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
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

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

<p>| Figure 1. | Variation of Specific Volume of Lithium | Page 3 |
| Figure 2. | Gas Bubble Formation by Segregation During the Freezing Process of Water and Metal | Page 6 |
| Figure 3. | Schematics of Void Formation in a Solidifying Lithium Coolant in an SP-100 System | Page 7 |
| Figure 4. | Variation of System Pressure and Saturation Concentration of He in Li with Lithium Temperature | Page 12 |
| Figure 5. | Homogeneous Nucleation Potential During the Cooldown Process of Li in SP-100 PHTS | Page 13 |
| Figure 6. | Heterogeneous Nucleation Geometric Factor | Page 14 |
| Figure 7. | Schematic Representation of Freezing and He Segregation Processes | Page 18 |
| Figure 8. | Calculated Temperature Profile | Page 24 |
| Figure 9. | Calculated Dimensionless Concentration Profile | Page 25 |
| Figure 10. | Variation of Solidification Velocity and Wall Temperature with Time for Different Coolant Channel Widths | Page 26 |
| Figure 11. | Variation of Frozen Fraction for Different Coolant Channel Widths | Page 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}) kg/m(^3) | Page 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}) kg/m(^3) | Page 29 |
| Figure 14. | Schematics of Shrinkage Void Formation in a Solidifying Lithium Coolant in an SP-100 System | Page 39 |
| Figure 15. | Variation of Freezing Constant, (\lambda), with Stefan Number | Page 44 |
| Figure 16. | Calculated Solid-Liquid Interface Velocity During Freeze of Li and LiF (Radiative BC, Ta = 250 K) | Page 45 |</p>
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>17</td>
<td>Temperature Variation in Wall Void Cases During Freeze of Li and LiF (Radiative BC, Ta = 250 K)</td>
<td>46</td>
</tr>
<tr>
<td>18</td>
<td>Calculated Heat Flux Ratio inside Void During Freeze of Li and LiF (Radiative BC, Ta = 250 K)</td>
<td>47</td>
</tr>
<tr>
<td>19</td>
<td>Temperature Variation, with Radiative BC Wall Void, Ta = 1350 K, During Thaw Process of Li and LiF</td>
<td>48</td>
</tr>
<tr>
<td>20</td>
<td>Heat Flux Variation During Thaw Process of Li and LiF (Wall Void, Radiative BC, Ta = 1350 K)</td>
<td>49</td>
</tr>
<tr>
<td>21</td>
<td>Variation of Heat Flux Ratio Inside Void During Thaw Process of Li and LiF (Wall Void, Radiative BC, Ta = 1350 K)</td>
<td>50</td>
</tr>
</tbody>
</table>
## LIST OF TABLES

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

(a) Bubbles in ice cube.

(b) Gas bubbles in a metal.
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, SSHN, necessary for HN of a gas nucleus of critical radius can be represented by:

\[ SS_{HN} = \frac{\Delta C_h}{C_{sat}} = \frac{2\sigma}{\varepsilon P_{L}}, \tag{1} \]

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

\[ SS_{HTN} = SS_{HN} F(\text{Geo}, \theta), \tag{2} \]

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

\[ F(\theta) = 1 - \frac{(2 + \cos \theta)(1 - \cos \theta)^2}{4}. \tag{3} \]

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 \( r_{cr} \) in equation (1) is (Cole 1974):
\[ r_{cr} = \left( \frac{3kT}{4\pi\sigma} \ln \left( \frac{n_c kT}{h} \right) \cdot \frac{E_d}{kT} \right)^{0.5} \]

(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 < \( E_d < 4\pi\sigma \rho^2/3 \)), and \( J \) can be assumed to lie somewhere between \( 10^1 \) and \( 10^{12} \) nuc./m\(^3\)-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 \( C_{\text{Sat}} \) are determined as functions of liquid Li pressure and temperature using the following correlation suggested by Slotnick et al. (1965):

\[ C_{\text{Sat}} = P_L \exp\left( \frac{1752}{T} \right) - 23.0 \]

(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:

\[ \frac{P_L V}{T} = \frac{P_0 V_0}{T_0} \]

(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:

\[ \text{BNP} = \frac{SS_{\text{act}}}{SS_{\text{HN}} \text{ (or SS}_{\text{HTN}})} \]

(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, \( C_0 \), is taken equal to saturation value, \( C_{\text{Sat}} \) 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 PL, Cs 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(θ) in Equation (3) needs to be as low as 2.5 x 10^{-3}, requiring a wetting angle θ = 150° (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

SUPERSATURATION FOR HETEROGENEOUS
NUCLEATION EQUALS F FACTOR TIMES
SUPERSATURATION REQUIRED FOR
HOMOGENEOUS NUCLEATION.

\[ R_S/R_{VN} = \]
SURFACE RADIUS OF CURVATURE/
RADIUS OF VAPOR NUCLEUS

\[ F(R_S/R_{VN}, \theta) \]

Legend:
- ■ PROJECTIONS, \( R_S/R_{VN} = 10 \)
- □ PROJECTIONS, \( R_S/R_{VN} = 1 \)
- ● FLAT PLANE
- ○ CAVITIES, \( R_S/R_{VN} = 1 \)
- △ CAVITIES, \( R_S/R_{VN} = 10 \)

WETTED

UNWETTED

0 50 100 150 200
WETTING ANGLE \( \theta \) (Degrees)

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(δ(t)), can be expressed as:

\[ J(\delta(t)) = (C(\delta, t) - C^*_s) V(t) . \]  

(8)

The solidification velocity, V(t) = dδ(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 $X_r = L - r\delta(t)$, $v(t) = -\Gamma(d\delta(t)/dt)$, 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 ($C_0 = 4.26 \times 10^{-6}$ 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 ($\delta \leq x \leq X_r$)

$$\rho_L C_{pl} \frac{\partial T_L}{\partial t} + \nabla \cdot (\rho_L C_{pl} \frac{\partial T_L}{\partial x}) = \frac{\partial}{\partial x}\left(k_L \frac{\partial T_L}{\partial x}\right),$$

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

$$\rho_S C_{ps} \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s \frac{\partial T_s}{\partial x}\right).$$
(C) **Initial and Boundary Conditions**

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

\[
k_x \frac{\partial T}{\partial x}(0, t) = -\varepsilon \sigma (T^a(0, t) - T^a_i) = h_f (T(0, t) - T_a), \quad (11b)
\]

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

\[
T_s(\delta, t) = T_f(\delta, t) = T_f, \quad (11d)
\]

\[
k_x \frac{\partial T}{\partial x}(\delta, t) - k_l \frac{\partial T}{\partial x}(\delta, t) = \rho_l \lambda \left( \frac{\delta^a(0) - \delta^a}{\alpha} - \frac{\alpha^a}{v} \right). \quad (11e)
\]

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, \( \Delta x \), 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)]:

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

The dimensionless nodal enthalpy and temperature are defined as:

\[
\theta = \frac{1}{\rho \Delta x} \int_{\Delta x} \rho \frac{(H - H_{sf})}{\lambda} \, dx, \quad \phi = \frac{\rho C_p (\tau - T_f)}{\lambda} \quad (13)
\]

It has been shown by Shamsunder and Sparrow (1975), that \( \theta \) and \( \phi \) have the following relationships:

\[
\phi = a + b \theta,
\]

where,

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

\[
a = 0, \ b = 0 \quad , \text{for} \quad 0 \leq \theta \leq 1.
\]
Figure 7. Schematic Representation of Freezing and He Segregation Processes
Using these dimensionless parameters, Equation (9) is transformed into:

\[
\frac{\partial \theta}{\partial t} = \frac{1}{\Delta x \rho [C_p \frac{\partial}{\partial x}]} \left[ k \frac{\partial \theta}{\partial x} \right]^{x+\Delta x} - v \frac{\partial \theta}{\partial x} - \theta \frac{\partial \phi}{\partial x}
\]

(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:

\[
\frac{\Theta^m - \Theta^{m-1}}{\Delta t} = \frac{1}{\Delta x \rho \left[ C_p \left( \frac{\partial}{\partial x} \right) \right]} \left[ \frac{k}{C_p} \left( \phi^m_{i+1} - \phi^m_i \right) \right] + \frac{1}{\Delta t} \left( \frac{\Theta^{m-1} - \Theta^m}{\Delta x} \right)
\]

(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, \( \delta \), is determined by \( \delta = x_i - \theta_i \Delta x_i \) when the value of \( \theta \) of the i-th node is less than 1 and greater than 0, since the frozen fraction of the node, \( \alpha \), can be conveniently related to \( \theta \) as \( \alpha = 1 - \theta \) from the definition of \( \theta \) 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 \( \theta \) and \( \phi \) 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:

\[
\frac{\partial C}{\partial t} + \nu \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2}
\]

(17)

\[C(x, 0) = C_0\] (18a)

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

\[\frac{\partial C(x_{e}, t)}{\partial x} = 0\] (18c)

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

\[
\frac{\Delta x_i (C_{i+1}^p - C_i^p)}{\Delta t} + J_{i,+} - J_{i,-} = 0.
\]

(19)

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

\[J_{i,\text{sign}} = \nu C_j + D_j^f F(\text{Pe}_j^f)(C_j - C_{j+1}), \quad (j = i \text{ for sign } = + \text{ and } j = i-1 \text{ for sign } = -)\] (20a)

where,

\[D_j^f = 2D(\Delta x_j + \Delta x_{j+1}),\] (20b)

\[F(\text{Pe}_j^f) = <0, (1 - 0.1|\text{Pe}_j^f|)^5> + <0, -\text{Pe}_j^f>,\] (20c)

\[\text{Pe}_j^f = \nu/D_j^f.\] (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:

$$V_{He} = \frac{n_{He}RT}{P},$$

where,

$$n_{He} = \frac{1}{A_w} \int (C(x, t) - C_h)dx.$$  \hspace{1cm} (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 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 (0.01 m, 0.05 m, and 0.1 m). 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 $8 \times 10^{-6}$ m/sec and $-2 \times 10^{-4}$ 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 PHIS 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 PHIS 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.
Figure 8. Calculated Temperature Profile
Figure 9. Calculated Dimensionless Concentration Profile

\[ L = 0.05 \text{ m}, \ Co = 4.26 \times 10^{-6} \text{ kg/m} \]

\[ X_L = L - (1+\Gamma)\delta \]

- \( t = 100 \text{ s} \)
- \( t = 400 \text{ s} \)
- \( t = 500 \text{ s} \)

\[ C(x, t)/Ch = 1.0 \]

Note: Bubble formation not considered in this run
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

[Diagram showing the variation of frozen fraction with time for different coolant channel widths (L = 0.01 m, L = 0.05 m, L = 0.10 m).]
Figure 12. Evolution of Voids During Lithium Coolant Cooldown and Freezing (Coolant Channel Width = 0.01 m, Initial He Concentration = 4.26 x 10^-6 kg/m^3)
Figure 13. Evolution of Voids During Lithium Coolant Cooldown and Freezing, (Coolant Channel Width = 0.05 m, Initial He Concentration = $4.26 \times 10^{-6}$ 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)
- $\Delta x$ : 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 $(6.26 \times 10^{-34}$ J/s)
- $h_r$ : Radiative heat transfer coefficient (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 (m³)

\( V_{He} \): Volume of He bubbles (m³)

\( v \): Material velocity due to volume shrinkage (m/s)

\( X_r \): Location of shrinkage void/liquid (or solid) interface (m)

\( x \): Spacial coordinate (m)

**Greek**

\( \delta \): Solid crust thickness (m)

\( \varepsilon \): Emissivity

\( \phi \): Dimensionless nodal temperature

\( \lambda \): Latent heat of fusion (J/kg)

\( \theta \): Dimensionless nodal enthalpy or Wetting angle

\( \alpha \): Frozen fraction of a node

\( \Gamma \): \( \rho_s/\rho_L - 1 \)

\( \rho \): Density (kg/m³)

\( \sigma \): Surface tension in Equation (1) (N/m)

\( \sigma \): Stefan-Boltzman constant (5.67 x 10⁻⁸ W/m² K⁴)

**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
i, j : 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.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>$3.5 \times 10^4$ Pa</td>
</tr>
<tr>
<td>Temperature</td>
<td>1350 K</td>
</tr>
<tr>
<td>Li Mass in the PHTS</td>
<td>110 kg</td>
</tr>
<tr>
<td>Li volume in the PHTS</td>
<td>255 Liter</td>
</tr>
<tr>
<td>Gas Separator/Accumulator volume</td>
<td>35 Liter</td>
</tr>
<tr>
<td>Average He concentration</td>
<td>$4.26 \times 10^{-6}$ kg/m$^3$</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Temperature</th>
<th>$\Delta F$ (kcal/mole)$^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) NbN Formation</td>
<td>$T &gt; 1273$ K</td>
<td>- 50.1</td>
</tr>
<tr>
<td>(2) Mixture of Nb2N and NbN Formation</td>
<td>$673 &lt; T &lt; 1273$ K</td>
<td>- 54.0</td>
</tr>
<tr>
<td>(3) LiT Formation</td>
<td>$773 &lt; T &lt; 973$ K</td>
<td>- 16.7</td>
</tr>
<tr>
<td>(4) Full Dissociation of LiT</td>
<td>$T &gt; 973$ K</td>
<td>- 3.2</td>
</tr>
<tr>
<td>(5) NbT Formation</td>
<td>$T &lt; 573$ K</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ 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

<table>
<thead>
<tr>
<th>Material</th>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Li</td>
<td>Thermal conductivity</td>
<td>42.8 J/s.m.K</td>
</tr>
<tr>
<td></td>
<td>Density</td>
<td>517 kg/m³</td>
</tr>
<tr>
<td></td>
<td>Heat capacity</td>
<td>4.384 x 10³ J/kg.K</td>
</tr>
<tr>
<td></td>
<td>Thermal diffusivity</td>
<td>1.89 x 10⁻⁵ m²/s</td>
</tr>
<tr>
<td>Solid Li</td>
<td>Thermal conductivity</td>
<td>75.8 J/s.m.K</td>
</tr>
<tr>
<td></td>
<td>Density</td>
<td>530 kg/m³</td>
</tr>
<tr>
<td></td>
<td>Heat capacity</td>
<td>3.78 x 10³ J/kg.K</td>
</tr>
<tr>
<td></td>
<td>Thermal diffusivity</td>
<td>3.78 x 10⁻⁵ m²/s</td>
</tr>
<tr>
<td>Base Case</td>
<td>Initial He concentration</td>
<td>4.26 x 10⁻⁶ kg/m³</td>
</tr>
<tr>
<td>Parameters</td>
<td>Diffusivity of He in liquid Li</td>
<td>5.96 x 10⁻⁹ m²/s</td>
</tr>
<tr>
<td></td>
<td>Diffusivity of He in solid Li</td>
<td>Negligible</td>
</tr>
<tr>
<td></td>
<td>Li Latent Heat of Fusion</td>
<td>4.321 x 10⁵ J/kg</td>
</tr>
<tr>
<td></td>
<td>Li Freezing Temperature</td>
<td>454 K</td>
</tr>
</tbody>
</table>
Table 4. Thermal Properties and Base Case Parameters used in the Analysis of Freeze and Thaw Processes of Li and LiF

<table>
<thead>
<tr>
<th>Material</th>
<th>Properties</th>
<th>Liquid</th>
<th>Solid</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>k</td>
<td>42.8</td>
<td>75.8</td>
<td>W/m.K</td>
</tr>
<tr>
<td></td>
<td>ρ</td>
<td>517</td>
<td>530</td>
<td>kg/m³</td>
</tr>
<tr>
<td></td>
<td>Cp</td>
<td>4384</td>
<td>3780</td>
<td>J/kg.K</td>
</tr>
<tr>
<td></td>
<td>α</td>
<td>1.89 x 10⁻⁵</td>
<td>3.78 x 10⁻⁵</td>
<td>m²/s</td>
</tr>
<tr>
<td></td>
<td>Hₘₗ</td>
<td>4.321 x 10⁵</td>
<td></td>
<td>J/kg</td>
</tr>
<tr>
<td></td>
<td>Tₘ</td>
<td>454</td>
<td></td>
<td>K</td>
</tr>
<tr>
<td>LiF</td>
<td>k</td>
<td>1.30</td>
<td>5.00</td>
<td>W/m.K</td>
</tr>
<tr>
<td></td>
<td>ρ</td>
<td>1376</td>
<td>1792</td>
<td>kg/m³</td>
</tr>
<tr>
<td></td>
<td>Cp</td>
<td>2779</td>
<td>2470</td>
<td>J/kg.K</td>
</tr>
<tr>
<td></td>
<td>α</td>
<td>3.40 x 10⁻⁵</td>
<td>2.94 x 10⁻⁵</td>
<td>m²/s</td>
</tr>
<tr>
<td></td>
<td>Hₘₗ</td>
<td>3.473 x 10⁵</td>
<td></td>
<td>J/kg</td>
</tr>
<tr>
<td></td>
<td>Tₘ</td>
<td>1122</td>
<td></td>
<td>K</td>
</tr>
<tr>
<td>PWC-11</td>
<td>k</td>
<td>23.9</td>
<td></td>
<td>W/m.K</td>
</tr>
<tr>
<td></td>
<td>ρ</td>
<td>6490</td>
<td></td>
<td>kg/m³</td>
</tr>
<tr>
<td></td>
<td>Cp</td>
<td>323.4</td>
<td></td>
<td>J/kg.K</td>
</tr>
<tr>
<td></td>
<td>α</td>
<td>1.14 x 10⁻⁵</td>
<td></td>
<td>m²/s</td>
</tr>
<tr>
<td></td>
<td>Tₘ</td>
<td>2740</td>
<td></td>
<td>K</td>
</tr>
<tr>
<td>LiF vapor</td>
<td>k</td>
<td>0.017</td>
<td></td>
<td>W/m.K</td>
</tr>
<tr>
<td>He gas</td>
<td>k</td>
<td>0.1678</td>
<td></td>
<td>W/m.K</td>
</tr>
</tbody>
</table>

**Base Case Parameters**

- Ambient Temperature of Space: 250 K
- Temperature of Wall or Heat Source: 250 K
  - Freeze: 1350 K
  - Thaw: 0.05 m
- Thickness of PCM at Liquid State: 7.6 x 10⁻⁴ m
- Emissivity: 0.8
  - at outer surface of the wall
  - 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, \( T_a \). 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. \( h_v = k_v/\delta_v \) [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**

\[
\rho_d C_{pd} \frac{\partial T_d}{\partial t} = \frac{\partial}{\partial x} \left( k_d \frac{\partial T_d}{\partial x} \right),
\]

(22)

**Heat Transfer Wall**

\[
\rho_c C_{pc} \frac{\partial T_c}{\partial t} = \frac{\partial}{\partial x} \left( k_c \frac{\partial T_c}{\partial x} \right),
\]

(23)

**Initial and Boundary Conditions**

\[
T(x, 0) = T_f,
\]

(24)

\[
T_d(S(0, t) = T_l(S(0, t)) = T_f,
\]

(25)

\[
k_c \frac{\partial T_c}{\partial x}(S(0, t)) - k_l \frac{\partial T_l}{\partial x}(S(0, t)) = \rho_l H_d \left( \frac{\partial X}{\partial x} \right),
\]

(26)

and

\[
k_c \frac{\partial T}{\partial x}(\cdot, 0) = \epsilon \sigma \left( T_f^4 - T_d^4 \right),
\]

(27)

\[
k_c \frac{\partial T}{\partial x}(X_n, t) = \epsilon \sigma \left( T_f^4 - T_f^4(0, t) \right) + \frac{k_v}{\delta_v} \left( T(X_n, t) - T(0, t) \right),
\]

for Fig 14a,

(28)

\[
\frac{\partial T}{\partial x}(X_n, t) = 0,
\]

for Fig 14b.

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

\[ q_i - q_{i+1} = \left[ \rho_d C_p \left( T_2^{n+1} - T_2^n \right) - \rho_d C_p T \left( \delta^{n+1} - \delta^n \right) \right] / \Delta t, \]  

(30)

where,

\[ q_i = -h_{01}(T_i^{n+1} - T_a), \]  

(31)

\[ q_{i+1} = -h_{12}(T_{i+1}^{n+1} - T_1^{n+1}), \]  

(32)

\[ q_2 = -h_2(T_f - T_2^{n+1}), \]  

(33)

\[ h_{01} = \frac{(T_1^2 + T_2^2)(T_1 + T_a)}{[1/\epsilon_\sigma + 4T_1/h_1]}, \]  

(34)

\[ h_1 = \frac{2K_y}{\epsilon}, \]  

(35)

\[ h_{12} = \left[ 1/h_1 + 1/h_2 + 1/h_2 \right]^{-1}, \]  

(36)

\[ h_2 = \frac{2K_y}{\delta}, \]  

(37)

\[ h_2 = \frac{K_y}{\delta} + \epsilon\sigma(T_3^2 + T_4^2)(T_3 + T_4), \]  

(38)

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

(39)

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

(40)

Heat Transfer Wall

\[ q_i - q_{i+1} = \rho_d C_p c \left( T_i^{n+1} - T_i^n \right) / \Delta t, \]  

(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, \( \delta \), should be known. An iterative procedure is used to determine \( \delta \) by solving the linearized heat balance at the S-L interface:
\[
\frac{2k_d}{\delta} \left( T_f - T_2^{n+1} \right) = (P_a) \rho_s H_{fs} \left( \frac{\delta^{n+1} - \delta^n}{\Delta t} \right),
\]

where, \( P_a \) 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 that 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, $\lambda$, with Stefan Number
(a) Freeze Velocity

Legend:
- Li-CV
- Li-WV
- LiF-CV
- LiF-WV

Figure 16. Calculated Solid-Liquid Interface Velocity During Freeze of Li and LiF (Radiative BC, Ta = 250 K)
Figure 17. Temperature Variation in Wall Void Cases During Freeze of Li and LiF (Radiative BC, Ta = 250 K)
Figure 18. Calculated Heat Flux Ratio inside Void During Freeze of Li and LiF (Radiative BC, Ta = 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, Ta = 1,350 K)
Figure 21. Variation of Heat Flux Ratio Inside Void During Thaw Process of Li and LiF (Wall Void, Radiative BC, Ta = 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

$\alpha$ : Thermal diffusivity (m$^2$/s)

$\Gamma$ : $\rho_s/\rho_L - 1$

$\delta$ : Solid crust thickness, (m)

$\delta_v$ : Void thickness, (m)

$\varepsilon$ : Emissivity

$\rho$ : Density (kg/m$^3$)

$\sigma$ : Stefan-Boltzman constant ($5.67 \times 10^{-8}$ W/m$^2$.K)
### Subscripts

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>c</td>
<td>Wall region</td>
</tr>
<tr>
<td>d</td>
<td>Developing phase</td>
</tr>
<tr>
<td>f</td>
<td>Fusion</td>
</tr>
<tr>
<td>L</td>
<td>Liquid</td>
</tr>
<tr>
<td>s</td>
<td>Solid</td>
</tr>
<tr>
<td>i</td>
<td>Initial</td>
</tr>
<tr>
<td>v</td>
<td>Void</td>
</tr>
<tr>
<td>01</td>
<td>Between wall and heat source (sink)</td>
</tr>
<tr>
<td>12</td>
<td>Between the centers of wall and developing phase</td>
</tr>
<tr>
<td>1</td>
<td>Within the half of the wall</td>
</tr>
<tr>
<td>2</td>
<td>Within the half of the developing phase</td>
</tr>
<tr>
<td>3</td>
<td>At the wall-void interface</td>
</tr>
<tr>
<td>4</td>
<td>At the PCM-void interface</td>
</tr>
</tbody>
</table>
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


55


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,
  HSF, HLF, CONDSF, CONDLF, RHOSF, RHOLF, EMIT
COMMON /CONV1/ EPS1, EPS2, EPS3
COMMON /OPTIN/ MLB, MRB, ILB, IRB, ICOMP, IENT, ITEM, SLOPT,
  PRTIME(20)
COMMON /MESHX/ X(0:500), DX(500), DT
COMMON /DIMS/ HX(0:500, 2), TX(0:500, 2), DELTA(0:2)
COMMON /DIMS/ 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 /DIMLV/ THETA(0:500, 2), PAI(0:500, 2), THEC(0:500)
COMMON /DIMLV/ THETA(0:500, 2), PAI(0:500, 2), THEC(0:500)
COMMON /TEMPO/ STHETA(0:500), STHEC(0:500), SPAI(0:500),
  SHX(0:500), STX(0:500)
COMMON /HERP/ RHO(50), CP(50), COND(50), TEM(50), ENT(50),
  DELTA(0:2)
COMMON /PROP/ HLS, CPL, CSL, CS, CONL, CONS, RHOS, RHL, RHS, TFF
NAMELIST /OPTION/ MLB, MRB, ILB, IRB, ICOMP, IENT, ITEM,
  SLOPT, NPRT, NStep
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 = ISOFLUX 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 = ISOFLUX WALL (TIME INDEPENDENT)
C 3 = CONVECTIVE BOUNDARY
C 4 = RADIATIVE BOUNDARY
CCCCCC9/26/1990 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 PRINT IS MADE ONCE AT THE TIME SPECIFIED BY
C INPUT VARIABLE 'TIME' IN THE NAMELIST 'INPUT'.
NAMELIST /INPUT1/ NT, TIME, NX, XL, HINIT, TINIT, TF, HSF, HLF,
  CONDSF, CONDLF, RHOSF, RHOLF, EMIT, TWALL, WNNALL, TA,
  CPS, CPL
NAMELIST /CONVER/ EPS1, EPS2, EPS3
OPEN(10, ERR=9999, FILE='COPHASE.INP', STATUS='OLD')
OPEN(11, ERR=9999, FILE='COPHASE.OUT', 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/5.670-08/

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 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.
DDELTADT = 0.
SDELTA = 0.
HF = HLF - HSF
HO = HWALL
SGAM = 1.0 - 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),RHOX(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)
C  **** INITIAL VALUES FOR CONSTANT TWALL< TF, PAIO = CONSTANT.
C
IF(ILB.EQ.1) THEN
   CALL PROPERTY(HWALL,TWALL,CPXO,RHOXO,CONDO)
   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  **** 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  **** 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  **** 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
30 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)
CONTINUE
SDELTA = DELTA(M-1)
C •••• OUTER ITERATION — DELTA ITERATION

IDITER = 0
DELTA(1) = DELTA(0) + DDELTADT*DT/2.  I ASSUMED CRUST THICKNESS

CONTINUE
IDITER = IDITER + 1
DDELTA = DELTA(1) - DELTA(0)

C •••• INNER ITERATION

C

CONVERGENCE ARE CHECKED IN EACH TIME STEP BY;
SUMDIF = SUM((F(I,M)-SF(I))*DX(I))*2.). I=ILEND,IREND
SUMASS = SUM((SF(I)*DX(I))*2.). I=ILEND,IREND

AND IF (SUMDIF/SUMASS)< EPS1.
THE CONVERGENCE ARE ACHIEVED

NITER = 0
SUMQINDT = QOLD

CONTINUE

NITER = NITER + 1
SUMDIF = 0.
SUMASS = 0.

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
ELSEIF(MLB .EQ. 1) THEN
  XLEND = SCAM*DELTA(M-1)
  XREND = XL
  ILEND = 1
  IF(XLEND .LT. XI(1)) THEN
    ILEND = 1
    GO TO 60
  ELSEIF(XLEND .GT. XI(NX)) 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
    ENDIF
  ENDIF

50
CONTINUE
DXI = XI(ILEND) - XLEND
IF(DXI .LT. DX1C1) THEN
  ILEN = IL + 1
  DXI = XI(ILEND) - XLEND
ENDIF
DX(ILEND) = DXI

C ***** LOCATION AND SIZE OF MOVING RIGHT BOUNDARY NODE: MRB = 1

ELSEIF(MRB .EQ. 1) THEN
  XREND = XL - SGAM*DELTA(M-1)
  XLEND = 0.
  ILEN = 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
    ENDDO
  CONTINUE
ENDIF

62 OXI = XREND - XI(IREND)
IF(DXI .LT. 0X101) THEN
  IREND = IL - 1
  OXI = XREND - XI(IREND)
ENDIF
OX(IREND) = DXI
ENDIF

K = ILEN
L = IREND
ILEND1 = ILEN + 1
IREND1 = IREND - 1
IREND2 = IREND - 2
DO 35 I = ILEN, IREND
  SUMASS = SUMASS + (HX(I,M-1)*DX(I))**2.
35

C ***** PRODUCTION RUN: LEFT BOUNDARY NODE

C ILB = 1 FOR CONSTANT WALL TEMPERATURE AT LEFT BOUNDARY
C
IF(ILB .EQ. 1) THEN
  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 = 1./ALO
A4 = 

CHECK = STHETA(K) + A1*(A2*PAI(K+1,M-1) + A3*PAI)

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

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

IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN
THETA(K,M) = CHECK
THEC(K) = -THETA(K,M)
ELSEIF(CHECK .GT. 1.) THEN
THETA(K,M) = ( STHETA(K)*rhoux(k)/rhox(k,m-1) - (1.-rhoux(k)/rhox(k,m-1))*Hsf/Hf + A1*(A2*PAI(K+1,M-1) + A3*PAI) - (A2+A3)*THEC(K) ) / (1.+A1*(A2+A3))
ELSE
THET(K) = 6.
THETA(K,M) = ( STHETA(K)*arhoux(k)/rhox(k.m-1) - (1.-arhoux(k)/rhox(k.m-1))*Hsf/Hf + A1*(A2*PAI(K+1,M-1) + A3*PAI) - (A2+A3)*THEC(K) ) / (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)

HDIF = (((HX(K,M) - HX(K,M-1))/HX(K,M-1))**2. 

ILB = 2 FOR CONSTANT WALL HEAT FLUX BOUNDARY AT LEFT BOUNDARY

ELSEIF(ILB .EQ. 2) THEN
PRINT ** ' CONSTANT WALL HEAT FLUX BOUNDARY ' 

ILB = 4 FOR CONVECTIVE BOUNDARY AT LEFT BOUNDARY

ELSEIF(ILB .EQ. 3) THEN
PRINT ** ' CONVECTIVE BOUNDARY ' 
ELSEIF(ILB .EQ. 4) THEN
  ALPA = 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.*ALPA*TX(K,M-1)**3.)
  STE = CPX(K,M-1)*TF - TA)/HF

  A1 = 2.*DT/(DX(K)*RHOX(K,M-1))
  A2 = 1./(ALO + ALP)
  A3 = HRR/CPX(K,M-1)/2.
  A4 =

  CHECK = STHETA(K) + 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) = 0.
      THETA(K,M) = (STHETA(K) + 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) + 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 *************** OPTIONS FOR OTHER BOUNDARY CONDITIONS ***************
HDIF = ((HX(K,M) - HX(K,M-1))/HX(K,M-1))**2.
SUMDIF = SUMDIF + ((HX(K,M) - HX(K,M-1)) + DX(K))**2.
HRNEW = HR

**** MAIN RUN: INTERIOR NODES

DO 200 I = ILEND1, IREND1

ALM = CPX(I-1,M-1)*DX(I-1)/CONDX(I-1,M-1)
ALO = CPX(I,M-1)*DX(I)/CONDX(I,M-1)
ALP = CPX(I+1,M-1)*DX(I+1)/CONDX(I+1,M-1)
A1 = 2.*DT/(DX(I)*RHOX(I,M-1))
A2 = 1./(ALO + ALP)
A3 = 1./(ALO + ALM)
A4 = CHECK = STHETA(I) + A1*(A2*PAI(I+1,M-1) + A3*PAI(I-1,M))

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

CHECK = STHETA(I)*srhox(i)/rhox(i.m-1)
& -(1.-srhox(i)/rhox(i.m-1))*Hsf/Hf
& + A1*(A2*PAI(I+1,M-1) + A3*PAI(I-1,M))

IF(CHECK .GE. 0. .AND. CHECK .LE. 1.) THEN
  THETA(I,M) = CHECK
  THEC(I) = -THETA(I,M)
ELSEIF(CHECK .GT. 1.) THEN
  THEC(I) = -1.
  THETA(I,M) = (STHETA(I)*srhox(i)/rhox(i.m-1)
  & -(1.-srhox(i)/rhox(i.m-1))*Hsf/Hf
  & + A1*(A2*PAI(I+1,M-1) + A3*PAI(I-1,M))
ELSE
  THETA(I,M) = (STHETA(I)*srhox(i)/rhox(i.m-1)
  & -(1.-srhox(i)/rhox(i.m-1))*Hsf/Hf
  & + A1*(A2*PAI(I+1,M-1) + A3*PAI(I-1,M))
ENDIF

HX(I,M) = HSF + THETA(I,M)*HF
CALL PROPERTY(HX(I,M),TX(1,M),CPX(1,M),RHOX(1,M),CONDX(1,M))
PAI(I,M) = THETA(I,M) + THEC(I)
**C ••• CHECK CONVERGENCE FOR THETA OR THEC WHICH EVER IS CONVENIENT**

\[
\text{HDF} = ((HX(I,M) - HX(I,M-1))/HX(I,M-1))^{**2}.
\]

\[
\text{SUMDIF} = \text{SUMDIF} + ((HX(I,M) - HX(I,M-1)) \times DX(I))^{**2}.
\]

**200 CONTINUE**

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

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

\[
\text{ALM} = \text{CPX}(L-1,M-1) \times DX(L-1)/\text{CONDX}(L-1,M-1)
\]

\[
\text{ALO} = \text{CPX}(L,M-1) \times DX(L)/\text{CONDX}(L,M-1)
\]

\[
\text{ALP} = \text{CPX}(L+1,M-1) \times DX(L+1)/\text{CONDX}(L+1,M-1)
\]

\[
\text{A1} = 2. \times DT/(DX(L) \times \text{RHOX}(L,M))
\]

\[
\text{A2} = 1. / (\text{ALO} + \text{ALO})
\]

\[
\text{A3} = 1. / (\text{ALO} + \text{ALM})
\]

\[
\text{A4} = 
\]

\[
\text{CHECK} = \text{STHETA}(L) + \text{A1} \times \text{A3} \times \text{PAI}(L-1,M) - \text{A4} \times \text{THETA}(L-1,M)
\]

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

\[
\text{THETA}(L,M) = \text{CHECK}
\]

\[
\text{THEC}(L) = -\text{THETA}(L,M)
\]

**ELSEIF(CHECK .GT. 1.) THEN**

\[
\text{THEC}(L) = -1.
\]

\[
\text{THETA}(L,M) = (\text{STHETA}(L) + \text{A1} \times \text{A3} \times (\text{PAI}(L-1,M) - \text{THEC}(L))
\]

\[
- \text{A4} \times \text{THETA}(L-1,M))/ (1. + A1 \times A3)
\]

**ELSE**

\[
\text{THEC}(L) = 0.
\]

\[
\text{THETA}(L,M) = (\text{STHETA}(L) + \text{A1} \times \text{A3} \times (\text{PAI}(L-1,M) - \text{THEC}(L))
\]

\[
- \text{A4} \times \text{THETA}(L-1,M))/ (1. + A1 \times A3)
\]

**ENDIF**

\[
\text{CHECK} = \text{STHETA}(L) * \text{SRHOX}(L,M-1)
\]

\[
- (1. - \text{SRHOX}(L,M-1)) \times \text{HSF}/\text{Hf}
\]

\[
+ \text{A1} \times \text{A3} \times \text{PAI}(L-1,M) - \text{A4} \times \text{THETA}(L-1,M)
\]

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

\[
\text{THETA}(L,M) = \text{CHECK}
\]

\[
\text{THEC}(L) = -\text{THETA}(L,M)
\]

**ELSEIF(CHECK .GT. 1.) THEN**

\[
\text{THEC}(L) = -1.
\]

\[
\text{THETA}(L,M) = (\text{STHETA}(L) * \text{SRHOX}(L,M-1)
\]

\[
- (1. - \text{SRHOX}(L,M-1)) \times \text{HSF}/\text{Hf}
\]

\[
+ \text{A1} \times \text{A3} \times (\text{PAI}(L-1,M) - \text{THEC}(L))
\]

\[
- \text{A4} \times \text{THETA}(L-1,M))/ (1. + A1 \times A3)
\]

**ELSE**

\[
\text{THEC}(L) = 0.
\]

\[
\text{THETA}(L,M) = (\text{STHETA}(L) * \text{SRHOX}(L,M-1)
\]

\[
- (1. - \text{SRHOX}(L,M-1)) \times \text{HSF}/\text{Hf}
\]

\[
+ \text{A1} \times \text{A3} \times (\text{PAI}(L-1,M) - \text{THEC}(L))
\]

\[
- \text{A4} \times \text{THETA}(L-1,M))/ (1. + A1 \times A3)
\]

**ENDIF**

\[
\text{HX}(L,M) = \text{HSF} + \text{THETA}(L,M) \times \text{Hf}
\]

**CALL PROPERTY(HX(L,M),TX(L,M),CPX(L,M),RHOX(L,M),CONDX(L,L))**
\[
\text{PAI}(L, M) = \text{THETA}(L, M) + \text{THEC}(L)
\]

**C **** CHECK CONVERGENCE FOR \text{THETA} OR \text{THEC} WHICH EVER IS CONVENIENT**

\[
\text{HDIF} = \left(\frac{\text{HX}(L, M) - \text{HX}(L, M-1)}{\text{HX}(L, M-1)}\right) \times 2.
\]

\[
\text{SUMDIF} = \text{SUMDIF} + \left(\frac{\text{HX}(L, M) - \text{HX}(L, M-1)}{\text{DX}(L)}\right) \times 2.
\]

**C **** LOCATION OF INTERFACE**

**C **** First, project \text{THETA} at \(x = 0\)**

\[
\begin{align*}
\text{hi} &= \text{dx}(1) \\
\text{h1} &= \text{dx}(2) \\
\text{h2} &= \text{dx}(3) \\
\text{hi1} &= \text{hi} \times \text{hi} \\
\text{hi2} &= \text{hi} + \text{hi} \\
\text{h2hi} &= \text{hi} + 2.0 \times \text{hi} \\
\text{h2hi2hi} &= \text{hi} + 2.0 \times \text{hi} + 2.0 \times \text{hi} \\
\text{theta}(0, m) &= \text{theta}(1, m) \times (2.0 \times \text{hi} + \text{hi}) \times \text{hi}2hi2hi / (\text{hi}1 \times \text{hi}2hi2hi) \\
&= \text{theta}(2, m) \times \text{hi} \times \text{hi}2hi2hi / (\text{hi}1 \times \text{hi}2hi) \\
&= \text{theta}(3, m) \times \text{hi} \times \text{hi}2hi2hi / (\text{hi}1 \times \text{hi}2hi2hi)
\end{align*}
\]

**C**

\[
\text{if} (\text{delta}(m-1) \leq 0.0 \text{ and } \text{theta}(0, m) \geq \text{SLOPT}) \text{ then}
\]

\[
\text{delta}(m) = 0.
\]

**C**

\[
\text{go to 550}
\]

**C**

**C**

\[
\text{ISL1} = 1
\]

**C**

\[
\text{IIEND1} = \text{IIEND} - 1
\]

**C**

\[
\text{DO} 541 \text{ I = IIEND, IREND1}
\]

**C**

\[
\text{IF} (\text{THETA}(I, M) \geq 0.0 \text{ and } \text{THETA}(I, M) \lt 1.0) \text{ THEN}
\]

**C**

\[
\text{ISL1} = I
\]

**C**

\[
\text{DELTA}(M) = \text{XI}(ISL1) - \text{DX}(ISL1) \times \text{THETA}(ISL1, M)
\]

**C**

\[
\text{GO TO 551}
\]

**C**

\[
\text{ELSEIF} (\text{THETA}(I, M) \leq \text{SLOPT} \text{ and } \text{THETA}(I+1, M) \geq \text{SLOPT}) \text{ THEN}
\]

**C**

\[
\text{ISL1} = I
\]

**C**

\[
\text{DELTA}(M) = \text{XI}(ISL1) - \text{DX}(ISL1) / 2.0 + 2.0 \times (\text{SLOPT} - \text{THETA}(ISL1, M)) \times
\]

\[
\left(\text{THETA}(ISL1+1, M) - \text{THETA}(ISL1, M)\right) / (\text{DX}(ISL1) + \text{DX}(ISL1+1))
\]

**C**

\[
\text{GO TO 551}
\]

**C**

\[
\text{ENDIF}
\]

**C**

\[
541 \text{ CONTINUE}
\]

**C**

\[
551 \text{ CONTINUE}
\]

**C**

\[
\text{If} (\text{theta}(\text{IREND}, M) \leq \text{SLOPT}) \text{ then}
\]

**C**

\[
\text{delta}(m) = \text{XREND}
\]

**C**

\[
\text{print} \text{,'Complete solidification of the system'}
\]

**C**

\[
\text{print} \text{,'Calculation Terminated'}
\]

**C**

\[
\text{go to 9999}
\]

**C**

\[
\text{go to 545}
\]

**C**

\[
\text{endif}
\]

**C**

\[
\text{if} (\text{ISL1} = 1) \text{ then}
\]

**C**

\[
\text{DELTA}(M) = \text{XI}(ISL1) - \text{DX}(ISL1) \times \text{THETA}(ISL1, M)
\]

**C**

\[
\text{ELSE}
\]

**C**

\[
\text{DELTA}(M) = \text{XI}(ISL1-1) - \text{DX}(ISL1-1) / 2.0 + 2.0 \times (\text{SLOPT} - \text{THETA}(ISL1-1, M)) \times
\]

\[
\left(\text{THETA}(ISL1-1, M) - \text{THETA}(ISL1, M)\right) / (\text{DX}(ISL1) + \text{DX}(ISL1-1))
\]

**C**

\[
\text{ENDIF}
\]

**C**

\[
\text{sumtheta} = 0.
\]

**C**

\[
\text{Do 555} \text{ I = IIEND, ISL1}
\]

**C555**

\[
\text{sumtheta} = \text{sumtheta} + \text{theta}(I, M) \times \text{DX}(I)
\]
avgtheta = sumtheta/(xi(isi1) - xendl)

delta(m) = (xi(isi1) - xendl)*(1-avgtheta)
isi1 = 1

DO 540 i = 1,LEND, IREND1

IF(THETA(I,M) .LE. SLOPT .AND. THETA(I+1,M) .GT. SLOPT) THEN

IS1 = 1

GO TO 545

ENDIF

C540 CONTINUE

C545 ximh = xi(isi1) - dx(isi1)/2.

xiph = xi(isi1) + dx(isi1+1)/2.

IF(isi1 .eq. 1) then

xim3h = 0.

else

xim3h = xi(isi1) - dx(isi1) - dx(isi1-1)/2.

endif

IF(ILB .eq. 1) then

ups1 = xrend

else

ups1 = 2.*xi(isi1)

endif

uns1 = 0.

liter = 0.

C546 Xo = (ups1+uns1)/2.

liter = liter+1

fx = theta(isi1-1,m)*(Xo - ximh)*(Xo - xiph)

& /((xim3h - ximh)*(xim3h - xiph))

& +theta(isi1,m)*(Xo - xim3h)*(Xo - xiph)

& /((xim3h - ximh)*(xim3h - xiph))

& +theta(isi1+1,m)*(Xo - xim3h)*(Xo - xiph)

& /((xiph - xim3h)*(xiph - ximh))

WRITE(*,2030) liter, isi1, snl(Xo), snl(fx)

C2030 format(2x,'Niter=' ,15,3, 'Nnode=' ,15,3, 'Xax=' ,e12.5, 3x,'fx=' ,e12.5)

dfx = fx - SLOPT

IF(fabs(fdx) .le. eps3) then

delta(m) = xa

GO TO 550

ELSE

ups1 = xa

GO TO 546

ENDIF

C550 CONTINUE

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

CONVERGE = SUMDIF/SUMASS

C **** CHECK ENERGY BALANCE

C DETERMINE THE ENERGY OUTPUT WITHIN DT

FIRST, BY HEAT FLUX
IF(ILB .EQ. 1) THEN
   DDXPAI = 2.*(PAI(K,M) - PAI0)/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.
DO 705 I = ILEN, IREND
   ETOTNEW = ETOTNEW + RHOX(I,M)*HX(I,M)*DX(I)
705 CONTINUE

ECOR = 0.
DO 706 I = ILEN, IREND
   ECOR = (RHOX(I,M) - SRHOX(I,M))*HSF*DX(I)
   EBALANCE = (QOUT - EOUT) / EOUT * 100.
   EBALRAT = ((QOUT - EOUT) / EOUT)**2.
   TSFRAT = QOUT/EOUT
706 CONTINUE

DIF = 0.
DO 560 I = ILEN, 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 = ILEN, IREND
      HX(JI,M-1) = HX(JI,M)
      CALL PROPERTY(HX(JI,M-1),TX(JI,M),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.
      PAI(JI,M-1) = THETA(JI,M-1) + THEC(JI)
801 CONTINUE
   GO TO 1050
ENDIF

WRITE(*, 610) SNGL(EOUT), SNGL(QOUT), SNGL(EBALANCE),
& SNGL(TOTEOUT), SNGL(OTOT),
& SNGL(TOTBAL), ISL1, SNGL(SMASS)
C WRITE(*,602) MA, IDITER, NITER, SNGL(CONVERGE), SNGL(SUMASS)
C OUTER ITERATION — DELTA ITERATION
C CONVERGENCE TEST FOR DELTA
C
IF(DIF Delta .GT. 1.D-5 .AND. DELTA(M-1) .GT. 1.D-5) THEN
   DIFDELTA = ((DELTA(M) - DELTA(M-1))/DELTA(M-1))**2.
ELSE
   DIFDELTA = DELTA(M) - DELTA(M-1)
ENDIF
C
DELTA(M-1) = (DELTA(M-1)+DELTA(M))/2.
C if(delta(m-1) .le. sdelta) delta(m-1)=sdelta
C IF(DIFDELTA .GT. EPS2) THEN
DO 816 I = IEND, IREN
HX(I,M-1) = HX(I,M)
CALL PROPERTY(HX(I,M-1),TX(I,M-1),CPX(I,M-1),RHOX(I,M-1),CONDX(I,M-1))
THETA(I-1,M-1) = (HX(I-1,M-1) - HSF)/HF
THEC(I) = -THETA(I,M-1)
IF(THEC(I) .GT. 0.) THEC(I) = 0.
IF(THEC(I) .LT. -1.) THEC(I) = -1.
PAI(I,M-1) = THETA(I,M-1) + THEC(I)
CONTINUE
GO TO 1025
END

C **** TRANSFORMATION INTO DIMENSIONED VARIABLES
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))
CONTINUE
TOTEOUT = ETOTINIT - ETOTNEW
QTOT = QTOT + QOUT
TOTBAL = QTOT/TOTEOUT

C **** STORE PRESENT STEP VALUES IN THE PREVIOUS STEP VARIABLES TO ADVANCE 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)
CONTINUE
DELTA(M-2) = SDELTA
DELTA(M-1) = DELTA(M)
DDELTADT = (DELTA(M-1) - DELTA(M-2))/DT
ETOTOLD = ETOTNEW
FROFRAC = DELTA(M)/XL
TIMEA = DT * DFLOAT(MA)
TIMEB = DT * DFLOAT(MA+1)
ma1 = ma/NpStp * NpStp
if(ma1 .LT. 20 .OR. ma1 .EQ. ma) then
deltaxl = delta(n)/XL
WRITE(11,1133) SNGL(TIMEA), SNGL(DDELTADT), SNGL(DeltaXL), SNGL(Tx(I,ILEND,m))
& WRITE(14,1130) SNGL(TIMEA), SNGL(Delta(W))
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)
FORMAT(2X,'FROZEN FRACTION = ',E12.5)
WRITE(*,712) SNGL(PRTIME(NK))
ITIME = ITIME + 1
WRITE(12,810) SNGL(EDOUT), SNGL(QOUT), SNGL(EBALANCE)
& SNGL(TOTEOUT), SNGL(QTOT),
& SNGL(TOTBAL), ISEL1, snl(dela(m))
WRITE(12, 1110) SNGL(EOUT), SNGL(QOUT), SNGL(EBALANCE)
& SNGL(TOTEOUT), SNGL(QTOT),
& SNGL(TOTBAL), ISEL1, snl(dela(m))
WRITE(12, 1110)
1110 FORMAT(/5X,'DIMENSIONLESS ENTHALPY DISTRIBUTION'/
& 4X,'POSITION ENTHALPY'/
& 5X,'TOTAL ENTHALPY')
DO 8010 IJ = ilend, irend
WRITE(12, 1120) SNGL(XI(IJ)), SNGL(THETA(IJ,M))
WRITE(13, 1111)
1111 FORMAT(/5X,'TEMPERATURE DISTRIBUTION'/
& 4X,'POSITION TEMPERATURE (K)'/
& 5X,'TOTAL TEMPERATURE (K)')
DO 8011 IJ = ilend, irend
WRITE(13, 1120) SNGL(XI(IJ)), SNGL(TX(IJ,M))
FORMAT(5X.E12.5,5X.E12.5)
FORMAT(5X.E12.5,5X.E12.5,5X.E12.5)
FORMAT(5X.E12.5,5X.E12.5,5X.E12.5,5X.E12.5)
END
CONTINUE
CONTINUE
C
C FORMAT STMTS
C
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/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/
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]'/
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.
NpStp = 5.
IDX = 0.
$END
$INPUT1
Fa = .5,
Ft = .5,
Fx = 1.05,
vopt = 0.,
Div = 1.,
NPRT = 10
$END
$CONVER
eps1 = 2.D-2
$END
Appendix B-1

List of Computer Program
SEGR.FOR
$OPTION
ILB = 4.
$END
$INPUT
NT = 13,
HINIT=1.132D6,
TINIT = 454.,
MSF=0.6999D6,
CPS=3.963D3,
CONDSF=71.20.
RHOSF=530..
EMIT=0.8.
TWALL = 100.,
$END
$CONVER
EPS1 = 1.D-30, EPS2 = 1.D-12, EPS3 = 1.D-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
   endif
   dx1 = 2.*Dc/Vmax/div
   sum = 1
   do 25 i=2,nx
      sum = sum + f*x**dfloat(i-1)
   25 sum = sum + f*x**dfloat(i-1)
   dxo = XL/sum
   Xi(0) = 0.
   do 30 i = 1, Nx
      dx(i) = dxo+f*x**dfloat(i-1)
      Xi(i) = Xi(i-1) + dx(i)
      if(dx1.lt.dx(1)) then
         nx = nx+1
         go to 20
      endif
   30      continue
   elseif(idx .eq. 1) then
      dxs = xsbl/Dfloat(Nx)
      do 35 i = 1, Nx
         dx(i) = dxs
      35 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
      sum = 1
      do 2511 i=2,nx
         sum = sum + f*x**dfloat(i-1)
      2511 sum = sum + f*x**dfloat(i-1)
      dxo = XL/sum
      Xi(0) = 0.
      do 3011 i = 1, Nx
         dx(i) = dxo+f*x**dfloat(i-1)
      3011 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
Nxl0 = Nx-10

C **** PREPARATION FOR INITIAL CONDITIONS

SGAM = RHOS/RHOL - 1.
IF(MRB .EQ. 0) SGAM = 8.

C **** INITIAL CONCENTRATION

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

C **** INITIAL TOTAL MASS OF GAS IN THE SYSTEM

CITOT = 0.
DO 50 I = 1, NX
50 CITOT = CITOT + CX(I,1)*DX(I)
CITOTOLD = CITOT

C **** Bubble Volume Calculation

EXCHE = CO*X/L/AWHE
VOLHETOT = EXCHE*R*TO/PO

CADM = 0.
CFLUX = 0.
DELTA = 0.
lend = 0
tr = 0.
itime = 0

C **** THE BEGINNING OF TIME LOOP

C 9000 Continue
C DO 9000 MA = 1, NT
itime = itime + 1
M = 1
mo = 1
tr = tr + dt
V(mo) = Av + BV + CV**2.

G = -(1.+SGAM)*V(mo)
DELTA = DELTA + V(mo)*DT
XLIQ = XLO-(1.+SGAM)*DELTA

IF(XLIQ .LE. DXEND) THEN
  lend = 1
ENDIF

PRINT *, ' S-L Front = ', SG1(Delta), ' [M]'
PRINT *, ' Liquid Length = ', SG1(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 ', SG1(XEND), ' [M]'
  PRINT *, ' Vol(Void)/Vol(Sys) = ', SG1(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 Patankar High Flux Function
C

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

C **** DETERMINE COEFFICIENTS FOR LEFT BOUNDARY NODE
C

DFL = Di(1)+The(1)
Dm1 = Dc/DX(1)
Pel = G/Dm1
FPel = FP(Pel)
DFl1 = Dm1*FPel
Aw(1) = 0.
Ae(1) = -Fo*DFL
IF(ILB .EQ. 1) THEN
Am(1) = DX(1)/dt + Fa*(DFL + G)
&
S(1) = Dx(1)/dt*Cx(1,M-1) - Cs*v(mo)
&
+ (1.-Fo)* (DFL*Cx(2,m-1) - (G + DFL)*Cx(1,m-1))
ELSEIF(ILB .EQ. 2) THEN
beta = 1./(1./v(mo) - DX(1)/2./Dc)
Am(1) = DX(1)/dt + Fa*(DFL + G - beta)
&
S(1) = Dx(1)/dt*Cx(1,M-1) - Cs*beta
&
+ (1.-Fo)* (DFL*Cx(2,m-1) + (beta - DFL - G)*Cx(1,m-1))
ELSEIF(ILB .EQ. 3) THEN
Am(1) = DX(1)/dt + Fa*(DFL + G)
&
S(1) = Dx(1)/dt*Cx(1,M-1)
&
+ (1.-Fo)* (DFL*Cx(2,m-1) - (DFL + G)*Cx(1,m-1))
ELSEIF(ILB .EQ. 4) THEN
Am(1) = DX(1)/dt + Fa*(DFL + G - v(mo))
&
S(1) = Dx(1)/dt*Cx(1,M-1) + (Co - Cs)*v(mo)
&
+ (1.-Fo)* (DFL*Cx(2,m-1) - (DFL + G - v(mo))*Cx(1,m-1))
ELSEIF(ILB .EQ. 5) THEN
Am(1) = DX(1)/dt + Fa*(DFL + G - v(mo))
&
S(1) = Dx(1)/dt*Cx(1,M-1) - Cs*v(mo)
&
+ (1.-Fo)* (DFL*Cx(2,m-1) - (DFL + G - v(mo))*Cx(1,m-1))
ELSE
Am(1) = DX(1)/dt + Fa*(DFL + G + DFl1)
&
S(1) = Dx(1)/dt*Cx(1,M-1) + (G + DFl1)*Co
&
+ (1.-Fo)* (DFL*Cx(2,m-1) - (DFL + G + DFl1)*Cx(1,m-1))
ENDIF

C **** DETERMINE COEFFICIENTS FOR INTERIOR NODES
DO 70 I = 2, Nx1
DF1 = Di(i)*FPi
DF1t = Di(i-1)*FPi(i-1)

Aw(i) = -Fo*(DF1t + G)
Ae(i) = -Fo*DF1
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) + Aw(i)*Cx(i-1,m-1))

70 CONTINUE

C •••• DETERMINE COEFFICIENTS FOR RIGHT BOUNDARY NODE

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

IF(IRB .EQ. 1) THEN
Am(Nx) = DX(Nx)/dt + Fo*DFR1
S(Nx) = Ddx(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
Am(Nx) = DX(Nx)/dt - Aw(Nx)
S(Nx) = Dx(Nx)/dt*Cx(Nx,M-1) + DFR*Co
& + (1.-Fo) + (DFR + G)*Cx(Nx1,m-1)
& - (DFR + G + DFR1)*Cx(Nx,m-1))
ELSEIF(IRB .EQ. 3) THEN
Am(Nx) = DX(Nx)/dt + Fo*DFR - Aw(Nx)
S(Nx) = Dx(Nx)/dt*Cx(Nx,M-1) + DFR*Co
& + (1.-Fo) + ((DFR + G)*Cx(Nx1,m-1)
& - (DFR + G + DFR1)*Cx(Nx,m-1))
ELSEIF(IRB .EQ. 4) THEN
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))
ELSE
Am(Nx) = DX(Nx)/dt + Fo*DF1*(Cl-Co)
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 •••• GET SOLUTION FOR PRESENT TIME STEP; TRIDIAGONAL MATRIX SOLVER

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. + sGom)*v(m)*dt/xl)
dx(i) = dx(i)/(1. - (1. + sGom)*v(m)*dt/xl)
100 CONTINUE
\[ x_i(i) = x_{i-1} + dx(i) \]  
CONTINUE

\[ C_{\text{max}} = C_x(1,m) \]
\[ I_{\text{max}} = 1 \]
Do 299 \( i = 1, N_x \)
if \((C_{\text{max}} \leq C_x(i,m))\) then
\[ C_{\text{max}} = C_x(i,m) \]
\[ I_{\text{max}} = i \]
end if
CONTINUE

\[ C_{x\text{ch}} = C_x(I_{\text{max}},m) / \text{Ch} \]
WRITE(11, 6030) SGLN(TR), CxCh
itime = itime/Npstp*Npstp
if (itime.eq. itime .lt. 20 .or. iend .eq. 1) then
WRITE(14, 6030) SGLN(TR), Delta
end if

PRINT *, ' '  
PRINT *, 'Time= ', SNGL(TR), ' Cx(1)= ', SGLN(Cx(1,m))
PRINT *, 'Max. C Appears at i = ', I_{\text{max}}, ' Cx(\text{I}_{\text{max}}) = ', SGLN(Cx(I_{\text{max}},m))

C *** CHECK MASS BALANCE

C *** DETERMINE MASS FLUX AT LEFT BOUNDARY

IF (ILB .EQ. 1) THEN
\[ \text{FluxL} = -C_x[v(ma)] \]
ELSEIF (ILB .EQ. 2) THEN
\[ \text{FluxL} = \beta_x(C_i - C_x) \]
ELSEIF (ILB .EQ. 3) THEN
\[ \text{FluxL} = 0. \]
ELSEIF (ILB .EQ. 4) THEN
\[ \text{FluxL} = (C_i - C_x)[d(delta)/dt] \]
ELSE
\[ \text{FluxL} = (G + DFL1)C_{x}G + DiFi(C_i - C_x) \]
ENDIF

C *** DETERMINE MASS FLUX AT RIGHT BOUNDARY

IF (IRB .EQ. 1) THEN
\[ \text{FluxR} = C_iG \]
ELSEIF (IRB .EQ. 2) THEN
\[ \text{FluxR} = G(C_{x}(N_x,m) + (1.-F_o)C_{x}(N_x,m-1)) \]
ELSEIF (IRB .EQ. 3) THEN
\[ \text{FluxR} = (G + DFR)(C_{x}(N_x,m) + (1.-F_o)C_{x}(N_x,m-1)) - DFR*C_{x} \]
ELSE
\[ \text{FluxR} = (G + DFR)(C_{x}(N_x,m) + (1.-F_o)C_{x}(N_x,m-1)) \]
ENDIF

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

ENDIF

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 - Citotold
BAL1 = Error1/Citotold *100.

C **** Bubble Volume Calculation

nnuc = 0.
sumdx = 0.
Cexcess = 0.
if(Cx(imax,m) .GT. Ch) then
if(i stop .eq.1) then
write(12, 2115) anol(tr)
do 2118 i = 1,nx,2
ccox = Cx(i,m)/co
xixliq = xi(i)/xliq/100.
2118 write(12, 2116) xixliq, ccox
2116 format(5x,d20.10,2x,d20.10)
2115 format(5x,'time = ',fie.3,' sec')
print *, 'optional stop at first occurrence of Cx(imax,m) > Ch'
stop
endif
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
AvailC = Cexcess - CADmass
AvailC = Cexcess
CADmass = 0.
do 2051 i = 1, Nx
if(Cx(i,m) .GE. Ch) then
Cx(i,m) = Ch
Sumdx = Sumdx + dx(i)
Nnuc = Nnuc + 1
Nucnode(Nnuc) = i
endif
2051 continue
endif

if(AvailC .GT. 0.) then
Mole = AvailC/AwHe
Mole = Mole/Trnuc
AddVol = Mole*Rg*To/Po
VolHe = VolHe + AddVol
endif
if(volHe .GT. VolHetot) then
   AdjCx = (VolHe - VolHetot)*Po*AwHe/(Rg*To)
   VolHe = VolHetot
   Redist = AdjCx/Sumdx
   DO 206 i = 1, Nnuc
      Cx(Nucnode(i),m) = Cx(Nucnode(i),m) + Redist*dx(Nucnode(i))
   else
      AdjCx = 0.
   endif
endif
VolSh = Delta*sGam
Voltot = VolHe + VolSh
WRITE(*, 6080) sngl(AddVoI), sngl(VolHe), sngl(VolSh), sngl(Voltot)
WRITE(*, 6020) SNGL(Citot), SNGL(Admass), SNGL(Ctotold), &
   SNGL(Errorl), SNGL(BALl)
C **** STORE PRESENT STEP VALUES IN THE PREVIOUS STEP VARIABLES TO ADVANCE
C NEXT TIME STEP
DO 300 1=1,NX
   Cx(I,M-1) = Cx(I,M)
300 CONTINUE
Ctotold = Citot - Cexcess + AdjCx
AvolIC = 0.
C **** TRANSFORMATION INTO DIMENSIONLESS VARIABLES
C
TB = Tr + DT
CxC = Cx(Inax,m)/Ch
itck = itime/NpStp+NpStp
if(itck .eq. itime .or. itime .eq. 1 &
   or. Inuc .EQ. 1 .or. end .eq.1) then
   WRITE(13,6090) angl(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) IFFlag = 1
   ENDF
500 CONTINUE
if(IFFlag .eq. 1) then
   do 400 ik = 1,nx,2
   CxC = 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
   write(12,2119) XiXLiq, CxCo, Anal
   400 write(12,2119) XiXLiq, CxCo, Anal
   format(5x,d20.10,2x,d20.10,2x,d20.10)
   IFFlag = 0
endif
Inuc = 0
CONTINUE

FORMAT STMTS

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]')
6060 FORMAT(3X,E12.5,3X,D20.10)
6070 FORMAT(3X,E12.5,3X,D20.10)
6080 FORMAT(3X,E12.5,3X,D20.10)
6090 FORMAT(2X,E12.5,2x,E12.5,2x,E12.5,2x,E12.5)
9999 STOP
END

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)

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

STOP
\[ Q(i) = \frac{(S(i) - oW(i) \cdot Q(i-1))}{DENUM} \]

\[ X(N) = Q(N) \]

\[ \text{DO 20 \ i=N-1,1,-1} \]
\[ X(i) = P(i) \cdot X(i+1) + Q(i) \]

\[ \text{CONTINUE} \]

\[ \text{RETURN} \]

\[ \text{END} \]
Appendix B-2

Input Data for Computer Program SEGR.FOR
PROGRAM SEGREGATE
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).
COMMON /VELOC/ v(0:1000), m(0:1000), tm(0:2)
COMMON /MATRX/ Aw(1000), Am(1000), Ae(1000), S(1000)
NAMELIST /INPUT1/ NT, TIME, NX, XL, Co, Cs, Ch, DC, vopt, 
& Av, Bv, Cv, Div, npct, fx, ft, Fa, dt, xsbi, Co
NAMELIST /CONVER/ EPS1, EPS2, EPS3
NAMELIST /OPTION/ MLB, MRB, ILB, IRB, Npct, IDX, istop
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): Patonckar High Flux
FP(z) = DMAX1(0.D0, -1.D0 - 0.1D0*DBS(z))*5.D0
& + DMAX1(O.DO, -z)
OPEN(10, ERR=9999, FILE='SEGRe.INP', STATUS='OLD')
OPEN(11, ERR=9999, FILE='SEGRe.Cm', STATUS='UNKNOWN')
OPEN(12, ERR=9999, FILE='SEGRe.Cxi', STATUS='UNKNOWN')
OPEN(13, ERR=9999, FILE='SEGRe.Vol', STATUS='UNKNOWN')
OPEN(14, ERR=9999, FILE='SEGRe.De', STATUS='UNKNOWN')
OPEN(15, ERR=9999, FILE='SEGRe.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/5.960-09/, Rho/530./, Rhol/517./
& Ch/1.7370-03/, Cs/1.59D-08/, Co/4.260-06/, Ce/1.59D-06/
DATA Po/7330./, To/454./, Rg/8.3143/, AwHe/4.0026D-03/
READ NAMELIST INPUT
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*V(i) + Cv*V(i)**2.
ENDIF
XL0 = XL
Nxo = Nx
C **** IDENTIFY PRINTOUT TIME
Appendix C

List of Computer Program
FREZ.FOR
if(iPCM/.ne.1) then  
        ! LiF calculation
C LiF properties
Ti=Tf
xKa=xKsf
xKf=xKsf
Cps=Cpsf
rhop=rhopf
rhoi=rhoif
xKv=xKvf
endif

n=5
nx=2

if(iopt .eq. 1) go to 9000

if(ivoid .eq. 1) then
  do -0.00001 slo do
  else do -0. slo do
  endif
  dos - do
do 10 l=1,n
  T0(l)=Ti
  Tt(l)=Tf
continue

H1 = Hsf + Cps+Tf
eps30 = eps3
eps0 = eps1
eps12 = dsqrt(eps1)
Gam = 1. - rhoi/rhop
rGam = Gam/(1.-Gam)

As = xKa/rhop/Cps
Ac = xKf/rhoc/Cpc
a1 = rhoi+Cps*tc/dt
a2 = rhoi+Cps/dt

hca = 2.*xKc/te
Ai = Emitout*Boltz/hca
SumLam=0.
do 50 it=1, nt

ind = It/npr+npr - It

if(lt .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 = rGm*ds
if( ivoid .eq. 1) then
  sis = ds + dvs
else
  sis = 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
  hcvss = xKv/dvs
  hr2s = Emitin*Boltz*(Ts(4)**2 + Ts(3)**2)*(Ts(4) + Ts(3))
  hv = hcvss + hr2s
C
  hv = hcvss

IF(IBC .eq. 1) THEN
C Overall between T1 and T2
C2 This considers heat transfer across the void
if( ivoid .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
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) = rhoa*H1/dt*(ds-do) + a2*do*To(2) + hss*Tf

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

  dT5 = Al*(Tn(1)**4.-Ta**4)/(1.44*Al*Tn(1)**3)
  Tn(5) = Tn(1)-dT5
C
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
\[ \begin{align*}
T_n(4) &= h_{12}(T_n(1)/h_{ss} + 1./h_{cs}T_n(2)) \\
T_n(3) &= h_{12}(T_n(2)/h_{ss} + 1./h_{cs}T_n(1)) \\
& \text{endif}
\end{align*} \]

ELSE

C BC2 Constant wall temperature
\[ \begin{align*}
T_n(1) &= T_o \\
T_n(2) &= T_n(1) \\
T_n(3) &= T_n(1)
\end{align*} \]

if(ivoid .eq. 1) then
C BC3 Constant wall temperature, with void
\[ \begin{align*}
h_{12} &= 1./(1./h_{ss} + 1./h_v)
\end{align*} \]
else
C BC2 Constant wall temperature, without void
\[ \begin{align*}
h_{12} &= h_{ss}
\end{align*} \]
endif

\[ \begin{align*}
T_n(2) &= (a_2*d_0*T_o(2) + \rho_{o}*H_{s}(d_s-d_o)/dt \\
&+ h_{ss}T_f + h_{12}T_n(1))/(h_{12} + h_{ss} + a_2*d_s)
\end{align*} \]
if(ivoid .eq. 1) then
\[ \begin{align*}
T_n(4) &= (h_vT_n(1) + h_{ss}T_n(2))/(h_{ss} + h_v)
\end{align*} \]
else
\[ \begin{align*}
T_n(4) &= T_n(1)
\end{align*} \]
endif

ENDIF

C Check energy balance of the system
C Heat flux at the left boundary of the system
\[ \begin{align*}
Q_{ls} &= -h_o1(T_n(1)-T_o)
\end{align*} \]
C Heat flux at the left boundary of the PCM
\[ \begin{align*}
Q_{lp} &= -h_{12}(T_n(2)-T_n(1))
\end{align*} \]
C For constant wall temperature only
if(!BC .eq. 2) \[ \begin{align*}
Q_{ls} &= Q_{lp}
\end{align*} \]
C Heat flux at the right boundary of the system, \( x=x_{LB} + \Delta x \)
C which is equal to Heat flux at the right boundary of the solid PCM
\[ \begin{align*}
Q_{rs} &= -\rho_{o}*H_s*(d_s-d_o)/dt
\end{align*} \]
C Total heat accumulated in the system within dt
C Fully implicit scheme
\[ \begin{align*}
E_{Qp} &= (Q_{lp} - Q_{rs})*dt \\
E_{Qs} &= (Q_{ls} - Q_{rs})*dt
\end{align*} \]
C Energy accumulated within the cladding
if(!BC .eq. 1) then
\[ \begin{align*}
E_c &= p_c*\rho_c*C_{pc}*(T_n(1) - T_o(1))
\end{align*} \]
else
\[ \begin{align*}
E_c &= 0.
\end{align*} \]
endif
C Energy accumulated within the solid crust
\[ \begin{align*}
E_p &= \rho_{o}*C_{ps}*(d_s*T_n(2) - d_o*T_o(2)) - (d_s-d_o)*\rho_{o}H_{s}
\end{align*} \]
C Total Energy accumulated in the system
\[ \begin{align*}
E_r &= E_c + E_p
\end{align*} \]
\[ \begin{align*}
E_r &= (E_{Qs} - E_o)/E_o
\end{align*} \]
Erp = (EQp - Ep)/Ep
REC = Ec/Ep
vel = (ds-do)/dt

if(it .eq. 1 .or. ind .eq. 0) then
write(*,6000) iout, sngl(Ec),sngl(Ep),sngl(REc),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 = ((sqrt(Cy)+do)/2.
Ero = (ds - dsc)/ds
AEro = dobs(Ero)
Erdn = dobs(ds - dsc)

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

iffErdn .LE. eps1) go to 30
if(dsc .GT. da) then
dm = da
Erdo = Erdn
goto 20
else
dm = ds
Erdo = Erdn
goto 20
endif
30 continue

if(ivoid .eq. 1) then
Qrin = -Emit*Eis/(Tn(4)**4 - Tn(3)**4)
Qcin = -hcv*(Tn(4)-Tn(3))
qrat = Qcin/Qrin
endif
Stef = Cps*(Tf - Tn(5))/Hsl
FC = (alis-as)/dt*sqrt(time/As)
SumLam = SumLam + FC

40 continue

if(lopt .ne. 1) then
if(it .eq. 1 .or. ind .eq. 0) then
print *,
print *,"Sol. converged"
oQls = dobs(Ols)
oQlp = dobs(Olp)
oQrs = dobs(Qrs)
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))
c
C This proc. calculates Average Freezing Temp. avgFC, for given time
C period
C in this proc. Wall Temp., Tw, is varied from 250 K to 450 K for Lithium ; Tff(Li) = 454 K
C to 1120 K for Lithium Fluoride ; Tff(LiF) = 1122 K
C
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 else
c  do = 0.
c endif
do = do
d = do

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

HI = Hsl + Cps*Tf
epasO = eps3
epso = eps1
eps12 = dsqrt(eps1)
Gam = 1. - rho1/rhos
\( r\Gamma_m = \frac{\Gamma_m}{(1 - \Gamma_m)} \)

\[ A_s = xK_s/rhos/Cps \]

\[ A_c = xK_c/rhoc/Cpc \]

\[ a1 = rhoc+Cpc*tc/dt \]

\[ a2 = rhos*Cps/dt \]

\[ hcs = 2.0*xKc/tc \]

\[ A_l = Emitout*Boltz/hcs \]

\[ \text{SumLam}=0. \]

\[ \text{do 150 it}=1, nt \]

\[ \text{ind} = \text{it}/npr*npr - 
\text{it time} = \text{dfloat(it)}*dt \]

\[ \text{Endo} = 1.030 \]

\[ \text{if(it .eq. 1) then} \]

\[ \text{dmax} = \text{do} + 2.0*eps3 \]

\[ \text{else} \]

\[ \text{dmax} = \text{do} + 2.0*vel*dt \]

\[ \text{endif} \]

\[ \text{dmin} = \text{do} \]

\[ \text{iout} = 0 \]

\[ \text{120 continue} \]

\[ \text{iout} = \text{iout} + 1 \]

\[ \text{C Assume ds; new solid crust thickness} \]

\[ ds = (dmax+dmin)/2. \]

\[ dvs = r\Gamma_m*ds \]

\[ \text{if( ivoid .eq. 1) then} \]

\[ \text{sis} = ds + dvs \]

\[ \text{else} \]

\[ \text{sis} = ds \]

\[ \text{endif} \]

\[ \text{C Equivalent heat transfer coefficients} \]

\[ \text{C At the outer wall of the cladding, ho1} \]

\[ \text{Den} = 1./Emitout/Boltz + 4.0*Ts(1)**3/hcs \]

\[ ho1 = (Ts(1)**2+To**2)*Ts(1)/Den \]

\[ \text{C within the void} \]

\[ hvs = 2.0*xKv/dvs \]

\[ hr2s = Emitin*Boltz*(Ts(4)**2 + Ts(3)**2)*(Ts(4) + Ts(3)) \]

\[ cv \]

\[ hv = hvs + hr2s \]

\[ hv = hvs \]

\[ \text{IF(!IBC .eq. 1) THEN} \]

\[ \text{C Overall between T1 and T2} \]

\[ \text{C2 This considers heat transfer across the void} \]

\[ \text{if(ivoid .eq. 1) then} \]

\[ h12 = 1./(1./hcs + 1./hv + 1./hss) \]

\[ \text{else} \]

\[ \text{C BC1 This does not consider heat transfer across the void} \]

\[ h12 = 1./(1./hcs + 1./hss) \]

\[ \text{endif} \]

\[ \text{C BC1 Radiative Boundary} \]

\[ \text{aw}(1) = 0. \]

\[ \text{ap}(1) = ho1 + h12 + a1 \]

\[ \text{ao}(1) = -h12 \]

\[ \text{a}(1) = \text{ao}(1)*To(1) + ho1*To \]
\[ \text{ow}(2) = -h_{12} \]
\[ \text{op}(2) = h_{12} + h_{ss} + a_2 \cdot ds \]
\[ \text{oe}(2) = 0. \]
\[ s(2) = \rho_{ss} \cdot h_{ss}/dt \cdot (ds - do) + a_2 \cdot do \cdot Tn(2) + h_{ss} \cdot Tf \]

\[ \text{call \ tdma}(Tn, ow, op, oe, s, nx) \]
\[ dT5 = A1 \cdot (Tn(1) \times 4 - Tn(4))/((1 \times A1 + Tn(1) \times 4) - Tn(4)) \]
\[ Tn(5) = Tn(1) - dT5 \]

**C BC1** This considers heat transfer across the void

if (ivoid .eq. 1) then
\[ Tn(4) = h_{12} \cdot (Tn(1)/h_{ss} + (1./h_{cs} + 1./h_{v}) \cdot Tn(2)) \]
\[ Tn(3) = h_{12} \cdot (Tn(2)/h_{cs} + (1./h_{ss} + 1./h_{v}) \cdot Tn(1)) \]
else
\[ Tn(4) = h_{12} \cdot (Tn(1)/h_{ss} + 1./h_{ss} \cdot Tn(2)) \]
\[ Tn(3) = h_{12} \cdot (Tn(2)/h_{cs} + 1./h_{ss} \cdot Tn(1)) \]
endif

**ELSE**

**C BC2** Constant wall temperature

\[ Tn(1) = T_{a} \]
\[ Tn(5) = Tn(1) \]
\[ Tn(3) = Tn(1) \]

if (ivoid .eq. 1) then
\[ Tn(4) = h_{12} \cdot (Tn(1)/h_{ss} + 1./h_{ss} \cdot Tn(2)) \]
else
\[ Tn(4) = Tn(1) \]
endif

**C BC3** Constant wall temperature, with void

\[ h_{12} = 1./((1./h_{ss} + 1./h_{v}) \cdot Tn(1)) \]

else

**C BC2** Constant wall temperature, without void

\[ h_{12} = h_{ss} \]

endif

\[ Tn(2) = (a_2 \cdot do \cdot Tn(2) + \rho_{ss} \cdot h_{ss} \cdot (ds - do)/dt \]
\[ + h_{ss} \cdot Tf + h_{12} \cdot Tn(1))/(h_{12} + h_{ss} + a_2 \cdot ds) \]

if (ivoid .eq. 1) then
\[ Tn(4) = (h_{v} \cdot Tn(1) + h_{ss} \cdot Tn(2))/(h_{ss} + h_{v}) \]
else
\[ Tn(4) = Tn(1) \]
endif

ENDIF

**C Check energy balance of the system**

**C Heat flux at the left boundary of the system**

\[ Q_{ls} = -h_{o1} \cdot (Tn(1) - T_{a}) \]

**C Heat flux at the left boundary of the PCM**

\[ Q_{lp} = -h_{12} \cdot (Tn(2) - Tn(1)) \]

**C For constant wall temperature only**

if (iBC .eq. 2) \[ Q_{ls} = Q_{lp} \]

**C Heat flux at the right boundary of the system, x=\alpha LB + \delta**

\[ Q_{rs} = -\rho_{ss} \cdot h_{ss} \cdot (ds - do)/dt \]

**C Total heat accumulated in the system within dt**

**C Fully implicit scheme**
\[ \text{E}_{Qp} = (Q_{lp} - Q_{rs}) \cdot dt \]
\[ \text{E}_{Qs} = (Q_{ls} - Q_{rs}) \cdot dt \]

C Energy accumulated within the cladding
\[
\text{if} \,(\text{iBC} \rightarrow \text{eq. 1}) \, \text{then} \\
\text{Ec} = t_{c} \cdot \rho_c \cdot C_p \cdot (T_n(1) - T_o(1)) \\
\text{else} \\
\text{Ec} = 0. \\
\text{endif} \\
\]

C Energy accumulated within the solid crust
\[
\text{Ep} = \rho_s \cdot C_p \cdot ((d_s - T_n(2)) - (d_s - T_o(2))) - (d_s - d_o) \cdot \rho_s \cdot H_l \\
\]

C Total Energy accumulated in the system
\[
\text{E}_a = \text{Ec} + \text{Ep} \\
\text{E}_{rs} = (\text{E}_{Qs} - \text{E}_a) / \text{E}_o \\
\text{E}_{rp} = (\text{E}_{Qp} - \text{E}_p) / \text{E}_p \\
\text{REcEp} = \text{Ec} / \text{Ep} \\
v_{el} = (d_s - d_o) / dt \\
\]

C Check the convergence
\[
\text{Cx} = 2. \cdot x \cdot k_s \cdot (T_f - T_n(2)) \cdot dt / \rho_s / H_s \\
\text{if} \,(\text{Cx} < 0.) \, \text{then} \\
\text{Cx} = 0. \\
\text{else} \\
\text{C} = (d_s - d_c) / 2. \\
\text{Ero} = d_c / d_s \\
\text{AEro} = \text{dabs}(\text{Ero}) \\
\text{Erdn} = \text{dabs}(d_s - d_c) \\
\text{endif} \\
\text{endif} \\
\text{if} \,(\text{it} = \text{eq. 1} \, \text{or} \, \text{ind} = \text{eq. 0}) \, \text{then} \\
\text{write}(*,6020) \, \text{angl}(\text{Ero}), \, \text{angl}(\text{Erdn}), \, \text{angl}(\text{Erp}), \, \text{angl}(\text{Ers}) \\
\text{endif} \\
\text{if} \,(\text{Erdn} < \text{eps}) \, \text{go to} \, 130 \\
\text{if} \,(d_m > d_s) \, \text{then} \\
\text{dmin} = d_s \\
\text{Erdn} = \text{Erdn} \\
\text{go to} \, 120 \\
\text{else} \\
\text{dmax} = d_s \\
\text{Erdn} = \text{Erdn} \\
\text{go to} \, 120 \\
\text{endif} \\
130 \text{ continue} \\
\text{Stef} = C_p \cdot (T_f - T_n(5)) / H_s \\
\text{FC} = (s_l - s_o) / dt \cdot \text{dsqrt} \,(\text{time} / A_s) \\
\text{c print *,'lt='',lt,'FC = ',FC} \\
\text{do} = d_s \\
\text{slo} = s_l \\
\text{dos} = d_s \\
\text{do} \, 140 \, i = 1,n \\\n\text{Tsl(i)=Tn(i)} \\\n\text{Tol(i)=Ts(i)} \\
140 \text{ continue} \\
\text{if} \,(\text{it} = \text{eq. 1} \, \text{or} \, \text{ind} = \text{eq. 0}) \, \text{then}
c print *
print *
print *,'Sol. converged'
continue

avgFC = SumLam/DFloat(nt)
write(11,6010) angl(Stef),angl(avgFC)
continue
write(11,8020)

STOP

format(2x,'Generate a plot./2x,'input data. ')
format(2x,'...T1...
format(2x,'...T2...
format(2x,'...T3...
format(2x,'...T4...
format(2x,'...T5...
format(2x,'...C1adding',"
format(2x,'...PCM-Void',"
format(2x,'...S-L Intf',"
format(2x,E12.5,2x,e14.7)
format(2x,'Erdm',E12.5,2x,'Erdn',E12.5,2x,'Erpn',e12.5,2x, &
'Ern',e12.5)
format(//2x,'lout=',15/
& 2x,'Ec=',e12.5,2x,'Ep=',e12.5,2x,'Ratio=',e12.5, &
2x,'vel=',e12.5)
format(2x,'end of data./2x,'title text is ',""."".Temperature', &
',"".K',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Freezing', &
',"".Constant St=',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Vsl, M/sec', &
',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Error in ', &
'Energy Balance',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Delta, M',""."" &
',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Heat Flux', &
'Ratio inside Void, Qcond/Qrad',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Energy Ratio', &
'in the System, dEc/dEs',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Heat Flux at', &
'Various Position, W/M*e2',"".""./2x,'go. ')
format(2x,'end of data./2x,'title text is ',""."".Freezing', &
'Constant vs Stefan Number',"".""./2x,'go. ')
end

c *******************************************************
SUBROUTINE TDMA(X, oW, oP, oE, S, N)
  implicit double precision (a-h, o-z)
  DIMENSION X(1), oW(1), oP(1), oE(1), S(1)
  DIMENSION P(1000), Q(1000)
  ( oW(1) = 0. , oE(N) = 0. )
  P(1) = -oE(1)/oP(1)
  Q(1) = S(1)/oP(1)
  DO 10 i=2,N
    DENUM = oP(i)+oW(i)*P(i-1)
    P(i) = -oE(i)/DENUM
    Q(i) = ( S(i)-oW(i)*Q(i-1) ) /DENUM
  10 CONTINUE
  X(N) = Q(N)
  DO 20 i=N-1,1,-1
    X(i) = P(i)*X(i+1)+Q(i)
  20 CONTINUE
  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
C =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
C Implicit double precision (a-h, o-z)
C
character*8 adum

dimension To(5),Te(5), Tn(5)
dimension ow(1000), op(1000), oe(1000), s(1000)
data To/250./, dt/.1/, nt/200/, Emitin/.8/, Emitout/.8/,
& Boltz/5.67D-08/, npr/10/, xSL/1./, lPr/500/

C Li properties
&C /1122./, Tif/1122./, xKsf/4.9997/, xKlf/1.3/,
&C Cpsf/2469.74/, rhoif/1792./, rholf/1376./, Hsif/347271./,
C Thermal conductivity of LiF vapor
&C xKv/0.016954/.
C Li properties
&C Tfk/454./, Ti/454./, xKsf/75.8/, xKlf/42.8/,
&C Cpsf/3780./, rhoif/538./, rholf/517./, Hsif/432100./,
C Thermal conductivity of He gas, at 200 F
&C xKv/0.16781/.
C Properties of cladding material
&C tc/0.00076/, Cpc/323.4/, rhoC/6490./, xKc/23.885/
&C eps1/1., eps2/1.75/, eps3/0.01/, tcm/2740./
C Initial size of void, thickness of the system
data i opt/1./, iPCM/2./, ivoid/1./, iBC/2./, q1/25000./

c
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='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='Qrot.dat', status='unknown')
open(16, err=9999, file='Qcld.dat', status='unknown')
open(17, err=9999, file='Qsol.dat', status='unknown')
open(18, err=9999, file='Qdel.dat', status='unknown')
open(19, err=9999, file='Ttot.dat', status='unknown')
open(20, err=9999, file='Qtot.dat', status='unknown')
open(21, err=9999, file='Tpro.dat', status='unknown')
open(22, err=9999, file='Tpro.dat', status='unknown')
open(23, err=9999, file='Tpro.dat', status='unknown')
open(24, err=9999, file='Tpro.dat', status='unknown')

c
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
C =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 To(5),Ts(5), Tn(5)
dimension aw(1000), ap(1000), ae(1000), a(1000)
data Ta/1350./, dt/1./, nt/20000./, Emitin/.5/, Emitout/.8/.
& Boltz/5.67D-08/, np/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./, Hslf/347271./,
C Thermal conductivity of LiF vapor
& xKvf/0.016954/,
C Li properties
& Tt/454./, Ti/454./, xKs/75.8/, xKI/42.8/, &
& Cps/3780/., rhos/530./., rhol/517./., Hsl/432100./,
C Thermal conductivity of He gas. at 260 F
& xKv/1.6751/,
C Properties of cladding material
& tc/0.00076/, Cpc/323.4/, rhoc/6498./, xKc/23.885/, &
& eps1/1.D-12/, eps2/1.75/, eps3/0.e1/, tcm/2740./
C Initial size of void, thickness of the system
& dvi/0.0001/, imochine/1/.
if(imochine .eq.1) then
open(6, err=9999, file='TTV.dot', status='unknown')
open(7, err=9999, file='TQR.dot', status='unknown')
else
open(6, err=9999, file='T1.dot', status='unknown')
open(7, err=9999, file='T2.dot', status='unknown')
open(8, err=9999, file='T3.dot', status='unknown')
open(9, err=9999, file='T4.dot', status='unknown')
open(10, err=9999, file='T5.dot', status='unknown')
open(11, err=9999, file='dv.dot', status='unknown')
open(12, err=9999, file='Vel.dot', 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='Qcld.dat', status='unknown')
open(18, err=9999, file='Qsol.dat', status='unknown')
open(19, err=9999, file='Qdel.dat', status='unknown')
endif

if(imochine .ne. 1) then
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', ' ')
10
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 1 LiF calculation

C LiF properties
Tf = Tff
Ti = Tif
xKs = xKsf
xKl = xKlf
Cps = Cpsf
rhos = rhosf
rhoi = rhoif
Hsl = Hsif
xKv = xKvf
endif

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

do = 0.000
dos = do

de 0.000

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

All = xKl/rhol/Cpi
As = xKs/rhos/Cps
Ac = xKc/rhoc/Cpc
al = rhoc*Cpc*tc/dt
\[ o_2 = \rho_01*C_p1/dt \]
\[ hcs = 2.*xKc/tc \]
\[ Al = Emitout*Boltz/hcs \]

\[
\begin{align*}
do & 3000 \text{ it}=1, \text{ nt} \\
\text{ind} & = \text{it}/npr*npr - \text{it} \\
\text{time} & = \text{dfloat(it)}*dT \\
Erdo & = 1.030 \\
\text{if}(\text{it} .eq. 1) & \text{then} \\
dmax & = do + 3.0*eps3 \\
\text{else} \\
dmax & = do + 3.0*vel*dt \\
\text{endif} \\
dmin & = do \\
lout & = 0 \\
\end{align*}
\]

100 continue
lout = lout + 1

C Assume ds; new solid crust thickness
\[ ds = (\text{dmax}+\text{dmin})/2. \]

C Equivalent heat transfer coefficients
C At the outer wall of the cladding, h01
\[ \begin{align*}
\text{Den} & = 1./\text{Emitout}/\text{Boltz} + 4.0*Ts(1)**3/hcs \\
h01 & = (Ts(1)**2+Ta**2)*(Ts(1)+Ta)/\text{Den} \\
\end{align*} \]

C within the void
\[ \begin{align*}
dvs & = dvo - (ds-do)^*\text{Gam} \\
\text{if}(dvo .lt. 1.d-06) & \text{then} \\
lvoid & = 0 \\
dvs & = 1.d-06 \\
\text{endif} \\
his & = 2.*xKl/ds \\
hcvs & = xKv/dvs \\
hr2s & = \text{Emitin}/\text{Boltz}*(Ts(4)**2 + Ts(3)**2)/(Ts(4) + Ts(3)) \\
hv & = hcvs + hr2s \\
\end{align*} \]

C Overall between T1 and T2
C2 This considers heat transfer across the void
\[ \begin{align*}
\text{IFMBC} .ne. 2) & \text{THEN} \\
\text{if}(!\text{void} .eq. 1) & \text{then} \\
h12 & = 1.0/((1./hcs + 1./hv + 1./hls) \\
\text{else} \\
C1 & \text{This does not consider heat transfer across the void} \\
h12 & = 1.0/((1./hcs + 1./hls) \\
\text{endif} \\
\end{align*} \]

C BC1 Radiative Boundary
\[ \begin{align*}
aw(1) & = 0. \\
aw(1) & = -h12 \\
\text{if}(\text{IBC} .eq. 1) & \text{then} \\
op(1) & = h01 + h12 + a1 \\
s(1) & = a1*To(1) + h01*To \\
\text{else} \\
op(1) & = h12 + a1 \\
s(1) & = a1*To(1) + a1 \\
\text{endif} \\
\end{align*} \]

C BC1
\[ \begin{align*}
aw(2) & = -h12 \\
op(2) & = h12 + his + a2*ds \\
aw(2) & = 0. \\
\end{align*} \]
\[ s(2) = \rho_{01}H_l/\text{d}t*(d_S-d_o) + a_2*d_o*To(2) + h_{ls}*T_f \]

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

if(iBC .eq. 1) then
  \[ dT5 = A_l*(Tn(1)**4-To**4)/(1.44+A_l*To**3) \]
  \[ Tn(5) = Tn(1)-dT5 \]
else
  \[ Tn(5) = Tn(1) + q1/h_c \]
endif

C BC1 This considers heat transfer across the void

if((void .eq. 1) then
  \[ Tn(4) = h_{12}*(Tn(1)/h_{ls} + (1./h_c + 1./h_v)*Tn(2)) \]
  \[ Tn(3) = h_{12}*(Tn(2)/h_c + (1./h_{ls} + 1./h_v)*Tn(1)) \]
else
  C BC1 This does not consider heat transfer across the void
  \[ Tn(4) = h_{12}*(Tn(1)/h_{ls} + 1./h_c*Tn(2)) \]
  \[ Tn(3) = h_{12}*(Tn(2)/h_c + 1./h_{ls}*Tn(1)) \]
endif

ELSE

C BC2 Constant wall temperature, without void

if((void .eq. 0) then
  \[ h_{12} = h_{ls} \]
C BC3 Constant wall temperature, with void
else
  \[ h_{12} = 1./(1./h_{ls} + 1./h_v) \]
endif

\[ Tn(1) = T_o \]
\[ Tn(2) = (a_2*d_o*To(2) + \rho_{01}H_l*(d_S-d_o)/\text{d}t \]
\[ + h_{ls}*T_f + h_{12}*(Tn(1))/(h_{12} + h_{ls} + a_2*d_S) \]

C BC2 Constant wall temperature,

\[ Tn(5) = Tn(1) \]
\[ Tn(3) = Tn(1) \]

C BC2 without void

if((void .eq. 0) then
  \[ Tn(4) = Tn(1) \]
else
  C BC2 with void
  \[ Tn(4) = (h_v*Tn(1) + h_{ls}*Tn(2))/(h_{ls} + h_v) \]
endif

ENDIF

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

\[ Q_{ls} = -h_{01}*(Tn(1)-T_o) \]

C Heat flux at the left boundary of the PCM

\[ Q_{lp} = -h_{12}*(Tn(2)-Tn(1)) \]

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) \[ Q_{ls} = Q_{lp} \]
if((IBC .eq. 3) \[ Q_{ls} = q_1 \]

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
\[ Q_{rs} = -hls*(Tf-Tn(2)) - \rho_{fl}*Hs*(ds-do)/dt \]

C for melting process, heat conducted at the RHS of liquid
C only by temperature gradient
\[ Q_{rs} = -hls*(Tf-Tn(2)) \]

C Total heat accumulated in the system within dt
C Fully implicit scheme
\[ EQp = (Qip - Qrs)*dt \]
\[ EQs = (Qis - Qrs)*dt \]

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)

\[ \text{if}(iBC \neq 2) \text{ then} \]
\[ Ec = tc*rhoc*Cpc*(Tn(1) - To(1)) \]
\[ \text{else} \]
\[ Ec = 0. \]
\[ \text{endif} \]

C Energy accumulated within the liquid PCM
\[ Ep = \rho_{fl}*Cpl*(ds*Tn(2) - do*To(2)) - (ds-do)*\rho_{fl}*Hs \]

C Total Energy accumulated in the system
\[ Eo = Ec + Ep \]
\[ Ers = (EQs - Eq)/Eo \]
\[ Erp = (EQp - Ep)/Ep \]
\[ RECp = Ec/Ep \]
\[ vel = (ds-do)/dt \]

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

C6080 format(///2x. 'it=', i5, 'iout=', i5, 'Ec-', e12.5, 2x, 'Ep-', e12.5, 2x, 'Ratio-', e12.5, 2x, 'vel-', e12.5)

C Check the convergence
\[ Cx = 2.*xKI*(Tn(2)-Tf)*dt/\rho_{fl}/Hs \]
\[ \text{if}(Cx \LT 0.) \text{ Cx = 0.} \]
\[ Cy = do**2 + 4.*Cx \]
\[ dsc = (dsqrt(Cy)+do)/2. \]
\[ Ero = (ds - dsc)/ds \]
\[ AErp = dabs(Ero) \]
\[ Erdn = dabs(ds - dsc) \]

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, 'Ers-', e12.5)

C if (Erdn .LE. eps1) go to 2000
C if (dsc .GT. ds) then
C dmin = ds
C Erdm = Erdn
C go to 100
C else
C dmax = ds
C Erdm = Erdn
C go to 100
```plaintext
2000 continue

if (tvoid .eq. 1) then
  Qrin = -Emitin*Boltz*(Tn(4)**4 - Tn(3)**4)
  Qcin = -hcvs*(Tn(4)-Tn(3))
  qrot = Qcin/Qrin
endif

do = ds
dos = ds

do = 170, i,n
  Ts(i) = Tn(i)
  To(i) = Ts(i)
  continue

if (it .le. 50 .or. ind .eq. 0 .or. do .gt. xSL) then
  print *,
  print *, 'Sol. converged'
  oQls = dabs(Qls)
  oQlp = dabs(Qlp)
  oQrs = dabs(Qrs)
  C for melting process, heat conducted at the RHS of liquid
  C only by temperature gradient
  C
  Qrs = dabs(Qrs)
  if (machine .eq. 1) then
    write(6, 6200) angl(time),angl(Tn(1)),angl(Tn(2)),angl(Tn(4)),
    & angl(vel)
    write(7, 6200) angl(time),angl(oQls),angl(oQlp),angl(oQrs),
    & angl(Qrot)
  else
    write(7, 6010) angl(time),angl(Tn(1))
    write(10, 6010) angl(time),angl(Tn(2))
    write(8, 6010) angl(time),angl(Tn(3))
    write(9, 6010) angl(time),angl(Tn(4))
    write(12, 6010) angl(time),angl(Tn(5))
    write(11, 6010) angl(time),angl(Tn(6))
    write(13, 6010) angl(time),angl(Ers)
    write(14, 6010) angl(time),angl(vel)
    write(15, 6010) angl(time),angl(RecEp)
    write(16, 6010) angl(time),angl(oQls)
    write(18, 6010) angl(time),angl(oQlp)
    write(19, 6010) angl(time),angl(oQrs)
  endif
endif

6010 format(2x,E12.5,2x,e14.7)
6200 format(1x,F8.2,1x,4e14.5)
if (do .gt. xSL) then
  write(6, 2990) format//2x,'Calculation Terminated on Complete melting of', & ' the System')
go to 3001
endif
if (Tn(1) .GE. tcm) then
  write(6, 2991) format//2x,'Calculation Terminated on Wall Temp. Exceeds', & ' Melting Temp. ')
go to 3001
```

endif
continue

if (machine .ne. 1) then
write(10,8010)
8010 format(2x,'end of data.','/2x,'title text is ','**','Temperature',
& ';','**','/2x,'go.')
write(11,8017)
8017 format(2x,'end of data.','/2x,'title text is ','**','Void',
& ';','Size, M**2**','/2x,'go.')
write(12,8011)
8011 format(2x,'end of data.','/2x,'title text is ','**','Val, M/sec',
& ';','/2x,'go.')
write(13,8012)
8012 format(2x,'end of data.','/2x,'title text is ','**','Error in ',
& 'Energy Balance',;',','/2x,'go.')
write(14,8013)
8013 format(2x,'end of data.','/2x,'title text is ','**','Delta, M',
& ';','/2x,'go.')
write(15,8014)
8014 format(2x,'end of data.','/2x,'title text is ','**','Heat Flux',
& ';','Ratio inside Void, Qcond/Qrad',;',','/2x,'go.')
write(16,8015)
8015 format(2x,'end of data.','/2x,'title text is ','**','Energy Ratio',
& ';','in the System, dEc/dEs',;',','/2x,'go.')
write(19,8016)
8016 format(2x,'end of data.','/2x,'title text is ','**','Heat Flux at ',
& 'Various Position, W/M**2',;',','/2x,'go.')
endif
9999 stop
end

**********************************************************************
*** TRIDIAGONAL MATRIX SOLVER : aWi.X(i-1) + oPi.X(i) + aEi.X(i+1) = Si
**********************************************************************
SUBROUTINE TDMA(X, oW,aP,oE,S, N)
implicit double precision (a-h, o-z)
DIMENSION X(1), oW(1),aP(1),oE(1),S(1)
DIMENSION P(1000),Q(1000)

P(1) = -oE(1)/aP(1)
Q(1) = S(1)/aP(1)

DO 10 i=2,N
  DENUM = oP(i)+oW(i)*P(i-1)
  P(i) = -oE(i)/DENUM
  Q(i) = ( S(i)-oW(i)*Q(i-1) ) /DENUM
10 CONTINUE

X(N) = Q(N)

DO 20 i=N-1,1,-1
  X(i) = P(i)*X(i+1)+Q(i)
20 CONTINUE