



**Institute for Space Nuclear Power Studies
Department of Chemical and Nuclear Engineering
The University of New Mexico
Albuquerque, New Mexico 87131**

**AN INVESTIGATION OF VOIDS FORMATION
MECHANISMS AND THEIR EFFECTS ON FREEZE
AND THAW PROCESSES OF LITHIUM AND
LITHIUM FLUORIDE**

MOHAMED S. EL-GENK AND JAE-YOUNG YANG

FINAL REPORT NO. UNM-ISNPS-NAG 3-1045

**NASA Grant No. NAG 3-1045
Performance Period May 1989 - January 1991**

(NASA-CR-188707) AN INVESTIGATION OF VOIDS
FORMATION MECHANISMS AND THEIR EFFECTS ON
FREEZE AND THAW PROCESSES OF LITHIUM AND
LITHIUM FLUORIDE Final Report, May 1989 -
Jan. 1991 (New Mexico Univ.) 116 pCSCL 07D G3/25

N91-30294

542241

Unclass 132P
0032347

August 1991



**Institute for Space Nuclear Power Studies
Department of Chemical and Nuclear Engineering
The University of New Mexico
Albuquerque, New Mexico 87131**

**AN INVESTIGATION OF VOIDS FORMATION
MECHANISMS AND THEIR EFFECTS ON FREEZE
AND THAW PROCESSES OF LITHIUM AND
LITHIUM FLUORIDE**

MOHAMED S. EL-GENK AND JAE-YOUNG YANG

FINAL REPORT NO. UNM-ISNPS-NAG 3-1045

**NASA Grant No. NAG 3-1045
Performance Period May 1989 - January 1991**

August 1991

TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT	iv
LIST OF FIGURES	vi
LIST OF TABLES	viii
1. INTRODUCTION	1
1.1 Background	1
1.2 Void Formation Mechanisms.....	2
1.3 Objectives	5
2. VOID FORMATION MECHANISMS DURING THE COOLDOWN AND FREEZING PROCESSES OF LITHIUM COOLANT IN THE SP-100 SYSTEM	8
2.1 Homogeneous and Heterogeneous Nucleation of He Gas Bubbles During the Cooldown Process of Li Coolant.....	8
2.1.1 Theoretical Background.....	8
2.1.2 Results and Discussion	9
2.2 Potential Formation of Intermetallic Compounds During the Cooldown Process of Li Coolant and Their Relation to the Formation of He Gas Bubbles	10
2.2.1 Potential Formation of Intermetallic Compounds	10
2.2.2 Discussion and Suggestion for Future Investigation	15
2.3 He Gas Bubble Formation by Segregation of He Gas atoms During the Freezing Process of Li Coolant	15
2.3.1 Physical Model.....	16
2.3.2 Results and Discussion	21
2.4 Nomenclature.....	30
3. THE EFFECTS OF SHRINKAGE VOID FORMATION ON THE FREEZING AND THAW PROCESSES OF LI COOLANT	36
3.1 Physical Model.....	36
3.2 Results and Discussion	41
3.2.1 Comparison with Available Analytical Solution	41
3.2.2 Freezing with Radiative Heat Transfer Boundary	41
3.2.3 Thaw with Radiative Heat Transfer Boundary.....	42
3.3 Nomenclature.....	51

4. SUMMARY AND CONCLUSIONS	53
ACKNOWLEDGEMENTS	54
REFERENCES	55
APPENDICES	
A-1 List of Computer Program COPHASE.FOR	57
A-2 Input Data For Computer Program COPHASE.FOR	58
B-1 List of Computer Program SEGR.FOR	59
B-2 Input Data For Computer Program SEGR.FOR	60
C List of Computer Program FREZ.FOR	61
D List of Computer Program MELT.FOR	62

**AN INVESTIGATION OF VOIDS FORMATION
MECHANISMS AND THEIR EFFECTS ON FREEZE AND THAW
PROCESS OF LITHIUM AND LITHIUM FLUORIDE**

ABSTRACT

In the first part of the research, the mechanisms of void formation during the cooldown and freezing of lithium coolant within the primary loop of SP-100 type systems are investigated. These mechanisms are: (a) homogeneous nucleation, (b) heterogeneous nucleation, (c) normal segregation of helium gas dissolved in liquid lithium, and (d) shrinkage of lithium during freezing. To evaluate the void formation potential due to segregation, a numerical scheme that couples the freezing and mass diffusion processes in both the solid and liquid regions is developed. The results indicated that the formation of He bubbles is unlikely by either homogeneous or heterogeneous nucleation during the cooldown process. However, homogeneous nucleation of He bubbles following the segregation of dissolved He in liquid Lithium ahead of the solid-liquid interface is likely to occur. Results also show that total volume of He void is insignificant when compared to that of shrinkage voids.

In viewing this, the subsequent research focuses on the effects of shrinkage void forming during freezing of lithium on subsequent thaw processes are investigated using a numerical scheme that is based on a single (solid/liquid) cell approach. The cases of lithium-fluoride are also investigated to show the effect of larger volume shrinkage upon freezing on the freeze and thaw processes. Results show that a void forming at the wall appreciably reduces the solid-liquid interface velocity, during both freeze and thaw, and causes a substantial rise in the wall temperature during thaw. However, in the case of Li, the maximum wall temperature was much lower than the melting temperature of PWC-

11, which is used as the structure material in the SP-100 system. Hence, it is concluded that a formation of hot spots is unlikely during the startup or restart of the SP-100 system.

LIST OF FIGURES

		<u>Page</u>
Figure 1.	Variation of Specific Volume of Lithium	3
Figure 2.	Gas Bubble Formation by Segregation During the Freezing Process of Water and Metal	6
Figure 3.	Schematics of Void Formation in a Solidifying Lithium Coolant in an SP-100 System	7
Figure 4.	Variation of System Pressure and Saturation Concentration of He in Li with Lithium Temperature	12
Figure 5.	Homogeneous Nucleation Potential During the Cooldown Process of Li in SP-100 PHTS	13
Figure 6.	Heterogeneous Nucleation Geometric Factor	14
Figure 7.	Schematic Representation of Freezing and He Segregation Processes	18
Figure 8.	Calculated Temperature Profile	24
Figure 9.	Calculated Dimensionless Concentration Profile	25
Figure 10.	Variation of Solidification Velocity and Wall Temperature with Time for Different Coolant Channel Widths	26
Figure 11.	Variation of Frozen Fraction for Different Coolant Channel Widths	27
Figure 12.	Evaluation of Voids During Lithium Coolant Cooldown and Freezing Coolant Channel Width = 0.01 m, Initial He Concentration = $4.26 \times 10^{-6} \text{ kg/m}^3$	28
Figure 13.	Evolution of Voids During Lithium Coolant Cooldown and Freezing, Coolant Channel Width = 0.05 m, Initial He Concentration = $4.26 \times 10^{-6} \text{ kg/m}^3$	29
Figure 14.	Schematics of Shrinkage Void Formation in a Solidifying Lithium Coolant in an SP-100 System	39
Figure 15.	Variation of Freezing Constant, λ , with Stefan Number	44
Figure 16.	Calculated Solid-Liquid Interface Velocity During Freeze of Li and LiF (Radiative BC, $T_a = 250 \text{ K}$)	45

Figure 17.	Temperature Variation in Wall Void Cases During Freeze of Li and LiF (Radiative BC, $T_a = 250$ K)	46
Figure 18.	Calculated Heat Flux Ratio inside Void During Freeze of Li and LiF (Radiative BC, $T_a = 250$ K)	47
Figure 19.	Temperature Variation, with Radiative BC Wall Void, $T_a = 1350$ K, During Thaw Process of Li and LiF	48
Figure 20.	Heat Flux Variation During Thaw Process of Li and LiF (Wall Void, Radiative BC, $T_a = 1,350$ K)	49
Figure 21.	Variation of Heat Flux Ratio Inside Void During Thaw Process of Li and LiF (Wall Void, Radiative BC, $T_a = 1350$ K)	50

LIST OF TABLES

	<u>Page</u>
Table 1. The SP-100 System Nominal Operating Conditions	33
Table 2. Temperature Ranges and the Free Energies of Formation of NbT, NbN and LiT in SP-100	33
Table 3. Thermal Properties and Base Case Parameters used in the Analysis of Helium Gas Segregation during Lithium Freezing.	34
Table 4. Thermal Properties and Base Case Parameters used in the Analysis of Freeze and Thaw Processes of Li and LiF.	35

1. INTRODUCTION

1.1 Background

The SP-100 Space Nuclear Power System, which is currently in the engineering development and testing phase, incorporates a fast flux, nuclear reactor which is cooled by a pumped liquid lithium (Li). The Li in the Primary Heat Transport System (PHTS), transports the reactor's thermal power to the Power Conversion Assemblies (PCAs), where it is partially converted into electricity. The residual heat is transported by liquid Li in the secondary loops from the Thermoelectric-Electromagnetic (TEM) pumps and the PCAs to the system's heat pipe radiator.

The operating temperatures of the primary and secondary Li coolants at the reactor nominal thermal power of 2.4 MW, are about 1350 K to 1375 K, and 800 K to 850 K, respectively. Because Li has a high melting point of -454 K, it will be frozen during launch and upon thawing and heating up to a nominal operating temperature of 1350 K, Li will undergo about 20-25% increase in volume (see Figure 1). To minimize the stresses in the walls of the reactor containment and/or the piping system during startup in orbit, voids are introduced throughout the PHTS and each primary and secondary loop is equipped with a gas separator/accumulator and an accumulator with gas loaded bellows, respectively.

Following a planned or an accidental shutdown, liquid Li in the primary and secondary coolant loops of the SP-100 system will eventually freeze. In the current SP-100 system design, the freezing process is controlled only by the natural law of cooling. The increase in the Li density during cooldown and freezing will stimulate formation of voids. Depending on the distribution of these voids, many different situations will arise

during the restart period of the SP-100 system. Homogeneously distributed voids within the solidified Li coolant, for example, would absorb the stress due to the volume increase of Li during the thaw process effectively. In this case, the stress in the walls of the coolant pipes, fuel pins and core container may not exceed those that cause deformation or failure of the materials. Ill posed voids, however, may lead to (a) mechanical failure of the coolant loop pipes and fuel elements due to excessive stresses, (b) thermal failure of structure or formation of hot spots during thaw. It is, therefore, important to understand their formation mechanisms and their effect on the system safety during rethaw.

1.2 Void Formation Mechanisms

In metal casting, volume shrinkage during freezing and bubble nucleation of dissolved gas atoms in the melt cause the formation of voids and results in a porous or leaky structure [Brick et al. (1977), Cahn & Haasen (1983)].

In the SP-100 system, helium (He) and tritium gas atoms are produced by neutron-lithium (n-Li) interactions in the reactor core. While tritium gas produced in the reactor core will readily diffuse through the niobium (Nb) walls to outer space, most of the He atoms will remain in the PHTS due to the very small diffusivity of He. McGhee, El-Genk and Rothrock (1989) have shown that Li coolant in the PHTS will be saturated with He gas within several days of operation and that the gas separators will only remove the amount of He gas in excess of the saturation concentration. It is, therefore, expected that He gas bubble might form, as in the metal casting process, during the cooldown and freeze processes of the Li coolant.

Variation of Specific Volume of Lithium

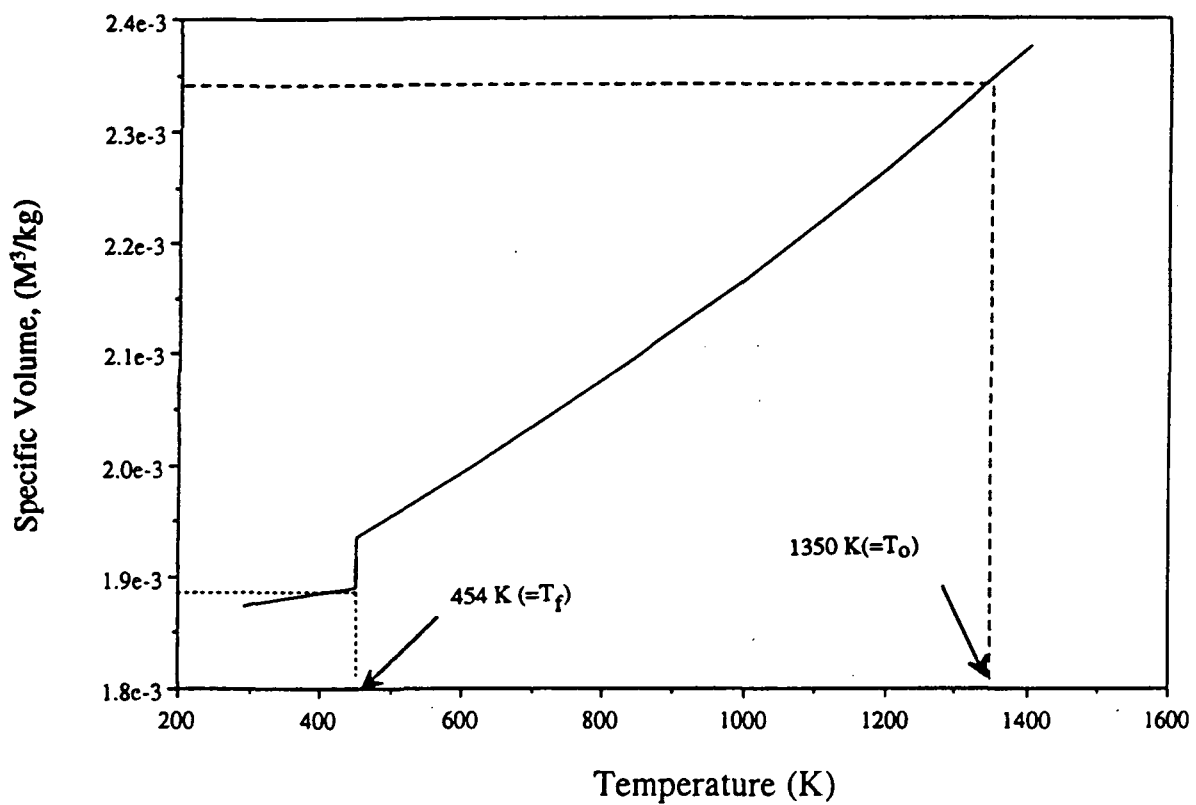


Figure 1. Variation of Specific Volume of Lithium

Two well known mechanisms of gas bubble formation are: (1) homogeneous nucleation (HN), and (2) heterogeneous nucleation (HTN). HN refers to the appearance of a gas nucleus in the bulk of liquid, away from container walls or suspended particles, while HTN refers to the formation of a gas nucleus on surfaces or suspended impurities. The gas concentration required for HN of bubbles could be orders of magnitude higher than the saturation concentration in Li. On the other hand, in a system rich in suspended impurities, the gas concentration required for bubble nucleation by HTN in liquid Li could be as low as the saturation concentration.

Another important mechanism of gas bubble formation during the freezing process is the segregation of dissolved gas atoms or molecules in a freezing medium. Segregation is a solute redistribution phenomenon during a freezing process. When the solubility limit of a solute in the solid phase is less than the solute concentration in the liquid phase, rejection of the solute by the S-L interface occurs as the freezing of the liquid progresses resulting in a buildup of the solute ahead of the S-L interface. Chalmers (1964) pointed out that in the case where gas is dissolved in a solidifying medium, segregation of gas in the liquid ahead of the solidification front can lead to the formation of gas voids. Figures 2a and 2b show gas void formation by segregation during the freezing processes of water and metal, respectively. In Chalmers (1964), seven different types of segregation are discussed including: (1) normal segregation, (2) grain boundary segregation, (3) cellular segregation, (4) dendritic segregation, (5) inverse segregation, (6) coring and intercrystalline segregation, and (7) gravity segregation. In microgravity, the last mechanism will not occur but the other six may occur, depending on the solidification process. The segregation of dissolved He atoms in liquid Li ahead of the solid-liquid (S-L) interface is expected to occur in the freezing process of Li coolant which may lead to the formation of gas bubbles during the process. The segregation mechanisms (2) - (6) require higher solidification velocities than that expected for normal

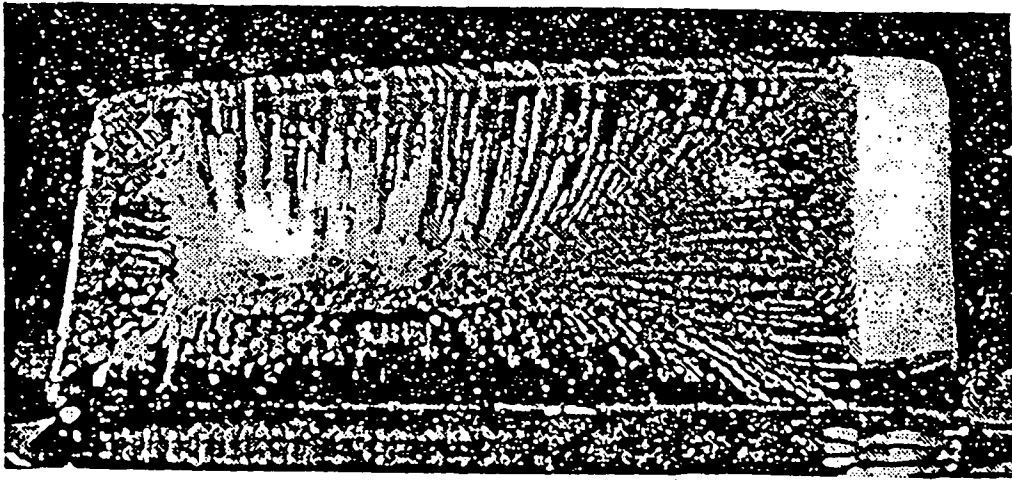
segregation, type (1). Because of the high heat capacity and latent heat of fusion of Li and the low heat rejection rate, since radiation is the only mode of heat rejection in the current design of the SP-100 system, the cooldown and freezing processes are expected to be very slow, hence normal segregation will be the more likely mechanism for formation of He gas bubbles in the SP-100 system.

The formation of He gas bubbles by normal segregation will be accompanied by volume shrinkage of Li upon freezing stimulating the formation of shrinkage voids. These voids may occur either at the solid/wall interface or at the liquid/wall interface (see Figure 3). While the former will occur in the absence of adhesion between solidified Li and Nb wall, the latter is expected if liquid Li poorly wets Nb.

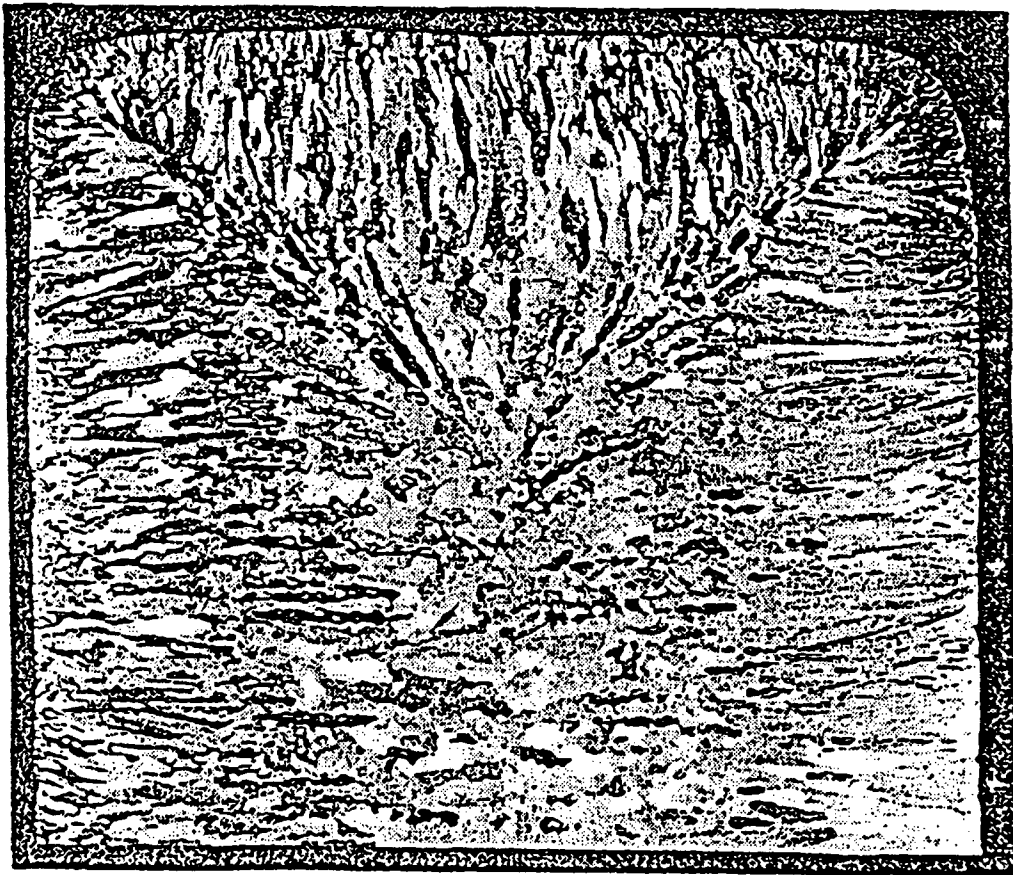
The potential for He gas bubble formation by HN, HTN, and normal segregation is investigated and the formation of voids due to volume shrinkage is quantified in Section 2. In Section 3, the research focuses on quantifying the thermal effects of shrinkage voids during the freeze and thaw processes.

1.3 Objectives

This research investigates: (1) the void formation mechanisms and the potential for forming voids during the cooldown and freezing processes of Li coolant in the SP-100 system after shutdown of the reactor in space, and (2) the thermal effect of void formation on the freeze and thaw processes of Li coolant. Also, investigated are the thermal effects of void formation on both freezing and subsequent thawing of LiF, which is being considered for thermal energy storage in space application by NASA. Results of Li and LiF are compared and discussed.

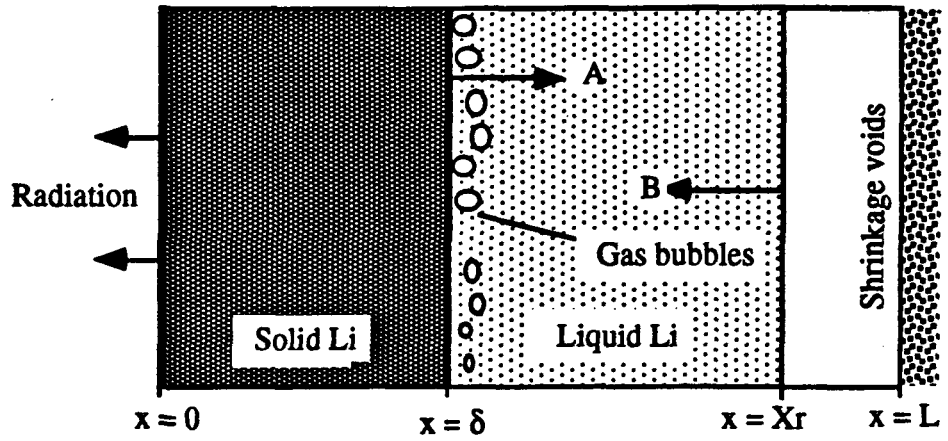


(a) Bubbles in ice cube .

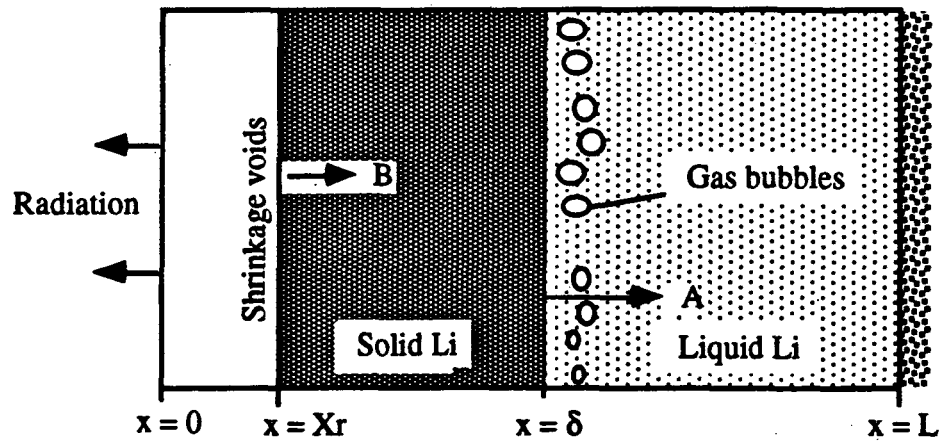


(b) Gas bubbles in a metal.

Figure 2. Gas Bubble Formation by Segregation during the Freezing Process of Water and Metal



(a) Shrinkage Void at Insulated Boundary



(b) Shrinkage Void at Wall /Solid Interface

Figure 3. Schematics of Void Formation in a Solidifying Lithium Coolant in a SP-100 System

2. VOID FORMATION MECHANISMS DURING THE COOLDOWN AND FREEZING PROCESSES OF LITHIUM COOLANT IN THE SP-100 SYSTEM

2.1 Homogeneous and Heterogeneous Nucleation of He Gas Bubbles During the Cooldown Process of Li Coolant

2.1.1 Theoretical Background

In order for a gas nucleus to be thermodynamically stable, its radius should be larger than a critical value. Van Stralen (1979) has shown that the supersaturation, SS_{HN} , necessary for HN of a gas nucleus of critical radius can be represented by:

$$SS_{HN} = \Delta C_h / C_{sat} = 2\sigma / r_c P_L, \quad (1)$$

where, $\Delta C_h = C_h - C_{sat}$. On the other hand, the supersaturation required for HTN of gas bubbles, SS_{HTN} , may be expressed as (Cole 1974):

$$SS_{HTN} = SS_{HN} F(\text{Geo}, \theta), \quad (2)$$

where F is a complex function of wetting angle, θ , and surface geometry. For a flat surface F is only a function of the liquid-solid wetting angle, θ

$$F(\theta) = 1 - \frac{(2 + \cos\theta)(1 - \cos\theta)^2}{4} \quad (3)$$

Since, F varies between 0 and 1, SS_{HTN} can be as small as 0 (when liquid Li does not wet the container's wall or when the liquid is rich in solid or gas impurities) and as large as SS_{HN} (when liquid Li perfectly wets the wall or the liquid is pure). An expression for r_{cF} in equation (1) is (Cole 1974):

$$r_{cr} = \left(\frac{3kT}{4\pi\sigma} \ln \left(\frac{n_s kT}{hJ} \right) - \frac{E_d}{kT} \right)^{0.5} \quad (4)$$

In this equation E_d can be reasonably taken to lie between 0 and the energy of formation of a gas cluster of radius r_{cr} ($0 < E_d < 4\pi r_{cr}^2 \sigma / 3$), and J can be assumed to lie somewhere between 10^1 and 10^{12} nuc./m³-s for what is normally thought of as a gas ebullition process. It can be shown that r_{cr} is approximately 1 nm, and is not a strong function of either J or E_d . Therefore, in the following assessment of the potential of He bubble nucleation during the cooldown process of liquid Li in SP-100 system, a value of $r_{cr} = 10^{-9}$ m is used. The values of C_{sat} are determined as functions of liquid Li pressure and temperature using the following correlation suggested by Slotnick et al. (1965):

$$C_{sat} = P_L \exp\left(-\frac{1752}{T} - 23.0\right) \quad (5)$$

The reduction of Li coolant volume during the cooldown process will be compensated for by volume increase in the gas separator/accumulator (GSA). If we assume an ideal gas system in the GSA, P_L in Equation (1) can be calculated from the ideal gas law:

$$\frac{P_L V}{T} = \frac{P_o V_o}{T_o} \quad (6)$$

The bubble nucleation potential (BNP) by either HN or HTN is defined as the ratio of actual supersaturation of the dissolved gas to supersaturation required for HN or HTN:

$$BNP = SS_{act}/SS_{HN} \text{ (or } SS_{HTN}), \quad (7)$$

He gas bubbles will nucleate when BNP is greater than or equal to unity.

2.1.2 Results and Discussion

In order to assess the potential of He gas bubble nucleation in the SP-100 PHTS, the initial He concentration in Li coolant, C_o , is taken equal to saturation value, C_{sat} , at

the nominal operating condition in the SP-100 prior to reactor shutdown (see Table 1). Using the system conditions listed in Table 1, the variations of P_L , C_s and BNP with Li temperature are calculated and the results are shown in Figures 4 and 5. In order for either HN or HTN of He bubble to occur the BNP should be higher than or equal to unity. However, as Figure 5 demonstrates, the BNP values for HN are much smaller than unity, hence HN of He gas bubbles is not possible throughout the entire cooldown process of Li coolant in SP-100. Furthermore, it can be deduced from Equation (2) and Figure 5 that in order for He gas bubbles to form by HTN, the value of $F(\theta)$ in Equation (3) needs to be as low as 2.5×10^{-3} , requiring a wetting angle $\theta = 150^\circ$ (see Figure 6). Such high wetting angle is not generally expected in a liquid metal-metal substrate system as in the SP-100. Liquid Li is known to perfectly wet metallic surfaces. Also, dewetting does not occur upon cooling of Li below the wetting temperature (673.5 K) once it is heated above the wetting temperature and maintained at the temperature for a while [Hoffman (1990)]. Therefore, it could be concluded that the formation of He bubbles by HTN during the cooldown process in the SP-100 PHTS is highly unlikely, provided all the system conditions are remaining as fabricated.

2.2 Potential Formation of Intermetallic Compounds During the Cooldown Process of Li Coolant and Their Relation to the Formation of He Gas Bubbles

It has been concluded in the previous section that the formation of He gas bubbles during the cooldown process of Li coolant is highly unlikely, provided all the system conditions are remaining as fabricated. However, should the characteristics of the metal substrate change due to the formation of intermetallic compounds, such as metal hydride or metal nitride of thickness as little as a few atom radii, the likelihood of dewetting of Li and the formation of He bubbles at the wall by HTN increases.

2.2.1 Potential Formation of Intermetallic Compounds

Because of their high compatibility with Li, Nb and Nb-1%Zr are used in the SP-100 system to fabricate the PHTS pipes and fuel cladding, respectively. As mentioned previously, the (n-Li) reactions in the reactor core produce tritium [McGhee, El-Genk and Rothrock (1989)]. Although the tritium's high diffusivity enables it to readily diffuse out from the PHTS, a small quantities of tritium may remain in the PHTS prior to reactor shutdown. The diffusivity of tritium in Nb rapidly decreases as the temperature of Nb is reduced [Alefeld and Volki (1978)], hence increasing the likelihood of Nb-T reaction during the cooldown process of Li in the SP-100 PHTS and the formation of Nb-T compounds at the inner surface of the pipes wall.

Another source for forming intermetallic compounds in SP-100 PHTS is nitrogen (N₂) gas in the nuclear fuel elements. Because, N₂ gas will be produced due to the dissociation of UN fuel during the operation of the SP-100 system. The amount of N₂ gas dissociated depends on the fuel temperature and burnup. Should the fuel cladding breach, N₂ gas will easily leak from the fuel into the Li coolant. It is also expected that N₂ gas will eventually diffuse through fuel cladding into Li coolant.

Table 2 shows that tritium and nitrogen readily react with Nb and form hydride and nitride at the reaction temperatures indicated. Since, the nominal operating temperature in the PHTS of the SP-100 system is about 1300 to 1350 K, formation of stable NbN is likely on the surface of fuel cladding or on the inner surfaces of the PHTS pipes. As the Li cools down after a reactor shutdown, within a temperature range of 673 <T<1273 K, the formation of a mixture of NbN and Nb₂N is expected. When the Li coolant temperature is below 973 K, the formation of LiT occurs and deposits saline LiT in the Li coolant. During the last stage of the cooldown process (T<573 K), the formation of NbT is expected.

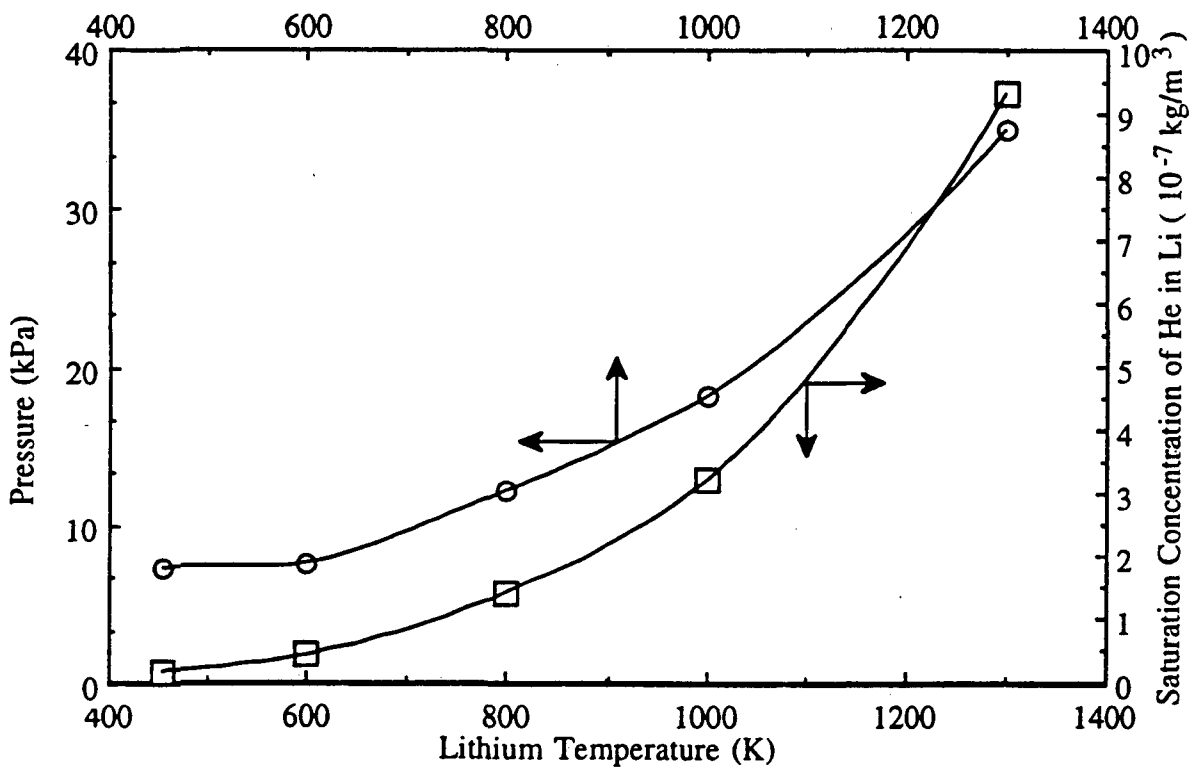


Figure 4. Variation of System Pressure and Saturation Concentration of He in Li with Lithium Temperature

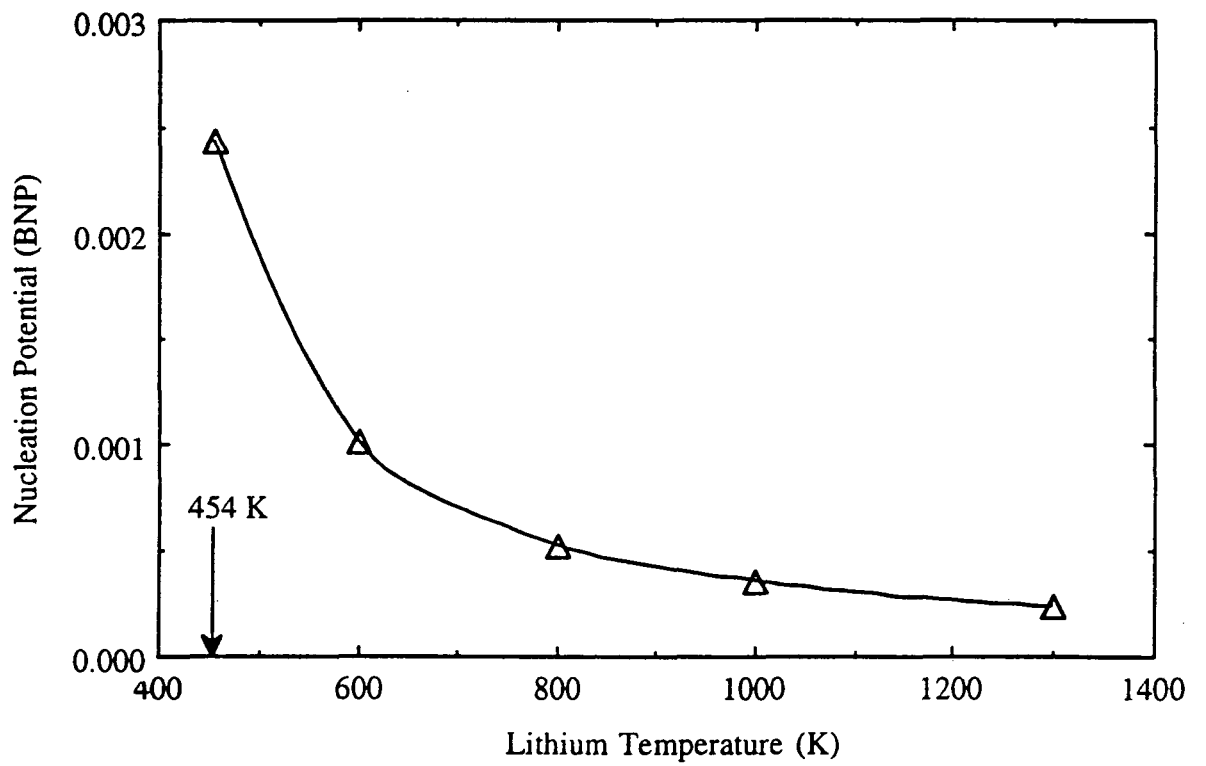


Figure 5. Homogeneous Nucleation Potential during the Cooldown Process of Li in SP-100 PHTS

HETEROGENEOUS NUCLEATION GEOMETRIC FACTOR

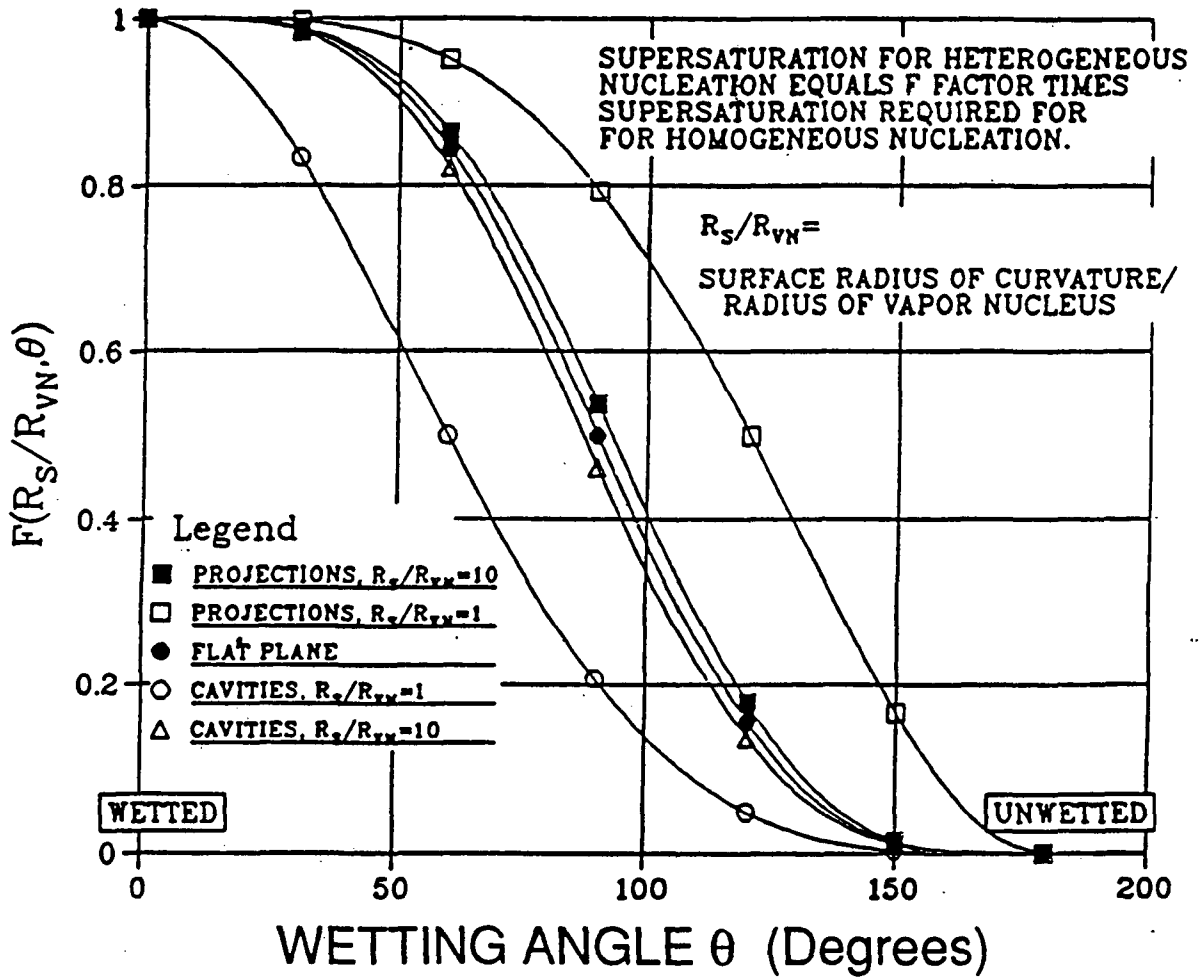


Figure 6. Heterogeneous Nucleation Geometric Factor

2.2.2 Discussion and Suggestion for Future Investigation

The deposit of LiT and the formation of NbT, NbN, and Nb₂N on inner surface of PHTS walls will increase the possibility of dewetting of Li from the walls, hence increasing the potential of void formation by HTN. However, in order to evaluate the potential, wetting angles of Li and mixture of Li and LiT on NbT, NbN, and Nb₂N are needed. Our literature search indicated that such information is not available, hence the potential of He gas bubble formation by HTN in conjunction with the formation and deposit of intermetallic compounds on the inner walls of coolant pipes, reactor core container, and the outer surface of fuel pins remain inconclusive. Experimental efforts to determine the wetting angles of Li on Nb-nitride and Nb-hydride substrates are, therefore, highly recommended.

2.3 He Gas Bubble Formation by Segregation of He Gas Atoms During the Freezing Process of Li Coolant

In the normal segregation process, the motion of He gas (solute) out of the solidified Li is in the direction of movement of solidification interface. The rate of He buildup ahead of the S-L interface is determined by the rate of He rejection from the solid at the solidification front and the rate of He diffusion away from the S-L interface into the liquid. The former process will tend to raise He concentration at the S-L interface, while the latter will reduce it. The rate of He rejection, $J(\delta(t))$, can be expressed as:

$$J(\delta(t)) = (C(\delta, t) - C_s^*) V(t) . \quad (8)$$

The solidification velocity, $V(t) (= d\delta(t)/dt)$, is obtained from the thermal analysis of the freezing process. In order to determine the potential of He gas formation by normal segregation, a physical model is developed in which the freezing of Li and the mass diffusion of He away from the S-L interface are coupled. In this model the void formation due to shrinkage of Li during freezing is also simulated.

2.3.1 Physical Model

For simplicity, a one dimensional system initially filled with liquid Li at its melting temperature is considered. The liquid Li is cooled by thermal radiation into space at one wall, $x = 0$, and is thermally insulated at the other wall, $x = L$. In Figure 3b, the shrinkage void forms at the wall/solidified crust interface, while in Figure 3a, it forms in the liquid at the insulated wall. In this chapter the model in Figure 3a is analyzed. The analysis of the model in Figure 3b will be described in chapter 3 in conjunction with the effect of shrinkage void formation on the freeze and thaw processes. In Figure 3a, the location and velocity of the boundary "B" of the liquid phase can be represented by $X_r = L - \Gamma\delta(t)$, $v(t) = -\Gamma(d\delta(t)/dt)$, respectively, where $\Gamma = (\rho_s/\rho_L - 1)$. The He concentration in liquid Li is assumed uniform prior to the initiation of the freezing process and equal to its saturation concentration in liquid Li at 1350 K ($C_0 = 4.26 \times 10^{-6} \text{ kg/m}^3$). The segregation model consists of two coupled models: (a) freezing model of liquid Li, and (b) mass diffusion model of He gas in liquid Li ahead of the S-L interface. Because the problem in Figure 3a entails two moving boundaries, S-L interface "A" and shrinkage void/liquid interface "B", and a boundary condition of the third kind (radiation), it is highly nonlinear. Hence, an exact analytical solution is not attainable. Instead, a numerical approach is used to solve coupled freezing and gas diffusion processes.

Freezing Model of Liquid Li

For the one dimensional system shown in Figures 3a and 7a, the heat balance equations in the liquid and solid Li and initial and boundary conditions can be written as:

(A) Liquid Li ($\delta \leq x \leq X_r$)

$$\rho_L C_{pL} \left(\frac{\partial T_L}{\partial t} + v \frac{\partial T_L}{\partial x} \right) = \frac{\partial}{\partial x} \left(k_L \frac{\partial T_L}{\partial x} \right) , \quad (9)$$

(B) Solid Li ($0 \leq x \leq \delta$)

$$\rho_s C_{ps} \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x} \left(k_s \frac{\partial T_s}{\partial x} \right) , \quad (10)$$

(C) Initial and Boundary Conditions

$$T(x,0) = T_f, \quad (11a)$$

$$k_s \frac{\partial T}{\partial x}(0, t) = \epsilon \sigma (T^4(0, t) - T_a^4) = h_r (T(0, t) - T_a), \quad (11b)$$

$$\frac{\partial T}{\partial x}(X_f, t) = 0, \quad (11c)$$

$$T_s(\delta, t) = T_L(\delta, t) = T_f, \quad (11d)$$

$$k_s \frac{\partial T_s}{\partial x}(\delta, t) - k_L \frac{\partial T_L}{\partial x}(\delta, t) = \rho_L \lambda \left(\frac{d\delta(t)}{dt} - v \right). \quad (11e)$$

Because of the high thermal conductivity of Li, the temperature differential in the frozen crust is expected to be small. Hence, constant properties can be assumed. When constant properties in each spatial mesh, Δx , within the solid and liquid Li are assumed, Equation 9 can be written in terms of enthalpy as [Shamsunder and Sparrow (1975), Hunter and Kuttler (1989)]:

$$\frac{\partial}{\partial t} \int_x^{x+\Delta x} \rho H dx + \left[\rho v H - k \frac{\partial T}{\partial x} \right]_{x+\Delta x} - \left[\rho v H - k \frac{\partial T}{\partial x} \right]_x = 0 \quad (12)$$

The dimensionless nodal enthalpy and temperature are defined as:

$$\theta \equiv \frac{1}{\rho \Delta x} \int_{\Delta x} \rho \frac{(H - H_{sf})}{\lambda} dx, \quad \phi \equiv \frac{C_p (T - T_f)}{\lambda} \quad (13)$$

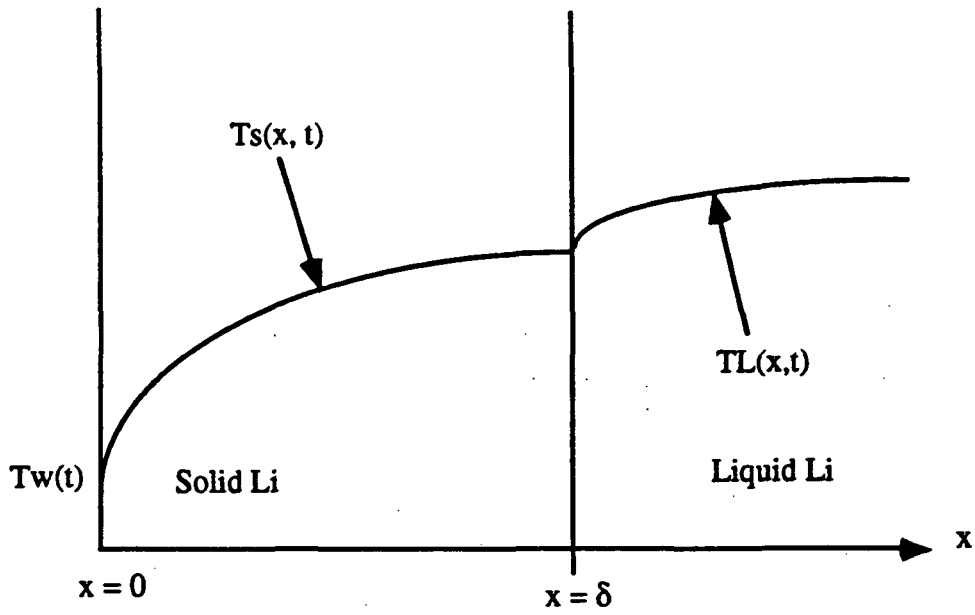
It has been shown by Shamsunder and Sparrow (1975), that θ and ϕ have the following relationships:

$$\phi = a + b\theta,$$

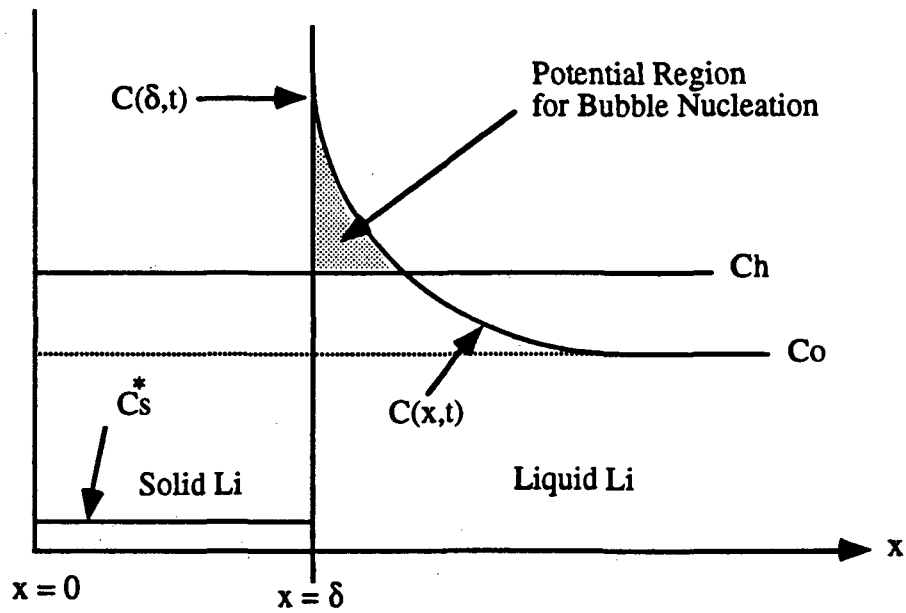
where,

$$a = 0, b = 1, \text{ for } \theta < 0 \quad (14)$$

$$a = 0, b = 0, \text{ for } 0 \leq \theta \leq 1.$$



(a) Freezing Process



(b) He Segregation Process

Figure 7. Schematic Representation of Freezing and He Segregation Processes

Using these dimensionless parameters, Equation (9) is transformed into:

$$\frac{\partial \theta}{\partial t} = \frac{1}{\Delta x \rho} \left[\frac{k}{C_p} \frac{\partial \phi}{\partial x} \right]_{x+\Delta x} - v \frac{\partial \theta}{\partial x} \quad (15)$$

It has been shown by Shamsunder and Sparrow (1975) that in the absence of convection term due to volume shrinkage, Equation (15) satisfies Equation (11e). It can also be shown that the same approach can be applied in the case with convection due to volume shrinkage to show that the energy conservation at the S-L interface is satisfied by Equation (15). Using backward finite difference formulation for the time derivative and forward difference formulation of the spacial derivatives Equation (15) is discretized as:

$$\frac{\theta_i^m - \theta_i^{m-1}}{\Delta t} = \frac{1}{\Delta x \rho} \left[\left(\frac{k}{C_p} \right)_e \frac{(\phi_{i+1}^{m-1} - \phi_i^m)}{\Delta x} - \left(\frac{k}{C_p} \right)_w \frac{(\phi_i^m - \phi_{i-1}^m)}{\Delta x} \right] + \Gamma \frac{(\delta^m - \delta^{m-1})}{\Delta t} \frac{(\theta_{i+1}^{m-1} - \theta_i^m)}{\Delta x} \quad (16)$$

The heat balance equation for the solid [Equation (10)] can be transformed and linearized as in Equations (15) and (16) by noting that v in the solid region is zero in and the last term of the Equation (16) drops out. The location of S-L interface, δ , is determined by $\delta = x_i - \theta_i \Delta x_i$ when the value of θ of the i -th node is less than 1 and greater than 0, since the frozen fraction of the node, α , can be conveniently related to θ as $\alpha = 1 - \theta$ from the definition of θ shown in Equation (13). The transformation and linearization of the initial and boundary conditions in Equation (11) are carried out consistently with those of the governing equations and the values of θ and ϕ at each time step are determined by a fully implicit scheme suggested by Shamsunder and Sparrow (1975). The program developed in accordance with the foregoing considerations (COPHASE.FOR) is listed in Appendix A-1 and input data required to run the program (COPHASE.INP) is listed in Appendix A-2.

Mass Diffusion Model of He Gas

The He segregation process during freezing of liquid Li is delineated in Figure 7b. The governing equation, initial and boundary conditions for He gas mass diffusion process in the liquid region ($x \geq \delta(t)$) are:

$$\frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}$$

(17)

$$C(x, 0) = C_0 \quad (18a)$$

$$J(\delta(t)) = (C(\delta, t) - C_s^*)V(t) \quad (18b)$$

$$\frac{\partial C}{\partial x}(X_r, t) = 0 \quad (18c)$$

Discretization of Equation (17) is done using Patankar's high flux approximation [Patankar (1980)], namely:

$$\frac{\Delta x_i}{\Delta t}(C_i^{n+1} - C_i^n) + J_{i,+} - J_{i,-} = 0 \quad (19)$$

The convection-diffusion flux at the left ($J_{i,-}$) and right ($J_{i,+}$) boundary of node i are defined as:

$$J_{i,\text{sign}} = vC_j + D_j^e F(\text{Pe}_j^e)(C_j - C_{j+1}), \quad (j = i \text{ for sign} = + \text{ and } j = i-1 \text{ for sign} = -) \quad (20a)$$

where,

$$D_j^e = 2D/(\Delta x_j + \Delta x_{j+1}), \quad (20b)$$

$$F(\text{Pe}_j^e) = \langle 0, (1 - 0.1|\text{Pe}_j^e|)^5 \rangle + \langle 0, -\text{Pe}_j^e \rangle, \quad (20c)$$

$$\text{Pe}_j^e = v/D_j^e. \quad (20d)$$

The operator $\langle a, b \rangle$ is the largest of a and b . After linearizing the initial and boundary conditions in a consistent manner with that of the governing equation, He concentration in the liquid ahead of S-L interface, $C(\delta, t)$, and the values of C_i at each time step are determined by using a tridiagonal matrix solver.

Volume Estimate of He Gas Voids

As shown in Figure 7b, when the He gas concentration ahead of the S-L interface, $C(\delta, t)$, reaches the HN concentration, He bubbles will nucleate and grow by absorbing gas atoms adjacent to them. The bubble growth will continue until all the gas atoms in excess of the solubility limit, or saturation concentration, C_{sat} , have diffused into the bubbles. Because detailed analysis of the bubble nucleation and growth processes is beyond the scope of this work, it is assumed that He gas atoms in excess of C_h will be instantaneously contained in bubbles. The volume of these bubbles is calculated as:

$$V_{He} = \frac{n_{He}RT}{P}, \quad (21)$$

where,

$$n_{He} = \frac{1}{A_w} \int (C(x, t) - C_h) dx \quad (22)$$

The numerical integration of the Equation (22) is carried out within the liquid region where the local He concentration, $C(x, t)$, is greater than C_h . The program simulating the segregation process and the gas bubble evolution (SEGR.FOR) is listed in Appendix B-1 and input data required to run the program (SEGR.INP) is listed in Appendix B-2.

2.3.2 Results and Discussion

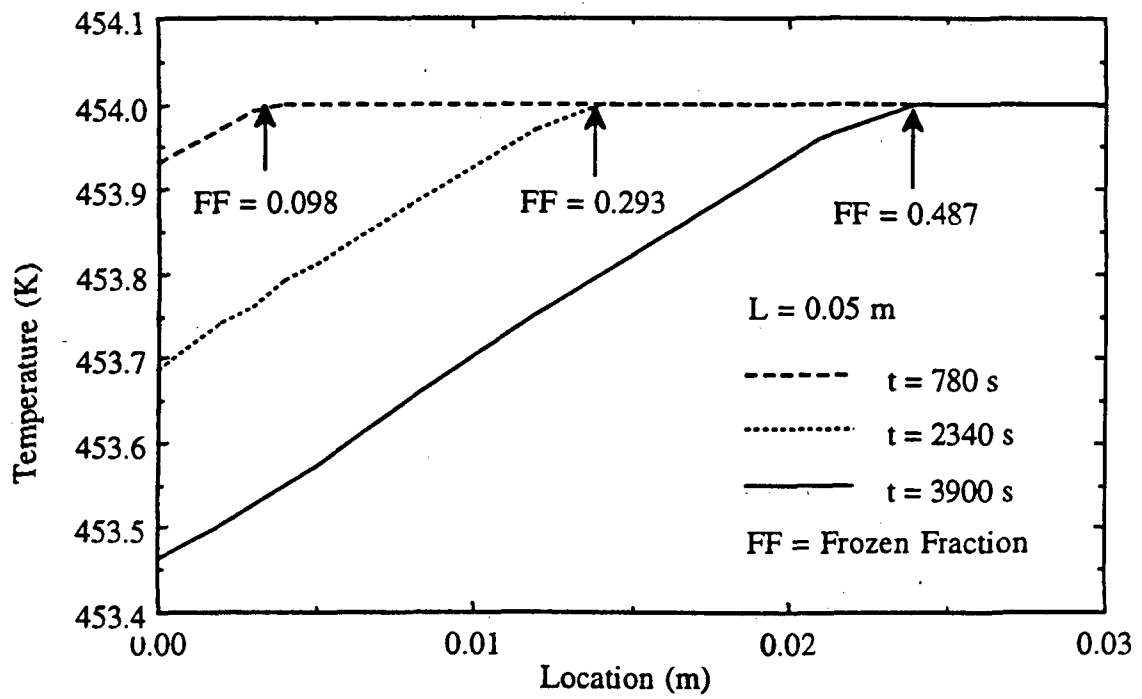
By using the thermal properties of Li, the base case parameters listed in Table 3 and the computer programs COPHASE.FOR and SEGR.FOR, the potential of He gas bubble formation by normal segregation and shrinkage of Li during the freezing of Li coolant in the SP-100 primary coolant system is assessed and the results are presented and discussed in this subsection.

The segregation model described earlier is applied to three different coolant channel widths (0.01m, 0.05m, and 0.1m). The results are presented in Figures 8, 9 and 10. Figure 8 delineates the calculated temperature profiles and Figure 9 shows the calculated He concentration profiles during the freezing process of liquid Li. It can be seen in Figure 8 that the temperature profile in the solid Li is almost linear. Also, the solidification velocities and the wall temperatures are independent of coolant channel width (see Figure 10). The solidification velocity and rate of change in the wall temperature are approximately 8×10^{-6} m/sec and -2×10^{-4} K/sec, respectively. Note that the freezing process of Li in SP-100 is extremely slow, suggesting a steady-state treatment of the problem could be sufficient. Also, a constant wall heat flux approximation may be used in the analysis of freezing process of Li with radiative heat transfer boundary. The low freezing velocity of Li is due to its high heat capacity and high latent heat of fusion as well as the low cooling rate at the wall. Figure 11 presents the calculated frozen fraction of the solidified liquid as a function of channel width, L.

The results in Figures 12 and 13 show the volume of He gas bubbles formed by normal segregation and that of shrinkage voids during the freezing process of Li. The results indicated that the onset of He bubble nucleation occurs approximately 350 seconds after the initiation of freezing at which the thickness of solidified Li is only about 3 mm. These results suggest that formation of He gas bubble by normal segregation would occur throughout the PHTS of the SP-100 system during the Li freezing. It can be also seen in Figure 12 that the contribution of segregation bubble is only about 2% of the total volume of the void at the completion of solidification of each coolant channel. This corresponds to 0.055% of the volume of the coolant channels considered.

One may argue that this amount of gas bubbles will not be sufficient to effectively remove the stress in the walls of PHTS during a subsequent restart of the SP-100. However, if these bubbles are captured by the freezing front into the solid Li, they will grow to compensate the volume shrinkage of Li. Thus, upon restart, the He

gas/shrinkage bubbles in the solid Li would effectively reduce the stress induced by the volume increase of Li. However, if the He gas bubbles are continuously driven by the solidification front, they will eventually collapse into the shrinkage voids. In order to minimize the stress during the restart of SP-100 and melting of Li, heating should be applied where the He/shrinkage void eventually form (see Figure 3). This would initially cause overheating of the wall (hot spot) due to the presence of the voids, but it will accommodate the increase in Li volume upon melting. It is not at all clear at present which of the two arrangement described in Figure 3 would occur in a solidifying Li in space. The subsequent research, therefore, focuses on the thermal effect of shrinkage void formation on the freeze and thaw processes of Li coolant in the SP-100 system.



(a) Temperature Profile

Figure 8. Calculated Temperature Profile

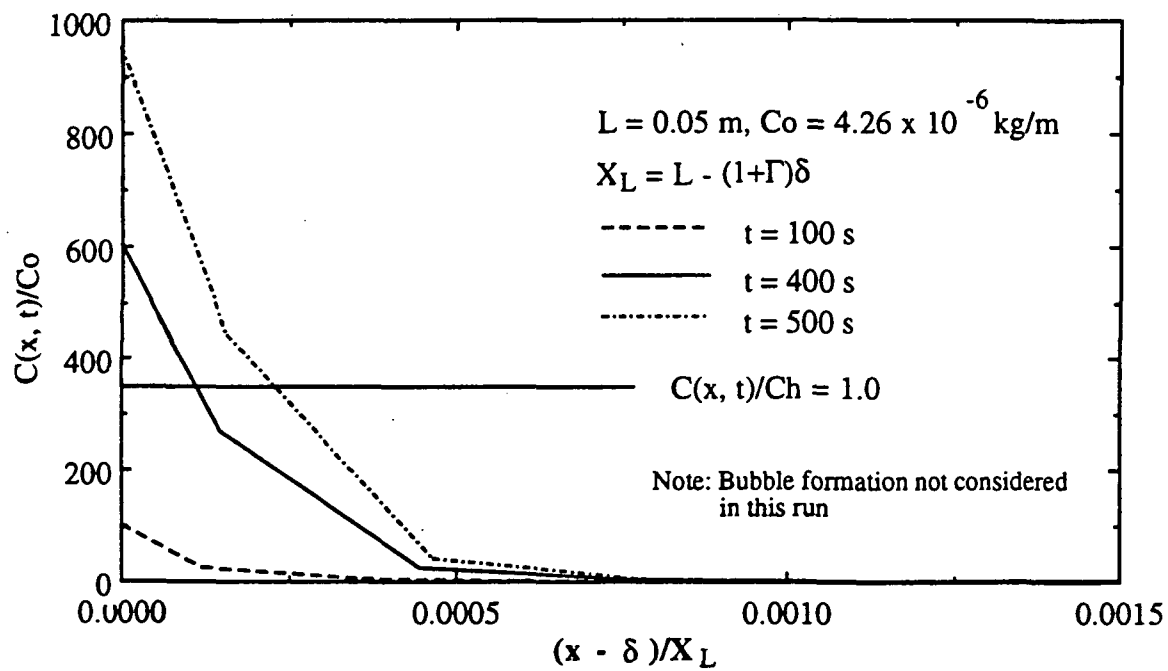


Figure 9. Calculated Dimensionless Concentration Profile

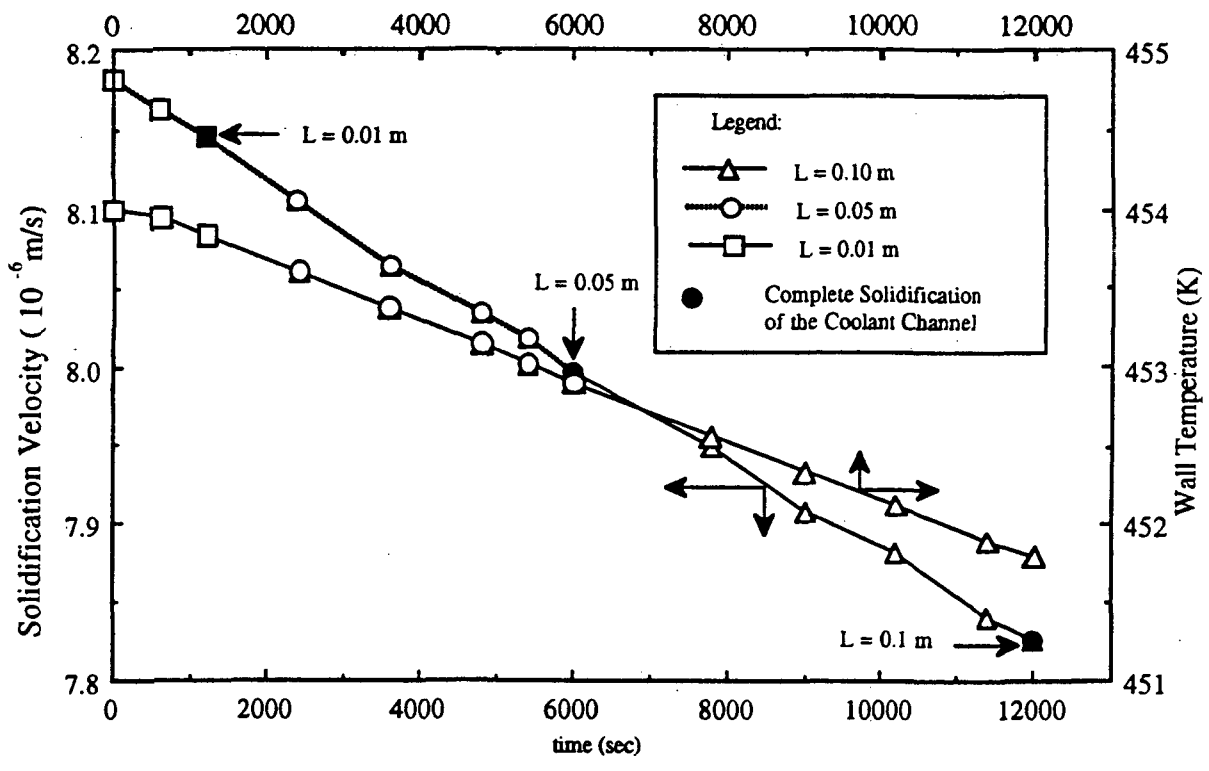


Figure 10. Variation of Solidification Velocity and Wall Temperature with Time for Different Coolant Channel Widths

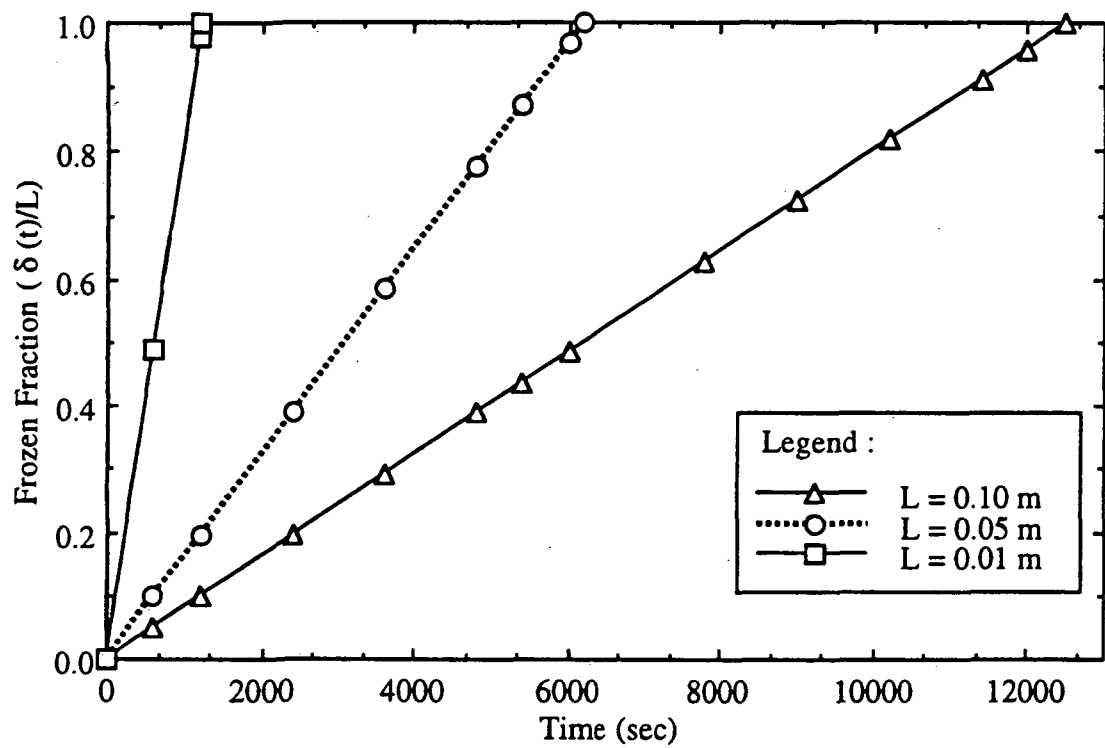


Figure 11. Variation of Frozen Fraction for Different Coolant Channel Widths

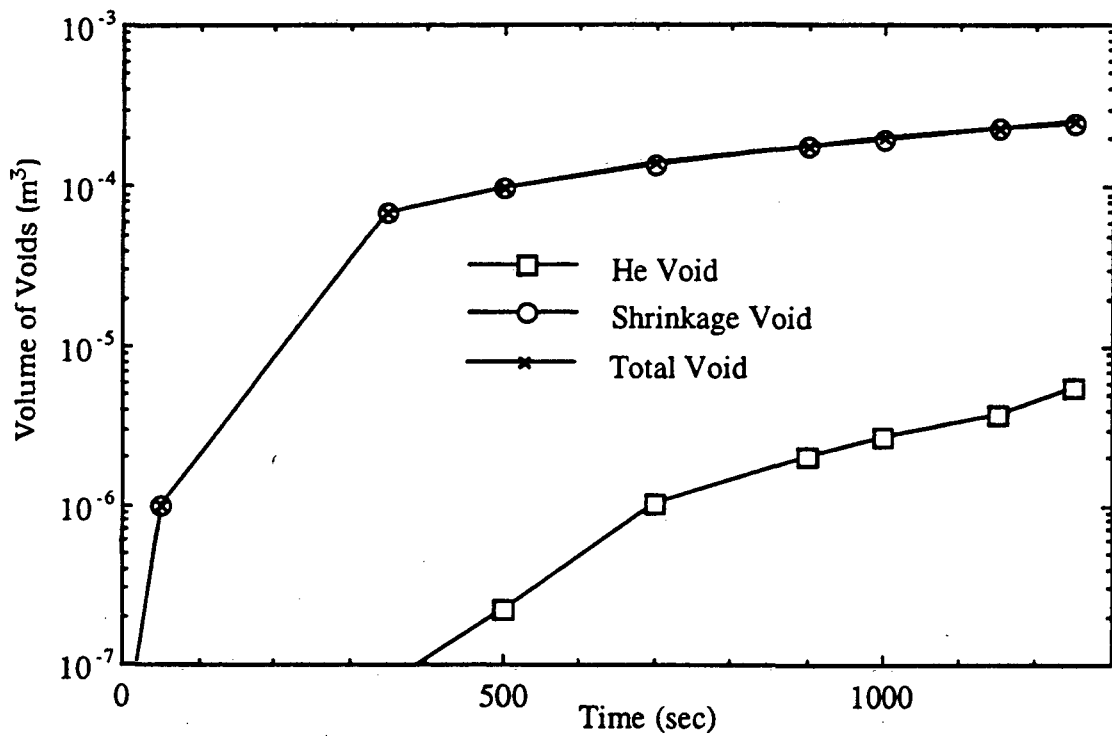


Figure 12. Evolution of Voids During Lithium Coolant Cooldown and Freezing (Coolant Channel Width = 0.01 m, Initial He Concentration = $4.26 \times 10^{-6} \text{ kg/m}^3$)

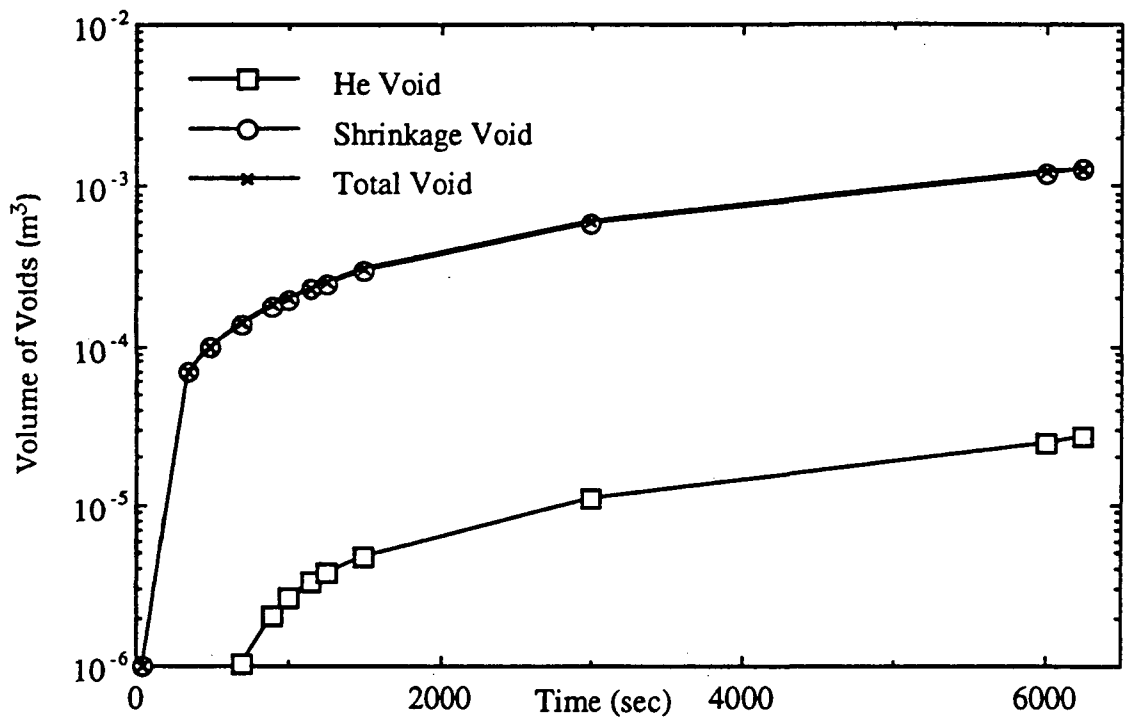


Figure 13. Evolution of Voids During Lithium Coolant Cooldown and Freezing, (Coolant Channel Width = 0.05 m, Initial He Concentration = $4.26 \times 10^{-6} \text{ kg/m}^3$)

2.4 Nomenclature

English

A_w	:	Atomic weight (g/mole)
BNP	:	Potential for bubble nucleation
C_p	:	Heat capacity (J/kg.K)
Δx	:	Spacial mesh size (m)
C_s^*	:	Solubility limit in the solid (kg/m ³)
C	:	Gas concentration concentration (kg/m ³)
D	:	Diffusion coefficient (m ² /s)
E_d	:	Activation energy for diffusion of a molecule of gas through the liquid (J)
H	:	Enthalpy (J/kg)
h	:	Boltzman constant (6.26×10^{-34} J/s)
h_r	:	Radiative heat transfer coefficient (W/m ² .K)W//m ² .K)
J	:	Nucleation rate in Equation (4) (Nucleations/s)
J	:	Convection-diffusion flux (kg/m ² .s)
n_t	:	Number density of gas molecules (molecules/m ³)
k	:	Thermal conductivity (J/m.K)
L	:	Coolant channel width (m)
n_{He}	:	Number of moles of He gas
P	:	Pressure (Pa)
Pe	:	Peclet number in Equation (20d)
R	:	Gas Constant (8.3144 J/mole.K)
r_{cr}	:	Critical radius of bubble (m)
T	:	Temperature (K)
t	:	Time (s)

$V(t)$:	S-L interface velocity (m/s)
V	:	Volume of the PHTS (m^3)
V_{He}	:	Volume of He bubbles (m^3)
v	:	Material velocity due to volume shrinkage (m/s)
X_r	:	Location of shrinkage void/liquid (or solid) interface (m)
x	:	Spacial coordinate (m)

Greek

δ	:	Solid crust thickness (m)
ϵ	:	Emissivity
ϕ	:	Dimensionless nodal temperature
λ	:	Latent heat of fusion (J/kg)
θ	:	Dimensionless nodal enthalpy or Wetting angle
α	:	Frozen fraction of a node
Γ	:	$\rho_s/\rho_L - 1$
ρ	:	Density (kg/m^3)
σ	:	Surface tension in Equation (1) (N/m)
σ	:	Stefan-Boltzman constant ($5.67 \times 10^{-8} W/m^2 K^4$)

Superscripts

e	:	Right boundary of a node
$n+1$ or m	:	Present time step
n or $m-1$:	Previous time step

Subscripts

a	:	Ambient
SS	:	Supersaturation
act	:	Actual
e	:	Right boundary of a node

f : At melting temperature
HN, h: Homogeneous nucleation
HTN : Heterogeneous nucleation
ij : i-th and j-th node, respectively
o : Initial condition
s : Solid
L : Liquid
sat : Saturation
w : Left boundary of a node

Table 1. The SP-100 System Nominal Operating Conditions.

Pressure	3.5 x 10 ⁴ Pa
Temperature	1350 K
Li Mass in the PHTS	110 kg
Li volume in the PHTS	255 Liter
Gas Separator/Accumulator volume	35 Liter
Average He concentration	4.26 x 10 ⁻⁶ kg/m ³

Table 2. Temperature Ranges and the Free Energies of Formation of NbT, NbN and LiT in SP-100.

Reaction	Temperature	$\Delta F(\text{kcal/mole})^a$
(1) NbN Formation	T > 1273 K	- 50.1
(2) Mixture of Nb ₂ N and NbN Formation	673 < T < 1273 K	- 54.0
(3) LiT Formation	773 < T < 973 K	- 16.7
(4) Full Dissociation of LiT	T > 973 K	
(5) NbT Formation	T < 573 K	- 3.2

a. The free energy of formation is the value at T = 298 K.

**Table 3. Thermal Properties and Base Case Parameters
Used in the Analysis of Helium Gas Segregation
During Lithium Freezing**

<u>Material</u>	<u>Property</u>	<u>Value</u>
<u>Liquid Li</u>	Thermal conductivity	42.8 J/s.m.K
	Density	517 kg/m ³
	Heat capacity	4.384 x 10 ³ J/kg.K
	Thermal diffusivity	1.89 x 10 ⁻⁵ m ² /s
<u>Solid Li</u>	Thermal conductivity	75.8 J/s.m.K
	Density	530 kg/m ³
	Heat capacity	3.78 x 10 ³ J/kg.K
	Thermal diffusivity	3.78 x 10 ⁻⁵ m ² /s
<u>Base Case Parameters</u>	Initial He concentration	4.26 x 10 ⁻⁶ kg/m ³
	Diffusivity of He in liquid Li	5.96 x 10 ⁻⁹ m ² /s
	Diffusivity of He in solid Li	Negligible
	Li Latent Heat of Fusion	4.321 x 10 ⁵ J/kg
	Li Freezing Temperature	454 K

Table 4. Thermal Properties and Base Case Parameters used in the Analysis of Freeze and Thaw Processes of Li and LiF

Material	Properties	Liquid	Solid	Units
Li	k	42.8	75.8	W/m.K
	ρ	517	530	kg/m ³
	C _p	4384	3780	J/kg.K
	α	1.89 x 10 ⁻⁵	3.78 x 10 ⁻⁵	m ² /s
		H _{sl}	4.321 x 10 ⁵	J/kg
	T _f	454		K
LiF	k	1.30	5.00	W/m.K
	ρ	1376	1792	kg/m ³
	C _p	2779	2470	J/kg.K
	α	3.40 x 10 ⁻⁵	2.94 x 10 ⁻⁵	m ² /s
		H _{sl}	3.473 x 10 ⁵	J/kg
	T _f	1122		K
PWC-11	k		23.9	W/m.K
	ρ		6490	kg/m ³
	C _p		323.4	J/kg.K
	α		1.14 x 10 ⁻⁵	m ² /s
	T _f		2740	K
LiF vapor	k	0.017		W/m.K
He gas	k	0.1678		W/m.K
<u>Base Case Parameters</u>				
	Ambient Temperature of Space		250	K
	Temperature of Wall or Heat Source			
	Freeze:		250	K
	Thaw:		1350	K
	Thickness of PCM at Liquid State		0.05	m
	PWC-11 Wall Thickness		7.6x10 ⁻⁴	m
	Emissivity			
	at outer surface of the wall		0.8	
	at inner surface of the wall		0.5	

3. THE EFFECTS OF SHRINKAGE VOID FORMATION ON THE FREEZE AND THAW PROCESSES OF LITHIUM COOLANT

3.1 Physical Model

As mentioned in the previous chapter, because the contribution of gas voids volume to total voids forms in the SP-100 system is small (~2%), its effect on the thermal behavior during the freeze and thaw processes is expected to be small and may be negligible. Therefore, in this chapter, only the effect of shrinkage void formation on the freeze and thaw processes is considered. Instead, cases with lithium-fluoride are analyzed for the comparison's purpose and to satisfy the practical interests, since LiF exhibits much larger volume shrinkage upon freezing (23.2% compared to 2.5% for the case of Li) and it is known as an excellent phase change material (PCM) for thermal energy storage (TES) for solar dynamic power system. In addition, it is important to show the temperature variation in the heat transfer surface, the model being used in this analysis considers the effect of heat transfer wall.

A simple numerical scheme is developed to simulate two different modes of shrinkage void formation in a finite one dimensional system, namely: (1) a shrinkage void forming at solid-wall interface (or wall void WV afterwards) (Figure 14a); and, (2) a shrinkage void forming at the center (or adiabatic boundary) of the system (center void or CV, afterwards) (Figure 14b). The former will occur in the absence of good adhesion between solidified PCM and the wall, while the latter is expected if liquid poorly wets the wall. Modeling this problem requires solving the heat transfer equations with two moving boundaries, namely, the solid-liquid (S-L) interface and the PCM-void (P-V) interface, subject to radiative heat transfer at the wall.

Because an analytical solution for such non-linear problems is not attainable, a numerical solution based on a single (solid/liquid) cell approach is used. The problem studied is that of a one dimensional slab initially filled with PCM at its fusion temperature in a container having a wall thickness, t_c , symmetric about $x = L$ (see Figure 14). The wall is either radiatively cooled into space or radiatively heated from an isothermal heat source (e.g. a thaw heat pipe) at a temperature, T_2 . The other side of the slab, $x = L$, is thermally insulated. The heat transfer within the void, that is forming during the freezing process, is by conduction and radiation. The conductance of the void is assumed to vary inversely with the size of void, i.e. $h_{vc} = k_v/\delta_v$ [Wilson and Solomon, 1986, Hunter and Kuttler, 1983]. The void is assumed to be filled with He gas and LiF vapor for the cases of Li and LiF, respectively. The sensible heat of the vapor is assumed negligible. Also, the temperature differential in the frozen crust is expected to be small because of the high thermal conductivity of Li. Hence, constant properties are assumed. During the freezing process, the location and velocity of the boundary "B" of the solid—represented by $X_r = \gamma S(t)$, $v(t) = \gamma(dS(t)/dt)$, respectively, where $\gamma = (1 - \rho_L/\rho_s)$. In Figure 14b, the boundary "B" representing the liquid-void interface moves in the opposite direction, hence $X_r = L - \Gamma\delta(t)$, and $v(t) = -\Gamma(d\delta(t)/dt)$, where $\Gamma = (\rho_s/\rho_L - 1)$.

During the thaw process, the location and velocity of the boundary "B" in Figure 14a can be represented as, $X_r = X_{ri} - \gamma\delta(t)$, and $v(t) = -\gamma(d\delta(t)/dt)$, respectively, where, X_{ri} is the initial thickness of void. In Figure 14b, $X_r = L - X_{ri} + \Gamma\delta(t)$, and $v(t) = \Gamma(d\delta(t)/dt)$.

Governing Equations

For the one-dimensional system shown in Figure 14 the temperature in the receding phases is uniform and equal to fusion temperature. The heat balance equations

in the developing phase (subscript d), and in the heat transfer wall (subscript c) are:

Developing Phase

$$\rho_d C_{pd} \frac{\partial T_d}{\partial t} = \frac{\partial}{\partial x} \left(k_d \frac{\partial T_d}{\partial x} \right), \quad (22)$$

Heat Transfer Wall

$$\rho_c C_{pc} \frac{\partial T_c}{\partial t} = \frac{\partial}{\partial x} \left(k_c \frac{\partial T_c}{\partial x} \right), \quad (23)$$

Initial and Boundary Conditions

$$T(x, 0) = T_f, \quad (24)$$

$$T_s(S(t), t) = T_L(S(t), t) = T_f, \quad (25)$$

$$k_s \frac{\partial T_s}{\partial x}(S(t), t) - k_L \frac{\partial T_L}{\partial x}(S(t), t) = \rho_L H_d \left(\frac{dS(t)}{dt} - v \right), \quad (26)$$

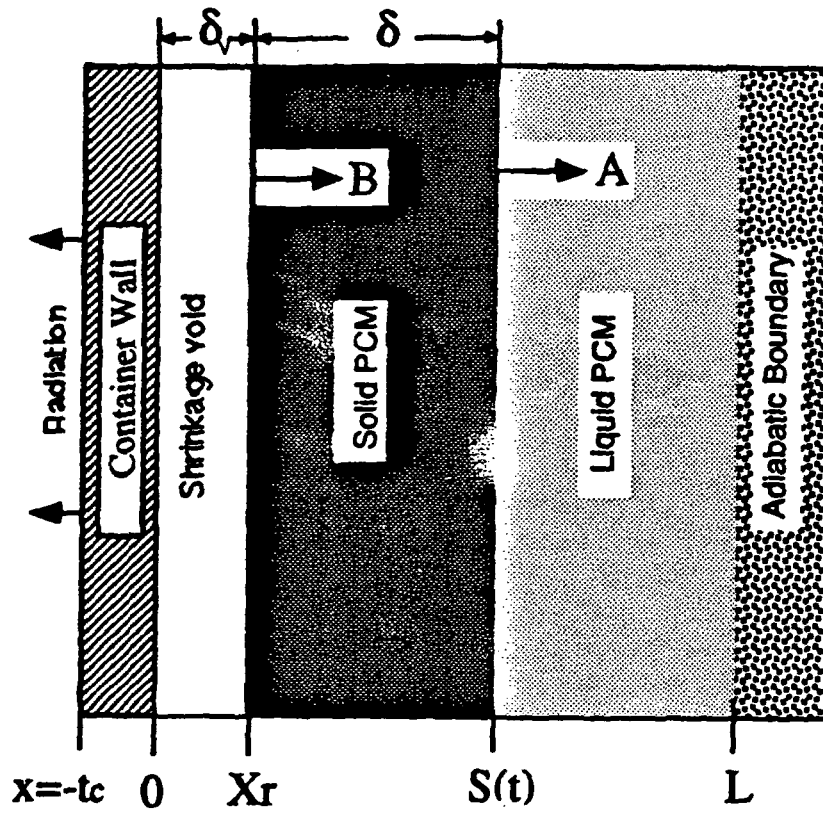
and

$$k_c \frac{\partial T}{\partial x}(-t_c, t) = \varepsilon \sigma (T^4(-t_c, t) - T_a^4), \quad (27)$$

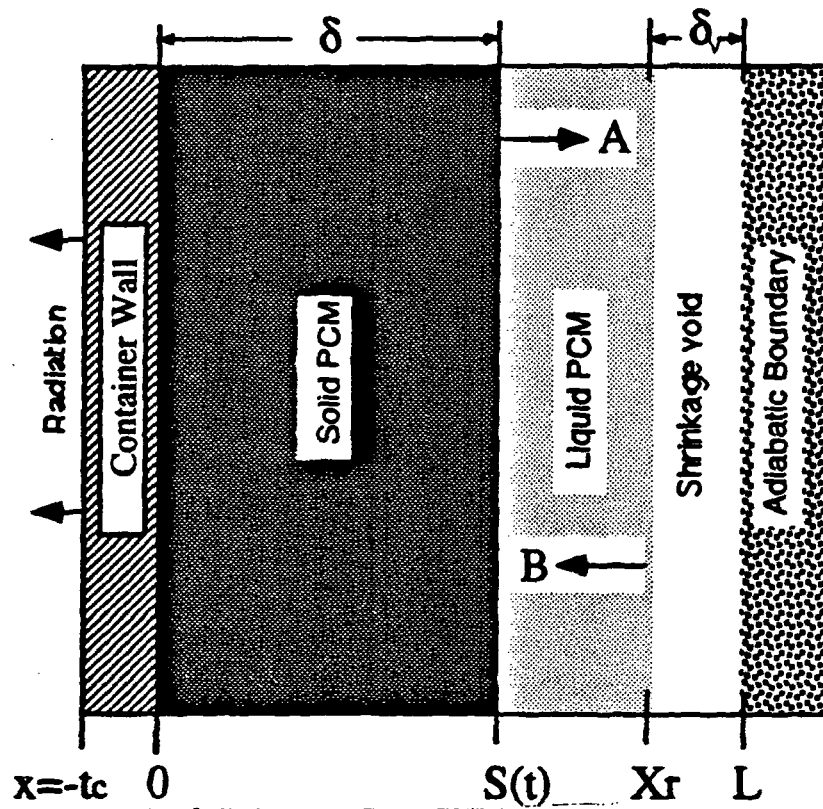
$$k_s \frac{\partial T}{\partial x}(X_r, t) = \varepsilon \sigma (T^4(X_r, t) - T^4(0, t)) + \frac{k_v}{\delta_v} (T(X_r, t) - T(0, t)), \quad \text{for Fig 14a,} \quad (28)$$

$$\frac{\partial T}{\partial x}(X_r, t) = 0, \quad \text{for Fig 14b.} \quad (29)$$

In a recent work by Yang and El-Genk (1991), it has been shown that when a radiative heat transfer boundary condition is applied to the freezing of Li, a linear temperature profile develops within the solid crust and quasi-steady state approximations can be used. When the thickness of a developing phase is small, a linear temperature profile may be used. The governing equations are linearized using a fully implicit scheme as follows:



(a) Shrinkage Void Forming at Solid/Wall Interface



(b) Shrinkage Void Forming at Center of System

Figure 14. Schematics of Shrinkage Void Formation in a Solidifying Lithium Coolant in a SP-100 System

Developing Phase

$$\dot{q}_1 - \dot{q}_{12} = [\rho_d C_{pd} (T_2^{n+1} \delta^{n+1} - T_2^n \delta^n) - \rho_d C_{pr} T_f (\delta^{n+1} - \delta^n)] / \Delta t, \quad (30)$$

where,

$$\dot{q}_1 = -h_{01} (T_1^{n+1} - T_a), \quad (31)$$

$$\dot{q}_{12} = -h_{12} (T_2^{n+1} - T_1^{n+1}), \quad (32)$$

$$\dot{q}_2 = -h_2 (T_f - T_2^{n+1}), \quad (33)$$

$$h_{01} = (T_1^2 + T_a^2) (T_1 + T_a) / [1/\epsilon\sigma + 4T_1/h_1], \quad (34)$$

$$h_1 = \frac{2K_c}{t_c}, \quad (35)$$

$$h_{12} = [1/h_1 + 1/h_v + 1/h_2]^{-1}, \quad (36)$$

$$h_2 = \frac{2K_d}{\delta}, \quad (37)$$

$$h_v = \frac{K_v}{\delta_v} + \epsilon\sigma (T_3^2 + T_4^2) (T_3 + T_4), \quad (38)$$

$$T_3 = h_{12} \left[\left(\frac{1}{h_2} + \frac{1}{h_v} \right) T_1 + \frac{T_2}{h_1} \right], \quad (39)$$

$$T_4 = h_{12} \left[\frac{T_2}{h_2} + \left(\frac{1}{h_1} + \frac{1}{h_v} \right) T_1 \right], \quad (40)$$

Heat Transfer Wall

$$\dot{q}_1 - \dot{q}_{12} = \rho_c C_{pc} t_c \frac{(T_1^{n+1} - T_1^n)}{\Delta t}. \quad (41)$$

The superscripts n and n+1 represent previous and present time steps. In order to solve for the temperatures of the wall and developing phase, the thickness of the developing phase, δ , should be known. An iterative procedure is used to determine δ by solving the linearized heat balance at the S-L interface:

$$\frac{2k_d(T_f - T_2^{n+1})}{\delta} = (Pa)\rho_s H_{sl} \left(\frac{\delta^{n+1} - \delta^n}{\Delta t} \right), \quad (42)$$

where, Pa is equal to 1 for freezing and -1 for thawing.

The computer program developed to assess the effect of shrinkage void on the freezing process of Li and LiF (FREZ.FOR) and that for melting process (MELT.FOR) are listed in the Appendices C and D, respectively.

3.2 Results and Discussion

3.2.1 Comparison with Available Analytical Solution

The accuracy of the numerical scheme is verified by making a comparison with Wilson & Solomon's analytical solution for a constant wall temperature (Wilson and Solomon, 1986). The thermal properties and base case parameters used in this comparison and in the subsequent analyses are shown in Table 4. In this comparison, it is assumed that conduction in the void is the only mode of heat transfer. The results are shown in Figure 15. This figure shows that the numerical solution is in reasonable agreement with the analytical solution for the base cases of interest (error of less than 10%). However, the error in the freezing constant for the cases with a wall void is larger (as much as 26%) than that with a center void. Figure 15 also shows that for base case conditions (St= 1.78 and 6.20 for Li and LiF, respectively) freezing constants for the wall void cases are approximately 34% and 19% of those for the center void cases. It is also shown that in the center void cases, Li and LiF have similar freezing constants, while in the wall void cases, LiF has a much lower freezing constant than that for Li, due to the larger void size of the former.

3.2.2 Freezing with Radiative Heat Transfer Boundary

The results of the freezing process with a radiative boundary condition are shown in Figures (16) through (18). Figure 16 shows that because the difference between the fusion temperature of Li (454 K) and the ambient (250 K) is relatively small and the

thermal conductivity of Li is high, the freezing velocity for Li is almost constant. Conversely, because of the high fusion temperature of the LiF (1122 K) the temperature differential between the wall and ambient is approximately three times higher than in the case of Li, the freezing velocity of LiF is an order of magnitude higher. As the void size and crust thickness increase (both have lower thermal conductance than in the case of Li), the wall temperature decreases, resulting in a lower freezing velocity. This velocity is still an order of magnitude higher than that of Li (see Figure 16). This figure also shows that while the location of the void negligibly affects the freezing of the Li, it significantly influences the freezing velocity of LiF. As Figure 16 demonstrates, the freezing velocity for LiF, in case of a void forming at the wall, is about half that in the case where the void forms at the opposite adiabatic boundary. Figures 17 and 18 shows that because the LiF fusion temperature is much higher and void size is larger than those of Li, the ratio of conduction to radiation heat transfer through the LiF void is about four orders of magnitude lower than that for Li.

3.2.3 Thaw with Radiative Heat Transfer Boundary

The thaw process with a radiative boundary has a practical importance to space applications. The thaw process begins by assuming that a shrinkage void has formed either at wall or at the center of a system (or adiabatic boundary). The size of void is equal to that resulting from a complete solidification of liquid initially filled in a container, having a width L . In the base case, void thickness is 1.23 mm for Li and 11.6 mm for LiF.

The results are delineated in Figures 19 through 21. At the start of the thaw process of Li the heat transfer to the frozen crust is limited by the heat transfer through the void. This causes a large fraction of the heat input to be absorbed in the wall, resulting in a higher wall temperature (see Figure 19). However, as the Li melts, reducing the size of the void, a smaller fraction of the heat input is absorbed in the wall,

causing the rise rate of the wall temperature to decrease. Eventually, when the heat transferring through the void equals the heat input, the wall temperature reaches a maximum value (see Figure 20). Beyond this point, the wall temperature decreases with time as the void size becomes very small. Subsequently, the heat transfer rate through the void exceeds the heat input; the difference is compensated for by the decrease in the sensible heat of the wall. The variation of the heat flux ratio inside the void during the thaw process is delineated in Figure 21.

In the case of LiF, because the initial void size is about an order of magnitude larger than that of Li, the thaw of LiF is always limited by the heat transfer through the void. This causes the wall temperature to rise monotonically as the thaw process continues. As shown in Figure 19, the maximum wall temperature during Li thaw (990 K) is about two-thirds that of LiF (1336 K). The peak wall temperature during Li thaw is much lower than the melting temperature of the wall materials in the SP-100 (PWC-11), suggesting that a development of hot spots is unlikely during thaw in the SP-100 system.

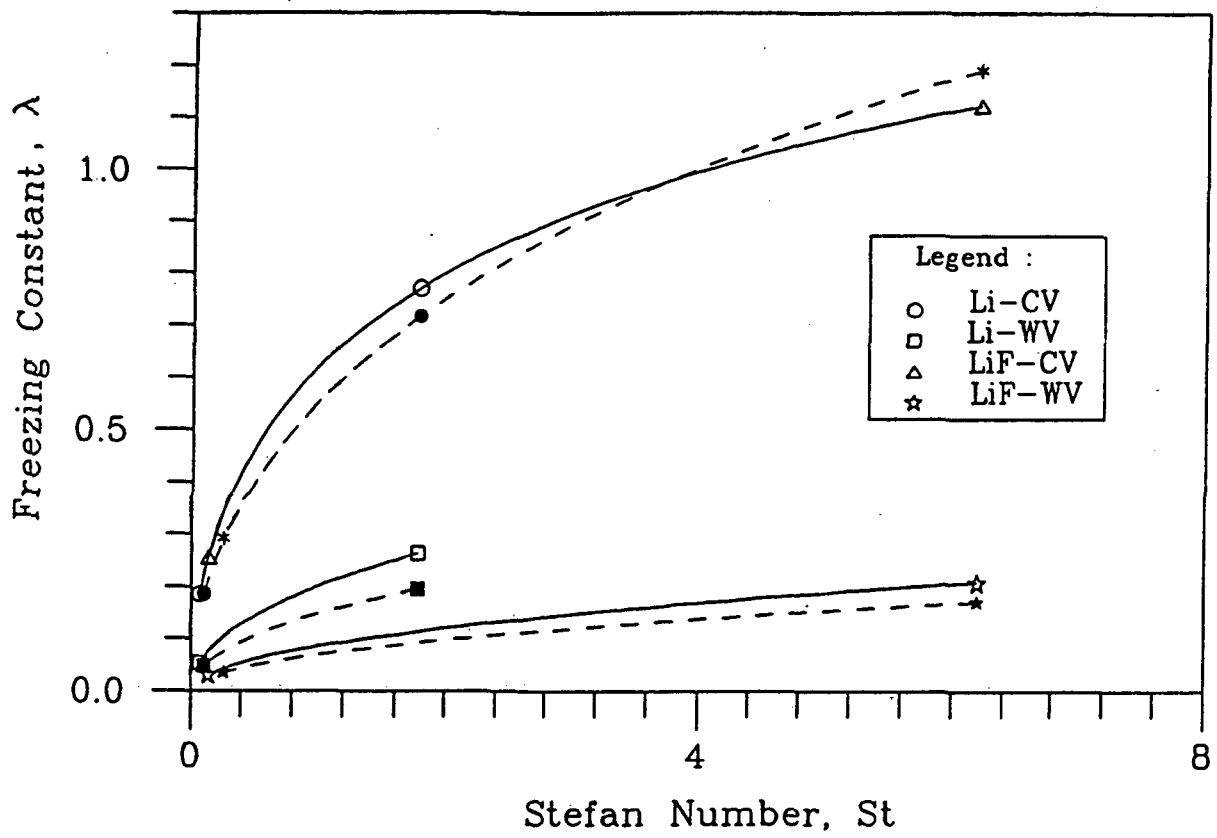


Figure 15. Variation of Freezing Constant, λ , with Stefan Number

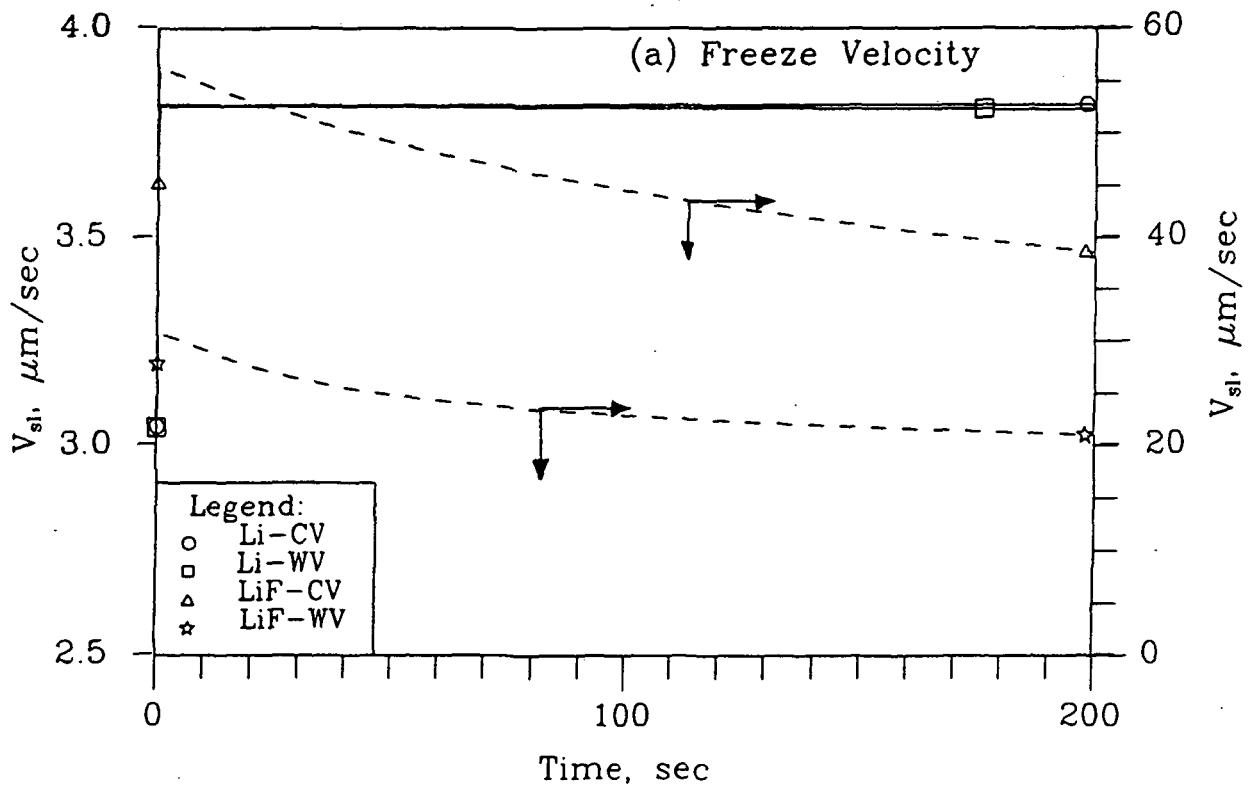


Figure 16. Calculated Solid-Liquid Interface Velocity During Freeze of Li and LiF (Radiative BC, $T_a = 250$ K)

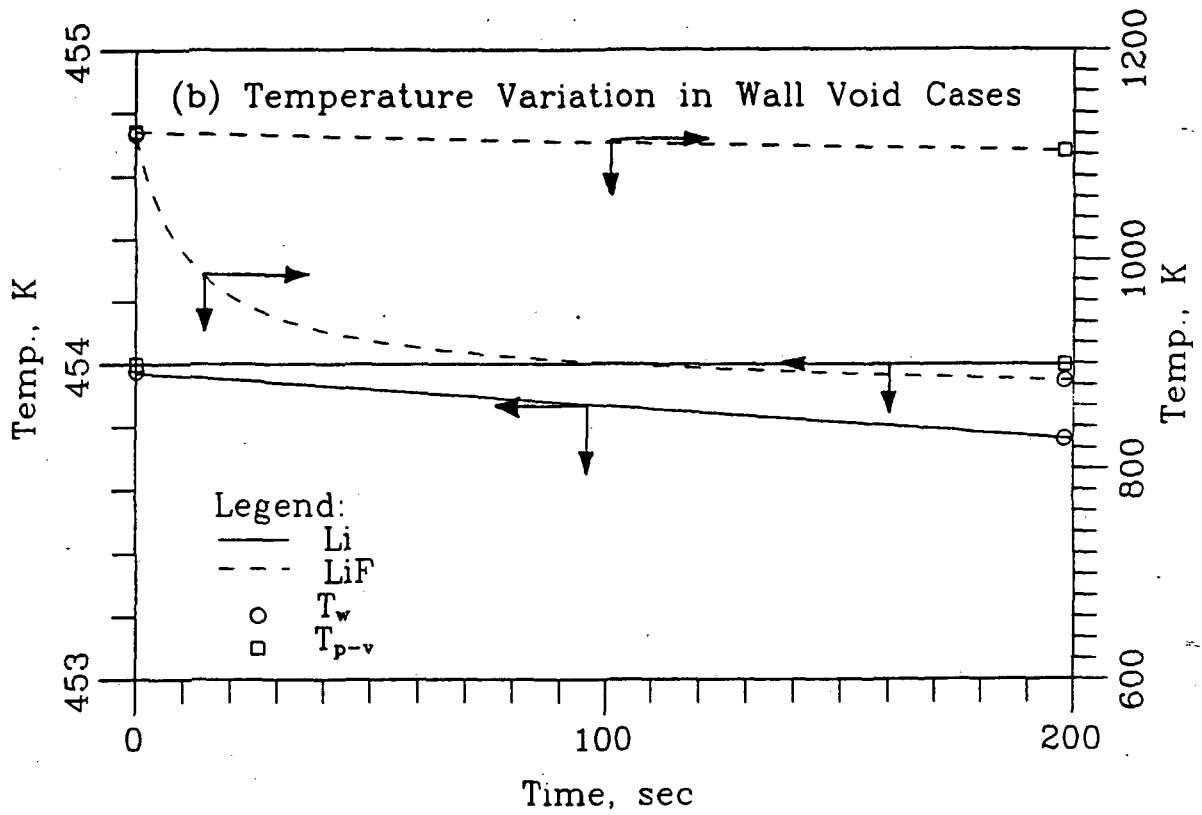


Figure 17. Temperature Variation in Wall Void Cases During Freeze of Li and LiF (Radiative BC, $T_a = 250$ K)

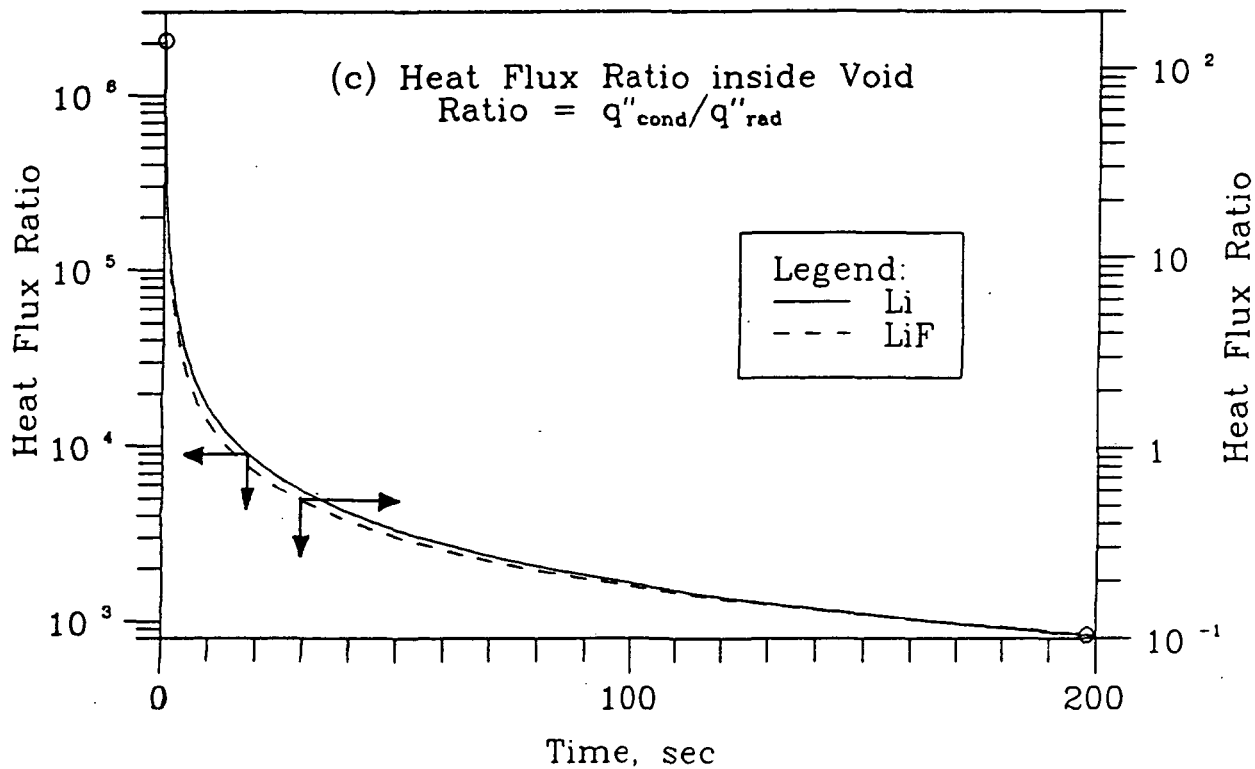


Figure 18. Calculated Heat Flux Ratio inside Void During Freeze of Li and LiF (Radiative BC, $T_a = 250$ K)

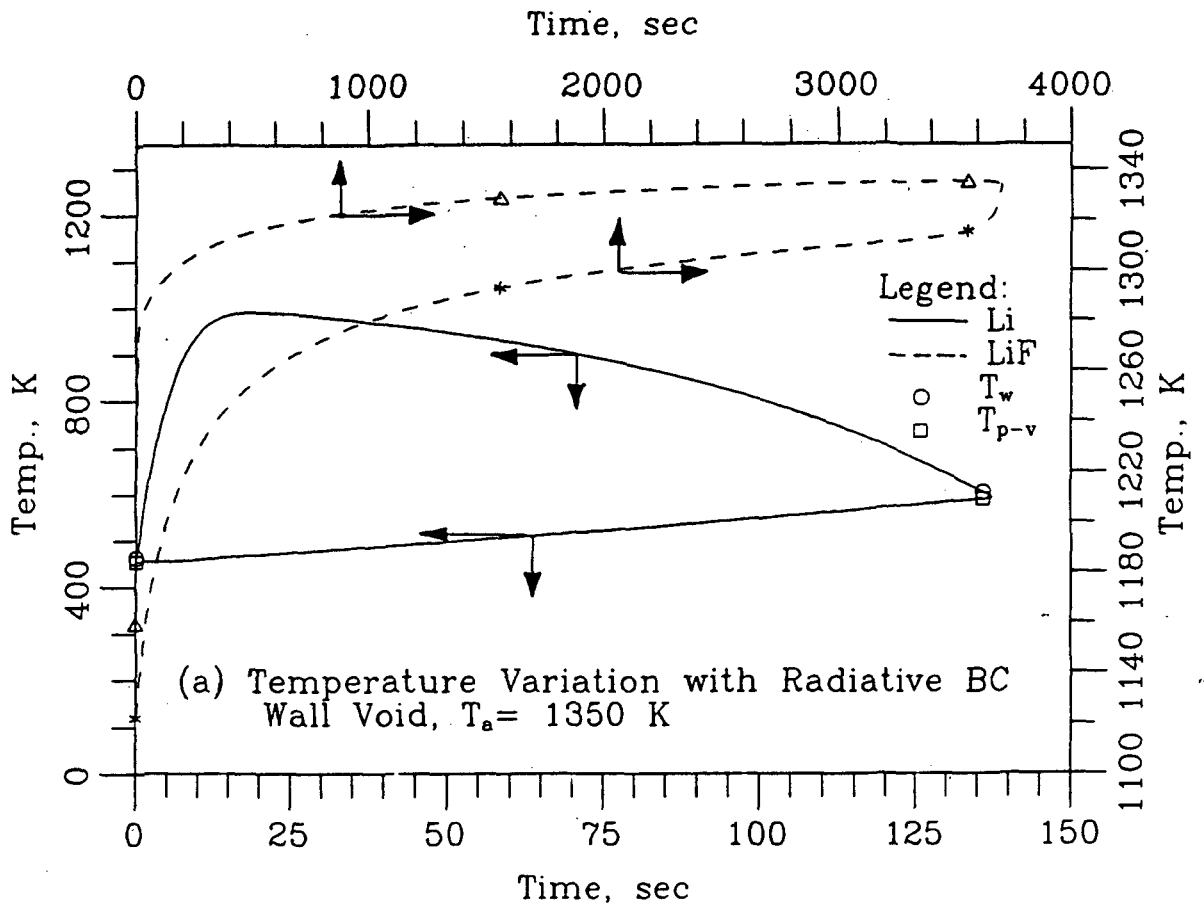


Figure 19. Temperature Variation, with Radiative BC Wall Void, $T_a = 1350$ K, During Thaw Process of Li and LiF

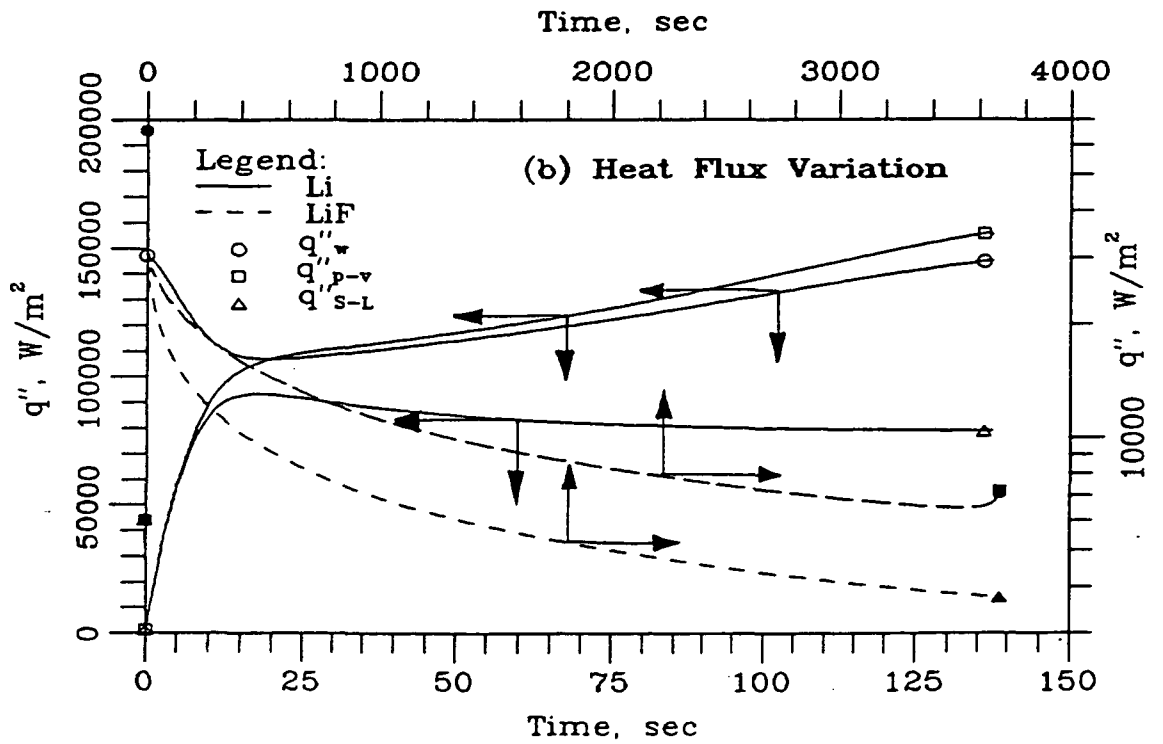


Figure 20. Heat Flux Variation During Thaw Process of Li and LiF (Wall Void, Radiative BC, $T_a = 1,350$ K)

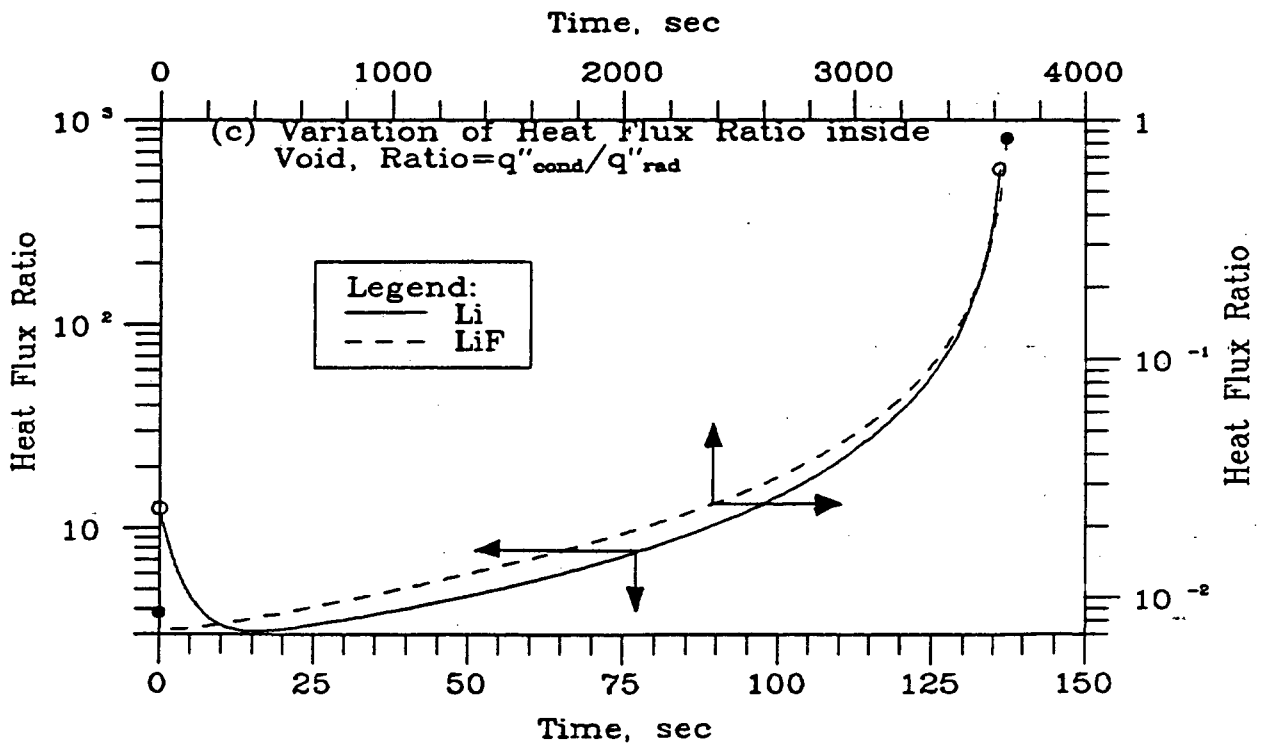


Figure 21. Variation of Heat Flux Ratio Inside Void During Thaw Process of Li and LiF (Wall Void, Radiative BC, $T_a = 1350$ K)

3.3 NOMENCLATURE

English

C_p	:	Heat capacity (J/kg.K)
H_{sl}	:	Latent heat of fusion (J/kg)
h_r	:	Radiative heat transfer coefficient (W/m ² .K)
h_{vc}	:	Thermal conductance of the void (W/m ² .K)
k	:	Thermal conductivity (J/m.K)
L	:	Coolant channel width (m)
st	:	Stefan number ()
T	:	Temperature (K)
T_1, T_2	:	Temperatures at the center of the wall and developing phase, respectively
t	:	Time (s)
t_c	:	Thickness of the wall (m)
v	:	Material velocity due to volume shrinkage (m/s)
X_r	:	Location of shrinkage void/liquid (or solid) interface (m)

Greek

α	:	Thermal diffusivity (m ² /s)
Γ	:	$\rho_s/\rho_L - 1$
δ	:	Solid crust thickness, (m)
δ_v	:	Void thickness, (m)
ϵ	:	Emissivity
ρ	:	Density (kg/m ³)
σ	:	Stefan-Boltzman constant (5.67 x 10 ⁻⁸ W/m ² .K)

Subscripts

c	:	Wall region
d	:	Developing phase
f	:	Fusion
L	:	Liquid
s	:	Solid
i	:	Initial
v	:	Void
01	:	Between wall and heat source (sink)
12	:	Between the centers of wall and developing phase
1	:	Within the half of the wall
2	:	Within the half of the developing phase
3	:	At the wall-void interface
4	:	At the PCM-void interface

4. SUMMARY AND CONCLUSIONS

It is shown that the formation of He gas voids either by HN or HTN during the cooldown process is unlikely. However, the formation of Nb-hydride and/or Nb-nitride in the SP-100 PHTS could increase the potential of Li-dewetting of the walls during cooldown, and hence the HTN of He bubbles. Analysis shows that HN of He bubble would occur by normal segregation during the freezing process of Li. Because of its high heat capacity and high latent heat of fusion as well as the low cooling rate of the wall, Li freezing is very slow. The results indicate that the total volume of He bubbles is insignificant (~2 %) compared to that due to volume shrinkage of Li during freezing. Hence the former is expected to play a minor role in relieving the stress in the walls during the restart of the SP-100 system. Depending on where heat is applied relative to the location of the shrinkage void, stress may or may not be induced in the PHTS structure during the restart of SP-100 system.

The effects of shrinkage void forming during freezing of lithium and lithium-fluoride on subsequent thaw processes are investigated using a numerical scheme that is based on a single (solid/liquid) cell approach. Results show that the formation or presence of a shrinkage void at the wall-PCM interface substantially reduces the S-L interface velocity while voids, forming at the center of the coolant ducts, do not influence the freeze and thaw processes.

Results also show that the presence of a void at the wall causes a substantial rise in the wall temperature during thaw. However, in the case of Li, the maximum wall temperature was much lower than the melting temperature of PWC-11, which is used as the

structure material in the SP-100 system. Hence, it is concluded that a formation of hot spots is unlikely during the startup or restart of the SP-100 system.

ACKNOWLEDGEMENTS

This research is supported by NASA Lewis Research Center under research Grant No. NAG. 3-1045 to the University of New Mexico's Institute for Space Nuclear Power Studies.

REFERENCES

- Alefeld, G. and J. Volki, Eds. (1978), *Hydrogen in Metals I*, Springer-Verlag, N.Y. pp 329-330.
- Brick, R. M., A. W. Pense, and R. B. Gordon (1977), *Structure and Properties of Engineering Materials*, 4th ed., McGraw-Hill.
- Cahn, R. W. and P. Haasen, Eds. (1983), *Physical Metallurgy*, 3rd ed., North-Holland Physics Publ., N.Y.
- Chalmers, B. (1964), *Principles of Solidification*, John Wiley & Sons, New York.
- Cole, R. (1974), "Boiling Nucleation," *Advances in Heat Transfer*, Vol. 10, pp 85-166, Academic Press, New York.
- Hoffman, N. (1990), *Private Communication*, ETEC Div., Rockwell International Corp., Canoga Park, CA, April, 1990.
- Hunter, L. W. and J. R. Kuttler (1983), "Cooling of a Slab with Thermal Contraction and Progressive Loss of Contact With a Cold Surface," *Trans. ASME*, 105, November 1983.
- Hunter, L. W. and J. R. Kuttler (1989), "The Enthalpy Method for Heat Conduction Problems with Moving Boundaries," *J. of Heat Transfer*, 111:239-242.
- McGhee, J., M. S. El-Genk, and R. B. Rothrock (1989), "An Assessment of Helium Gas in SP-100 Class Reactors," *24th IECEC Conf.*, Crystal City, Washington, D.C., Aug. 1989.
- Patankar, S. V. (1980). *Numerical Heat Transfer and Fluid Flow*, Hemisphere Pub. Co., Washington, D.C.

- Shamsunder, N. and E. M. Sparrow (1975). "Analysis of Multidimensional Conduction Phase Change Via the Enthalpy Model," *J. of Heat Transfer*, August 1975.
- Slotnick, H. et al. (1965), *The Solubility of Helium in Lithium and Potassium*, PWAC - 380, Pratt & Whitney Aircraft Co., Middletown, Conn., 24 February 1965.
- van Stralen, Sjoerd and R. Cole, (1979), *Boiling Phenomena*, Vol. I & II, Hemisphere, Washington, D.C., pp 259 - 260.
- Wilson, D. G. , and A. D. Solomon (1986). "A Stefan-Type Problem with Void Formation and its Explicit Solution," *IMA J. of Applied Mathematics*, 37, [1].
- Yang, J. Y. and M. S. El-Genk (1991), "Mechanisms of Void Formation During Cooldown and Freezing of Lithium in SP-100 Type Systems," *Proc. of the 8th Symposium on Space Nuclear Power Systems*, Albuquerque, NM, 6-10 January 1991.

Appendix A-1

List of Computer Program COPHASE.FOR



```

PROGRAM COPHASE
IMPLICIT REAL*8 (A-H, O-Z)
COMMON /INPT1/ NT, TIME, NX, XL, HINIT, TINIT, TA, TF, TWALL,
1 HSF, HLF, CONDSF, CONDLF, RHOSF, RHOLF, EMIT
COMMON /CONVE1/ EPS1, EPS2, EPS3
COMMON /OPTIN/ MLB, MRB, ILB, IRB, ICOMP, IENT, ITEM, SLOPT,
& PRTIME(20)
COMMON /MESHX/ XI(0:500), DX(500), DT
COMMON /DIMSV/ HX(0:500, 2), TX(0:500, 2), DELTA(0:2)
COMMON /DIMLV/ THETA(0:500, 2), PAI(0:500, 2), THEC(0:500)
COMMON /LOCPR/ RHOX(0:500,2), CPX(0:500,2), CONDX(0:500,2)
COMMON /TEMPO/ STHETA(0:500), STHEC(0:500), SPAI(0:500),
& SRHOX(0:500), SCPX(0:500), SCONDX(0:500), SHX(0:500),
& STX(0:500)
COMMON /THERP/ RHO(50), CP(50), COND(50), TEM(50), ENT(50)
COMMON/PROP/HL,HS,CL,CS,CONL,CONS,RHL,RHS,TFF

NAMELIST /OPTION/ MLB, MRB, ILB, IRB, ICOMP, IENT, ITEM,
& SLOPT, NPRT, NpStp
C **** MLB = 1 FOR MOVING LEFT BOUNDARY
C MRB = 1 FOR MOVING RIGHT BOUNDARY
C ILB = INDEX FOR LEFT BOUNDARY CONDITIONS
C 0 = ADIABATIC BOUNDARY
C 1 = ISOTHERMAL WALL (TIME INDEPENDENT)
C 2 = ISOFUX WALL (TIME INDEPENDENT)
C 3 = CONVECTIVE BOUNDARY
C 4 = RADIATIVE BOUNDARY
C IRB = INDEX FOR LEFT BOUNDARY CONDITIONS
C 0 = ADIABATIC BOUNDARY
C 1 = ISOTHERMAL WALL (TIME INDEPENDENT)
C 2 = ISOFUX WALL (TIME INDEPENDENT)
C 3 = CONVECTIVE BOUNDARY
C 4 = RADIATIVE BOUNDARY
CCCCCC*** 9/26/1990 OPTION FOR IRB = 1 - 4 ARE NOT USED
C
C ICOMP = 1 FOR COMPARISON WITH ANALYTICAL RESULT IF AVAILABLE
C IENT = 1 FOR UNIFORM INITIAL ENTHALPY DISTRIBUTION
C 2 FOR NON-UNIFORM INITIAL ENTHALPY DISTRIBUTION
C (INPUT REQUIRED)
C ITEM = 1 FOR UNIFORM INITIAL TEMPERATURE DISTRIBUTION
C 2 FOR NON-UNIFORM INITIAL TEMPERATURE DISTRIBUTION
C (INPUT REQUIRED)
C SLOPT = OPTION FOR LOCATION OF INTERFACE
C THREE DIFFERENT POSITION CAN BE CONSIDERED AS THE INTERFACE
C = 0. FOR DELTA BASED ON THETA(X,T) = 0
C = .5 FOR DELTA BASED ON THETA(X,T) = 1/2
C = 1. FOR DELTA BASED ON THETA(X,T) = 1
C PRTIME(I) = PRINT OUT RESULTS AT TIME PRTIME(I) (SEC)
C IF NO INPUT IS MADE FOR THIS VARIABLE,
C PRINT IS MADE ONCE AT THE TIME SPECIFIED BY
C INPUT VARIABLE 'TIME' IN THE NAMELIST 'INPUT1'.

NAMELIST /INPUT1/ NT, TIME, NX, XL, HINIT, TINIT, TF, HSF, HLF,
1 CONDSF, CONDLF, RHOSF, RHOLF, EMIT, TWALL, HWALL, TA,
2 CPS, CPL
NAMELIST /CONVER/ EPS1, EPS2, EPS3
OPEN(10, ERR=9999, FILE='COPHASE.INP', STATUS='OLD')
OPEN(11, ERR=9999, FILE='COPHASE.VEL', STATUS='UNKNOWN')
OPEN(12, ERR=9999, FILE='COPHASE.ENT', STATUS='UNKNOWN')
OPEN(13, ERR=9999, FILE='COPHASE.TEM', STATUS='UNKNOWN')
OPEN(14, ERR=9999, FILE='COPHASE.CRS', STATUS='UNKNOWN')

C **** DEFAULT VALUES FOR OPTIONS
DATA MLB/0/, MRB/0/, ILB/1/, IRB/0/, SLOPT/0./, IFLAG/0/

```

```

C ***** CONSTANTS
DATA PHI/3.1415926/, BOLTZ/5.67D-08/
C ***** READ INPUT
READ(10,OPTION)
READ(10,INPUT1)
READ(10,CONVER)
HL = HLF
HS = HSF
CL = CPL
CS = CPS
CONL = CONDLF
CONS = CONDSF
RHL = RHOLF
RHS = RHOSF
TFF = TF

C ***** IDENTIFY TIME FOR PRINTOUT
DPRT = TIME/DFLOAT(NPRT)
PRTIME(1) = 0.
DO 5 I=1,NPRT
5 PRTIME(I+1) = PRTIME(I)+DPRT
C ***** MESH GENERATION:
C NX = NUMBER OF NODES
NX1 = NX - 1
DX1 = XL/DFLOAT(NX)
DX101 = DX1 * 0.1

XI(0) = 0.
XI(NX) = XL

DO 10 I=1,NX
10 DX(I) = DX1
   XI(I) = XI(I-1) + DX(I)

C ***** THE TIME STEP SIZE: UNIFORM
DT = TIME/DFLOAT(NT)

C ***** PREPARATION FOR INITIAL CONDITIONS

DELTA(0) = 0.
DELTA(1) = 0.
DELTA(2) = 0.
DDELTA DT = 0.
SDELTA = 0.
HF = HLF - HSF
HO = HWALL
SGAM = 1. - RHOLF/RHOSF
IF(MLB .EQ.1) SGAM = -SGAM
IF(MLB .EQ.0) SGAM = 0.

C ***** INITIAL TEMPERATURE, HEAT CAPACITY, THERMAL CONDUCTIVITY, &
C DENSITY
C DIMENSIONLESS ENTHALPY, THETA(I,M), TEMPERATURE, PAI(I,M)
C AND ENTHALPY CORRECTION FACTOR, THEC(I)

DO 20 J = 1,2
DO 20 I = 1, NX
HX(I,J) = HINIT
CALL PROPERTY(HX(I,J),TX(I,J),CPX(I,J),RHGX(I,J),CONDX(I,J))
THETA(I,J) = (HX(I,J) - HSF)/HF
THEC(I) = - THETA(I,J)
IF(THEC(I) .GT. 0.) THEC(I) = 0.
IF(THEC(I) .LT. -1.) THEC(I) = -1.
PAI(I,J) = THETA(I,J) + THEC(I)
20 CONTINUE

```

```

RHOIN=RHOX(1,1)
WRITE(*.1001) SNGL(RHOX(1,1)),SNGL(RHOX(2,1)),
& SNGL(RHOX(NX-1,1)),SNGL(RHOX(NX,1))
1001 FORMAT(/5X,'DENSITIES',E12.5,2X,E12.5,2X,E12.5,2X,E12.5)
C
C **** INITIAL VALUES FOR CONSTANT TWALL< TF, PAIO = CONSTANT.
C
IF(ILB .EQ. 1) THEN
CALL PROPERTY(HWALL,TWALL,CPXO,RHOXO,CONDXO)
THETAO = (HWALL - HSF)/HF
PAIO = CPXO*(TWALL - TF)/HF
THECO = PAIO - THETAO
HO = HWALL
QOLD = 0.
WRITE(*.21) SNGL(TWALL),SNGL(THETAO), SNGL(PAIO)
C
C **** INITIAL VALUES FOR RADIATIVE BOUNDARY
C
ELSEIF(ILB .EQ. 4) THEN
THETOLD = THETA(1,1)
TWOLD = TX(1,1)
PAIOLD = PAI(1,1)
HROLD = EMIT*BOLTZ*(TINIT**2. + TA**2.)*(TINIT + TA)
QOLD = HROLD*(TINIT - TA)
STE = CPX(1,1)*(TF - TA)/HF
TA2 = TA**2.
WRITE(*.22) SNGL(TWOLD),SNGL(THETOLD), SNGL(PAIOLD)
ENDIF
C
C **** TOTAL SYSTEM ENERGY [Joule]
C
ETOT = 0.
DO 25 I = 1, NX
25 ETOT = ETOT + RHOX(I,1)*HX(I,1)*DX(I)
ETOTOLD = ETOT
ETOTINIT = ETOT
QTOT = 0.
WRITE(12,26) SNGL(TF),SNGL(HF),SNGL(HLF),SNGL(HSF),
& SNGL(CPL),SNGL(CPS),
& SNGL(CONL),SNGL(CONS),SNGL(RHOLF),SNGL(RHOSF)
WRITE(*.26) SNGL(TF),SNGL(HF),SNGL(HLF),SNGL(HSF),
& SNGL(CPL),SNGL(CPS),
& SNGL(CONL),SNGL(CONS),SNGL(RHOLF),SNGL(RHOSF)
C
C **** THE BEGINNING OF TIME LOOP *****
DO 9000 MA = 1, NT
M=2
C **** STORE PREVIOUS STEP VALUES IN THE TEMPORARY STORAGE VARIABLES
DO 30 I=1,NX
SHX(I) = HX(I,M-1)
STHEC(I) = THEC(I)
STHETA(I) = THETA(I,M-1)
SPAI(I) = PAI(I,M-1)
SRHOX(I) = RHOX(I,M-1)
SCPX(I) = CPX(I,M-1)
SCONDX(I) = CONDX(I,M-1)
30 CONTINUE
SDELTA = DELTA(M-1)

```

```

C-----
C **** OUTER ITERATION ----- DELTA ITERATION
C-----
      IDITER = 0
      DELTA(1) = DELTA(0) + DDELTA*DT/2.      I ASSUMED CRUST THICKNESS
1025  CONTINUE
      IDITER = IDITER + 1
      DDELTA = DELTA(1) - DELTA(0)

```

```

C-----
C      INNER ITERATION
C-----
C
C      CONVERGENCE ARE CHECKED IN EACH TIME STEP BY:
C      SUMDIF = SUM(F(I,M)-SF(I))*DX(I)**2.), I=ILEND,IREND
C      SUMASS = SUM(SF(I)*DX(I)**2.), I=ILEND,IREND
C
C      AND IF (SUMDIF/SUMASS)<= EPS1,
C      THE CONVERGENCE ARE ACHIEVED
C-----

```

```

      NITER = 0
      SUMQINDT = QOLD
1050  CONTINUE

      NITER = NITER + 1

      SUMDIF = 0.
      SUMASS = 0.

```

```

C-----
C **** ADJUSTMENTS OF THE SIZE AND LOCATION OF THE BOUNDARY NODES
C-----

```

```

C **** INITIAL LOCATION OF BOUNDARY NODES
      IF(MLB .EQ. 0 .AND. MRB .EQ. 0) THEN
          XLEND = 0.
          XREND = XL
          ILEND = 1
          IREND = NX

```

```

C **** LOCATION AND SIZE OF MOVING LEFT BOUNDARY NODE; MLB = 1
C
      ELSEIF(MLB .EQ. 1) THEN
          XLEND = SGAM*DELTA(M-1)
          XREND = XL
          ILEND = 1

          IF(XLEND .LT. XI(1)) THEN
              ILEND = 1
              GO TO 60

          ELSEIF(XLEND .GT. XI(NX1)) THEN
              ILEND = NX
              GO TO 60

          ELSE
              DO 50 IL=2,NX
              IF(XLEND .GT. XI(IL-1) .AND. XLEND .LE. XI(IL)) THEN
                  ILEND = IL
                  GO TO 60
              50  CONTINUE
          ENDIF
      CONTINUE

```

```

ENDIF
60      DXI = XI(ILEND) - XLEND
        IF(DXI .LT. DX101) THEN
            ILEND = IL + 1
            DXI = XI(ILEND) - XLEND
        ENDIF
        DX(ILEND) = DXI
C
C ***** LOCATION AND SIZE OF MOVING RIGHT BOUNDARY NODE; MRB = 1
C
        ELSEIF(MRB .EQ. 1) THEN
            XREND = XL - SGAM*DELTA(M-1)
            XLEND = 0.
            ILEND = 1

            IF(XREND .GT. XI(NX1)) THEN
                IREND = NX
                GO TO 62

            ELSEIF(XREND .LE. XI(1)) THEN
                IREND = 1
                GO TO 62

            ELSE

                DO 61 IL=1,NX1
                    IF(XREND .GT. XI(IL-1) .AND. XLEND .LE. XI(IL)) THEN
                        IREND = IL
                        GO TO 62
                    ENDIF
                CONTINUE
            ENDIF

61      CONTINUE
        ENDIF

62      DXI = XREND - XI(IREND)
        IF(DXI .LT. DX101) THEN
            IREND = IL - 1
            DXI = XREND - XI(IREND)
        ENDIF
        DX(IREND) = DXI

ENDIF

K = ILEND
L = IREND

ILEND1 = ILEND + 1
IREND1 = IREND - 1
IREND2 = IREND - 2

DO 35 I = ILEND, IREND
35      SUMASS = SUMASS + (HX(I,M-1)*DX(I))*2.
C
C ***** PRODUCTION RUN: LEFT BOUNDARY NODE
C
C ILB = 1 FOR CONSTANT WALL TEMPERATURE AT LEFT BOUNDARY
C
        IF(ILB .EQ. 1) THEN
C
            ALM = CPX(K-1,M-1)*DX(K-1)/CONDX(K-1,M-1)
            ALO = CPX(K,M-1)*DX(K)/CONDX(K,M-1)
            ALP = CPX(K+1,M-1)*DX(K+1)/CONDX(K+1,M-1)

            A1 = 2.*DT/(DX(K)*RHOX(K,M-1))
            A2 = 1./(ALO + ALP)

```

```

C      A3 = 1./ALO
C      A4 =

c      CHECK = STHETA(K) + A1*(A2*PAI(K+1,M-1) + A3*PAIO)
c
c      IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN
c      THETA(K,M) = CHECK
c      THEC(K) = -THETA(K,M)
c
c      ELSEIF(CHECK .GT. 1.) THEN
c      THEC(K) = -1.
c      THETA(K,M) = ( STHETA(K) + A1*(A2*PAI(K+1,M-1)
c      &      + A3*PAIO - (A2+A3)*THEC(K)) ) / (1.+A1*(A2+A3))
c
c      ELSE
c      THEC(K) = 0.
c      THETA(K,M) = ( STHETA(K) + A1*(A2*PAI(K+1,M-1)
c      &      + A3*PAIO - (A2+A3)*THEC(K)) ) / (1.+A1*(A2+A3))
c      ENDIF

c      CHECK = STHETA(K)*srhox(k)/rhox(k,m-1)
c      &      -(1.-srhox(k)/rhox(k,m-1))*Hsf/Hf
c      &      + A1*(A2*PAI(K+1,M-1) + A3*PAIO)

c      IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN
c      THETA(K,M) = CHECK
c      THEC(K) = -THETA(K,M)

c      ELSEIF(CHECK .GT. 1.) THEN
c      THEC(K) = -1.
c      THETA(K,M) = ( STHETA(K)*srhox(k)/rhox(k,m-1)
c      &      -(1.-srhox(k)/rhox(k,m-1))*Hsf/Hf
c      &      + A1*(A2*PAI(K+1,M-1)
c      &      + A3*PAIO - (A2+A3)*THEC(K)) ) / (1.+A1*(A2+A3))

c      ELSE
c      THEC(K) = 0.
c      THETA(K,M) = ( STHETA(K)*srhox(k)/rhox(k,m-1)
c      &      -(1.-srhox(k)/rhox(k,m-1))*Hsf/Hf
c      &      + A1*(A2*PAI(K+1,M-1)
c      &      + A3*PAIO - (A2+A3)*THEC(K)) ) / (1.+A1*(A2+A3))
c      ENDIF

c      HX(K,M) = HSF + THETA(K,M)*HF
c      CALL PROPERTY(HX(K,M),TX(K,M),CPX(K,M),RHOX(K,M),CONDX(K,M))

c      PAI(K,M) = THETA(K,M) + THEC(K)

c      HDIF = ((HX(K,M) - HX(K,M-1))/HX(K,M-1))*2.
-----
C      ILB = 2 FOR CONSTANT WALL HEAT FLUX BOUNDARY AT LEFT BOUNDARY
-----
C      ELSEIF(ILB .EQ. 2) THEN
C      PRINT *,' '
C      PRINT *,' CONSTANT WALL HEAT FLUX BOUNDARY '
-----
C      ILB = 4 FOR CONVECTIVETIVE BOUNDARY AT LEFT BOUNDARY
-----
C      ELSEIF(ILB .EQ. 3) THEN
C      PRINT *,' '
C      PRINT *,' CONVECTIVE BOUNDARY '

```



```

C
C ILB = 4 FOR RADIATIVE BOUNDARY AT LEFT BOUNDARY
C
ELSEIF(ILB .EQ. 4) THEN
ALPHA = BOLTZ*EMIT*DX(K)/CONDX(K,M-1)/2.
HRR = BOLTZ*EMIT*(TX(K,M-1)**2. + TA2)*(TX(K,M-1) + TA)
& /((1. + 4.*ALPHA*TX(K,M-1)**3.)
STE = CPX(K,M-1)*(TF - TA)/HF
C
ALM = CPX(K-1,M-1)*DX(K-1)/CONDX(K-1,M-1)
ALO = CPX(K,M-1)*DX(K)/CONDX(K,M-1)
ALP = CPX(K+1,M-1)*DX(K+1)/CONDX(K+1,M-1)
A1 = 2.*DT/(DX(K)*RHOX(K,M-1))
A2 = 1./(ALO + ALP)
A3 = HRR/CPX(K,M-1)/2.
C
A4 =
CHECK = STHETA(K) + A1*(A2*PAI(K+1,M-1) - A3*Ste)
c
c IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN
c THETA(K,M) = CHECK
c THEC(K) = -THETA(K,M)
c
c ELSEIF(CHECK .GT. 1.) THEN
c THEC(K) = -1.
c THETA(K,M) = ( STHETA(K) + A1*(A2*PAI(K+1,M-1) - (A2+A3)
& * THEC(K) - A3*Ste) )/(1.+ A1*(A2+A3))
c
c ELSE
c THEC(K) = 0.
c THETA(K,M) = ( STHETA(K) + A1*(A2*PAI(K+1,M-1) - (A2+A3)
& * THEC(K) - A3*Ste) )/(1.+ A1*(A2+A3))
c
c ENDIF
c
CHECK = STHETA(K)*srhox(k)/rhox(k,m-1)
& -(1.-srhox(k)/rhox(k,m-1))*Hsf/Hf
& + A1*(A2*PAI(K+1,M-1) - A3*Ste)
IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN
THETA(K,M) = CHECK
THEC(K) = -THETA(K,M)
ELSEIF(CHECK .GT. 1.) THEN
THEC(K) = -1.
THETA(K,M) = ( STHETA(K)*srhox(k)/rhox(k,m-1)
& -(1.-srhox(k)/rhox(k,m-1))*Hsf/Hf
& + A1*(A2*PAI(K+1,M-1) - (A2+A3)
& * THEC(K) - A3*Ste) )/(1.+ A1*(A2+A3))
ELSE
THEC(K) = 0.
THETA(K,M) = ( STHETA(K)*srhox(k)/rhox(k,m-1)
& -(1.-srhox(k)/rhox(k,m-1))*Hsf/Hf
& + A1*(A2*PAI(K+1,M-1) - (A2+A3)
& * THEC(K) - A3*Ste) )/(1.+ A1*(A2+A3))
ENDIF
HX(K,M) = HSF + THETA(K,M)*HF
CALL PROPERTY(HX(K,M),TX(K,M),CPX(K,M),RHOX(K,M),CONDX(K,M))
PAI(K, M) = THETA(K, M) + THEC(K)
ENDIF
C ..... 1 ..... OPTIONS FOR OTHER BOUNDARY CONDITIONS .....

```


C CHECK CONVERGENCE FOR THETA OR THEC WHICH EVER IS CONVENIENT
HDIF = ((HX(I,M) - HX(I,M-1))/HX(I,M-1))*2.

SUMDIF = SUMDIF + ((HX(I,M) - HX(I,M-1))*DX(I))*2.

200 CONTINUE

C
C CLOSING RUN: RIGHT BOUNDARY NODE (IDIABATIC BC ONLY)
C

DX01 = DX(L) + DX(L-1)

ALM = CPX(L-1,M-1)*DX(L-1)/CONDX(L-1,M-1)

ALO = CPX(L,M-1)*DX(L)/CONDX(L,M-1)

C ALP = CPX(L+1,M-1)*DX(L+1)/CONDX(L+1,M-1)

A1 = 2.*DT/(DX(L)*RHOX(L,M-1))

A2 = 1./(ALO + ALO)

A3 = 1./(ALO + ALM)

C A4 =

C CHECK = STHETA(L) + A1*A3*PAI(L-1,M) - A4*THETA(L-1,M)

C IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN

C THETA(L,M) = CHECK

C THEC(L) = -THETA(L,M)

C ELSEIF(CHECK .GT. 1.) THEN

C THEC(L) = -1.

C THETA(L,M) = (STHETA(L) + A1*A3*(PAI(L-1,M) - THEC(L))
& - A4*THETA(L-1,M))/(1. + A1*A3)

C ELSE

C THEC(L) = 0.

C THETA(L,M) = (STHETA(L) + A1*A3*(PAI(L-1,M) - THEC(L))
& - A4*THETA(L-1,M))/(1. + A1*A3)

C ENDIF

C CHECK = STHETA(L)*srhox(L)/rhox(L,m-1)
& - (1.-srhox(L)/rhox(L,m-1))*Hsf/Hf
& + A1*A3*PAI(L-1,M) - A4*THETA(L-1,M)

C IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN

C THETA(L,M) = CHECK

C THEC(L) = -THETA(L,M)

C ELSEIF(CHECK .GT. 1.) THEN

C THEC(L) = -1.

C THETA(L,M) = (STHETA(L)*srhox(L)/rhox(L,m-1)
& - (1.-srhox(L)/rhox(L,m-1))*Hsf/Hf
& + A1*A3*(PAI(L-1,M) - THEC(L))
& - A4*THETA(L-1,M))/(1. + A1*A3)

C ELSE

C THEC(L) = 0.

C THETA(L,M) = (STHETA(L)*srhox(L)/rhox(L,m-1)
& - (1.-srhox(L)/rhox(L,m-1))*Hsf/Hf
& + A1*A3*(PAI(L-1,M) - THEC(L))
& - A4*THETA(L-1,M))/(1. + A1*A3)

C ENDIF

C HX(L,M) = HSF + THETA(L,M)*HF

C CALL PROPERTY(HX(L,M),TX(L,M),CPX(L,M),RHOX(L,M),CONDX(L,M))

```

      PAI(L, M) = THETA(L, M) + THEC(L)
C **** CHECK CONVERGENCE FOR THETA OR THEC WHICH EVER IS CONVENIENT
      HDIF = ((HX(L,M) - HX(L,M-1))/HX(L,M-1))**.2.
      SUMDIF = SUMDIF + ((HX(L,M) - HX(L,M-1))*DX(L))**.2.

```

```

C **** LOCATION OF INTERFACE

```

```

C **** First, project THETA at x = 0.
      hi = dx(1)
      h1 = dx(2)
      h2 = dx(3)
      hih1 = hi+h1
      h1h2 = h1 + h2
      h12hi = h1 + 2.*hi
      hi2h1h2 = hi + 2.*h1 + h2
      h22hi2h1 = h2 + 2.*h1 + 2.*hi
      theta(0,m) = theta(1,m)*(2.*hi + h1)*h22hi2h1/(hih1*hi2h1h2)
&      - theta(2,m)*hi*h22hi2h1/(hih1*h1h2)
&      + theta(3,m)*hi*h12hi/(h12h1h2*h1h2)

c      if (delta(m-1) .le. 0. .and. theta(0,m) .ge. SLOPT) then
c      delta(m) = 0.
c      go to 550
c      endif

      ISL1 = 1
c      ilendm1 = ilend - 1
      DO 541 I = ILEND, IREND1
      IF(THETA(I,M) .GE. 0. .AND. THETA(I,M) .LT. 1.) THEN
      ISL1 = I
      DELTA(M) = XI(ISL1) - DX(ISL1)*THETA(ISL1,M)
      GO TO 551
c      ELSEIF(THETA(I,M) .LE. SLOPT .AND. THETA(I+1,M) .GT. SLOPT) THEN
c      IF(THETA(I,M) .LE. SLOPT .AND. THETA(I+1,M) .GT. SLOPT) THEN
c      ISL1 = I
c      DELTA(M) = XI(ISL1) - DX(ISL1)/2. + 2.*(SLOPT - THETA(ISL1,M))*
c      & (THETA(ISL1+1,M)-THETA(ISL1,M))/(DX(ISL1)+DX(ISL1+1))
c      GO TO 551
c      ENDIF
541 CONTINUE
551 CONTINUE

      if(theta(irend,m) .le. slopt) then
      delta(m) = xrend
      print *, 'Complete solidification of the system'
      print *, 'Calculation Terminated'
      go to 9999
c      go to 545
      endif

c      if(isl1 .eq. 1) then
c      DELTA(M) = XI(ISL1) - DX(ISL1)*THETA(ISL1,M)
c      ELSE
c      DELTA(M) = XI(ISL1-1) - DX(ISL1-1)/2.
c      & + 2.*(SLOPT - THETA(ISL1-1,M))*
c      & (THETA(ISL1,M)-THETA(ISL1-1,M))/(DX(ISL1)+DX(ISL1-1))
c      endif

C      sumtheta = 0.
C      Do 555 i = ilend, isl1
C555 sumtheta = sumtheta + theta(i,m)*dx(i)

```

```

C      avgtheta = sumtheta/(xi(isl1) - xlend)
C      delta(m) = (xi(isl1) - xlend)*(1.-avgtheta)

c      isl1 = 1
c      DO 540 I = ILEND, IREND1
c      IF(THETA(I,M) .LE. SLOPT .AND. THETA(I+1,M) .GT. SLOPT) THEN
c      ISL1 = I
c      go to 545
c      ENDF
c540  CONTINUE
c
c545  ximh = xi(isl1) - dx(isl1)/2.
c      xiph = xi(isl1) + dx(isl1+1)/2.
c
c      if(isl1 .eq. 1) then
c      xim3h = 0.
c      else
c      xim3h = xi(isl1) - dx(isl1) - dx(isl1-1)/2.
c      endif
c
c      if(ILB .eq. 1) then
c      upsl = xrend
c      else
c      upsl = 2.*xi(isl1)
c      endif
c
c      unsl = 0.
c      liter = 0
c546  Xa = (upsl+unsl)/2.
c      iiter = iiter+1
c      fx = theta(isl1-1,m)*(Xa - ximh)*(Xa - xiph)
c      &      /((xim3h - ximh)*(xim3h - xiph))
c      &      +theta(isl1,m)*(Xa - xim3h)*(Xa - xiph)
c      &      /((ximh - xim3h)*(ximh - xiph))
c      &      +theta(isl1+1,m)*(Xa - xim3h)*(Xa - ximh)
c      &      /((xiph - xim3h)*(xiph - ximh))
c
c      write(*,2030) iiter, isl1 ,sngl(Xa), sngl(fx)
c2030  format(2x,'Niter=',i5,3x,'Nnode=',i5,3x,'Xa=',e12.5,
c      &      3x,'fx=',e12.5)

c      dfx = fx - SLOPT
c      if(dabs(dfx) .le. eps3) then
c      delta(m) = xa
c      go to 550
c      elseif(dfx .lt. 0.) then
c      unsl = xa
c      go to 546
c      else
c      upsl = xa
c      go to 546
c      endif
c550  CONTINUE

C      WRITE(*,609) SNGL(THETA(K,M)),SNGL(THETA(K+1,M)),
C      &      SNGL(THETA(L-1,M)),SNGL(THETA(L,M))

      CONVERGE = SUNDIF/SUMASS

C


---


C **** CHECK ENERGY BALANCE


---


C
C      DETERMINE THE ENERGY OUTPUT WITHIN DT
C      FIRST, BY HEAT FLUX

```

```

IF(ILB.EQ.1) THEN
DDXPAI = 2.*(PAI(K,M) - PAIO)/DX(K)
QNEW = CONDX(K,M)*HF/CPX(K,M)*DDXPAI

ELSEIF(ILB.EQ.4) THEN
QNEW = HRR*(TX(K,M) - TA)
ENDIF

SUMQINDT = SUMQINDT + QNEW
QOUT = QNEW*DT
C **** THEN, BY TOTAL SYSTEM ENERGY [JOULE]
ETOTNEW = 0.
705 DO 705 I = ILEND, IREND
ETOTNEW = ETOTNEW + RHOX(I,M)*HX(I,M)*DX(I)

ECOR = 0.
706 DO 706 I = ILEND, IREND
ECOR = (RHOX(I,M) - SRHOX(I))*HSF*DX(I)
EOUT = ETOTOLD - ETOTNEW + ECOR
EBALANCE = (QOUT - EOUT) / EOUT *100.
EBALRAT = ((QOUT - EOUT) / EOUT)**2.
TSTPRAT = QOUT/EOUT

DIF = 0.
DO 560 I = ILEND, IREND
DIF = DIF + ((HX(I,M) - HX(I,M-1))/HX(I,M-1))**2.
560 CONTINUE

IF(DIF .GT. EPS1) THEN

DO 801 JI = ILEND, IREND
HX(JI,M-1) = HX(JI,M)
CALL PROPERTY(HX(JI,M-1),TX(JI,M-1),CPX(JI,M-1),
& RHOX(JI,M-1),CONDX(JI,M-1))
THETA(JI,M-1) = (HX(JI,M-1) - HSF)/HF
THEC(JI) = -THETA(JI,M-1)
IF(THEC(JI) .GT. 0.) THEC(JI) = 0.
IF(THEC(JI) .LT. -1.) THEC(JI) = -1.
801 PAI(JI, M-1) = THETA(JI, M-1) + THEC(JI)
CONTINUE
GO TO 1050

ENDIF

WRITE(*, 610) SNGL(EOUT), SNGL(QOUT), SNGL(EBALANCE),
& SNGL(TOTEOUT), SNGL(QTOT),
& SNGL(TOTBAL), IS11, SNGL(delta(m))

C WRITE(*, 602) MA, IDITER, NITER, SNGL(CONVERGE), SNGL(SUMASS)

C OUTER ITERATION — DELTA ITERATION
C CONVERGENCE TEST FOR DELTA
C
C IF(DELTA(M).GT.1.D-5 .AND. DELTA(M-1) .GT. 1.D-5) THEN
C DIFDELTA = ((DELTA(M) - DELTA(M-1))/DELTA(M-1))**2.
C ELSE
C DIFDELTA = DELTA(M) - DELTA(M-1)
C ENDIF
C
C DELTA(M-1) = (DELTA(M-1)+DELTA(M))/2.
C If(delta(m-1) .ie. sdelta) delta(m-1)=sdelta
C
C IF(DIFDELTA .GT. EPS2) THEN

```

```

C      DO 816 I = ILEND, IREND
C      HX(I,M-1) = HX(I,M)
C      CALL PROPERTY(HX(I,M-1),TX(I,M-1),CPX(I,M-1),
C      &      RHOX(I,M-1),CONDX(I,M-1))
C
C      THETA(I,M-1) = (HX(I,M-1) - HSF)/HF
C      THEC(I) = -THETA(I,M-1)
C      IF(THEC(I) .GT. 0.) THEC(I) = 0.
C      IF(THEC(I) .LT. -1.) THEC(I) = -1.
C      PAI(I, M-1) = THETA(I, M-1) + THEC(I)
C816  CONTINUE
C      GO TO 1025
C      ENDF

C-----
C **** TRANSFORMATION INTO DIMENSIONED VARIABLES
C-----
      DO 700 I = 1, NX

      HX(I,M) = THETA(I,M)*HF + HSF
      CALL PROPERTY(HX(I,M),TX(I,M),CPX(I,M),RHOX(I,M),CONDX(I,M))

700  CONTINUE

      TOTEOUT = ETOTINIT - ETOTNEW
      QTOT = QTOT + QOUT
      TOTBAL = QTOT/TOTEOUT

C **** STORE PRESENT STEP VALUES IN THE PREVIOUS STEP VARIABLES TO ADVANCE
C      NEXT TIME STEP

      DO 710 I=1,NX
      THETA(I,M-1) = THETA(I,M)
      PAI(I,M-1) = PAI(I,M)
      TX(I,M-1) = TX(I,M)
      HX(I,M-1) = HX(I,M)
      RHOX(I,M-1) = RHOX(I,M)
      CPX(I,M-1) = CPX(I,M)
      CONDX(I,M-1) = CONDX(I,M)
710  CONTINUE
      DELTA(M-2) = SDELTA
      DELTA(M-1) = DELTA(M)
      DDELTADT = (DELTA(M-1) - DELTA(M-2))/DT
      QOLD = QNEW
      ETOTOLD = ETOTNEW
      FROFRAC = DELTA(M)/XL
      TIMEA = DT * DFLOAT(MA)
      TIMEB = DT * DFLOAT(MA+1)
      ma1 = ma/NpStp * NpStp
      if(ma .lt. 20 .or. ma1 .eq. ma) then
      deltaxi = delta(m)/XL
      WRITE(11,1133) SNGL(TIMEA), SNGL(DDELTADT), SNGL(DeltaXL),
      &      SNGL(Tx(ILEND,m))
      WRITE(14,1130) SNGL(TIMEA), SNGL(DELTA(M))
      endif
      DO 770 NK = 1,NPRT
      IF(TIMEA.LE.PRTIME(NK) .AND. TIMEB .GT.PRTIME(NK)) THEN
      WRITE(12,712) SNGL(PRTIME(NK))
      WRITE(13,712) SNGL(PRTIME(NK))
      WRITE(13,713) SNGL(FROFRAC)
713  FORMAT(2X,'FROZEN FRACTION = ',E12.5)
      WRITE(*,712) SNGL(PRTIME(NK))

      ITIME = ITIME + 1
      WRITE(12, 610) SNGL(EOUT), SNGL(QOUT), SNGL(EBALANCE)

```

```

&          , SNGL(TOTEOUT), SNGL(QTOT),
&          SNGL(TOTBAL), Is11, angl(delta(m))
WRITE(*, 610) SNGL(EOUT), SNGL(QOUT), SNGL(EBALANCE)
&          , SNGL(TOTEOUT), SNGL(QTOT),
&          SNGL(TOTBAL), Is11, angl(delta(m))
1110 WRITE(12, 1110)
FORMAT(/5X, 'DIMENSIONLESS ENTHALPY DISTRIBUTION' /
&      4X, '-----' /
&      5X, 'POSITION          ENTHALPY')
DO 8010 IJ = ilend, irend
8010 WRITE(12, 1120) SNGL(XI(IJ)), SNGL(THETA(IJ,M))
WRITE(13, 1111)
1111 FORMAT(/5X, 'TEMPERATURE DISTRIBUTION' /
&      4X, '-----' /
&      5X, 'POSITION          TEMPERATURE (K)')
DO 8011 IJ = ilend, irend
8011 WRITE(13, 1120) SNGL(XI(IJ)), SNGL(TX(IJ,M))
1120 FORMAT(5X, E12.5, 3X, E12.5)
1130 FORMAT(5X, E12.5, 3X, E12.5, 3X, E12.5)
ENDIF
770 CONTINUE
9000 CONTINUE

```

```

C
C   FORMAT STMTS

```

```

21  FORMAT(/5X, 'CONSTANT WALL TEMPERATURE LEFT BOUNDARY' /
&      4X, '-----' /
&      5X, 'Twall              =', F10.5, ' [K]' /
&      5X, 'Dimless Wall Enthalpy =', E12.5 /
&      5X, 'Dimless Wall Temperature =', E12.5)

22  FORMAT(/5X, 'RADIATIVE LEFT BOUNDARY' /
&      4X, '-----' /
&      5X, 'Initial Twall          =', F10.5, ' [K]' /
&      5X, 'Dimless Wall Enthalpy =', E12.5 /
&      5X, 'Dimless Wall Temperature =', E12.5)

26  FORMAT(/5X, 'MATERIAL PROPERTIES' /
&      4X, '-----' /
&      5X, 'Tm [K] = ', F10.3, 5X, 'DHf [J/Kg] = ', F10.3 /
&      5X, '          LIQUID          SOLID' /
&      4X, '-----' /
&      5X, 'H          [J/Kg]', 3X, F10.2, 2X, F10.2 /
&      5X, 'Cp          [J/Kg-K]', 3X, F10.2, 2X, F10.2 /
&      5X, 'K          [J/s-M-K]', 3X, F10.2, 2X, F10.2 /
&      5X, 'Rho        [Kg/M**3]', 3X, F10.2, 2X, F10.2)

602 FORMAT(/5X, 'TIME STEP NO. =', 15 /
&      5X, 'NO. OF DELTA ITERATION =', 15 /
&      5X, 'NO. OF INNER ITERATION =', 15 /
&      5X, 'CONVERGENCE =', E12.5, ' SUMASS =', E12.5)

609 FORMAT(/5X, 'DIMENSIONLESS ENTHALPY DISTRIBUTION AT' /
&      5X, 'ILEND          ILEND+1          IREND-1          IREND' /
&      4X, E12.5, 2X, E12.5, 2X, E12.5, 2X, E12.5)

610 FORMAT(/5X, 'ENERGY BALANCE AT THIS TIME STEP' /
&      4X, '-----' /
&      5X, 'EOUT          =', E12.5, ' [JOULES]' /
&      5X, 'QOUT          =', E12.5, ' [JOULES]' /
&      5X, '% ERROR      =', E12.5 //
&      5X, 'TOTAL ENERGY BALANCE UPTO NOW' /
&      4X, '-----' /
&      5X, 'EOUT          =', E12.5, ' [JOULES]' /

```



```
&          5X,'QOUT      = '.E12.5,' [JOULES]'/
&          5X,'QOUT/EOUT = '.E12.5//
&          5X,'NODE FREEZING=''.I5/
&          5X,'CRUST THICKNESS ='.E12.5//)
712  FORMAT(/5X,'COMPUTED RESULTS AT TIME =',F12.2,' [SEC]')
1133  FORMAT(2X,E12.5,2X,E12.5,2X,E12.5,2X,E12.5)
```

```
9999  STOP
      END
```

```
SUBROUTINE PROPERTY(H,T,CP,RHO,CON)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/PROP/HL,HS,CPL,CPS,CONL,CONS,RHOL,RHOS,TF
IF(H .GT. HL) THEN
  T = TF + (H - HL)/CPL
  CP = CPL
  RHO = RHOL
  CON = CONL
ELSEIF(H .GE. HS) THEN
  T = TF
  CP = CPL - (HL - H)*(CPL - CPS)/(HL-HS)
  CON = CONL - (HL - H)*(CONL - CONS)/(HL-HS)
  RHO = RHOL - (HL - H)*(RHOL - RHOS)/(HL-HS)
ELSE
  T = TF + (H - HS)/CPS
  CP = CPS
  RHO = RHOS
  CON = CONS
ENDIF
RETURN
END
```

Appendix A-2

Input Data for the Computer Program COPHASE.FOR



```
$OPTION
MRB = 1.      ILB = 0.      IRB = 1.
NpStp = 5.
IDX = 0.
$END
$INPUT1
Fa = .5.      Xsbl = 0.05.
Ft = .5.      NT = 200.      TIME = 2.,      dt = .0005.
Fx = 1.05.    NX = 325.      XL = .05.
vopt = 0.,    Av = 7.80D-06.  Bv = 0. .      Cv = 0. .
Div = 1.,     CO = 4.26D-06.
NPRT = 10
$END
$CONVER
eps1 = 2.D-2
$END
```

Appendix B-1

List of Computer Program SEGR.FOR



```
$OPTION
ILB = 4,      NPRT = 10,      NpStp = 1
$END
$INPUT1
NT = 13,      TIME = 7800.,    NX=50, XL = .05,
HINIT=1.132D6,
TINIT = 454., Tf=454.,      TA=250.,
HSF=0.6999D6, HLF=1.132D6,
CPS=3.963D3 , CPL=4.384D3,
CONDSF=71.20, CONDLF=42.80,
RHOSF=530.,  RHOLF=517.,
EMIT=0.8,
TWALL=100.,  HWALL=.6D6
$END
$CONVER
EPS1 = 1.0-30, EPS2 = 1.0-12, EPS3 = 1.0-14
$END
```

```

dtprt = time/dfloat(nprt)
DO 5 I=1,nprt
PRTIME(I) = dfloat(i)*dtprt
5 CONTINUE

C **** MESH GENERATION: STABILITY OF SOLUTION
C find maximum velocity, Vmax
if(idx .eq. 0) then
Vmax = V(1)
do 10 i = 1,nt
if(Vmax .le. V(i)) then
Vmax = V(i)
endif
10 continue
dx1 = 2.*Dc/Vmax/div

20 sum = 1
do 25 i=2,nx
25 sum = sum + fx**dfloat(i-1)

dxo = XL/sum
Xi(0) = 0.
do 30 i = 1, Nx
30 dx(i) = dxo*fx**dfloat(i-1)
Xi(i) = Xi(i-1) + dx(i)

if(dx1.lt.dx(1)) then
nx = nx+1
go to 20
endif

elseif(idx .eq.1) then
dxs = xsbl/Dfloat(Nx)
DO 35 i = 1,Nx
35 dx(i) = dxs
Xi(i) = Xi(i-1) + dx(i)

else
Vmax = V(1)
do 1011 i = 1,nt
if(Vmax .le. V(i)) then
Vmax = V(i)
endif
1011 continue
dx1 = 2.*Dc/Vmax/div

2011 sum = 1
do 2511 i=2,nx
2511 sum = sum + fx**dfloat(i-1)

dxo = XL/sum
Xi(0) = 0.
do 3011 i = 1, Nx
3011 dx(i) = dxo*fx**dfloat(i-1)
Xi(i) = Xi(i-1) + dx(i)

if(dx1.lt.dx(1)) then
nx = nx+1
go to 2011
endif

endif
dxend = dx(1)/20.
Nx1 = Nx-1

```

```

Nx10 = Nx-10

C **** PREPARATION FOR INITIAL CONDITIONS

SGAM = RHOS/RHOL - 1.
IF(MRB .EQ.0) SGAM = 0.

C **** INITIAL CONCENTRATION

DO 40 J = 1,2
DO 40 I = 1, NX
Cx(I,J) = Co
40 CONTINUE

C -----
C **** INITIAL TOTAL MASS OF GAS IN THE SYSTEM
C -----
Citot = 0.
DO 50 I = 1, NX
50 Citot = Citot + Cx(I,1)*DX(I)
Ctotold = Citot
c Co*XL

C **** Bubble Volume Calculation
ExcHe = Co*XL/AwHe
VolHetot = ExcHe*Rg*To/Po

CADmass = 0.
Cflux = 0.
DELTA = 0.
iend = 0
tr = 0.
itime = 0

C -----
C **** THE BEGINNING OF TIME LOOP *****
C -----
9000 Continue
c DO 9000 MA = 1, NT
itime = itime + 1
M=2
ma = 1
tr = tr + dt
V(ma) = Av + Bv*tr + Cv*tr**2.

G = -(1.+sGam)*V(ma)
DELTA = DELTA + v(ma)*DT
Xliq = Xlo-(1.+sGam)*Delta

if(xliq .le. dxend) then
iend = 1
endif

print *, '
print *, ' S-L Front = ', Sngl(delta), ' [M]'
print *, ' Liquid Length = ', Sngl(Xliq), ' [M]'

if(MRB .eq. 1) then

Xend = XLo - sGam*DELTA
Vf = (XLo-Xend)/XLo
print *, ' Void Forming At Right Boundary'
print *, ' Void Location is ', sngl(Xend), ' [M]'
print *, ' Vol(Void)/Vol(Sys) = ', sngl(Vf)

else

```

```

Xend = XLo
Vf = 0.
print *, ' No Void Formation'
print *, ' Void Location is ', sngl(Xend), ' [M]'
print *, ' Vol(Void)/Vol(Sys) = ', sngl(Vf)

endif

```

```

C **** Determine Equivalent Interface Diffusion Coefficients and
C Patanckar High Flux Function

```

```

DO 60 I = 1, Nx
Di(i) = 2.*Dc/(DX(i)+DX(i+1))
Pe = G/Di(i)
Fpe(i) = FP(Pe)
60 Continue

```

```

C **** DETERMINE COEFFICIENTS FOR LEFT BOUNDARY NODE

```

```

DFL = Di(1)*FPe(1)
Dm1 = Dc/DX(1)
Pe1 = G/Dm1
FPe1 = FP(Pe1)
DFL1 = Dm1*FPe1
Aw(1) = 0.
Ae(1) = -Fo*DFL

IF(ILB .EQ. 1) THEN                                | J- = -Cs*[d(delta)/dt]
Am(1) = DX(1)/dt + Fo*(DFL + G)
S(1) = Dx(1)/dt*Cx(1,M-1) - Cs*v(ma)
&      + (1.-Fa)*(DFL*Cx(2,m-1) - (G + DFL)*Cx(1,m-1))

ELSEIF(ILB .EQ. 2) THEN                             | J- = beta*(Ci - Cs)
beta = 1./(1./v(ma) - DX(1)/2./Dc)
Am(1) = DX(1)/dt + Fo*(DFL + G - beta)
S(1) = Dx(1)/dt*Cx(1,M-1) - Cs*beta
&      + (1.-Fa)*(DFL*Cx(2,m-1) + (beta - DFL - G)*Cx(1,m-1))

ELSEIF(ILB .EQ. 3) THEN                             | J- = 0.
Am(1) = DX(1)/dt + Fo*(DFL + G)
S(1) = Dx(1)/dt*Cx(1,M-1)
&      + (1.-Fa)*(DFL*Cx(2,m-1) - (DFL + G)*Cx(1,m-1))

ELSEIF(ILB .EQ. 4) THEN                             | J- = (Co - Cs)*[d(delta)/dt]
Am(1) = DX(1)/dt + Fo*(DFL + G)
S(1) = Dx(1)/dt*Cx(1,M-1) + (Co - Cs)*V(ma)
&      + (1.-Fa)*(DFL*Cx(2,m-1) - (DFL + G)*Cx(1,m-1))

ELSEIF(ILB .EQ. 5) THEN                             | J- = (C1 - CS)*[d(delta)/dt]
Am(1) = DX(1)/dt + Fo*(DFL + G - v(ma))
S(1) = Dx(1)/dt*Cx(1,M-1) - Cs*V(ma)
&      + (1.-Fa)*(DFL*Cx(2,m-1) - (DFL + G - v(ma))*Cx(1,m-1))

ELSE                                                | C(0, T) = Ch
Am(1) = DX(1)/dt + Fo*(DFL + G + DFL1)
S(1) = Dx(1)/dt*Cx(1,M-1) + (G + DFL1)*Ca
&      + (1.-Fa)*(DFL*Cx(2,m-1) - (DFL + G + DFL1)*Cx(1,m-1))

ENDIF

```

```

C **** DETERMINE COEFFICIENTS FOR INTERIOR NODES

```


C

```
DO 70 I = 2, Nx1
DFi = Di(i)*FPe(i)
DFi1 = Di(i-1)*FPe(i-1)

Aw(i) = -Fo*(DFi1 + G)
Ae(i) = -Fo*DFi
Am(i) = DX(i)/dt - (Ae(i) + Aw(i))
S(i) = Dx(i)/dt*Cx(i,M-1) - (1.-Fo)/Fo*(Ae(i)*Cx(i+1,m-1)
&      -(Ae(i)+Aw(i))*Cx(i,m-1) + Aw(i)*Cx(i-1,m-1))
```

70 CONTINUE

C

C **** DETERMINE COEFFICIENTS FOR RIGHT BOUNDARY NODE

C

```
DFR = Di(Nx)*FPe(Nx)
DFR1 = Di(Nx1)*FPe(Nx1)
Aw(Nx) = -Fo*(DFR1 + G)
Ae(Nx) = 0.

IF(IRB .EQ. 1) THEN                                ! J+ = Co*G
Am(Nx) = DX(Nx)/dt + Fo*DFR1
S(Nx) = Dx(Nx)/dt*Cx(Nx,M-1) - Co*G
&      + (1.-Fo) * ((G+DFR1)*Cx(Nx1,m-1)
&      - DFR1*Cx(Nx,m-1))

ELSEIF(IRB .EQ. 2) THEN                             ! Ci+1 = Ci
Am(Nx) = DX(Nx)/dt - Aw(Nx)
S(Nx) = Dx(Nx)/dt*Cx(Nx,M-1)
&      + (1.-Fo)/Fo*Aw(Nx)*(Cx(Nx1,m-1) - Cx(Nx,m-1))

ELSEIF(IRB .EQ. 3) THEN                             ! Ci+1 = Co
Am(Nx) = DX(Nx)/dt + Fo*DFR - Aw(Nx)
S(Nx) = Dx(Nx)/dt*Cx(Nx,M-1) + DFR*Co
&      + (1.-Fo)*((DFR1 + G)*Cx(Nx1,m-1)
&      - (DFR + G + DFR1)*Cx(Nx,m-1))

ELSEIF(IRB .EQ. 4) THEN                             ! Ci+1 = 0.
Am(Nx) = DX(Nx)/dt + Fo*DFR - Aw(Nx)
S(Nx) = Dx(Nx)/dt*Cx(Nx,M-1)
&      + (1.-Fo)*((DFR1 + G)*Cx(Nx1,m-1)
&      - (DFR + G + DFR1)*Cx(Nx,m-1))

ELSE                                                ! J+ = Co*G + Di*Fi(Ci-Co)
Am(Nx) = DX(Nx)/dt + Fo*(DFR + DFR1 + G)
S(Nx) = Dx(Nx)/dt*Cx(Nx,M-1) - Co*(G - DFR)
&      + (1.-Fo)*((DFR1 + G)*Cx(Nx1,m-1)
&      - (DFR + DFR1 + G)*Cx(Nx,m-1))

ENDIF
```

C

C **** GET SOLUTION FOR PRESENT TIME STEP; TRIDIAGONAL MATRIX SOLVER

C

```
CALL TDMA(sCx, Aw, Am, Ae, S, Nx)

C **** STORE CALCULATED VALUES IN THE PRESENT VARIABLES
DO 100 I=1,NX
Cx(I,M) = sCx(I)
c Cx(i,m) = Cx(i,m)/(1. - (1. + sGam)*v(m)*dt/x1)
dx(i) = dx(i)*(1. - (1. + sGam)*v(m)*dt/x1)
```



```

FluxR = Co*(G - DFR)
&      + (G + DFR)*(Fo*Cx(Nx,m) + (1.-Fo)*Cx(Nx,m-1))

```

```
ENDIF
```

```

C
C Obtain total mass at the time step

Citot = 0.
DO 200 I = 1,Nx
Citot = Citot + Cx(i,m)*dx(i)
200 continue
avgCi = Citot/Xliq

Admass = (FluxL - FluxR)*dt
CAdmass = CAdmass + Admass
Error1 = Citot - Admass - Ctotold
BAL1 = Error1/Ctotold *100.

C **** Bubble Volume Calculation
nnuc = 0
sumdx = 0.
Cexcess = 0.
if(Cx(imax,m) .GT. Ch) then
if(istop .eq.1) then
write(12, 2115) sngl(tr)
do 2118 i = 1,nx,2
cxco = cx(i,m)/co
xixliq = xi(i)/xliq/100.
2118 write(12, 2116) xixliq, cxco
2116 format(5x,d20.10,2x,d20.10)
2115 format(5x,'time = ',f10.3,' sec')
print *, 'optional stop at first occurrence of Cx(imax,m) > Ch'
stop
endif

DO 205 i = 1, Nx
if(Cx(i,m) .GE. Ch) then
Cexcess = Cexcess + (Cx(i,m) - Ch)*dx(i)
endif
205 continue

if(Cexcess .GT. CAdmass) then
c AvailC = Cexcess - CAdmass
AvailC = Cexcess
c CAdmass = 0.
do 2051 i = 1, Nx

if(Cx(i,m) .GE. Ch) then
Cx(i,m) = Ch
Sumdx = Sumdx + dx(i)
Inuc = 1
Nnuc = Nnuc + 1
Nucnode(Nnuc) = i
endif

2051 continue
endif

if(AvailC .GT. 0.) then
TheMole = AvailC/AwHe
HeMole = TheMole/Trnuc
AddVol = HeMole*Rg*To/Po
VolHe = VolHe + AddVol

```

```

        if(volHe .GT. VolHetot) then
AdjCx = (VolHe - VolHetot)*Po*AwHe/(Rg*To)
VolHe = VolHetot
Redist = AdjCx/Sumdx
206 Cx(Nucnode(i),m) = Cx(Nucnode(i),m) + Redist*dx(Nucnode(i))

        else
AdjCx = 0.
endif

endif

endif

VolSh = Delta*sGam
Voltot = VolHe + VolSh
Write(*,6080) sngl(AddVol), sngl(VolHe), sngl(VolSh), sngl(Voltot)
WRITE(*, 6020) SNGL(Citot), SNGL(Admass), SNGL(Ctotold),
& SNGL(Error1), SNGL(BAL1)

C **** STORE PRESENT STEP VALUES IN THE PREVIOUS STEP VARIABLES TO ADVANCE
C NEXT TIME STEP
DO 300 I=1,NX
Cx(I,M-1) = Cx(I,M)
300 CONTINUE
Ctotold = Citot - Cexcess + AdjCx
AvailC = 0.

C
C **** TRANSFORMATION INTO DIMENSIONLESS VARIABLES
C

TB = Tr + DT
CxCh = Cx(Imax,m)/Ch
itck = itime/NpStp*NpStp

& if(itck .eq. itime .or. itime .eq. 1
.or. Inuc .EQ. 1 .or. iend .eq.1) then
Write(13,6090) sngl(TR), sngl(VolHe), sngl(VolSh), sngl(Voltot)
endif
print *,' '
print *,'Time=', SNGL(TR),' Cx(1)=' , Cx(1,m)

DO 500 IJ = 1,NPRT

IF(TR .LE. PRTIME(IJ) .AND. TB .GT.PRTIME(IJ)) THEN
WRITE(*,6050) SNGL(Tr)
WRITE(12,6050) SNGL(Tr)
WRITE(12,6040)
IPFlag = 1
ENDIF
500 CONTINUE
if(IPFlag .eq. 1) then
do 400 ik = 1,nx,2
CxCh=Cx(ik,m)/Ch
CxCo = Cx(ik,m)/Co
XiXLIq = Xi(ik)/XLIq
Arg = (xi(ik)-dx(ik)/2.)/(2.*DSQRT(Dc*tr))
Anal = (Co*(1. - DERF(Arg)) + Co*DERF(Arg))/Co
400 write(12,2119) XiXLIq, CxCo, Anal
2119 format(5x,d20.10,2x,d20.10,2x,d20.10)

IPFlag = 0
endif
Inuc = 0

```

```

        if(iend .ne. 1) then
          go to 9000
        endif
c9000  CONTINUE

```

```

C
C   FORMAT STMTS
C

```

```

5010  FORMAT(5X,D12.5,3X,D12.5)
6001  format(1x,'L =',F10.4, ' m')
6010  FORMAT(/5X,'INITIAL CONCENTRATION DISTRIBUTION'/
&      5x,E12.5,2X,E12.5,2X,E12.5,2X,E12.5)
6020  FORMAT(/5X,'MASS BALANCE AT THIS TIME STEP'/
&      4x, '-----'/'
&      5X,' Total Mass = ',E12.5,' [Kg/M**3]'/
&      5X,' Accumulation = ',E12.5/'
&      5X,' Initial Mass = ',E12.5/'
&      4x, '-----'/'
&      5X,' Difference = ',E12.5,' [Kg/M**3]'/
&      5X,' % ERROR = ',E12.5)
6030  FORMAT(3X,E12.5,3X,D20.10)
6040  FORMAT(/5X,'He Concentration Distribution'/
&      4x, '-----'/'
&      5X,'Position(M)  Concentration [Kg/M**3]'/
&      4x, '-----')
6050  FORMAT(/5X,'COMPUTED RESULTS AT TIME =',E12.5,' [SEC]')
6070  FORMAT(3X,E12.5,3X,D20.10)
6080  format( 5x,'Information for Void'/
&      4x, '-----'/'
&      5x,'Added He Vol.      =',e12.5,' [M**3]'/
&      5x,'Total He Vol.      =',e12.5/'
&      5x,'Vol. of Shrinkage Void =',E12.5/'
&      5x,'Total Void Volume  =',E12.5//)
6090  format(2x,e12.5,2x,e12.5,2x,e12.5,2x,e12.5)
9999  STOP
      END

```

```

c *****
c TRIDIAGONAL MATRIX SOLVER : aWi.X(i-1) + aPi.X(i) + aEi.X(i+1) = Si
c *****

```

```

SUBROUTINE TDMA(X, aW,aP,aE,S, N)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DIMENSION X(1), aW(1),aP(1),aE(1),S(1)
DIMENSION P(1000),Q(1000)

```

```

c
c   ( aW(1) = 0. , aE(N) = 0. )
c

```

```

c
c   P(1) = -aE(1)/aP(1)
c   Q(1) = S(1)/aP(1)
c

```

```

c
c   DO 10 i=2,N
c     DENUM = aP(i)+aW(i)*P(i-1)
c     P(i) = -aE(i)/DENUM

```

```
      Q(i) = ( S(i)-oW(i)*Q(i-1) ) /DENUM
10  CONTINUE
c
      X(N) = Q(N)
c
      DO 20 i=N-1,1 , -1
          X(i) = P(i)*X(i+1)+Q(i)
20  CONTINUE
c
      RETURN
      END
```

Appendix B-2

Input Data for Computer Program SEGR.FOR



```

PROGRAM SEGRGATE
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION PRTIME(20), Nucnode(1000)
COMMON /CONVE1/ EPS1, EPS2, EPS3
COMMON /MESHX/ Xi(0:1000), dx(1000), sdx(1000), DT
COMMON /CONCE/ Cx(0:1000,2), Di(0:1000), FPe(0:1000),
& sCx(1000)
COMMON /VELOC/ v(0:1000), T(0:1000), vel(0:2), tm(0:2)
COMMON /MATRIX/ Aw(1000), Am(1000), Ae(1000), S(1000)
NAMELIST /INPUT1/ NT, TIME, NX, XL, Co, Cs, Ch, Dc, vopt,
& Av, Bv, Cv, Div, nprt, fx, ft, Fa, dt, xsbl, Ca
NAMELIST /CONVER/ EPS1, EPS2, EPS3
NAMELIST /OPTION/ MLB, MRB, ILB, IRB, Npstp, IDX, istop

C **** IRB = 0 ; Adiabatic Right Boundary
C          = 1 ; Constant supply of gas at initial concentration
c          with the speed of (solidification+volume shrinkage)

C **** Function F(Pe): Patancker High Flux
FP(z) = DMAX1(0.D0, 1.D0 - 0.1D0*DABS(z))*5.D0
&      + DMAX1(0.D0, -z)

OPEN(10, ERR=9999, FILE='SEGR6.INP', STATUS='OLD')
OPEN(11, ERR=9999, FILE='SEGR6.Cmt', STATUS='UNKNOWN')
OPEN(12, ERR=9999, FILE='SEGR6.Cxi', STATUS='UNKNOWN')
OPEN(13, ERR=9999, FILE='SEGR6.Vol', STATUS='UNKNOWN')
OPEN(14, ERR=9999, FILE='SEGR6.Del', STATUS='UNKNOWN')
OPEN(15, ERR=9999, FILE='SEGR6.Tem', STATUS='UNKNOWN')
OPEN(20, ERR=9999, FILE='vel.Tem', STATUS='old')

C **** DEFAULT VALUES FOR OPTIONS
DATA MLB/0/, MRB/0/, ILB/1/, IRB/0/, Vopt/0/
DATA dt/ 5./

C **** CONSTANTS
DATA PHI/3.1415926/, Dc/5.96D-09/, Rhos/530./, Rhol/517./
DATA Ch/1.737D-03/, Co/4.26D-06/, Cs/1.59D-08/,
&      Csat/1.59D-08/
DATA Po/7330./, To/454./, Rg/8.3143/, AwHe/4.0026D-03/

C **** READ NAMELIST INPUT
READ(10,OPTION)
READ(10,INPUT1)
READ(10,CONVER)
write(11,6001) XL
write(12,6001) XL
write(13,6001) XL
write(14,6001) XL
write(15,6001) XL

C **** THE TIME STEP SIZE: UNIFORM

DTin = TIME/DFLOAT(NT)

IF(VOPT .GT. 0.) THEN
DO 1 I=1,NT
1      READ(20,5010) T(I),V(I)
ELSE
DO 2 I=1,NT
2      T(I) = dFLOAT(I)*dtin
V(I) = Av + Bv*t(i) + Cv*t(i)**2.
ENDIF

XLo = XL
Nxo = Nx

C **** IDENTIFY PRINTOUT TIME

```


Appendix C

List of Computer Program FREZ.FOR



```

c      write(6, 6002)
      write(7, 6003)
c      write(8, 6004)
      write(9, 6005)
      write(10, 6006)
      write(17, 6007)
      write(18, 6008)
      write(19, 6009)
      endif

      if(ipcm .ne. 1) then      ! LiF calculation
C LiF properties
      Tf=Tff
      Ti=Tif
      xKs=xKsf
      xKi=xKif
      Cps=Cpsf
      rhos=rhosf
      rhoi=rhoif
      Hsl=Hslf
      xKv=xKvf
      endif

      n=5
      nx=2

      if(iopt .eq. 1) go to 9000

c      if(ivoid .eq. 1) then
c      do = 0.00001
c      slo = do
c      else
c      do = 0.
c      slo = do
c      endif
      dos = do

      do 10 i=1,n
      To(i)=Ti
      Ts(i)=Ti
10      continue

      HI = Hsl + Cps*Tf
      eps3o = eps3
      epso = eps1
      eps12 = dsqrt(eps1)
      Gam = 1. - rhoi/rhos
      rGam = Gam/(1.-Gam)

      As = xKs/rhos/Cps
      Ac = xKc/rhoc/Cpc
      a1 = rhoc*Cpc*tc/dt
      a2 = rhos*Cps/dt

      hcs = 2.*xKc/tc
      Al = Emitout*Boltz/hcs
      SumLam=0.
      do 50 it=1, nt

      ind = it/nprenpr - it
      time = dfloat(it)*dt
      Erdo = 1.D30
      if(it .eq. 1) then
      dmax = do + 2.*eps3

```

```

else
dmax = do + 2.*vel*dt
endif
dmin = do
iout = 0

20 continue
iout = iout + 1

C Assume ds; new solid crust thickness
ds = (dmax+dmin)/2.
dvs = rGam*ds
if( ivoi .eq. 1) then
sis = ds + dvs
else
sis = ds
endif

C Equivalent heat transfer coefficients
C At the outer wall of the cladding, hot

Den = 1./Emitout/Boltz + 4.*Ts(1)**3/hcs
ho1 = (Ts(1)**2+Ta**2)*(Ts(1)+Ta)/Den

C within the void

hss = 2.*xKs/ds
hcvs = xKv/dvs
hr2s = Emitin*Boltz*(Ts(4)**2 + Ts(3)**2)*(Ts(4) + Ts(3))
hv = hcvs + hr2s
c hv = hcvs

IF(IBC .eq. 1) THEN

C Overall between T1 and T2
C2 This considers heat transfer across the void
if(ivoi .eq. 1) then
h12 = 1./(1./hcs + 1./hv + 1./hss)
else
C BC1 This does not consider heat transfer across the void
h12 = 1./(1./hcs + 1./hss)
endif

C BC1 Radiative Boundary
aw(1) = 0.
ap(1) = ho1 + h12 + a1
ae(1) = -h12
s(1) = a1*To(1) + ho1*Ta

aw(2) = -h12
ap(2) = h12 + hss + a2*ds
ae(2) = 0.
s(2) = rhos*Hl/dt*(ds-do) + a2*do*To(2) + hss*Tf

call tdma(Tn,aw,ap,ae,s,nx)

dT5 = A1*(Tn(1)**4.-Ta**4)/(1.+4.*A1*Tn(1)**3)
Tn(5) = Tn(1)-dT5

C BC1 This considers heat transfer across the void
if(ivoi .eq. 1) then
Tn(4) = h12*(Tn(1)/hss + (1./hcs + 1./hv)*Tn(2))
Tn(3) = h12*(Tn(2)/hcs + (1./hss + 1./hv)*Tn(1))
else
C BC1 This does not consider heat transfer across the void

```

```

Tn(4) = h12*(Tn(1)/hss + 1./hcs*Tn(2))
Tn(3) = h12*(Tn(2)/hcs + 1./hss*Tn(1))
endif

ELSE
C BC2 Constant wall temperature
Tn(1) = Ta
Tn(5) = Tn(1)
Tn(3) = Tn(1)

if(ivoid .eq. 1) then
C BC3 Constant wall temperature, with void
h12 = 1./(1./hss + 1./hv)
else
C BC2 Constant wall temperature, without void
h12 = hss
endif

Tn(2) = (a2*do*To(2) + rhos*Hl*(ds-do)/dt
& + hss*Tf + h12*Tn(1))/(h12 + hss + a2*ds)

if(ivoid .eq. 1) then
Tn(4) = (hv*Tn(1) + hss*Tn(2))/(hss + hv)
else
Tn(4) = Tn(1)
endif

ENDIF

C Check energy balance of the system
C Heat flux at the left boundary of the system

Qls = -ho1*(Tn(1)-Ta)

C Heat flux at the left boundary of the PCM

Qlp = -h12*(Tn(2)-Tn(1))
C For constant wall temperature only
if(iBC .eq. 2) Qls = Qlp

C Heat flux at the right boundary of the system, x=xLB + delta
C which is equal to Heat flux at the right boundary of the solid PCM

Qrs = -rhos*Hsl*(ds-do)/dt

C Total heat accumulated in the system within dt
c Fully implicit scheme
EQp = (Qlp - Qrs)*dt
EQs = (Qls - Qrs)*dt

C Energy accumulated within the cladding
if(iBC .eq. 1) then
Ec = tc*rhoc*Cpc*(Tn(1) - To(1))
else
Ec = 0.
endif

C Energy accumulated within the solid crust
Ep = rhos*Cps*(ds*Tn(2) - do*To(2))-(ds-do)*rhos*Hl

C Total Energy accumulated in the system
Ea = Ec + Ep

Ers = (EQs - Ea)/Ea

```

```

Erp = (EQp - Ep)/Ep
REcEp = Ec/Ep
vel = (ds-do)/dt

if(it .eq. 1 .or. ind .eq. 0) then
c write(*,6080) iout, sngl(Ec),sngl(Ep),sngl(REcEp),sngl(vel)
endif

C Check the convergence

Cx = 2.*xKs*(Tf-Tn(2))*dt/rhos/Hsl
if(Cx .LT. 0.) Cx = 0.
Cy = do**2 + 4.*Cx
dsc = (dsqrt(Cy)+do)/2.

Ero = (ds - dsc)/ds
AEro = dabs(Ero)
Erdn = dabs(ds - dsc)

if(it .eq. 1 .or. ind .eq. 0) then
c write(*,6020) sngl(Erdo), sngl(Erdn), sngl(Erp),sngl(Ers)
endif

if(Erdn .LE. eps1) go to 30
if(dsc .GT. ds) then
dmin = ds
Erdo = Erdn
go to 20
else
dmax = ds
Erdo = Erdn
go to 20
endif

30 continue

if(ivoid .eq. 1) then
Qrin = -Emitin*Boltz*(Tn(4)**4 - Tn(3)**4)
Qcin = -hcvs*(Tn(4)-Tn(3))
qrat = Qcin/Qrin
endif
Stef = Cps*(Tf - Tn(5))/Hsl
FC = (sis-sio)/dt*dsqrt(time/As)
SumLam = SumLam + FC
do = ds
sio = sis
dos = ds
do 40 i=1,n
Ts(i)=Tn(i)
To(i)=Ts(i)
40 continue
if(iopt .ne. 1) then
if(it .eq. 1 .or. ind .eq. 0) then

print *, ' '
print *, ' '
print *, 'Sol. converged'
aQls = dabs(Qls)
aQlp = dabs(Qlp)
aQrs = dabs(Qrs)
write(7, 6010) sngl(time),sngl(Tn(1))
write(10, 6010) sngl(time),sngl(Tn(2))
c write(8, 6010) sngl(time),sngl(Tn(3))
write(9, 6010) sngl(time),sngl(Tn(4))

```

```

c      write(6, 6010) sngl(time),sngl(Tn(5))
      write(11, 6010) sngl(time),sngl(FC)
      write(12, 6010) sngl(time),sngl(vel)
      write(13, 6010) sngl(time),sngl(Ers)
      write(14, 6010) sngl(time),sngl(ds)
      write(15, 6010) sngl(time),sngl(qrot)
      write(16, 6010) sngl(time),sngl(REcEp)
      write(17, 6010) sngl(time),sngl(oQ1s)
      write(18, 6010) sngl(time),sngl(oQ1p)
      write(19, 6010) sngl(time),sngl(oQrs)
      endif
      endif
50     continue

      avFC = SumLam/DFloat(nt)
      write(10,8010)
      write(11,8011) Sngl(Stef)
      write(12,8012)
      write(13,8013)
      write(14,8014)
      write(15,8015)
      write(16,8016)
      write(19,8017)
      go to 9999

9000   continue
C This proc. calculates Average Freezing constant, avgFC, for given time
C period
C      in this proc. Wall Temp., Tw, is varied from 250 K
C      to 450 K for Lithium      ; Tf(Li) = 454 K
C      to 1120 K for Lithium Fluoride ; Tf(LiF) = 1122 K
      if(iPCM .eq. 1) then
      Tu = 450.
      else
      Tu = 1120.
      endif
      Tl = 250.

      dTe = (Tu-Tl)/25.
      Tlow = Tl - dTe

      do 160 iTw=1,25
      Tw = Tlow + dTe*Dfloat(iTw)
      Ta = Tw
      print *, 'Tw = ',sngl(Tw)
c      if(ivoid .eq. 1) then
c      do = 0.00001
c      slo = do
c      else
c      do = 0.
c      slo = do
c      endif
      dos = do

      do 110 i=1,n
      To(i)=Ti
      Ts(i)=Ti
110     continue

      Hl = Hsl + Cps*Tf
      eps3o = eps3
      epso = eps1
      eps12 = dsqrt(eps1)
      Gam = 1. - rho1/rhos

```

```

rGam = Gam/(1.-Gam)

As = xKs/rhos/Cps
Ac = xKc/rhoc/Cpc
a1 = rhoc*Cpc*tc/dt
a2 = rhos*Cps/dt

hcs = 2.*xKc/tc
Al = Emitout*Boltz/hcs
SumLam=0.
do 150 it=1, nt

    ind = it/npr*npr - it
    time = dfloat(it)*dt
    Erdo = 1.D30
    if(it .eq. 1) then
        dmax = do + 2.*eps3
    else
        dmax = do + 2.*vel*dt
    endif
    dmin = do
    iout = 0

120    continue
    iout = iout + 1

C Assume ds; new solid crust thickness
ds = (dmax+dmin)/2.
dvs = rGam*ds
if( ivoi .eq. 1) then
    sls = ds + dvs
else
    sls = ds
endif

C Equivalent heat transfer coefficients
C At the outer wall of the cladding, ho1

    Den = 1./Emitout/Boltz + 4.*Ts(1)**3/hcs
    ho1 = (Ts(1)**2+Ta**2)*(Ts(1)+Ta)/Den

C within the void

    hss = 2.*xKs/ds
    hcvs = xKv/dvs
    hr2s = Emitin*Boltz*(Ts(4)**2 + Ts(3)**2)*(Ts(4) + Ts(3))
c    hv = hcvs + hr2s
    hv = hcvs

    IF(IBC .eq. 1) THEN

C Overall between T1 and T2
C2    This considers heat transfer across the void
    if(ivoi .eq. 1) then
        h12 = 1./(1./hcs + 1./hv + 1./hss)
    else
C BC1    This does not consider heat transfer across the void
        h12 = 1./(1./hcs + 1./hss)
    endif

C BC1 Radiative Boundary
    aw(1) = 0.
    ap(1) = ho1 + h12 + a1
    ae(1) = -h12
    s(1) = a1*To(1) + ho1*Ta

```

```

aw(2) = -h12
ap(2) = h12 + hss + a2*ds
ae(2) = 0.
s(2) = rhos*Hl/dt*(ds-do) + a2*do*To(2) + hss*Tf

call tdma(Tn,aw,ap,ae,s,nx)

dT5 = A1*(Tn(1)**4.-To**4)/(1.+4.*A1*Tn(1)**3)
Tn(5) = Tn(1)-dT5

C BC1 This considers heat transfer across the void
if(ivoid .eq. 1) then
Tn(4) = h12*(Tn(1)/hss + (1./hcs + 1./hv)*Tn(2))
Tn(3) = h12*(Tn(2)/hcs + (1./hss + 1./hv)*Tn(1))
else
C BC1 This does not consider heat transfer across the void
Tn(4) = h12*(Tn(1)/hss + 1./hcs*Tn(2))
Tn(3) = h12*(Tn(2)/hcs + 1./hss*Tn(1))
endif

ELSE
C BC2 Constant wall temperature
Tn(1) = To
Tn(5) = Tn(1)
Tn(3) = Tn(1)

if(ivoid .eq. 1) then
C BC3 Constant wall temperature, with void
h12 = 1./(1./hss + 1./hv)
else
C BC2 Constant wall temperature, without void
h12 = hss
endif

Tn(2) = (a2*do*To(2) + rhos*Hl*(ds-do)/dt
& + hss*Tf + h12*Tn(1))/(h12 + hss + a2*ds)

if(ivoid .eq. 1) then
Tn(4) = (hv*Tn(1) + hss*Tn(2))/(hss + hv)
else
Tn(4) = Tn(1)
endif

ENDIF

C Check energy balance of the system
C Heat flux at the left boundary of the system

Qls = -ho1*(Tn(1)-To)

C Heat flux at the left boundary of the PCM

Qlp = -h12*(Tn(2)-Tn(1))
C For constant wall temperature only
if(iBC .eq. 2) Qls = Qlp

C Heat flux at the right boundary of the system, x=xLB + delta
C which is equal to Heat flux at the right boundary of the solid PCM

Qrs = -rhos*Hsl*(ds-do)/dt

C Total heat accumulated in the system within dt
c Fully implicit scheme

```



```
EQp = (Qlp - Qrs)*dt
EQs = (Qls - Qrs)*dt
```

```
C Energy accumulated within the cladding
if(IBC .eq. 1) then
Ec = tc*rhoc*Cpc*(Tn(1) - To(1))
else
Ec = 0.
endif
```

```
C Energy accumulated within the solid crust
Ep = rhos*Cps*(ds*Tn(2) - do*To(2))-(ds-do)*rhos*Hl
```

```
C Total Energy accumulated in the system
Ea = Ec + Ep
```

```
Ers = (EQs - Ea)/Ea
Erp = (EQp - Ep)/Ep
```

```
REcEp = Ec/Ep
vel = (ds-do)/dt
```

```
C Check the convergence
```

```
Cx = 2.*xKs*(Tf-Tn(2))*dt/rhos/Hsl
if(Cx .LT. 0.) Cx = 0.
Cy = do**2 + 4.*Cx
dsc = (dsqrt(Cy)+do)/2.
```

```
Ero = (ds - dsc)/ds
AEro = dabs(Ero)
Erdn = dabs(ds - dsc)
```

```
c if(it .eq. 1 .or. ind .eq. 0) then
write(*,6020) sngl(Erdo), sngl(Erdn), sngl(Erp),sngl(Ers)
endif
```

```
if(Erdn .LE. eps1) go to 130
if(dsc .GT. ds) then
dmin = ds
Erdo = Erdn
go to 120
else
dmax = ds
Erdo = Erdn
go to 120
endif
```

```
130 continue
```

```
Stef = Cps*(Tf - Tn(5))/Hsl
FC = (s1s-s1o)/dt*dsqrt(time/As)
c FC = s1s/2./dsqrt(As*time)
SumLam = SumLam + FC
c print *, 'It=',it,' Fc = ',FC
```

```
do = ds
s1o = s1s
dos = ds
do 140 i=1,n
Ts(i)=Tn(i)
To(i)=Ts(i)
140 continue
```

```
if(it .eq. 1 .or. ind .eq. 0) then
```


c TRIDIAGONAL MATRIX SOLVER : $aW_i \cdot X(i-1) + aP_i \cdot X(i) + aE_i \cdot X(i+1) = S_i$
c

```
      SUBROUTINE TDMA(X, aW,aP,aE,S, N)
         implicit double precision (a-h, o-z)
         DIMENSION X(1), aW(1),aP(1),aE(1),S(1)
         DIMENSION P(1000),Q(1000)
c
c      ( aW(1) = 0. , aE(N) = 0. )
c
         P(1) = -aE(1)/aP(1)
         Q(1) = S(1)/aP(1)
c
         DO 10 i=2,N
            DENUM = aP(i)+aW(i)*P(i-1)
            P(i) = -aE(i)/DENUM
            Q(i) = ( S(i)-aW(i)*Q(i-1) ) /DENUM
10      CONTINUE
c
         X(N) = Q(N)
c
         DO 20 i=N-1,1,-1
            X(i) = P(i)*X(i+1)+Q(i)
20      CONTINUE
c
         RETURN
         END
```

```

program freeze
C This program uses dichotomic search for S-L front
C
C This program calculates temperatures T(i), i=1,5
C i=1, outer surface of the wall
C =2, middle of the solid crust
C =3, inner surface of cladding
C =4, PCM-Void interface
C =5, outer surface of cladding
C
      implicit double precision (a-h, o-z)
      character*8 adum
      dimension Tst(2,2000),Qst(3,2000), Timst(2000), Vst(2000)
      dimension To(5),Ts(5), Tn(5)
      dimension aw(1000), ap(1000), ae(1000), s(1000)
      data To/250./, dt/.1/, nt/2000/, Emitin/.8/, Emitout/.8/,
      & Boltz/5.67D-08/, npr/10/, xSL/1./, iTpr/500/
C LIF properties
      & Tff/1122./, Tif/1122./, xKsf/4.9997/, xKlf/1.3/,
      & Cpsf/2469.74/, rhosf/1792./, rhoif/1376./, Hsif/347271./
C Thermal conductivity of LiF vapor
      & xKvf/0.016954/,
C Li properties
      & Tf/454./, Ti/454./, xKs/75.8/, xKI/42.8/,
      & Cps/3780./, rhos/530./, rhoI/517./, HsI/432100./
C Thermal conductivity of He gas, at 200 F
      & xKv/0.16781/,
C Properties of cladding material
      & tc/0.00076/, Cpc/323.4/, rhoc/6490./, xKc/23.885/,
      & eps1/1.0-12/, eps2/1.75/, eps3/0.01/, tcm/2740./
C Initial size of void, thickness of the system
      data iopt/1/, iPCM/2/, ivoid/1/, iBC/2/, q1/25000./

```

```

c      open(6, err=9999, file='T1.dat', status='unknown')
c      open(7, err=9999, file='T2.dat', status='unknown')
c      open(8, err=9999, file='T3.dat', status='unknown')
      open(9, err=9999, file='T4.dat', status='unknown')
      open(10, err=9999, file='T5.dat', status='unknown')
      open(11, err=9999, file='FC.dat', status='unknown')
      open(12, err=9999, file='Vel.dat', status='unknown')
      open(13, err=9999, file='Ers.dat', status='unknown')
      open(14, err=9999, file='SL.dat', status='unknown')
      open(15, err=9999, file='Qrat.dat', status='unknown')
      open(16, err=9999, file='Erat.dat', status='unknown')
      open(17, err=9999, file='Qcid.dat', status='unknown')
      open(18, err=9999, file='Qsol.dat', status='unknown')
      open(19, err=9999, file='Qdel.dat', status='unknown')
      open(20, err=9999, file='Ttot.dat', status='unknown')
      open(21, err=9999, file='Qtot.dat', status='unknown')
c      open(22, err=9999, file='Tpro.dat', status='unknown')
c      open(23, err=9999, file='Tpro.dat', status='unknown')
c      open(24, err=9999, file='Tpro.dat', status='unknown')

```

```

write(11,6001)
IF(iopt.ne.1) then

```

```

write(7, 6001)
write(12,6001)
write(13,6001)
write(14,6001)
write(15,6001)
write(16,6001)
write(17,6001)

```

Appendix D

List of Computer Program MELT.FOR



```

        program melt
C This program uses dichotomic search for S-L front
C
C This program calculates temperatures T(i), i=1,5
C i=1, middle of the wall
C =2, middle of the liquid
C =3, inner surface of cladding
C =4, PCM-Void interface
C =5, outer surface of cladding
C
C during a melting processes
    implicit double precision (a-h, o-z)
    character*8 adum
    dimension Tst(2,2000),Qst(3,2000), Timst(2000), Vst(2000)
    dimension To(5),Ts(5), Tn(5)
    dimension aw(1000), ap(1000), ae(1000), s(1000)
    data Ta/1350./, dt/1./, nt/20000/, Emitin/.5/, Emitout/.8/,
    & Boltz/5.67D-08/, npr/10/, xSL/0.05/, iTpr/500/
C LiF properties
    & Tff/1122./, Tif/1122./, xKsf/4.9997/, xKlf/1.3/,
    & Cpsf/2469.74/, rhosf/1792./, rholf/1376./, Hs1f/347271./,
C Thermal conductivity of LiF vapor
    & xKvf/0.016954/,
C Li properties
    & Tf/454./, Ti/454./, xKs/75.8/, xKl/42.8/,
    & Cps/3780./, rhos/530./, rho1/517./, Hs1/432100./,
C Thermal conductivity of He gas, at 200 F
    & xKv/0.16781/,
C Properties of cladding material
    & tc/0.00076/, Cpc/323.4/, rhoc/6490./, xKc/23.885/,
    & eps1/1.D-12/, eps2/1.75/, eps3/0.01/, tcm/2740./
C Initial size of void, thickness of the system
    data lopt/0/,lPCM/2/, lvoid/1/, iBC/1/, q1/30000./
    data dvi/0.0001/, imachine/1/
    if(imachine .eq.1) then
        open(6, err=9999, file='TTV.dat', status='unknown')
        open(7, err=9999, file='TQR.dat', status='unknown')
    else
        open(6, err=9999, file='T1.dat', status='unknown')
        open(7, err=9999, file='T2.dat', status='unknown')
        open(8, err=9999, file='T3.dat', status='unknown')
        open(9, err=9999, file='T4.dat', status='unknown')
        open(10, err=9999, file='T5.dat', status='unknown')
        open(11, err=9999, file='dv.dat', status='unknown')
        open(12, err=9999, file='Vel.dat', status='unknown')
        open(13, err=9999, file='Ers.dat', status='unknown')
        open(14, err=9999, file='SL.dat', status='unknown')
        open(15, err=9999, file='Qrat.dat', status='unknown')
        open(16, err=9999, file='Erat.dat', status='unknown')
        open(17, err=9999, file='Qcid.dat', status='unknown')
        open(18, err=9999, file='Qsol.dat', status='unknown')
        open(19, err=9999, file='Qdel.dat', status='unknown')
    endif

1      format(2x,'Generate a plot. '/2x,'input data.')
2      format(2x,'...', 'T1', '...')
3      format(2x,'...', 'T2', '...')
4      format(2x,'...', 'T3', '...')
5      format(2x,'...', 'T4', '...')
6      format(2x,'...', 'T5', '...')
7      format(2x,'...', 'Cladding', '...')
8      format(2x,'...', 'PCM-Void', '...')
9      format(2x,'...', 'S-L Intf', '...')

    if(imachine .ne. 1) then

```

```
write(6,1)
write(11,1)
write(12,1)
write(13,1)
write(14,1)
write(15,1)
write(16,1)
write(17,1)
```

```
write(6,2)
write(7,3)
write(8,4)
write(9,5)
write(10,6)
write(17,7)
write(18,8)
write(19,9)
endif
```

```
n=5
nx=2
```

```
      if(IPCM .ne. 1) then      ! LIF calculation
C LIF properties
Tf=Tff
Ti=Tif
xKs=xKsf
xKl=xKlf
Cps=Cpsf
rhos=rhosf
rhoI=rhoIf
Hsl=Hslf
xKv=xKvf
endif
```

```
Hs = Cps*Tf
Hl = Hsl + Hs
Cpl = Hl/Tf
eps3o = eps3
eps1 = eps1
eps12 = dsqrt(eps1)
Gam = 1. - rhoI/rhos
rGam = (1.-Gam)/Gam
```

```
do = 0.000
dos = do
```

```
C Estimate the thickness of PCM and void
C based on the assumption that the system was originally filled with liquid
C at its fusion temperature
```

```
dvi = xSL*Gam
xPCM = xSL - dvi
dvo = dvi
```

```
do 10 i=1,n
To(i)=Ti
Ts(i)=Ti
continue
```

10

```
Ali = xKl/rhoI/Cpl
As = xKs/rhos/Cps
Ac = xKc/rhoc/Cpc
a1 = rhoc*Cpc*tc/dt
```

```

a2 = rho1*Cpl/dt

hcs = 2.*xKc/tc
A1 = Emitout*Boltz/hcs

do 3000 it=1, nt

ind = it/nprenpr - it
time = dfloat(it)*dt
Erdo = 1.D30
if(it .eq. 1) then
dmax = do + 3.*eps3
else
dmax = do + 3.*vel*dt
endif
dmin = do
iout = 0

100 continue
iout = iout + 1

C Assume ds; new solid crust thickness
ds = (dmax+dmin)/2.

C Equivalent heat transfer coefficients
C At the outer wall of the cladding, ho1

Den = 1./Emitout/Boltz + 4.*Ts(1)**3/hcs
ho1 = (Ts(1)**2+Ta**2)*(Ts(1)+Ta)/Den

C within the void
dvs = dvo - (ds-do)*Gam
if(dvo .lt. 1.d-06) then
ivoid = 0
dvs = 1.d-06
endif
h1s = 2.*xKl/ds
hcvs = xKv/dvs
hr2s = Emitin*Boltz*(Ts(4)**2 + Ts(3)**2)*(Ts(4) + Ts(3))
hv = hcvs + hr2s

C Overall between T1 and T2
C2 This considers heat transfer across the void
IF(IBC .ne. 2) THEN
if(ivoid .eq. 1)then
h12 = 1./(1./hcs + 1./hv + 1./h1s)
else
C1 This does not consider heat transfer across the void
h12 = 1./(1./hcs + 1./h1s)
endif

C BC1 Radiative Boundary
aw(1) = 0.
ae(1) = -h12
if(IBC .eq. 1) then
ap(1) = ho1 + h12 + a1
s(1) = a1*To(1) + ho1*Ta
else
ap(1) = h12 + a1
s(1) = a1*To(1) + q1
endif

C BC1
aw(2) = -h12
ap(2) = h12 + h1s + a2*ds
ae(2) = 0.

```



```

s(2) = rho1*Hl/dt*(ds-do) + a2*do*To(2) + hls*Tf
C BC1
call tdma(Tn,ow,ap,ae,s,nx)

if(IBC .eq. 1) then
dT5 = A1*(Tn(1)**4.-To**4)/(1.+4.*A1*Tn(1)**3)
Tn(5) = Tn(1)-dT5
else
Tn(5) = Tn(1) + q1/hcs
endif

C BC1 This considers heat transfer across the void
if(ivoid .eq. 1) then
Tn(4) = h12*(Tn(1)/hls + (1./hcs + 1./hv)*Tn(2))
Tn(3) = h12*(Tn(2)/hcs + (1./hls + 1./hv)*Tn(1))
else
C BC1 This does not consider heat transfer across the void
Tn(4) = h12*(Tn(1)/hls + 1./hcs*Tn(2))
Tn(3) = h12*(Tn(2)/hcs + 1./hls*Tn(1))
endif

ELSE

C BC2 Constant wall temperature, without void
if(ivoid .eq. 0) then
h12 = hls
C BC3 Constant wall temperature, with void
else
h12 = 1./(1./hls + 1./hv)
endif

Tn(1) = Ta
Tn(2) = (a2*do*To(2) + rho1*Hl*(ds-do)/dt
& + hls*Tf + h12*Tn(1))/(h12 + hls + a2*ds)

C BC2 Constant wall temperature.
Tn(5) = Tn(1)
Tn(3) = Tn(1)
C BC2 without void
if(ivoid .eq. 0) then
Tn(4) = Tn(1)
else
C BC2 with void
Tn(4) = (hv*Tn(1) + hls*Tn(2))/(hls + hv)
endif

ENDIF

C Check energy balance of the system
C Heat flux at the left boundary of the system

Qls = -ho1*(Tn(1)-To)

C Heat flux at the left boundary of the PCM

Qlp = -h12*(Tn(2)-Tn(1))
C For constant wall temperature heat flux at the outer surface of
C cladding should be equal to that for inner surface of cladding

if(IBC .eq. 2) Qls = Qlp
if(IBC .eq. 3) Qls = q1

C Heat flux at the right boundary of the system, x=xLB + delta
C which is equal to Heat flux at the right boundary of the solid PCM

```

```

      Qrs = -hls*(Tf-Tn(2)) - rho1*Hsl*(ds-do)/dt
C for melting process, heat conducted at the RHS of liquid
C only by temperature gradient
      Qrs1 = -hls*(Tf-Tn(2))

C Total heat accumulated in the system within dt
c Fully implicit scheme
      EQp = (Qlp - Qrs)*dt
      EQs = (Qls - Qrs)*dt

C Energy accumulated within the cladding (Temperature variation in the
C cladding is considered only when the radiative and constant heat flux
C boundary conditions)
      if(IBC .ne. 2) then
          Ec = tc*rhoc*Cpc*(Tn(1) - To(1))
C For constant wall temp Ec = 0.
          else
              Ec = 0.
          endif

C Energy accumulated within the liquid PCM
      Ep = rho1*Cpl*(ds*Tn(2) - do*To(2))-(ds-do)*rho1*Hs

C Total Energy accumulated in the system
      Ea = Ec + Ep

      Ers = (EQs - Ea)/Ea
      Erp = (EQp - Ep)/Ep

      REcEp = Ec/Ep
      vel = (ds-do)/dt

c      if(it .eq. 1 .or. ind .eq. 0) then
c          write(*,6080) it,iout,sngl(Ec),sngl(Ep),sngl(REcEp),sngl(vel)
c      endif
c6080      format(///2x,'it=',i5,'          iout=',i5/
c          & 2x,'Ec=',e12.5,2x,'Ep=',e12.5,2x,'Ratio=',e12.5,
c          & 2x,'vel=',e12.5)

C Check the convergence

      Cx = 2.*xKl*(Tn(2)-Tf)*dt/rho1/Hsl
      if(Cx .LT. 0.) Cx = 0.
      Cy = do*2 + 4.*Cx
      dsc = (dsqrt(Cy)+do)/2.

      Ero = (ds - dsc)/ds
      AEro = dabs(Ero)
      Erdn = dabs(ds - dsc)

c      if(it .eq. 1 .or. ind .eq. 0) then
c          write(*,6020) sngl(Erdo), sngl(Erdn), sngl(Erp),sngl(Ers)
c      endif
c6020      format(2x,'Erdo=',E12.5,2x,'Erdn=',E12.5,2x,'Erp=',e12.5,2x,
c          & 'Ers=',e12.5)

      if(Erdn .LE. eps1) go to 2000
      if(dsc .GT. ds) then
          dmin = ds
          Erdo = Erdn
          go to 100
      else
          dmax = ds
          Erdo = Erdn
          go to 100

```

```

endif
2000 continue
if(ivoid .eq. 1) then
Qrin = -Emitin*Boltz*(Tn(4)**4 - Tn(3)**4)
Qcin = -hcv*(Tn(4)-Tn(3))
qrat = Qcin/Qrin
endif

do = ds
dos = ds
dvo = dvs
do 170 i=1,n
Ts(i)=Tn(i)
Tc(i)=Ts(i)
170 continue
if(it .le. 50 .or. ind .eq. 0 .or. do .gt. xSL) then

c print *, '
c print *, '
c print *, 'Sol. converged'

aQls = dabs(Qls)
aQlp = dabs(Qlp)

c aQrs = dabs(Qrs)
C for melting process, heat conducted at the RHS of liquid
C only by temperature gradient
aQrs = dabs(Qrs1)
if(imachine .eq. 1) then
write(6, 6200) sngl(time),sngl(Tn(1)),sngl(Tn(2)),sngl(Tn(4)),
& sngl(vel)
write(7, 6200) sngl(time),sngl(aQls),sngl(aQlp),sngl(aQrs),
& sngl(Qrat)
else
write(7, 6010) sngl(time),sngl(Tn(1))
write(10, 6010) sngl(time),sngl(Tn(2))
write(8, 6010) sngl(time),sngl(Tn(3))
write(9, 6010) sngl(time),sngl(Tn(4))
write(6, 6010) sngl(time),sngl(Tn(5))
write(11, 6010) sngl(time),sngl(dvs)
write(12, 6010) sngl(time),sngl(vel)
write(13, 6010) sngl(time),sngl(Ers)
write(14, 6010) sngl(time),sngl(ds)
write(15, 6010) sngl(time),sngl(qrat)
write(16, 6010) sngl(time),sngl(REcEp)
write(17, 6010) sngl(time),sngl(aQls)
write(18, 6010) sngl(time),sngl(aQlp)
write(19, 6010) sngl(time),sngl(aQrs)
endif
endif
6010 format(2x,E12.5,2x,e14.7)
6200 format(1x,f8.2,1x,4e14.5)
if(do .gt. xSL)then
write(*,2990)
2990 format(//2x,'Calculation Terminated on Complete melting of',
& ' the System')
go to 3001
endif
if(Tn(1) .GE. tcm) then
write(*,2991)
2991 format(//2x,'Calculation Terminated on Wall Temp. Exceeds',
& ' Melting Temp.')
go to 3001

```

