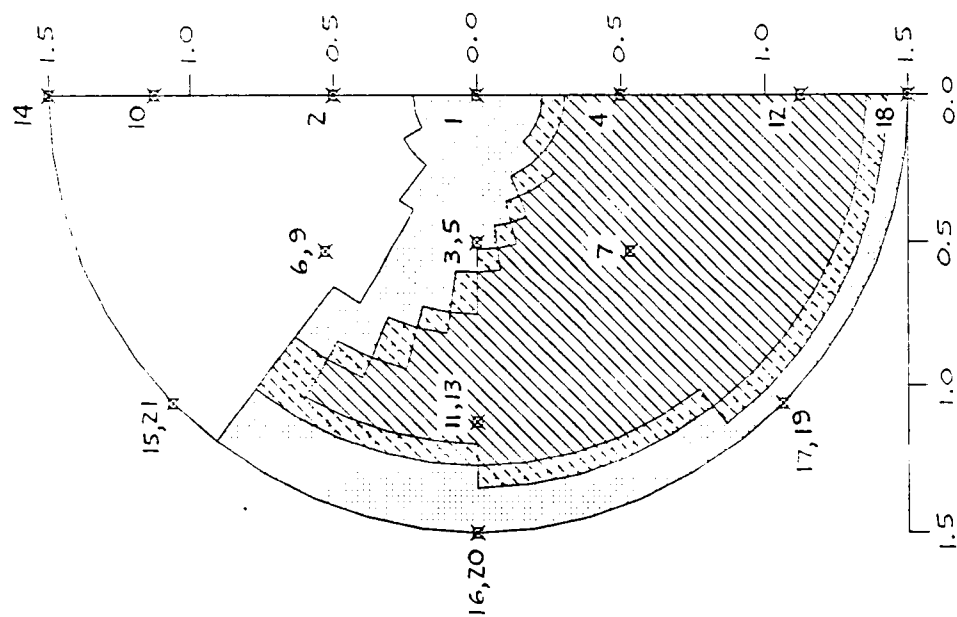
Figure 31 (continued)

Thermocouple Number(s)	Measured Temperature(s) ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	1091.4	†	†
2	1138.3	†	†
3,5	1313.0, 1281.4	1260.0	37.2
4	1091.6	1177.0	182.4
6,9	1239.9, 1258.7	†	†
7	1129.7	1153.9	424.2
10	1263.1	†	†
11,13	1207.0, 1213.1	1225.8	45.8
12	1161.4	1141.8	-22.6
14	1388.2	1388.2	*
15,21	1326.8, 1315.5	1321.1	*
16,20	1332.8, 1317.2	1340.0	*
17,19	1290.7, 1322.8	1306.8	*
18	1289.5	1289.5	*

* Boundary Condition
 † Temperatures not calculated in void.

Thermocouple Number(s)	Measured Temperature ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	1218.4	1263.1	+14.7
2	1255.7	†	†
3,5	1282.6, 1339.7	1261.0	-100.2
4	1219.9	1206.4	-13.5
6,9	1252.6, 1301.0	†	†
7	1215.2	1307.1	-8.1
10	1353.4	†	†
11,13	1252.0, 1251.8	1251.7	-0.2
12	1207.2	1211.1	+3.9
14	1469.0	1468.6	*
15,21	1375.6, 1124.2	1399.2	*
16,20	1368.9, 1395.8	1382.2	*
17,19	1328.1, 1353.4	1340.7	*
18	1330.9	1330.7	*

* Boundary Condition
† Temperatures not calculated in void.

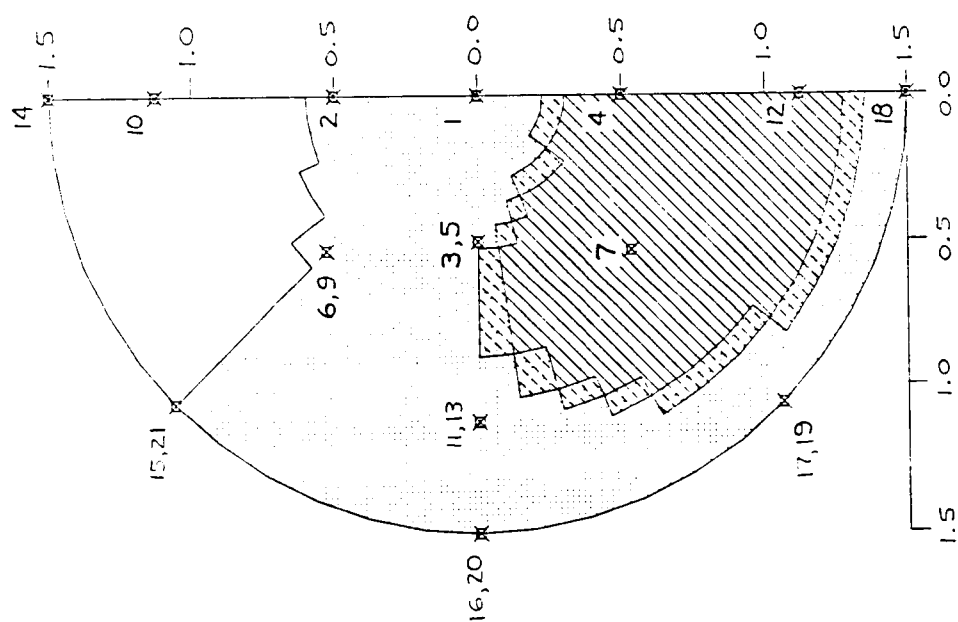


(D) Time = 600 s.

Figure 31 (continued)

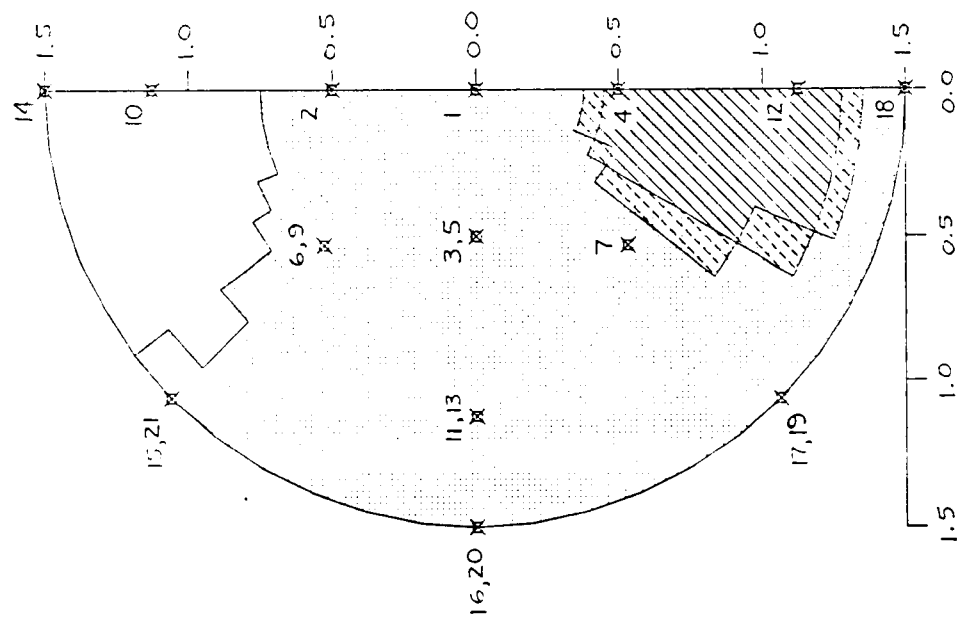
Thermocouple Number(s)	Measured Temperature(s) (°F)	Calculated Temperature (°F)	Calculated - Average - Measured
1	1311.3	1301.1	-10.2
2	1393.8	1360.7	33.1
3,5	1431.9, 1378.5	1396.7	-98.5
4	1214.1	1235.9	-8.2
6,9	1267.4, 1337.6	1267.5	+65.0
7	1238.1	1239.3	+1.2
10	1413.6	†	†
11,13	1337.6, 1302.1	1343.0	+23.2
12	1234.0	1242.3	+8.3
14	1516.1	1515.8	*
15,21	1447.7, 1461.6	1452.7	*
16,20	1407.2, 1436.7	1421.7	*
17,19	1319.0, 1374.0	1361.5	*
18	1364.7	1364.6	*

* Boundary Condition
† Temperatures not calculated in void.



(E) Time = 700 s.

Figure 31 (continued)



(F) Time = 800 s.

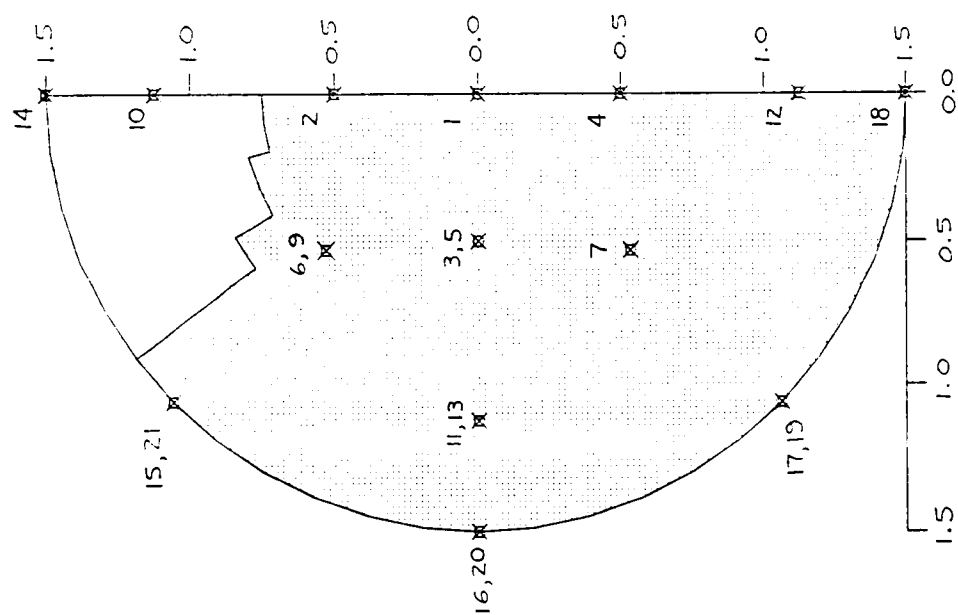
Figure 31 (continued)

Thermocouple Number(s)	Measured Temperature ($^{\circ}F$)	Calculated Temperature ($^{\circ}F$)	Calculated - Average Measured
1	1397.2	1428.5	+31.3
2	1508.0	1478.8	-29.2
3,5	1472.5, 1414.2	1428.7	-44.7
4	1290.8	1255.3	-35.5
6,9	1287.5, 1376.0	1479.8	+148.1
7	1282.5	1371.5	+88.7
10	1558.4	†	†
11,13	1400.4, 1353.8	1435.2	+58.1
12	1257.9	1254.4	-3.5
14	1584.2	1583.9	*
15,21	1551.6, 1550.4	1550.6	*
16,20	1451.0, 1514.2	1482.3	*
17,19	1361.7, 1395.3	1378.4	*
18	1379.2	1379.2	*

* Boundary Condition
† Temperatures not calculated in void.

Thermocouple Number(s)	Measured Temperature(s) (°F)	Calculated Temperature (°F)	Calculated -Average -Measured
1	1454.6	1528.1	-473.5
2	1575.9	1561.4	-11.5
3,5	1503.3, 1452.5	1529.5	-451.6
4	1305.6	1473.7	-1168.1
6,9	1311.1, 1393.4	1564.8	-4212.6
7	1350.4	1476.0	-125.6
10	1618.0	†	†
11,13	1495.5, 1431.5	1532.2	-467.2
12	1385.1	1395.0	-109.9
14	1632.0	1631.9	*
15,21	1627.1, 1617.6	1622.1	*
16,20	1528.0, 1587.6	1557.5	*
17,19	1374.8, 1401.9	1388.5	*
18	1380.6	1380.6	*

* Boundary Condition
† Temperatures not calculated in void.



(G) Time = 900 s. (Completely melted.)

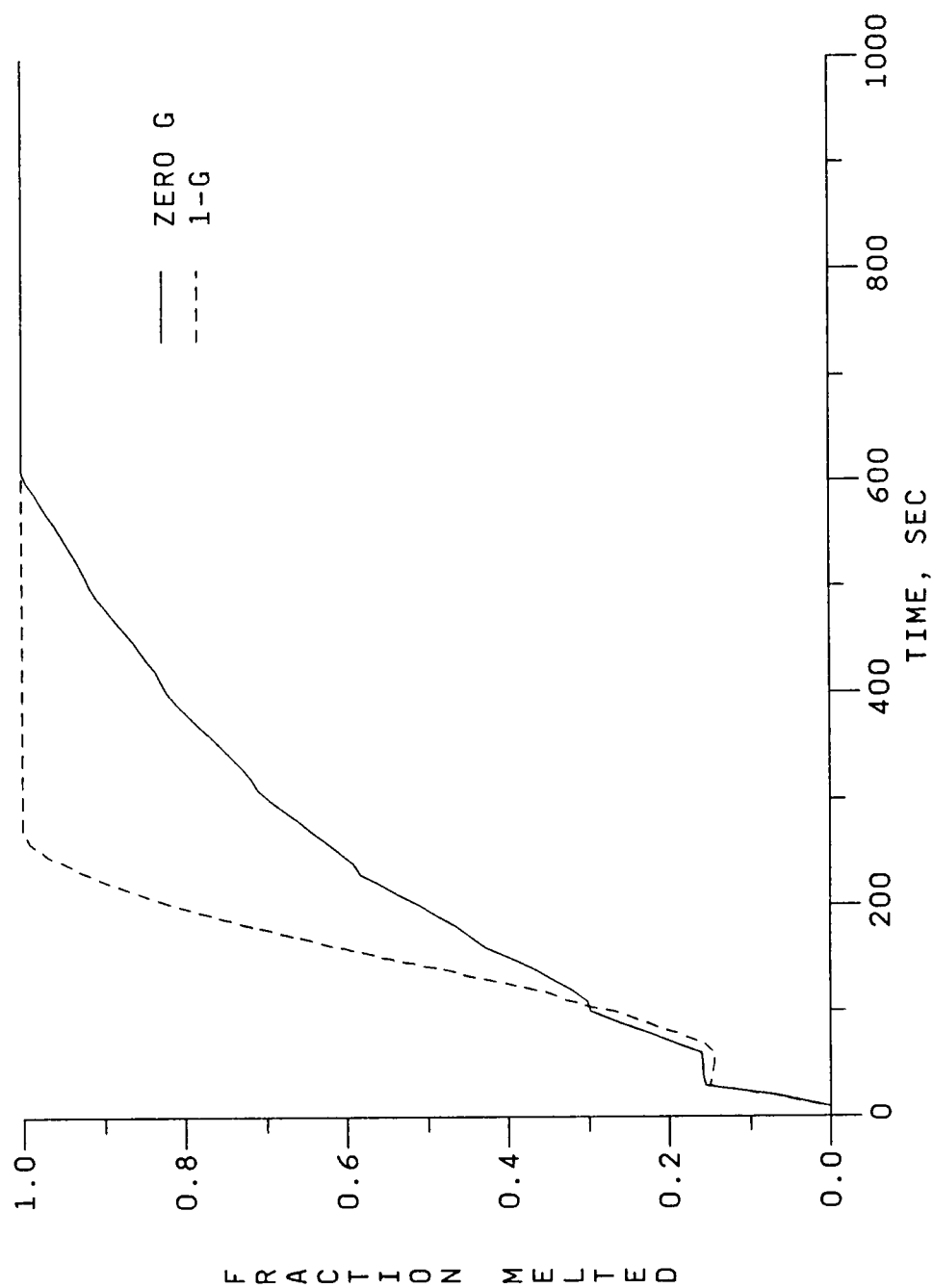
Figure 31 (continued)

The values for LiH physical properties listed in Table I were used for the calculations. The value for solid thermal conductivity was 50 percent of the nominal value, based on the test results. For the zero-gravity case with zero contact angle, the vapor would be contained in a spherical bubble which would have no affinity for the container wall. The void in a completely frozen container would therefore be expected to be a concentric sphere, with a spherical shell of salt completely surrounding it. This greatly simplifies the heat transfer model, as the problem becomes one-dimensional. In addition, natural convection driven by surface tension gradients (usually referred to as Marangoni flow), which can be very significant in zero-gravity situations, would not be expected to be important, since the heated liquid would have no free surface.

An assumption must be made as to how the volume expansion due to the phase change is accommodated, since the liquid is not directly in contact with the void. The possibilities are for the excess liquid to leak through cracks in the solid into the void, or for the solid to be crushed inward. Due to the tendency of solid LiH to crack when cooling, it is thought that the former is actually the case. In experiments conducted at Oak Ridge National Laboratory, concentric voids were formed in spherical capsules containing LiH by slowly rotating the containers about a horizontal axis during cooling [27]. The containers were then heated enough to partly melt the LiH near the shell, allowed to cool, and radiographed. The radiographs tended to confirm that the excess liquid flows into the void through cracks, as the overall concentric appearance of the solid remained intact and additional frozen salt was noted in the lower part of the void.

Based on the above results, a one-dimensional model was used for the zero-gravity calculations. Natural convection effects were not considered, and the excess liquid produced by melting was assumed to leak into the void through cracks

in the solid. The means by which the liquid makes its way through the solid was not modeled. The necessary amount of liquid was simply removed from the melting volume on the outer surface of the solid, reappearing in the two-phase volume at the inner solid surface. Results of the zero-gravity and normal gravity calculations are compared in Figures 32 and 33. The total time required for melting in the zero-gravity case was 610 seconds, as opposed to 270 seconds for the normal gravity case. The difference is mostly due to the effect of natural convection in the normal gravity case. It is interesting to note that the rate of energy gain is initially slightly greater for the zero-gravity case. This is due to the distribution of salt in the container, with more salt being directly in contact with the shell in the zero-gravity case.



3 INCH DIA SPHERE WITH CONVECTION BC

Figure 32. Fraction of Salt Melted vs. Time for Zero-Gravity and Normal Gravity Cases.

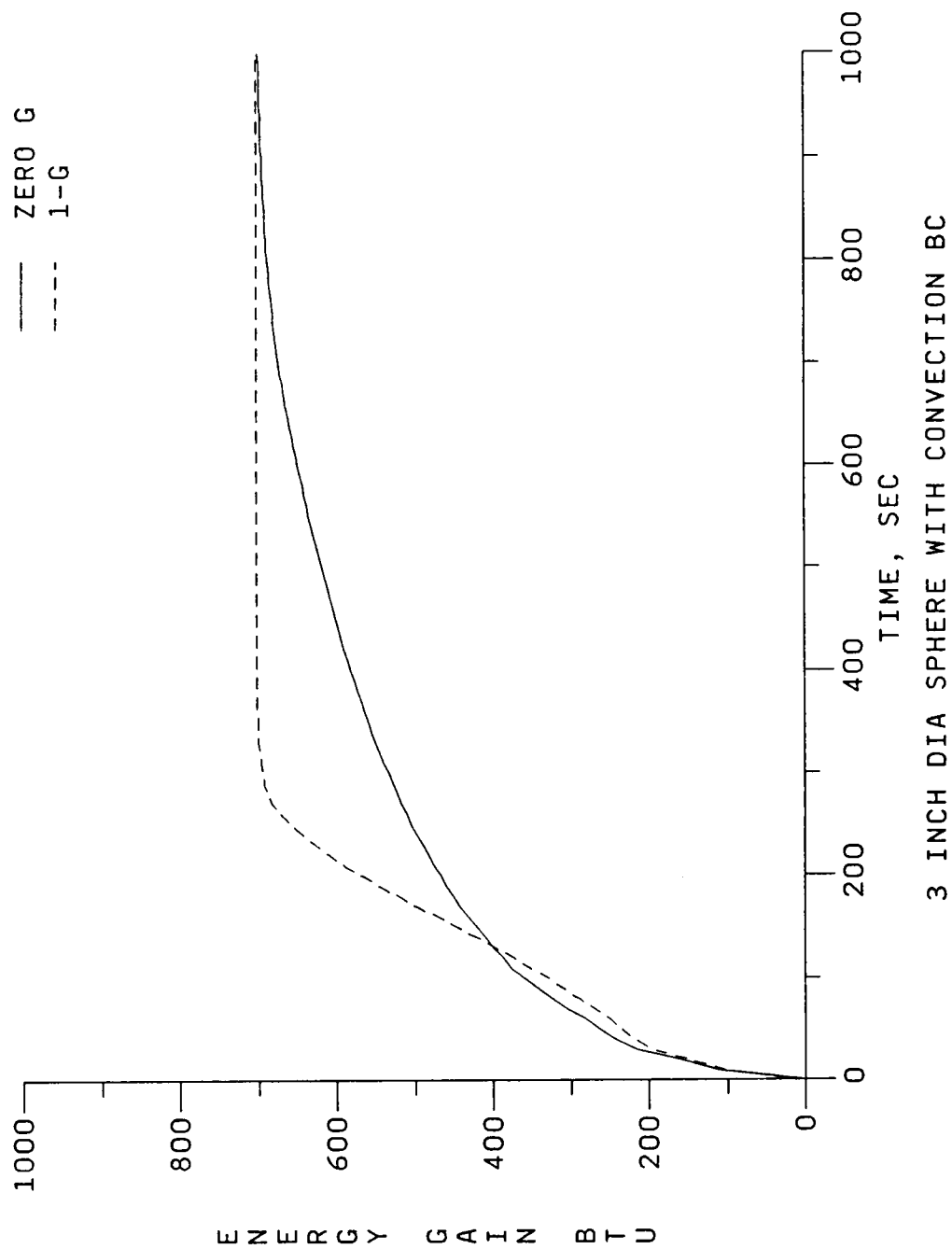


Figure 33. Energy Gain vs. Time for Zero-Gravity and Normal Gravity Cases.

CHAPTER VI

SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS FOR FURTHER STUDY

A theoretical and experimental study of the heat transfer characteristics of spherically encapsulated lithium hydride salt was carried out. A numerical heat transfer model was developed to simulate the heat transfer performance of individual spherical LiH capsules under normal-gravity and zero-gravity conditions for an axisymmetric (two-dimensional) case, including effects due to the solid-liquid phase change. The model employs a finite difference formulation and uses an enthalpy-based method to account for phase change. The model also predicts the void that forms as the salt freezes, using a vertical force balance on the liquid-vapor interface to predict the interface shape. Natural convection flow in the melted salt is also modeled; the equations of motion are solved to determine the velocity field in the liquid. Calculations were carried out on a uniform, fixed finite difference grid.

Experiments were carried out in which instrumented spherical containers filled with LiH were heated rapidly in a high-flux induction furnace to simulate as closely as possible a typical heating cycle in a real thermal energy storage system. Thirteen Type K thermocouples were suspended inside the containers to measure temperatures in the salt, while eight thermocouples were attached to the outside of the shell. A total of three thermal characterization tests were carried out. The second and third tests were both successful, providing repeatable thermal data over several heating cycles. The data obtained during these experiments was used to determine the physical behavior of the capsules during melting and solidification, and the experimental data was compared with results of the

numerical calculations in order to validate the numerical model. Numerical results for zero-gravity and normal-gravity cases were also compared, and conclusions were drawn about the effects of gravity on the thermal behavior of these systems.

Based on the comparison between the heat transfer model predictions and the experimental results, it appears that the heat transfer performance of encapsulated LiH can be adequately modeled using the approach taken in the present study. The performance of the numerical model in predicting temperature-time histories of thermocouples embedded in the salt was generally satisfactory, but the model underpredicted the total time required for melting by ten to fifteen percent. The void behavior predicted by the model was also in reasonable agreement with the experimentally observed behavior. However, much work remains to resolve the differences between the model results and the observed behavior.

A parametric study of the effects of the various LiH physical property values (k_s , k_l , c_s , c_l) on the model results would be of great help. Unfortunately, it was not practical to perform such a study at present, since a full solution of the heating model with natural convection calculations included required over 20 hours of CPU time on the UTSI VAX 11/785 computer for each case. Such a parametric study would be much easier if the model could be installed on a faster computer. In addition, no effort was made to optimize the speed of the fluid flow calculation procedure. It may be that a more efficient solution method could be adopted without excessive effort. It would also be helpful to compare results from the fluid flow model with experimentally measured velocity distributions for some test cases, if such experimental data can be located.

More thermal characterization tests, perhaps with containers of different geometries and different heating cycles, would be helpful in providing a better data base for comparison with model calculations. The reason for the erratic

thermocouple readings experienced during the tests needs to be investigated, in order to determine if the problem can be corrected, and also to provide a better method for determining when the measured data is reliable.

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VITA

John Paul Foote was born in Jackson, Tennessee in 1957 and grew up in Martin, Tennessee, attending the public schools there until his graduation from Martin Westview High School in 1975. He entered the University of Tennessee at Martin the following fall, and transferred to the University of Tennessee, Knoxville in 1978, receiving a Bachelor of Science in Mechanical Engineering in June of 1980. In the fall of 1980, he received a graduate research assistantship at the University of Tennessee Space Institute (UTSI) in the Energy Conversion Research and Development Programs. He received a Master of Science in Mechanical Engineering from UTSI in December of 1982, then began work in the PhD program at UTSI as a part-time student while working at UTSI as a research engineer in the Energy Conversion Programs. He received a research fellowship at the Oak Ridge National Laboratory (ORNL) in 1986, and spent 15 months working on his dissertation in the ORNL Engineering Technology Division while on leave from UTSI. He Received the Doctor of Philosophy degree from UTSI in August, 1989.