NUMERICAL MODELING OF A LEAD MELTING FRONT UNDER THE INFLUENCE OF NATURAL CONVECTION

by
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A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in fulfillment of the requirements for the degree of Master of Science (Nuclear Engineering).

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ABSTRACT

This work presents a study of the Effective Heat Capacity (EHC) method applied to the numerical simulation of the interface between a solid and a naturally convecting pool of liquid lead under pseudo-steady-state and transient conditions using COMSOL Multiphysics. The EHC method is implemented as a temperature dependent pseudo-material with discontinuities in the heat capacity, dynamic viscosity, and thermal conductivity to simulate the melting front. The approach is validated with experimental data for a vertical melting front between two walls. The hot wall heat flux and the cold wall temperature are adjusted until the numerical model that best matches the experimental data is found. The best case boundary conditions then serve as the control in subsequent studies of key modeling parameters, including the mesh refinement, the discontinuity width and location, the maximum allowable time step, and the jump in dynamic viscosity. An extra fine mesh with a maximum element size of $1.24 \times 10^{-3}$ m$^2$ results in the most accurate model. For pseudo-steady-state models the width and location of the discontinuity does not affect the results substantially but it does affect the settling times and transient behavior of the models. The maximum allowable time step is dependent on the mesh resolution. The behavior of the pseudo-solid transitions from solid to liquid when the dynamic viscosity is less then $1.0 \times 10^4$ Pa·s.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF FIGURES.</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>xi</td>
</tr>
<tr>
<td>CHAPTER 1 INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>CHAPTER 2 BACKGROUND</td>
<td>3</td>
</tr>
<tr>
<td>2.1. The Need for Small Modular Reactors</td>
<td>3</td>
</tr>
<tr>
<td>2.2. Design Considerations for Lead and Lead-Bismuth Eutectic Reactors</td>
<td>4</td>
</tr>
<tr>
<td>2.3. Lead &amp; LBE Cooled Reactors</td>
<td>5</td>
</tr>
<tr>
<td>2.4. Natural Convection Coupled with Phase Change in Liquid Metals</td>
<td>12</td>
</tr>
<tr>
<td>2.4.1. Laminar Natural Convection</td>
<td>13</td>
</tr>
<tr>
<td>2.4.2. Turbulent Natural Convection</td>
<td>13</td>
</tr>
<tr>
<td>2.4.3. Numerical Solution for Conduction Only</td>
<td>14</td>
</tr>
<tr>
<td>2.4.4. Phase Change with Natural Convection</td>
<td>16</td>
</tr>
<tr>
<td>CHAPTER 3 MODEL DEVELOPMENT AND VALIDATION</td>
<td>19</td>
</tr>
<tr>
<td>3.1. Pseudo-material Thermophysical Definitions</td>
<td>19</td>
</tr>
<tr>
<td>3.2. Description of the Validation Experiments</td>
<td>23</td>
</tr>
<tr>
<td>3.3. Representative COMSOL Model</td>
<td>26</td>
</tr>
<tr>
<td>3.4. Validation Methodology</td>
<td>29</td>
</tr>
<tr>
<td>3.5. Pseudo-Steady-State Model Validation Results</td>
<td>31</td>
</tr>
<tr>
<td>CHAPTER 4 MODEL RESULTS AND DISCUSSION</td>
<td>48</td>
</tr>
<tr>
<td>4.1. Mesh Refinement</td>
<td>48</td>
</tr>
</tbody>
</table>
## LIST OF FIGURES

2.1 Cross-sectional view of the SSTAR's thermal hydraulic system (Halsey et al., 2005). ................................................................. 8
2.2 The Gen4 Energy LBE cooled SMR. (Gen4 Energy, January 2010). ....... 9
2.3 SVBR monoblock reactor installation (Zrodnikov et al., 2008). ............ 10
2.4 The lead-cooled BREST-300 (International Atomic Energy Agency, 2002). .... 10
2.5 The ELSY Project design overview (Cinotti et al., 2007). .................... 11

3.1 Pseudo material dynamic viscosity as a function of temperature. .......... 20
3.2 Pseudo material heat capacity as a function of temperature. ............... 21
3.3 Pseudo material thermal conductivity as a function of temperature. ...... 22
3.4 Experimental apparatus used to study solid-liquid interface for lead under horizontal heat flux (based on Szekely and Chhabra 1970). ............... 23
3.5 First set of experimental data used to validate the numerical model (derived from Szekely and Chhabra 1970). ......................... 24
3.6 Second set of experimental data used to validate the numerical model (derived from Szekely and Chhabra 1970). ......................... 25
3.7 The experimental melting front location as the system transitions from one pseudo-steady-state to another. ................................. 26
3.8 Material assignments and boundary conditions for the two dimensional representative COMSOL model. ............................. 27
3.9 Progression of the COMSOL model from the initial state to a pseudo-steady-state. ......................................................... 28
3.10 The Modified Total Temperature RSS and the Cold Wall RSS versus hot wall heat flux for the first set of data. ......................... 32
3.11 The Melting Front RSS versus the hot wall heat flux for the first set of data. 32
3.12 The Average RSS versus hot wall heat flux for the first set of data. 33
3.13 The Modified Total Temperature RSS versus cold wall temperatures for a range of inlet heat fluxes. 34
3.14 The Cold Wall RSS versus cold wall temperatures for a range of inlet heat fluxes. 34
3.15 The Melting Front RSS versus cold wall temperatures for a range of inlet heat fluxes. 35
3.16 The Average RSS versus cold wall temperatures for a range of inlet heat fluxes. 35
3.17 The Average RSS versus hot wall heat flux for a range of cold wall temperatures. 36
3.18 The minimum Average RSS points form each hot wall heat flux series versus cold wall temperature. 37
3.19 The minimum Average RSS points from each cold wall temperature series versus hot wall heat flux. 37
3.20 Temperature field and velocity field with the EHC transition zone contours for the conditions derived for the first validation case. 38
3.21 The numerical model's time averaged temperature probe readings for the last 500 seconds of the best case boundary condition run compared with the horizontal temperature plots from the first set of experimental data. 39
3.22 Total Temperature RSS versus hot wall heat flux for the second set of experimental data. 40
3.23 The Average RSS versus hot wall heat flux for the second set of data. 41
3.24 The Total Temperature RSS versus cold wall temperature for the second set of data for a range of inlet heat fluxes. 42
3.25 The Cold Wall RSS versus cold wall temperatures for the second set of data for a range of inlet heat fluxes. 42
3.26 The Melting Front RSS versus cold wall temperature for the second set of data for a range of inlet heat fluxes. .................................................. 43
3.27 The Average RSS versus cold wall temperatures for the second set of data for a range of inlet heat fluxes. .................................................. 43
3.28 The Average RSS versus hot wall heat flux for the second set of data for a range of cold wall temperatures. .................................................. 44
3.29 The minimum Average RSS points from each hot wall heat flux series versus cold wall temperature for the second set of data. ....................... 44
3.30 The minimum Average RSS points from each cold wall temperature series versus hot wall heat flux for the second set of data. ...................... 45
3.31 Temperature and velocity fields with the EHC transition zone contours for the second best case model. .................................................. 46
3.32 The numerical model’s time averaged temperature probe readings for the last 500 seconds of the second set of best case boundary conditions compared with the horizontal temperature plots from the second set of experimental data. ... 47

4.1 The Modified Total Temperature RSS for the first validation case as a function of mesh refinement. .................................................. 49
4.2 The Cold Wall RSS for the first validation case as a function of mesh refinement. 49
4.3 The Melting Front RSS for the first validation case as a function of mesh refinement. .................................................. 50
4.4 The Average RSS for the first validation case as a function of mesh refinement. 50
4.5 Pseudo material heat capacity as a function of temperature. ................. 52
4.6 The Modified Total Temperature RSS as a function of the EHC transition zone width. .................................................. 53
4.7 The Cold Wall RSS as a function of the EHC transition zone width. ......... 53
4.8 The Melting Front RSS as a function of the EHC transition zone width. ... 54
4.9 The Average RSS as a function of the EHC transition zone width. .......... 54
4.10 The experimental and predicted melting front locations as the cold wall
temperature is decreased. .................................................. 55
4.11 The melting front location at the high temperature probe elevation as a
function of the transition zone width. .................................. 56
4.12 The melting front location at the mid-low temperature probe elevation as a
function of the transition zone width. ................................. 56
4.13 Modified Total Temperature RSS as a function of the latent heat of melting
location relative to the melting temperature. ....................... 58
4.14 Cold Wall RSS as a function of the latent heat of melting location relative to
the melting temperature. .................................................... 58
4.15 Melting Front RSS as a function of the latent heat of melting location relative
to the melting temperature. ............................................... 59
4.16 Average RSS as a function of the latent heat of melting location relative to
the melting temperature. .................................................... 59
4.17 The melting front location at the high temperature probe elevation as
a function of the latent heat of melting location relative to the melting
temperature................................................................. 60
4.18 The melting front location at the mid-low temperature probe elevation as
a function of the latent heat of melting location relative to the melting
temperature................................................................. 61
4.19 The formation of a singularity in the validation model caused by too large of
a time step. ..................................................................... 63
4.20 The Modified Total Temperature RSS as the pseudo material definition of the
solid’s dynamic viscosity is varied from 1 to $10^7$ Pa · s. ............ 65
4.21 The Cold Wall RSS as the pseudo material definition of the solid’s dynamic
viscosity is varied from 1 to $10^7$ Pa · s. ............................... 65
4.22 The Melting Front RSS as the pseudo material definition of the solid’s dynamic viscosity is varied from 1 to $10^7$ Pa·s. ............................................. 66
4.23 The average RSS as the pseudo material definition of the solid’s dynamic viscosity is varied from 1 to $10^7$ Pa·s. ............................................. 66
LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Basic characteristics of reactor coolants (Todreas et al., 2004; Etherington and Etherington, 1958).</td>
<td>4</td>
</tr>
<tr>
<td>2.2</td>
<td>Key characteristics of several lead and lead bismuth cooled reactors.</td>
<td>7</td>
</tr>
<tr>
<td>3.1</td>
<td>Constant values chosen for material properties of the numerical model.</td>
<td>20</td>
</tr>
<tr>
<td>4.1</td>
<td>Parameters of various mesh resolutions.</td>
<td>48</td>
</tr>
<tr>
<td>4.2</td>
<td>Maximum allowable time step for various mesh resolutions.</td>
<td>62</td>
</tr>
</tbody>
</table>
Greek Symbols

$\alpha$ Thermal Diffusivity
$\beta$ Coefficient of volumetric expansion
$\Delta$ Difference between two values
$\delta$ Error value
$\lambda$ Thermal conductivity
$\lambda$ Thermal conductivity
$\nu$ Dynamic viscosity
$\rho$ Density
$\sigma$ Microscopic cross section

Latin Symbols

$\bar{u}$ Generic time averaged field parameter
$\bar{T}$ Time averaged temperature probe reading
$\bar{X}$ Time averaged melting front location
$F$ Externally applied force
$I$ Identity matrix
$u$ Directional fluid flow velocity
$C$ Heat capacity
$CF$ Nusselt number correction factor
$d$ Characteristic Diameter
$dT$ Temperature transition zone
$g$ Acceleration of gravity
$Gr$ Local Grashof number
Characteristic height

Elevation

Number of samples used in error estimation

Nusselt number

Pressure

Prandtl number

Latent heat of fusion

Rate of freezing or melting

Rayleigh number

Reynolds number

Temperature

Magnitude of fluid flow velocity

Location of melting front

Horizontal Cartesian coordinate

Vertical Cartesian coordinate

Cold Wall

Fluid Boundary

Hot Wall

Subscripts

Latent heat of melting zone location

Boiling

Latent heat of melting zone width

Empirically determined value

Experimentally determined value

Numerically determined value

Scattering
th  Thermal
a  Absorption
b  Bulk fluid property
c  Cold wall
e  Electrical
l  Liquid
m  Melting
p  Constant pressure
s  Solid
y  Component of value in the y direction
CHAPTER 1
INTRODUCTION

There is interest in heavy metal coolants for nuclear reactor applications since materials with heavy nuclei allow for a fast flux neutron spectrum. This is due to an inherently small cross section for neutron down scattering to thermal energies. Such a spectrum is favorable for many nuclear applications, including: transmutation of transuranic materials into shorter lived radio-isotopes, long-life Small Modular Reactors (SMRs) for remote applications, and for breeding fissile fuel.

This work presents a study of the Effective Heat Capacity (EHC) method applied to the numerical simulation of the interface between a solid and a naturally convecting pool of liquid heavy metal. The EHC method is a fixed grid numerical modeling technique often used to solve phase change systems dominated by transient heat conduction (Basak and Ayappa, 1997; Voller et al., 1990). A COMSOL Multiphysics based modeling technique implements this method for lead subject to these conditions. A pseudo-material with discontinuous temperature dependent material properties near the melting temperature simulates the melting front. The technique is validated with experimental data for a vertical melting front between two walls. Key modeling parameters of the model are studied parametrically to understand the limitations of the EHC method.

This project is focused on understanding the limitations of the EHC modeling strategy to provide useful guidelines for implementation of this technique. This goal is accomplished by the following objectives:

1. Develop a numerical modeling approach to simulate naturally convecting lead in contact with a moving solid-liquid phase change boundary;
2. validate the modeling approach by comparing numerical results with published experimental results;
3. parametrically study the key modeling parameters to explore the limitations of the modeling approach; and,
4. document the limitations of the modeling approach to provide guidelines for future researchers.

The project’s implementation of the EHC method in COMSOL multiphysics uses finite element analysis to model the phase change of lead under the influence of natural convection. The modeling approach is validated by reproducing published experimental data. Lead subject to phase change with laminar natural convection in the presence of a horizontal
temperature gradient has been studied experimentally and a theoretical model exists for the shape of the melting front (Szekely and Chhabra, 1970).

The EHC based model that simulates the phase change of lead has several key parameters that effect the behavior of the melting front and temperature field discontinuities. The mesh resolution, maximum time step, width and location of the temperature transition zone, and the magnitude of the jump in dynamic viscosity all have limits beyond which the model departs from meaningful results. Parametric sweeps of these parameters provide guidelines for accurate phase change modeling using the EHC method.

The following Chapter presents the need for SMRs, the design considerations for liquid metal cooled reactors, previous designs of liquid metal reactors, and a detailed literature review of previous modeling techniques used to study natural convection coupled with freezing/thawing metals. Development and validation of the numerical modeling approach is presented in Chapter 3. Parametric studies of key modeling parameters are presented in Chapter 4 to fully understand the limitations of the EHC method. Finally, conclusions about the acceptable parameter limits are given in Chapter 5, followed by recommendations for future research in Chapter 6.
CHAPTER 2
BACKGROUND

This Chapter presents foundational material for this project starting with the justification for Small Modular Reactors (SMRs) in Section 2.1. Section 2.2 discusses design considerations for lead and lead-bismuth eutectic cooled reactors. Next, Section 2.3 gives an overview of Lead-cooled Fast Reactors (LFRs) which use lead and lead-bismuth eutectic coolant. Finally, Section 2.4 presents a detailed literature review of previous modeling approaches used to study natural convection coupled to freezing/thawing metals.

2.1. The Need for Small Modular Reactors

Nuclear power production is expected to increase by a factor of four by 2050 (Tucek et al., 2006; Wider et al., 2005). This increase is partially attributed to increased energy security and climate concerns of the developed world, but it is mainly attributed to the ambitions of the developing world (Smith et al., 2008; Tucek et al., 2006; Wider et al., 2005; Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007a). As the developing world strives to increase its standard of living in the coming decades, the demand for small or moderate increments of power (10-700 MW) will grow in areas with little to no grid infrastructure (Smith et al., 2008; Kuznetsov, 2008; Nakicenovic et al., 1998; Buongiorno, 2001). In a carbon-conscious society this growth demands new and advanced energy sources.

A key objective of the Global Nuclear Energy Partnership (GNEP) is the development and demonstration of concepts for SMRs that can be globally deployed while meeting four criteria: proliferation resistance, defense-in-depth-safety, sustainable use of fissile material, and economic viability (Smith et al., 2008; Cinotti et al., 2007; Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007a). The IPCC’s special report on emission scenarios has several scenarios which call for a large increase in nuclear power (Wider et al., 2005). This increase will require reprocessing and fast reactors in order to use fuel more efficiently and to burn minor actinides (Wider et al., 2005). Fast reactors under consideration by the Generation IV International Forum are lead cooled fast reactors, gas, and sodium cooled reactors (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007a; Wider et al., 2005). Lead cooled fast reactors are a competitive option to meet the GNEP criteria.
2.2. Design Considerations for Lead and Lead-Bismuth Eutectic Reactors

Table 2.1 compares lead to other potential coolants based on their fundamental characteristics. The low relative moderating power of lead, lead-bismuth eutectic, sodium, and helium is ideal for maintaining a fast flux neutron spectrum in a reactor. Relative moderating power is an average of the elastic and inelastic scattering cross-sections over the fission spectrum (Todreas et al., 2004; Etherington and Etherington, 1958). For comparison, all moderating powers in Table 2.1 have been normalized to that of lead. Helium has a lower heat capacity than lead, lead-bismuth eutectic and sodium thus degrading its performance as a coolant. Sodium is highly reactive with water and air which raises safety concerns about its use as a coolant. Lead and lead-bismuth eutectic coolants are not chemically reactive with water or air, and are prime candidates for small modular reactors.

Heavier nuclei are generally more transparent to fast neutrons and thus promote a better fast flux neutron economy (Todreas et al., 2004). Another benefit to heavy liquid metal coolants is their high heat capacity (147 J·kg⁻¹·K⁻¹ for liquid lead). Higher heat capacity coolants absorb heat during transient conditions and increase the time until peak cladding temperatures are reached (Hejzlar et al., 2009). A disadvantage of heavy liquid metal coolants is a relatively high neutron absorption cross-section which could lead to a reactivity insertion in the event of coolant voiding (Lafuente and Pera, 2010).

The natural circulation achievable with lead and lead-bismuth eutectic is widely exploited in the reactor designs detailed in Section 2.3. Many lead fast reactor and accelerator driven systems use natural circulation in the primary loop (Abanades and Pena, 2009). Natural circulation is the preferred method of decay heat removal since it would continue removing heat even in the event that on-site power is disrupted (Abanades and Pena, 2009). In particular, lead and lead-bismuth eutectic have favorable thermal-hydraulic characteristics as coolants due to the natural circulation pumping power achievable (Abanades and Pena,

<table>
<thead>
<tr>
<th>Atomic Mass (g·mol⁻¹)</th>
<th>Relative Atomic Mass</th>
<th>Relative at 1 MeV Power (m barn)</th>
<th>σ₂E at 1 MeV (barn)</th>
<th>σ₂H at 1 MeV (barn)</th>
<th>Melting Point (°C)</th>
<th>Boiling Point (°C)</th>
<th>Chemical Reactivity (air &amp; H₂O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb 207</td>
<td>1</td>
<td>6.001</td>
<td>6.4</td>
<td>327</td>
<td>1737</td>
<td>Inert</td>
<td></td>
</tr>
<tr>
<td>LBE 208</td>
<td>0.82</td>
<td>1.492</td>
<td>6.9</td>
<td>125</td>
<td>1970</td>
<td>Inert</td>
<td></td>
</tr>
<tr>
<td>Na 23</td>
<td>1.80</td>
<td>0.230</td>
<td>3.2</td>
<td>98</td>
<td>883</td>
<td>Reactive</td>
<td></td>
</tr>
<tr>
<td>H₂O 18</td>
<td>421</td>
<td>0.1056</td>
<td>3.5</td>
<td>0</td>
<td>100</td>
<td>Inert</td>
<td></td>
</tr>
<tr>
<td>D₂O 20</td>
<td>49</td>
<td>0.0002115</td>
<td>2.6</td>
<td>0</td>
<td>100</td>
<td>Inert</td>
<td></td>
</tr>
<tr>
<td>He 2</td>
<td>0.27</td>
<td>0.007953</td>
<td>3.7</td>
<td>-</td>
<td>-269</td>
<td>Inert</td>
<td></td>
</tr>
</tbody>
</table>
The pressure difference, $P$, generated in the primary coolant loop of a pool-type reactor is defined by Equation 2.1, where the elevation difference, $h$, is between the thermal center of the core and the heat exchanger (Abanades and Pena, 2009). The temperature difference, $\Delta T$, is between the hot and cold legs of the coolant circulation loop (Abanades and Pena, 2009):

$$\Delta P = \beta \cdot h \cdot g \cdot \Delta T.$$  

(2.1)

Lead-bismuth eutectic has a lower melting temperature than lead (397.7 K at 0.1 MPa) which lowers the operating range of the coolant (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007b). Despite the better operating range, lead is favored over lead-bismuth eutectic because of several drawbacks. Bismuth is rare, expensive, and has neutron activation issues (Carlin, 2012; International Atomic Energy Agency, 2002, 2003; Li, 2008; Loewen, 2005; Loewen and Bisanz, 2003). Furthermore, swelling of solid lead-bismuth eutectic is an issue (Wider et al., 2005; Zuccini et al., 2005; Agostini et al., 2004; Foletti et al., 2006). Also, lead-bismuth eutectic is more corrosive than lead, although oxygen control systems which maintain the oxygen content in lead-bismuth eutectic between $10^7$ and $10^{-6}$ at. pct. slow the corrosion process (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007b; Schullenberg et al., 2005; Gromov et al., 1998; Zhang, 2009; Gorynin et al., 1998). The issues associated with lead-bismuth eutectic have swayed the focus of this work toward modeling lead only.

2.3. Lead & LBE Cooled Reactors

In the early 1950’s, both the USSR and the US nearly simultaneously began to develop liquid metals as coolants for nuclear submarine power plants (Gromov et al., 1998). While the US developed a sodium cooled reactor for the USS Sea Wolf (SSN 575), the Soviets developed (starting in 1952) an LBE cooled LFR for the Alpha-class submarines (Gromov et al., 1998; Schullenberg et al., 2005; Todreas et al., 2004). The sodium cooled reactor in the Sea Wolf was eventually decommissioned and replaced with a pressurized water cooled reactor between 1958 and 1960 (Todreas et al., 2004). The Alpha-class submarines went on to demonstrate over eighty reactor years of LBE experience (Wider et al., 2005; Zrondonkov et al., 2008; Todreas et al., 2004). This experience was made public at a comprehensive conference in 1998 which sparked a global revival of interest in LBE technology (Wade, 2000).

More recently, LFRs have received renewed global interest as potential future commercial reactors (Spencer et al., 2000; Todreas et al., 2004). The literature reveals
several trends in the design of lead cooled reactors. LFR technology will make future commercial reactors modular, economic, safe, and proliferation resistant (Spencer et al., 2000). Modularity is achieved since fast flux cores can be made smaller than thermal reactors. Smaller sizes make LFRs economic through mass production. The strong reactivity feedback of a fast flux reactor gives most LFRs the ability to load follow autonomously, thus minimizing operator intervention and reducing accident scenarios. Furthermore, in the event of an accident, most LFRs are able to remove decay heat from the core via natural convection. Proliferation resistance is archived in LFR designs by designing cores to last the lifetime of the entire system thus eliminating the need to access the nuclear inventory of the core.

There are three main applications of lead coolants: lead cooled small modular reactors, accelerator driven systems, and high temperature reactors. Since there is considerable overlap in the research and development of these three applications, several research facilities are currently engaged in lead and LBE technological advancements. Phase change is mainly an issue for LFRs in remote locations and not for accelerator driven systems or high temperature reactors, thus LFRs are the focus of this literature review.

Table 2.2 provides a summary of the key characteristics of several LFRs. Because of the many parallels between lead and LBE coolants, both types of reactor designs are covered. The thermal and electric power rating, size, and lifetime of each reactor is included since the demand for SMRs is mainly attributed to these features.

Lead cooled SMRs are a novel approach to meeting the developing world’s growing energy demands. The realization that SMRs are greatly needed has led to the development of approximately sixty different SMR designs (Kuznetsov, 2008; International Atomic Energy Agency, 2006). Approximately thirty of these designs will operate without on-site refueling (Kuznetsov, 2008; International Atomic Energy Agency, 2005, 2006). Reactors in this category are designed to be mass produced in a factory and delivered via rail, ship, or, via semi truck. Mass production should bring the cost of nuclear power reactors down to competitive levels (Gen4 Energy, January 2010; Kuznetsov, 2008; Allen and Crawford, 2007; Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2002; International Atomic Energy Agency, 2003; Wade, 2000).

Reactors in the SMR class require long-life core designs to eliminate the need for refueling, fuel handling, and on-site fuel storage (Allen and Crawford, 2007). Long-life cores are beneficial from a non-proliferation standpoint because a developing country will not need access to enrichment or refueling technologies and will not accumulate large amounts of spent fuel (LaFuenteme and Piera, 2010; Halsey et al., 2005; International Atomic Energy Agency, 2002; Kuznetsov, 2008). One plan to serve the majority of the developing worlds needs calls
for centralized support facilities to be placed in locations controlled by the Italian National Agency for New Technologies, Energy and the Environment. Spent reactors would be shipped to these locations, or back to the factory of origin at the end of their lives (Dostal et al., 2008). Country users would not have access to the fissile material or enrichment technology which could be used in weapons proliferation (International Atomic Energy Agency, 2003).

Many SMR designs have eliminated the intermediate heat exchanger loop by placing steam generators or CO$_2$ heat exchangers directly in the reactor vessel, reducing the cost and size of the plant while increasing overall efficiency (Allen and Crawford, 2007; Cinotti et al., 2007). The high density of liquid metal coolant and provisions for an escape path for vapors prevent any bubbles caused by steam generator tube rupture from entering the reactor core (Sienicki and Spencer, 2002; Allen and Crawford, 2007; Loewen and Tokuhiko, 2003).

The LFR program has been transferred from the GEN IV LFR Working Group to the GNEP Reactor Campaign (Smith et al., 2008; Halsey et al., 2005; Sienicki and Petkov, 2002a; Tzanos et al., 2008). Before the US LFR program was refocused the Secure, Transportable, Autonomous Reactor (STAR) family of LFRs was developed (Smith et al., 2008; Allen and Crawford, 2007). The SSTAR can provide incremental energy generation to developing nations and remote communities without electrical grid connections (Smith et al., 2008;)

<table>
<thead>
<tr>
<th>Designation</th>
<th>Coolant Convection</th>
<th>Coolant Type</th>
<th>Power (MW$_{th}$)</th>
<th>Power (MW$_e$)</th>
<th>Size ($d \times h$) (m)</th>
<th>Lifetime (yr)</th>
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<tbody>
<tr>
<td>Small Modular Reactors</td>
<td></td>
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</tr>
<tr>
<td>SSTAR</td>
<td>Natural</td>
<td>Pb</td>
<td>45</td>
<td>20</td>
<td>3.2 x 12</td>
<td>15-30</td>
</tr>
<tr>
<td>STAR-LM</td>
<td>Natural</td>
<td>Pb</td>
<td>400</td>
<td>181</td>
<td>5.5 x 16.9</td>
<td>15-30</td>
</tr>
<tr>
<td>G4M</td>
<td>Forced</td>
<td>LBE</td>
<td>70</td>
<td>25</td>
<td>1.5 x 2.5</td>
<td>7-10</td>
</tr>
<tr>
<td>Alpha’s</td>
<td>Forced</td>
<td>LBE</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SVBR-75\100</td>
<td>Forced</td>
<td>LBE</td>
<td>280</td>
<td>101.5</td>
<td>4.53 x 6.92</td>
<td>~ 8</td>
</tr>
<tr>
<td>BREST-300</td>
<td>Forced</td>
<td>Pb</td>
<td>700</td>
<td>300</td>
<td>5.5 x 15</td>
<td>5</td>
</tr>
<tr>
<td>BREST-600</td>
<td>Forced</td>
<td>Pb</td>
<td>1400</td>
<td>600</td>
<td>6.2 x 17</td>
<td>5-6</td>
</tr>
<tr>
<td>ELSY &amp; ARR</td>
<td>Forced</td>
<td>LBE</td>
<td>1500</td>
<td>600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RTLHR</td>
<td>Forced</td>
<td>LBE</td>
<td>50</td>
<td>15</td>
<td>3 x 3.85</td>
<td>15</td>
</tr>
<tr>
<td>INEE/L/MIT</td>
<td>Forced</td>
<td>LBE</td>
<td></td>
<td>300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Accelerator Driven Systems</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>MYRRHA ADS</td>
<td>Forced</td>
<td>LBE</td>
<td></td>
<td>50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Italian XADS</td>
<td>Natural</td>
<td>LBE</td>
<td></td>
<td>80</td>
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<td></td>
</tr>
<tr>
<td>High Temperature Reactors</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>STAR-H2</td>
<td>Natural</td>
<td>Pb</td>
<td>400</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ULLFRD</td>
<td>Forced</td>
<td>LBE</td>
<td>200</td>
<td>core: 0.157$^2$</td>
<td>20</td>
<td></td>
</tr>
</tbody>
</table>
Figure 2.1. Cross-sectional view of the SSTAR’s thermal hydraulic system (Halsey et al., 2005).

Allen and Crawford, 2007). This design uses a very efficient (44 %) CO$_2$ Brayton cycle with in-vessel heat exchangers (Smith et al., 2008; Kuznetsov, 2008). Figure 2.1 is a basic thermal hydraulic schematic for the SSTAR (Halsey et al., 2005). Lead coolant entering the bottom of the reactor core is heated, thus decreasing in density. The lighter coolant rises through the chimney to the top of the vessel where it enters the in-core CO$_2$ heat exchangers and is cooled. Figure 2.1 also shows the decay heat removal system which will use naturally convecting air to cool the outside wall of the vessel (Sienicki and Petkov, 2002b).

Gen4 Energy (previously known as Hyperion Power) and Los Alamos National Laboratory designed an LBE cooled fast flux reactor called the Gen4 Module (G4M) which is significantly smaller than the SSTAR (Gen4 Energy, January 2010) (Figure 2.2). The biggest difference between the SSTAR and the G4M is that the SSTAR uses natural circulation in the primary coolant circuit, while the G4M will use forced convection (Gen4 Energy, January 2010). The uranium nitride (UN) core is intended to last the lifetime of the entire G4M (7 to 10 years) (Gen4 Energy, January 2010). Burying the reactor in a vault greatly restricts access to the fissile inventory in the core and protects the system from accidental and deliberate
Figure 2.2. The Gen4 Energy LBE cooled SMR. (Gen4 Energy, January 2010).

facility breaches (Gen4 Energy, January 2010). The G4M is able to load follow (Gen4 Energy, January 2010). As power demands increase over time additional units could be deployed incrementally increasing the power plants capacity (Gen4 Energy, January 2010).

Building on their experience with lead and LBE coolants, Russian engineers have designed several LFRs, although the funding has been cut (Wider et al., 2005). The SVBR75/100 modular reactor is currently the most advanced LBE cooled reactor (Wider et al., 2005). The SVBR-75/100 is designed to operate at 75-100 MW$_e$ depending on the power conversion parameters (Zrodnikov et al., 2008). Possible multi-purpose applications of this reactor include modular installations and autonomous power sources (Zrodnikov et al., 2008). This reactor is cheaper than a Light Water Reactor (LWR) and cheaper to run than a gas-fired plant (Wider et al., 2005). Figure 2.3 shows the basic elements of the SVBR design including the monoblock vessel design, the Control and Protection System (CPS), the Main Circulation Pumps (MCPs), the Steam Generators (SG), and the reactor core (Zrodnikov et al., 2008).

Research and Development Institute of Power Engineering and the Russian Research Center Kurchatov Institute developed the Russian BREST-300 and BREST-600 LFRs (International Atomic Energy Agency, 2002). The BREST reactors have an epithermal
Figure 2.3. SVBR monoblock reactor installation (Zrodnikov et al., 2008).

Figure 2.4. The lead-cooled BREST-300 (International Atomic Energy Agency, 2002).
neutron spectrum. The systems are intended to address safety, economics, proliferation resistance and waste disposal (Allen and Crawford, 2007). A diagram of the BREST-300 is shown in Figure 2.4. Both reactor variants use forced convection of lead in the primary loop to transfer heat to a supercritical steam loop (International Atomic Energy Agency, 2002).

The European Lead-cooled System (ELSY), shown in Figure 2.5, is a pool-type lead-cooled 600 MW$_e$ fast reactor (Cinotti et al., 2007). ELSY has been under development by the Sixth EURATOM Framework Programme since 2006 (Cinotti et al., 2007). ELSY will be used for transmutation of waste, central power generation, and irradiation testing of advanced fuels and structural materials (Tzanos et al., 2008).

The current focus of the United States LFR program is the Advanced Research Reactor (ARR) which incorporates features and operating conditions of the ELSY system (Tzanos et al., 2008). This effort is a collaboration between Argonne National Laboratory (ANL),
En te Nazionale per le Nuove Tecnologie (ENEA), and Del Fungo Giera Energia (DFGE) (Tzanos et al., 2008). This reactor is in the initial design stages and is very similar to ELSY (Tzanos et al., 2008).

Until recently Japan was researching LFR systems using LBE (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007b). One of the LFR designs is a Rail Transportable LBE cooled Reactor (RTL) which has been proposed by researchers at Tokyo Institute of Technology (TIT) (Dostal et al., 2008). This reactor was designed to be modular to keep the target country form having to deal with spent fuel (Dostal et al., 2008). Rapid development using existing technology, rather than optimized design was the focus of this concept (Dostal et al., 2008).

The Idaho National Laboratory (INL) and the Massachusetts Institute of Technology (MIT) have proposed three LBE cooled, 300 MW, actinide burning reactor systems (Allen and Crawford, 2007). The Actinide Burning Reactor (ABR) is a fertile-free actinide burner for incineration of transuranics from Light Water Reactors (LWRs) (Allen and Crawford, 2007). The fertile free Minor Actinide-Burning Reactor (MABR) works in tandem with LWRs or gas-cooled thermal reactors and is intended to burn minor actinides (Allen and Crawford, 2007). The Actinide-Burning Reactor with Thorium (ABR T) is aimed at reducing electricity generation costs by increasing the time between refueling intervals (Allen and Crawford, 2007). All three systems operate at identical power ratings and use a CO$_2$ Brayton cycle as the secondary system (Allen and Crawford, 2007). Rail transportability is possible with these designs (Allen and Crawford, 2007). Actinide burning incinerates long-lived fission products by transmutation, thus decreasing the amount and half life of high level waste to be placed in long term geological repositories (Abderrahim and D'Hondt, 2007; Foletti et al., 2006).

2.4. Natural Convection Coupled with Phase Change in Liquid Metals

The role that natural convection plays in the solidification and melting of metals is important in many metallurgical processes, and has been the focus of many studies. Both laminar and turbulent natural convection must be considered to fully understand the possibilities encountered in the study of naturally convecting liquid metals in the presence of a melting or freezing front. Early numerical models of the Stephan problem (also known as the moving boundary problem) ignored natural convection and assumed that conduction was the main heat transfer mechanism (Zalba et al., 2003). This assumption was later proven to be inaccurate (Zalba et al., 2003). The literature describes many fundamentally different numerical approaches for the analysis of solid-liquid interaction in the presence of natural
convection (Zalba et al., 2003). The following subsections summarize the main contributors to this field of study as it pertains to the numerical modeling of two-phase liquid metals.

### 2.4.1. Laminar Natural Convection

Natural convection in a finite vessel with a vertical temperature gradient was first considered by Benard in 1900 and is known as Benard convection (Benard, 1900; Chiesa and Guthrie, 1971). Benard found that there was a critical temperature gradient marking the onset of natural convection and that the initial flow had a steady cellular character (Benard, 1900; Chiesa and Guthrie, 1971). The theoretical explanation of natural convection was first described by Rayleigh who obtained the well-known dimensionless Rayleigh Number (Rayleigh, 1916; Chiesa and Guthrie, 1971). Separation of variables found an exact solution to the system of linearized equations of motion describing natural convection (Pellew and Southwell, 1940). This analysis led to a critical Rayleigh Number (Ra=1708) below which there is only the trivial solution to the problem: fluid at rest (Pellew and Southwell, 1940; Chiesa and Guthrie, 1971). Liang et al. (1969) numerically studied the wall effects introduced by finite sized vessels and found two solutions for laminar fluid flow in a cylindrical container with a height to diameter ratio of about one. One solution corresponds to fluid flowing up the axis of the cylinder; the other solution corresponds to fluid flowing downward along the axis (Liang et al., 1969; Chiesa and Guthrie, 1971).

### 2.4.2. Turbulent Natural Convection

Several researchers have studied turbulent natural convection in liquid mercury and saw no wall effects (Globe and Dropkin, 1959; Catton and Edwards, 1967; Chiesa and Guthrie, 1971). Catton and Edwards (1967) studied a wide range of cell aspect ratios and demonstrated significant wall effects; however, they used high Prandtl Number fluids which do not include typical liquid metals. Chiesa and Guthrie (1971) demonstrated that the aspect ratio does play a significant role in turbulent naturally convecting liquid metal systems and that turbulent convection tends to prevail over laminar convection.

Equation 2.2 relates the Rayleigh number to the Nusselt number empirically for a given height to diameter ratio \((h/d)\) and is valid over the range \(0 \leq h/d \leq 1.5\) and \(2 \cdot 10^4 \leq Ra \leq 1 \cdot 10^7\) (Chiesa and Guthrie, 1971):

\[
Nu_{emp} = 0.78(0.68)^{h/d}Ra^{1/3}.
\]  
(2.2)

On the smallest scales, local properties of a turbulent flow field fluctuate rapidly; while
on larger scales, properties are more constant in time (COMSOL, 2012). The Reynolds number (given by Equation 2.3) is a dimensionless number indicating the likelihood that the turbulent regime has been entered into (COMSOL, 2012). As the Reynolds number increases, fluid flow tends to become more turbulent (COMSOL, 2012):

\[ Re = \frac{\rho ul}{\nu}. \]  

(2.3)

Naturally convecting liquid transitions from laminar flow to turbulent flow as the temperature gradient is increased, thus increasing the velocity of the convecting liquid. Turbulent flow can be simulated with the Navier-Stokes equations (Equation 2.4), but requires a large number of mesh elements to capture all the scales in the flow (COMSOL, 2012):

\[
\rho \frac{\partial u}{\partial t} + \rho (u \cdot \nabla) u = \nabla \cdot (-P \mathbf{I} + \nu (\nabla u + (\nabla u)^T)) + \mathbf{F}, \\
\rho \nabla \cdot \mathbf{u} = 0.
\]  

(2.4)

Furthermore, all quantities fluctuate in time and space for turbulent flow, resulting in extreme computational costs (COMSOL, 2012). Equation 2.4 assumes that the flow is incompressible and Newtonian (COMSOL, 2012). To deal with the high computational cost of modeling Equation 2.4 numerically, an alternative approach is applied which divides the flow into large resolved scales and small unresolved scales which can be modeled with a turbulence model (COMSOL, 2012). This significantly reduces the computational cost of resolving all the scales present in the model (COMSOL, 2012). Dividing each quantity into an averaged part and a fluctuating part and then averaging the values leads to the Reynolds-Averaged Navier-Stokes (RANS) equations (Equation 2.5) (COMSOL, 2012):

\[
\rho \frac{\partial \mathbf{U}}{\partial t} + \rho (\mathbf{U} \cdot \nabla) \mathbf{U} + \rho (\mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (-p \mathbf{I} + \nu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) + \mathbf{F}, \\
\rho \nabla \cdot \mathbf{u} = 0.
\]  

(2.5)

2.4.3. Numerical Solution for Conduction Only

Zalba et al. (2003) provides an in-depth summary of numerical heat transfer techniques used to simulate phase change materials. Solving moving boundary problems is complicated due to the fact that the solid/liquid boundary moves depending on the rate of latent heat released or absorbed at the boundary (Zalba et al., 2003).

Pure conduction was considered before convection was included in the solution.
techniques. The first one dimensional numerical solution to the moving boundary problem was published by London and Seban in 1943 (Zalba et al., 2003; London and Seban, 1943). Shamsundar and Srinivasan (1978) showed that London and Seban’s approach led to increased errors as the solidification process progressed, and a two-dimensional formulation was more appropriate (Zalba et al., 2003; Shamsundar and Srinivasan, 1978).

Lazaridis (1970) developed a numerical solution of the multidimensional solidification (or melting) problem which solved the pertinent heat transfer equations and found the temperature distribution throughout the phase change material (Lazaridis, 1970; Zalba et al., 2003). Shamsundar and Sparrow (1975) laid the foundation for the analysis of multidimensional conduction phase change via the enthalpy model (Shamsundar and Sparrow, 1975; Zalba et al., 2003). Shamsundar and Sparrow’s finite difference method is valid for pure substances having a single melting temperature and for alloys having a temperature transition zone (Shamsundar and Sparrow, 1975; Zalba et al., 2003). Shamsundar and Sparrow extended their work to include the effects of density change and they concluded that the rate of heat transfer and the Biot number is linked with the convection in the liquid region (Shamsundar and Sparrow, 1976; Zalba et al., 2003).

The finite difference method allowed Goodling to solve the moving boundary problem for outward solidification from a cylinder in one dimension (Goodling and Khader, 1975; Zalba et al., 2003). Shamsundar and Srinivasan proposed a two-dimensional method of solving solidification around a cylinder which had an axial term, thus approaching a three-dimensional solution (Shamsundar and Srinivasan, 1980; Zalba et al., 2003). Sparrow and Hsu confirmed the influence of the axial term on the outside of a cylinder carrying coolant. He then developed an analytical solution which uses a coordinate transformation to immobilize the transition boundary (Sparrow and Hsu, 1981; Zalba et al., 2003). Shamsundar continued previous works and developed analytical solutions which are solved using Sparrow’s boundary immobilization technique (Shamsundar, 1982; Sparrow and Hsu, 1981; Zalba et al., 2003).

Achard et al. compared a purely convective finite difference enthalpy method with experimental data and found significant discrepancies thus deducing that it is necessary to consider natural convection (Achard et al., 1983; Zalba et al., 2003). The enthalpy method was shown to be the most suitable moving boundary method (Hunter and Kuttler, 1989; Zalba et al., 2003).
2.4.4. Phase Change with Natural Convection

Szekely and Chhabra (1970) considered the solid-liquid interface of pure lead subject to natural convection driven by a horizontal temperature gradient. The steady-state experimental analysis concluded that the location of the solid-liquid interface could be accurately predicted using Ostrach’s analysis of laminar natural convection from a surface immersed in an infinite medium, by which Eckert’s correlation (Equation 2.6) is derived (Ostrach, 1952; Eckert and Carlson, 1961; Szekely and Chhabra, 1970):

\[ X(y) = \frac{\lambda_s y(T_m - T_c)}{0.508Gr^{1/4}Pr^{1/2} (0.952 + Pr)^{1/4} \lambda_l (T_b - T_m)}. \] (2.6)

Analyzing the time it took the system to transition between two steady states allowed the prediction of the rate of movement of the solid-liquid interface with the appropriate transient conduction equation and empirical heat transfer coefficients (Szekely and Chhabra, 1970; Chiesa and Guthrie, 1974).

Chiesa and Guthrie (1974) extended their Benard convection study to include melting and solidification of both pure metals and alloys. These experiments considered a vertical cylindrical vessel with heating from the bottom and cooling from the top (Chiesa and Guthrie, 1974). The work includes the effect of interface morphology on heat transfer rates caused by dendrite formation at the solid-liquid interface for lead-tin alloys (Chiesa and Guthrie, 1974). The numerical solution found predicts the freezing rates and interface location, batch cooling curves at any location in the solid, temperature profiles in the solid, and transition times for when the pure conduction regime is entered and \( Nu = 1 \) (Chiesa and Guthrie, 1974). Chiesa and Guthrie (1974) also demonstrated that the rate of freezing (or melting) affects the measured Nusselt number. The deviation from the steady state Nusselt number is accounted for with a correction factor applied to Equation 2.2:

\[ Nu = CF * Nu_{emp} = e^{(-7.2 \frac{h_R}{\alpha Nu})} * Nu_{emp}. \] (2.7)

Equation 2.7 implies that as the rate of freezing (or melting) is increased, the steady state Nusselt number under predicts the measured Nusselt number. Experiments including convection in paraffin were published by Sparrow et al. and Bathelt et al. (Sparrow et al., 1978; Bathelt et al., 1979; Zalba et al., 2003). These experiments used imaging techniques and temperature probes to demonstrate that natural convection plays a significant role in the melting process. Another method for the inclusion of convection in simulations is to use an
effective thermal conductivity which accounts for the increased rate of heat transfer caused by convection with a higher thermal conductivity in the liquid region (Farid and Husian, 1990; Farid et al., 1998; Rieger et al., 1983; Zalba et al., 2003).

Methods for solving the moving boundary problem can be classified by two methods: fixed grid methods based on enthalpy, and moving grid methods utilizing interface immobilization techniques (Ismail and Stuginsky, 1999; Zalba et al., 2003). Literature provides information on several specific classifications of these techniques (Ozisik, 1993; Ismail and Stuginsky, 1999; Zalba et al., 2003). Furzerland concluded that, in general, enthalpy methods are better suited for numerical studies of phase change materials (Furzerland, 1980; Zalba et al., 2003). Ozisik classifies the numerical solutions with both conduction and convection in the following way (Ozisik, 1993):

1. Exact solutions, limited to a few idealized situations,
2. integral methods,
3. heat moving source methods,
4. perturbation methods,
5. electrical analogies,
6. finite differences methods, and
7. finite elements methods.

Ultimately, the choice of which method to use depends on the context of the problem and the preference of the investigator (Voller et al., 1990). Finite element analysis is used in this work since COMSOL Multiphysics is designed to solve coupled systems of equations which are inherent in modeling the melting front under the influence of natural convection. Furthermore, finite element analysis is better suited to handle complex boundaries than finite difference methods (Dalhuijesn and Segal, 1986). The Effective Heat Capacity (EHC) method (also known as the enhanced or apparent heat capacity method) is a popular choice used to solve fixed grid phase change problems since it is implemented in existing numerical heat transfer codes with simple modifications (Voller et al., 1990). Voller et. al. (1990) provide the derivation of the EHC method from first principles and compares the EHC method to other fixed grid methods (Voller et al., 1990).

In the following Chapter the EHC method is coupled with natural convection in COMSOL. A step function in the dynamic viscosity makes it possible to define the entire system with a single pseudo-material. The resulting model is then used to simulate
experiments performed by Szekely and Chhabra. Two sets of pseudo-steady-state data and one set of transient data are simulated with the model to demonstrate its validity.
CHAPTER 3
MODEL DEVELOPMENT AND VALIDATION

Modeling the phase change of lead under the influence of natural convection for horizontal heat flux is accomplished in COMSOL multiphysics with the Effective Heat Capacity (EHC) method and finite element analysis (Voller et al., 1990). This modeling approach uses a pseudo material with an increased heat capacity near the melting temperature that simulates the latent heat of fusion. The pseudo material is discussed in Section 3.1. The complete description of the validation experiment is given in Section 3.2. In Section 3.3, the non-isothermal laminar flow physics module is used to construct a representative COMSOL model of the experiments performed by Szekely and Chhabra (Section 2.4.4.). Section 3.4. presents the method for comparing the COMSOL model to experimental and theoretical data. Finally, in Section 3.5., the numerical model is validated with two sets of experimental data.

3.1. Pseudo-material Thermophysical Definitions

The Working Party on Scientific Issues of the Fuel Cycle (WPFC), established under the protection of the Nuclear Science Committee (NSC) of the Nuclear Energy Agency (NEA) created the Working Group on Lead-bismuth Eutectic (WG-LBE) in 2002 (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007b). The WG-LBE released a state-of-the-art handbook on lead, bismuth, and LBE which is a critical review of existing data and discrepancies. The thermophysical property definitions for lead and LBE used in the present models are given in Appendix A.

Hot and cold temperatures in the experiments performed by Szekely and Chhabra were not reported to have varied more than 30 K from each other (Szekely and Chhabra, 1970). The thermophysical properties of lead do not vary significantly over a 30 K range except for discontinuities at the melting temperature, thus they are defined as constant in the present models (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007b). This assumption reduces the computational requirements greatly (COMSOL, 2012). Table 3.1 gives the values for the material properties used in the models.

The EHC method is applied as a pseudo material which includes the discontinuities in the material properties at the phase transition. The entire region of lead in the model is defined as a liquid that has the pseudo material definitions defined below. COMSOL is ‘tricked’ into treating the liquid like a solid when it is below the melting temperature by defining the dynamic viscosity as a step function. The step function for the dynamic
viscosity is defined by Equation 3.1, and is shown graphically in Figure 3.1:

\[ \nu(T) = \begin{cases} 10^7, & T < T_m \\ \nu_l, & T > T_m \end{cases} \tag{3.1} \]

The EHC method simulates the latent heat of melting with a temperature dependent heat capacity that has a transition zone near the melting temperature (Voller et al., 1990).

Table 3.1. Constant values chosen for material properties of the numerical model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Solid</th>
<th>Liquid</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho )</td>
<td>11,340</td>
<td>10,650</td>
<td>kg m(^{-1})</td>
</tr>
<tr>
<td>( C_p )</td>
<td>0.125</td>
<td>0.161</td>
<td>kJ kg(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>34.6</td>
<td>16.3</td>
<td>W m(^{-1}) K(^{-1})</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>24.3</td>
<td>9.5</td>
<td>mm(^2) s(^{-1})</td>
</tr>
<tr>
<td>( T_m )</td>
<td>600.3</td>
<td>-</td>
<td>K</td>
</tr>
<tr>
<td>( Q_m )</td>
<td>23.34</td>
<td>-</td>
<td>kJ kg(^{-1})</td>
</tr>
<tr>
<td>( \nu )</td>
<td>-</td>
<td>0.00241</td>
<td>N s m(^{-2})</td>
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<tr>
<td>( \beta )</td>
<td>-</td>
<td>-1.14 \times 10^{-4}</td>
<td>K(^{-1})</td>
</tr>
<tr>
<td>( Pr )</td>
<td>-</td>
<td>0.0239</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 3.1. Pseudo material dynamic viscosity as a function of temperature.
In this model a step function with a width of $dT_{C_p}$ is used to define this zone. This high heat capacity region essentially takes a phenomena that occurs explicitly at the melting temperature of pure substances and spreads it out enough that it can be modeled numerically. By defining the magnitude of the modified heat capacity zone as the latent heat of melting divided by the temperature width of the modified heat capacity zone the region absorbs the same amount of heat as the latent heat does during phase transition (Voller et al., 1990). As the transition zone width is decreased a narrow spike in the heat capacity forms which can lead to erroneous solutions as the effects of the latent heat of melting begin to skip node points (Voller et al., 1990). It is demonstrated in subsequent sections that the heat capacity step cannot occur at the same location as the dynamic viscosity step. An additional temperature step separates these two interfaces ($dT_\nu$). The magnitude of the modified heat capacity region is defined as $Q_m/dT_{C_p}$ to assure that the latent heat of melting is accurately accounted for. Thus, the modified heat capacity is defined by equation 3.2, and is shown graphically in Figure 3.2:

$$C_p(T) = \begin{cases} 
C_{p,s}, & T < T_m - dT_{C_p} - dT_\nu \\
C_{p,s} + Q_m/dT_{C_p}, & T_m - dT_{C_p} - dT_\nu < T < T_m - dT_\nu \\
C_{p,l}, & T_m - dT_\nu < T
\end{cases}.$$ (3.2)

The difference between the thermal conductivity of the liquid and solid is also defined

![Figure 3.2. Pseudo material heat capacity as a function of temperature.](image-url)
with a temperature dependent step function as defined by Equation 3.3, and is shown graphically in Figure 3.3:

\[
\lambda(T) = \begin{cases} 
\lambda_s, & T < T_m \\
\lambda_l, & T > T_m 
\end{cases} \tag{3.3}
\]

The value of the density does not effect the behavior of the solid so the density of the entire lead region is defined as that of liquid lead near its melting temperature. The temperature dependent liquid lead function from Appendix A is used to simulate natural convection. Natural convection is driven by temperature dependent density gradients in the presence of a gravitational field, thus convection is included in the model as a volumetric force proportional to the product of the temperature dependent density and the acceleration of gravity, Equation 3.4:

\[
F_y(T) = -g \ast \rho(T). \tag{3.4}
\]

The volumetric force is applied to the entire two-phase lead region.

Figure 3.3. Pseudo material thermal conductivity as a function of temperature.
3.2. Description of the Validation Experiments

Validation of the modeling approach is accomplished by comparing results from the numerical model with experimental and theoretical data from Szekely and Chhabra’s work in which they studied the location of the melting front of pure lead under pseudo-steady state and transient conditions (Szekely and Chhabra, 1970).

The apparatus used by Szekely and Chhabra consisted of a furnace with the outside dimensions of 12 inches by 12 inches by 3.5 inches deep (Szekely and Chhabra, 1970). The furnace contained partially solidified lead (Figure 3.4). The furnace walls were 1/8 inch thick stainless steel coated on the outside with an 1/8 inch of copper (Szekely and Chhabra, 1970). The copper coating unified the wall temperatures since it has a high thermal conductivity (Szekely and Chhabra, 1970). The hot wall of the furnace was heated with eight Chromalox strip elements and the cold wall was cooled with a blower (Szekely and Chhabra, 1970). All remaining surfaces were insulated (Szekely and Chhabra, 1970). Hot and cold wall temperatures were measured with five thermocouples per side, and the temperature field in the lead was measured by twenty four 1/8 inch calibrated chromel-alumel thermocouples (Szekely and Chhabra, 1970).

The lead was melted by applying heat to the hot wall with the Chromalox strip elements while the cold wall was insulated. Once the lead was completely melted the insulation was removed from the cold wall and the blower was turned on. The liquid-phase lead circulated by

Figure 3.4. Experimental apparatus used to study solid-liquid interface for lead under horizontal heat flux (based on Szekely and Chhabra 1970).
natural convection, and a freezing front formed on the cold wall and progressed into the liquid region. The resulting temperature field in the lead was measured by thermocouples at various locations throughout the apparatus. The lead was considered to be in pseudo-steady-state when the thermocouples inside the lead reported constant temperatures for at least thirty minutes.

There are two complete sets of pseudo-steady-state data in Szekely and Chhabra’s paper. Figures 3.5 and 3.6 show this data presented in two different ways. Figure 3.5a shows the location of the temperature probes, probe designations, recorded temperatures, extrapolated melting front and theoretical melting front for the first set of data. Figure 3.5b shows the horizontal temperature profiles at various heights through the apparatus for the same set of data. Szekely and Chhabra did not report experimental uncertainty in their data.

Figure 3.6a shows the location of the temperature probes, probe designations, recorded temperatures, extrapolated melting front and theoretical melting front for the second set of data. Figure 3.6b shows the horizontal temperature profiles at various heights through the apparatus for the second set of data used to validate the numerical model (derived from Szekely and Chhabra 1970).

(a) Probe locations and temperature field

Figure 3.5. First set of experimental data used to validate the numerical model (derived from Szekely and Chhabra 1970).
Szekely and Chhabra also studied the melting front location during the transition from one pseudo-steady-state to another pseudo-steady-state (Szekely and Chhabra, 1970). The experimental apparatus was allowed to reach pseudo-steady-state. Next, the cold wall temperature was decreased and held at a lower temperature (Szekely and Chhabra, 1970). The growth of the melting front into the liquid was shown to lag behind the applied cold wall temperature (Szekely and Chhabra, 1970). Three experimental studies are presented in Szekely and Chhabra’s work. Szekely and Chhabra did not report which set of temperature probes was used to extrapolate the melting front location (Szekely and Chhabra, 1970). Also, Szekely and Chhabra did not use the boundary conditions from the two pseudo-steady-state sets of data. The boundary conditions were chosen to have a relatively thin solid region for the first pseudo-steady-state, and a relatively thick solid region for the second pseudo-steady-state. Figure 3.7 shows the applied cold wall temperature and the resulting melting front location for a transient experimental run transitioning between two pseudo-steady-states (based on Szekely and Chhabra, 1970).
Figure 3.7. The experimental melting front location as the system transitions from one pseudo-steady-state to another.

3.3. Representative COMSOL Model

A two-dimensional representation of the mid-plane of the experiment is assumed to be valid in this case since the vessel is much wider than it is thick (COMSOL, 2012). The non-isothermal laminar flow physics module in COMSOL allows for the implementation of heat transfer between fluids and solids (COMSOL, 2012). This module provides the necessary tools to define all the parameters required to accurately reconstruct the validation experiment (COMSOL, 2012). Specifically, it is used to define and implement the pseudo-material definition for the two phase lead (Figure 3.8a). Also, it is used to define the solid regions, thermally insulated boundaries, walls, initial conditions, the volumetric buoyancy force, pressure constraints, and non adiabatic boundaries (Figure 3.8a and 3.8b).

COMSOL uses finite element analysis to solve the system of equations implemented by the physics module. A free-triangular mesh is generated by COMSOL. The mesh refinement is one of the key modeling parameters. The effect that mesh resolution has on the results is explored in Section 4.1.

A uniform temperature is applied to the cold wall of the furnace, and a uniform heat flux is applied to the hot wall. The top and bottom boundaries are adiabatic. Since the
fluid flow is assumed to be laminar a no-slip fluid flow condition is applied at the walls. The initial temperature field for the model varies linearly in the $x$ direction between the hot wall the cold wall. All of the models are run for 2000 seconds to assure that pseudo-steady-state conditions have been reached. The applied boundary conditions and material definitions are shown in Figure 3.8.

Figure 3.9a shows the initial temperature field, and Figures 3.9b-3.9d illustrate the progression of the freeze front as the model approaches pseudo-stead-state for a typical run. The fluid behaves in a cellular manner as eddies form and merge. As this happens the

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Figure 3.8. Material assignments and boundary conditions for the two dimensional representative COMSOL model.
Figure 3.9. Progression of the COMSOL model from the initial state to a pseudo-steady-state.
convecting liquid alters the shape and position of the melting front by increasing the local heat transfer rates. White arrows show the relative velocity in these plots, and the black contour lines mark the pseudo-material discontinuities. The right contour line shows the melting front where the viscosity is increased. Between the center and right contour lines is the $dT_v$ zone. The region between the left and center contour lines shows the high heat capacity $dT_{C_p}$ zone.

To compare the experimental and numerical results, temperature probes in the model are used to extract the temperature at the locations of the experimental thermocouples. Temperature probes located in the fluid tend to oscillate as eddies form and merge, therefore the average of the last 500 seconds of every run provides a better validation value. Each run reached pseudo-steady-state at around 1500 seconds. Temperature fluctuations after 1500 seconds are seen; however, they are mainly due to eddies in the fluid flow and do not alter the melting front significantly.

### 3.4. Validation Methodology

This Section develops four metrics to compare how well the numerical model is reproducing Szekely and Chhabra’s experimental results (Szekely and Chhabra, 1970). These metrics are based on the square Root of the Sum of the Squares (RSS). The RSS method is used to compare the entire temperature field (Total Temperature RSS), the temperature near the cold wall (Cold Wall RSS), and the location of the melting front (Melting Front RSS). These three metrics are averaged resulting in the Average RSS metric.

The Total Temperature RSS is computed by Equation 3.5 across all of the available temperature probe data:

$$
\delta T = \sqrt{\frac{\Sigma (T_{\exp} - \bar{T}_{\num})^2}{N - 1}}.
$$

Using the RSS error formula in this way indicates that the numerical model is approaching the experimental results as the error value goes to zero. Essentially, Equation 3.5 is the square root of the sum of the squares of the difference between the experimental value and the numerical, time averaged, value. The $(N - 1)$ term normalizes the expression by the number of probe locations making it possible to compare the error from data sets where different numbers of probes are considered.

Much better results are obtained by ignoring the three probes nearest the hot wall. The justification for ignoring these three temperature probes is that the reported temperatures
in Figure 3.5a were not given numerically in Szekely and Chhabra’s work; they were only available graphically in (Figure 3.5b). The values presented in Figure 3.5a were extracted from Figure 3.5b using graphical analysis software. Additionally, in all of the numerical models, the increase in the horizontal temperature profiles near the hot wall is less sharp then reported in the experimental results. It seems reasonable to assume that there was an error in the experimental measurement of the hot wall temperatures. Furthermore, Szekely and Chhabra omitted these three values in the figures that form the basis for Figures 3.6a and 3.6b. The calculation of the Total Temperature RSS without these three values will be referred to as the Modified Total Temperature RSS in this work. The Modified Total Temperature RSS will be used for the first set of data, and the Total Temperature RSS will be used for the second set of data.

Another way to analyze how well the numerical model can simulate experimental results is to evaluate the location of the melting front. The Melting Front RSS is found by linear extrapolation of the horizontal temperature profiles measured by the thermocouples in the solid region out to the melting temperature. The assumption that the temperature profile is linear in the solid is valid as long as the heat flux is predominately horizontal and no heat is being generated in the material. Temperature probes in the solid region of the numerical model are used to extrapolate where the melting front would be located if the experimental probes were reading the same values. Equation 3.5 expressed in terms of position leads to Equation 3.6:

$$\delta X = \sqrt{\frac{\sum(X_{\text{exp}} - X_{\text{num}})^2}{N - 1}}.$$  \hspace{1cm} (3.6)

Equation 3.6 compares the extrapolated melting front location from the model with the experiment. The true melting front location can be extracted from the numerical data; however, the experimental procedure was limited to extrapolation of the melting front from the probe locations. For consistency the numerically extrapolated melting front will be compared to the experimentally extrapolated melting front.

In some of the numerical models, cases were encountered where two probes were not available in the solid region from which to extrapolate the location of the melting front. In these cases, the melting front error for that particular point is not included in the total melting front error estimation.

Although Szekely and Chhabra measured the cold wall temperature to verify that it was uniform they did not report the cold wall temperature. Consequently, the four temperature probes nearest the cold wall are used as the Cold Wall RSS metric. Equation 3.5 is used
to find the combined error of these four temperature probes. This metric is more sensitive to the cold wall temperature than it is to the other heat transfer mechanisms in the model. Non-zero values for the cold wall error estimation indicates that the cold wall temperature needs to be adjusted. This error estimator allows the cold wall temperature in the model to be set to match the experimental results.

Both the Cold Wall RSS and the Melting Front RSS metrics are extracted from localized regions of the model; therefore, boundary condition cases exist which result in small RSS values for these localized metrics that may not agree with the other metrics or the experimental data. Combining all the metrics into an Average RSS metric provides a tool which indicates the model’s overall consistency with the experimental data. Units are ignored in the calculation of the Average RSS since it brings together metrics based on temperature with the Melting Front RSS metric which is based on distance.

3.5. Pseudo-Steady-State Model Validation Results

The first step in validating the model was to find the thermal boundary conditions and loads that best reproduce the experimental conditions. A parametric sweep of the hot wall heat flux determined the most likely experimental range to within a few thousand W/m$^2$. The hot wall heat flux was varied from 5000 W/m$^2$ to 20000 W/m$^2$ in increments of 1000 W/m$^2$. The cold wall temperature was initially set to 590.5 K; subsequent runs of the model indicated that this was a reasonable value. The first transition zone ($dT_v$) was arbitrarily set to 1 K. The second transition zone ($dT_{cp}$) was set to 0.6 K. The COMSOL mesh resolution was set to Extra Fine with a maximum element size of $1.24 \times 10^{-3}$ m$^2$.

Figures 3.10-3.12 show the Modified Total Temperature RSS, the Cold Wall RSS, the Melting Front RSS, and the Average RSS respectively for incremental heat additions to the hot wall. In Figure 3.10 there is a minimum in the Modified Total Temperature RSS at 12000 W/m$^2$, and a minimum in the Cold Wall RSS at 11000 W/m$^2$. The minimum in the Melting Front RSS (Figure 3.11) also occurs near 11000 W/m$^2$ indicating that the experimental hot wall heat flux was likely in the range of 10000-13000 W/m$^2$ for the first set of experimental data. The minimum Average RSS value of 0.586 occurs when the hot wall heat flux is 12000 W/m$^2$. The minimum Average RSS roughly agrees with the Modified Total Temperature RSS and the Cold Wall RSS.

Since the numerical model is sensitive to both the hot wall heat flux and the cold wall temperature, a two parameter parametric sweep of the cold wall temperature and the heat flux refined the boundary conditions of the experiment. The hot wall heat flux varied from
Figure 3.10. The Modified Total Temperature RSS and the Cold Wall RSS versus hot wall heat flux for the first set of data.

Figure 3.11. The Melting Front RSS versus the hot wall heat flux for the first set of data.
Figure 3.12. The Average RSS versus hot wall heat flux for the first set of data.

8500 W/m\(^2\) to 14500 W/m\(^2\) in increments of 1000 W/m\(^2\). The cold wall temperature varied from 588.5 K to 591.5 K in increments of 0.5 K. Some combinations of the two parameters were omitted to reduce computational time (approximately 11 hours per case). The goal of the following study was to identify minimums to find the relationship between the two parameters. Once a relationship was found, the best case boundary conditions were extracted and used as the control variables in subsequent studies.

Figures 3.13-3.16 show the Modified Total Temperature RSS, the Cold Wall RSS, the Melting Front RSS, and the Average RSS versus the cold wall temperature, respectively, for various hot wall heat flux values. The minimum Modified Total Temperature RSS of 1.06 K occurs when the hot wall heat flux is 13500 W/m\(^2\) and the cold wall temperature is 589.5 K. The minimum Cold Wall RSS value of 0.236 K occurs when the hot wall heat flux is 10500 W/m\(^2\) and the cold wall temperature is 590.5 K. The minimum Melting Front RSS value of 0.313 occurs when the hot wall heat flux is 12500 W/m\(^2\) and the cold wall temperature is 589.5 K. The minimum Average RSS value of 0.625 occurs when the hot wall heat flux is 11500 W/m\(^2\) and the cold wall temperature is 590.5 K. There are several boundary condition cases where the Melting Front RSS and the Cold Wall RSS reach local minimums, but the Average RSS indicates that these cases are deviating from the experimental boundary.
Figure 3.13. The Modified Total Temperature RSS versus cold wall temperatures for a range of inlet heat fluxes.

Figure 3.14. The Cold Wall RSS versus cold wall temperatures for a range of inlet heat fluxes.
Figure 3.15. The Melting Front RSS versus cold wall temperatures for a range of inlet heat fluxes.

Figure 3.16. The Average RSS versus cold wall temperatures for the a range of inlet heat fluxes.
conditions.

Figure 3.17 shows the Average RSS versus hot wall heat flux for the parametric sweep of the boundary conditions. Transposing the data in this way shows that the model's boundary condition parameter space is sufficiently explored. Additional data points in the cold wall temperature series for $T_c = 590.5$ K are included from the initial hot wall heat flux parameter sweep. The minimum Average RSS of 0.586 occurs when the hot wall heat flux is 12000 W/m$^2$ and the cold wall temperature is 590.5 K.

Figures 3.18 and 3.19 show the minimum Average RSS values from Figures 3.16 and 3.17 respectively. A least squares regression is used to fit a third order polynomial function to this data with an $R^2$ value of 0.99 for both data sets. The polynomial function in Figure 3.18 describes how the model's Average RSS is effected by the hot wall heat flux, and the polynomial function in Figure 3.19 describes how the model's Average RSS is effected by the cold wall temperature. Setting the first derivatives of these polynomial functions equal to zero finds the best case boundary conditions of 11180 W/m$^2$ for the hot wall heat flux, and 590.4 K for the cold wall temperature.

Running the simulation with the best case boundary conditions for the first set of data results in a modified total temperature RSS of 1.08 K, a Cold Wall RSS of 0.252 K, a Melting
**Figure 3.18.** The minimum Average RSS points form each hot wall heat flux series versus cold wall temperature.

\[ y = -5.96 \times 10^{-12} x^3 + 2.46 \times 10^{-7} x^2 - 3.27 \times 10^{-3} x + 1.48 \times 10^1 \]

\[ R^2 = 9.91 \times 10^{-1} \]

**Figure 3.19.** The minimum Average RSS points from each cold wall temperature series versus hot wall heat flux.

\[ y = 2.61 \times 10^{-2} x^3 - 4.61 \times 10^1 x^2 + 2.71 \times 10^4 x - 5.30 \times 10^6 \]

\[ R^2 = 9.89 \times 10^{-1} \]
Front RSS of 0.364 cm, and an Average RSS of 0.565. The Average RSS is lower than the polynomial fit predicts indicating that the numerical model is in excellent agreement with the first set of experimental data. The temperature field of the validation model is shown in Figure 3.20a after a 2000 second run. Figure 3.20b shows the velocity field for the same conditions.

Figure 3.20. Temperature field and velocity field with the EHC transition zone contours for the conditions derived for the first validation case.
model.

The time averaged temperature probe readings for the last 500 seconds of the best case numerical model is compared to the horizontal temperature profiles of the first set of experimental data in Figure 3.21. Figure 3.21 shows very good agreement in the solid region and tends to have lower temperatures in the liquid region. Lower liquid temperatures may be an indication that the implementation of the EHC method overestimates the heat transfer rates of through the melting front transition zone or that the model is transferring heat through the liquid too efficiently.

The validation metrics are used to compare the numerical model with the second set of experimental data. It is reasonable to assume that the only difference between the two sets of data is the thermal loads on the system. Figure 3.22 shows the Total Temperature

Figure 3.21. The numerical model’s time averaged temperature probe readings for the last 500 seconds of the best case boundary condition run compared with the horizontal temperature plots from the first set of experimental data.
Figure 3.22. Total Temperature RSS versus hot wall heat flux for the second set of experimental data.

RSS and the Cold Wall RSS versus hot wall heat flux obtained by comparing the second set of data with the initial hot wall heat flux sweep from 5000 W/m² to 2000 W/m². The Total Temperature RSS is used instead of the Modified Total Temperature RSS because the readings from the three temperature probes that are ignored in the calculation of the Modified Total Temperature RSS are not documented for the second set of experimental data thus no modifications were necessary (Szekely and Chhabra, 1970). The minimum Total Temperature RSS of 1.05 occurs when the hot wall heat flux is 10000 W/m². The Cold Wall RSS increases with increasing hot wall heat flux indicating that a cold wall temperature of 590.5 K is too warm for a hot wall heat flux of 10000 W/m².

Figure 3.23 shows the Average RSS versus hot wall heat flux for the second set of data. The minimum Average RSS of 0.522 occurs when the heat flux is 10000 W/m². Figures 3.22 and 3.23 show that there is agreement between the numerical data and the second set of experimental data for a hot wall heat flux of 10000 W/m² and a cold wall temperature of 590.5 K, however, the Cold Wall RSS in Figure 3.23 indicates that cold wall boundary condition should be lowered for better agreement. Fortunately, the second set of data has thermal loads close enough to the first set of data that the boundary condition parameter
sweep conducted for the first set of data can be analyzed for this second case.

Figures 3.24-3.27 show the Total Temperature RSS, the Cold Wall RSS, the Melting Front RSS, and the Average RSS versus cold wall temperature, respectively, for the second set of data over a range of inlet heat fluxes. It is difficult to tell from Figures 3.24 and 3.26 where the minimums are located, however Figure 3.27 indicates that the cold wall heat flux parameter space is wide enough to find the minimum of each hot wall heat flux data series. By comparing Figures 3.25 and 3.27 to Figures 3.14 and 3.16 it becomes apparent that the cold wall temperature of the second set of experimental data was about 1 K cooler then it was for the first set of data. Figure 3.28 shows the Average RSS versus hot wall heat flux for the second set of data to confirm that the parameter space has been adequately explored in both parameter spaces.

Figures 3.29 and 3.30 show the minimum Average RSS from each hot wall heat flux and cold wall temperature series, respectively. For the second set of data, Figures 3.29 and 3.30, were used to find the best case boundary conditions of 11525.7 W/m² for the hot wall heat flux, and 589.4 K for the cold wall temperature.
Figure 3.24. The Total Temperature RSS versus cold wall temperature for the second set of data for a range of inlet heat fluxes.

Figure 3.25. The Cold Wall RSS versus cold wall temperatures for the second set of data for a range of inlet heat fluxes.
Figure 3.26. The Melting Front RSS versus cold wall temperature for the second set of data for a range of inlet heat fluxes.

Figure 3.27. The Average RSS versus cold wall temperatures for the second set of data for a range of inlet heat fluxes.
Figure 3.28. The Average RSS versus hot wall heat flux for the second set of data for a range of cold wall temperatures.

Figure 3.29. The minimum Average RSS points from each hot wall heat flux series versus cold wall temperature for the second set of data.
Figure 3.30. The minimum Average RSS points from each cold wall temperature series versus hot wall heat flux for the second set of data.

Figure 3.31a shows the temperature profile after a 2000 second run for the model with the boundary conditions that best fit the second set of experimental data ($Q_{in} = 11525.7 \text{ W/m}^2$, and $T_c = 589.4 \text{ K}$). The best case boundary conditions for the second set of data result in a Total Temperature RSS of 1.05 K, a Cold Wall RSS of 0.43 K, a Melting Front RSS of 0.60 cm, and an Average RSS of 0.69. Figure 3.31b shows the velocity field for the same model at the end of a 2000 second run.

Figure 3.32 compares the temperature probe values from best case numerical model with the horizontal temperature profiles from the second set of experimental data. It is interesting to note that the hot wall heat flux for both sets of data were found to be very close to one another, and the cold wall temperature only differed by about 1 K, yet the temperature profiles for each case (Figures 3.21 and 3.32) differ significantly.

The resolution of the experimental data is too coarse to fully verify some of the effects observed in the numerical models. The experimental melting front presented by Szekely and Chhabra for both data sets was much more parabolic and smooth than that predicted by any of the numerical models (Szekely and Chhabra, 1970). The experimental melting front is a hand drawn fit to four data points which are extrapolated from temperature probes in the solid region. It is possible that the experiment had a wavy melting front like that of the
Figure 3.31. Temperature and velocity fields with the EHC transition zone contours for the second best case model.

Another observed discrepancy is that the experiment was reported to have a more steady temperature field in the liquid than the one observed in the numerical model. The researchers reported that the sampling frequency of the temperature probes was one second, which should be sufficient enough to see the fluctuations observed in the numerical model but lacked the resolution to observe it. Fitting a curve to the four points in the numerical melting front would smooth over the observed features in the melting front.
Figure 3.32. The numerical model’s time averaged temperature probe readings for the last 500 seconds of the second set of best case boundary conditions compared with the horizontal temperature plots from the second set of experimental data.

(Szekely and Chhabra, 1970). Perhaps there was thermal capacitance in the temperature probes that was not accounted for which resulted in a time averaged reading that did not have the resolution to see the fluctuations. Another possibility is that the two-dimensional representation of the model is inadequate to fully account for mixing in the fluid.

In the following chapter the EHC method’s key modeling parameters are studied parametrically. The first set of experimental data is compared with the numerical model while the boundary conditions remain fixed \((Q_{in} = 11195.8 \text{ W/m}^2, \text{ and } T_c = 590.4 \text{ K})\) and key modeling parameters are varied. Transient boundary conditions are used to study the models behavior under non-steady-state conditions. The limitations of this modeling approach are documented, and the recommended ranges for the key model parameters are presented.
CHAPTER 4
MODEL RESULTS AND DISCUSSION

Documentation of the limitations of the Effective Heat Capacity (EHC) modeling approach is a major goal of this work. The parametric sweeps of key modeling parameters discussed in the following sections provide guidelines for phase change modeling. The mesh refinement is shown to play a major role in the accuracy of EHC models in Section 4.1. In Section 4.2, the width and location of the EHC transition zone is shown to have little effect on pseudo-steady-state models, although the width and location is shown to play a significant role in transient cases. The maximum allowable time step’s importance in EHC modeling is discussed in Section 4.3. Finally, in Section 4.4, the jump in dynamic viscosity used to simulate the solid behavior of the pseudo-material is varied to find the threshold between solid and liquid behavior.

4.1. Mesh Refinement

A parametric sweep of mesh resolution provides information about the sensitivity of the EHC method to the mesh resolution. COMSOL’s mesh routine has preset mesh resolution settings. The element size that each setting will produce is model specific. Table 4.1 shows important parameters of the various meshes studied in this section for the validation model. The mesh has been varied from Coarse to Extremely Fine. As the mesh resolution is increased the numerical model approaches the experimental data. Figures 4.1-4.4 show how the model’s error metrics are effected by mesh refinement.

The EHC method cannot be implemented in COMSOL using the Reynolds Averaged Navier-Stokes (RANS) equation (Section 2.4.) due to the non-linearities used to simulate the melting front, thereby limiting this work to the use of the full blown Navier-Stokes equations in the non-isothermal fluid flow physics module (COMSOL, 2012). Consequently, higher

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<th>Table 4.1. Parameters of various mesh resolutions.</th>
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Figure 4.1. The Modified Total Temperature RSS for the first validation case as a function of mesh refinement.

Figure 4.2. The Cold Wall RSS for the first validation case as a function of mesh refinement.
Figure 4.3. The Melting Front RSS for the first validation case as a function of mesh refinement.

Figure 4.4. The Average RSS for the first validation case as a function of mesh refinement.
mesh resolution is required for good results (COMSOL, 2012). Parametric mesh refinement sweeps indicate that the validation model was on the threshold of turbulence. As the mesh resolution is increased the model increasingly agrees with the experiment because an extremely fine mesh is needed to accurately represent turbulent flow with the Navier-Stokes equations. The mesh refinement plays a crucial role in capturing the full effect of the latent heat of melting and is thus a critical modeling parameter. In addition to providing adequate resolution to describe the melting front, mesh refinement also affects the behavior of the naturally convecting liquid.

The EHC method implies that the mesh must be fine enough that the zone of high heat capacity material between the solid and liquid regions is continuous in order to account for the latent heat of fusion (Voller et al., 1990). When the mesh is too coarse, the high heat capacity region becomes discontinuous, resulting in gaps of lower heat capacity material (Voller et al., 1990). These gaps tend to allow the melting front to deform faster under transient conditions. Additionally, as the heat flux through the transition zone is increased, the temperature gradient of the transition zone is increased. For higher heat flux situations, the mesh resolution must also be increased to avoid gap formation.

The naturally convecting liquid region is very sensitive to mesh refinement. As the mesh refinement is increased, and with it the degrees of freedom of the matrix, smaller eddies form. Although the laminar physics module is used, extremely fine mesh refinement begins to reveal that the fluid may be undergoing turbulent convection. Szekely and Chhabra alluded to the possibility that the fluid may be turbulent (Szekely and Chhabra, 1970). It is interesting to note that the lower region of the melting front in the numerical model is not very close to the experimentally and theoretically determined location until the mesh refinement is increased to Finer. When a coarser mesh is used, the lower solid region progresses much further into the liquid region. The progression of the solid into the lower liquid region is not as predominant in refined mesh models because eddies form near the bottom and transfer heat from the hot wall to the melting front by convection more efficiently. When these eddies are not present, there is little fluid flow in the lower region so most of the heat transfer is by conduction. The decrease in the in all four RSS metrics for the coarse mesh indicates that a purely conductive model may lead to reasonable results for horizontal heat flux between two vertical walls.

The increased Modified Total Temperature RSS, Melting Front RSS, and Average RSS in Figures 4.1, 4.3 and 4.4 respectively, for the extremely fine mesh case may indicate that the boundary conditions found in the previous chapter may be slightly off. The best case boundary conditions were found with a extra fine mesh. In the mesh refinement study
the extra fine mesh resulted in the lowest RSS values. A three parameter sweep including the mesh refinement, the hot wall heat flux and the cold wall may lead to better agreement between the experimental and numerical data; however, this work is left to future researchers.

4.2. Transition Zone Width and Location

Parametric studies of the width and location of the discontinuous transition zone (Figure 4.5) indicate that the transition zone has little affect on the results of the pseudo-steady-state models. The transition zone width and location may play larger roles in transient modeling.

4.2.1. Latent Heat of Melting Transition Zone Width

Figures 4.6-4.9 show the effect of varying the width of the EHC zone \((dT_{C_p})\) from 0.5 K to 100 K. A logarithmic x-axis is used in these plots since the width of the EHC zone varies over several orders of magnitude. The relatively flat trends in Figures 4.6-4.9 suggest that the width of the EHC zone \((dT_{C_p})\) is not a critical modeling parameter under pseudo-steady-state conditions.

A transient study shows that the EHC width is a critical modeling parameter under transient conditions. One set of transient experimental data from Szekely and Chhabra’s work was reproduced in COMSOL (Szekely and Chhabra, 1970). The hot wall heat flux was

![Figure 4.5. Pseudo material heat capacity as a function of temperature.](image)
Figure 4.6. The Modified Total Temperature RSS as a function of the EHC transition zone width.

Figure 4.7. The Cold Wall RSS as a function of the EHC transition zone width.
Figure 4.8. The Melting Front RSS as a function of the EHC transition zone width.

Figure 4.9. The Average RSS as a function of the EHC transition zone width.
Figure 4.10. The experimental and predicted melting front locations as the cold wall temperature is decreased.

assumed to be 11195.8 W/m² (the best case hot wall heat flux for the first set of data). The cold wall temperature was set to 592.8 K for 2000 seconds. After 2000 seconds the cold wall temperature was decreased to 589.1 K over the next 1200 seconds. The cold wall temperature is held constant for the remainder of the 6000 second run. The melting front location at each temperature probe elevation is extracted directly from the model. Figure 4.10 shows the applied cold wall temperature, the experimental melting front location, and the numerical melting front location at each temperature probe elevation. The modeling parameters are the same as those used in the first validation experiment.

The numerical melting front location is not as stable as the experimental melting front, and it over predicts the growth of the solid region, but qualitatively the melting front location for the high and mid-low sets of temperature probe elevations agree with the experimental curve. The location of the melting front lags behind the cold wall transition. In order to examine the sensitivity of the melting front evolution to the transition zone width, the width was increased by factors of 8, 64, and infinity, representing a $dT_{Cp}$ of 4.8 K, 38.4 K, and constant heat capacity, respectively. Figures 4.11 and 4.12 show the resulting melting front distance predictions for the high and mid-low temperature probe elevations, respectively, for
Figure 4.11. The melting front location at the high temperature probe elevation as a function of the transition zone width.

Figure 4.12. The melting front location at the mid-low temperature probe elevation as a function of the transition zone width.
each value of $dT_C$. Each model is started from the same initial state, 2000 seconds into a pseudo-steady-state run, and terminates after 6000 seconds.

The locations of the melting front in Figures 4.11 and 4.12 for the 0.6 K and 4.8 K transition zone widths are very similar, although the 4.8 K data set is slightly more variable. When the transition zone is large (38.4 K) or omitted, the melting front location becomes very unstable. Additionally, the transition between states occurs faster than observed experimentally. Based on the performance of the model in this study the smaller transition zone widths are more accurate, and the transition zone width is a key modeling parameter in transient studies.

4.2.2. Latent Heat of Melting Transition Zone Location

Figures 4.13-4.16 show how the modeling metrics are affected by the location of the latent heat of melting transition zone, relative to the melting temperature. The location of the latent heat of melting transition zone is defined by $dT_\nu$ in Figure 4.5. Increasing the value of $dT_\nu$ decreases the temperature of the latent heat of melting transition zone. For pseudo-steady-state runs the width of $dT_\nu$ had little effect on the behavior of the model.

The value of $dT_\nu$ cannot be greater than the difference between the melting temperature and the cold wall temperature. There is very little change in the modeling metrics as the latent heat of melting location relative to the melting temperature varies from 0.5 K to 16 K. This result is surprising, and indicates that the details of the EHC method are not important in pseudo-steady-state models. The latent heat of melting transition zone location could not coincide with the location of the discontinuous dynamic viscosity or singularities would form. Trial and error found that values of $dT_\nu$ less than 0.5 K destabilize the model at the melting front causing singularities.

The EHC transition zone width and location studies studies show that the EHC zone does not effect the accuracy of the validation model. The thermal loads on this model are fixed, resulting in a pseudo-steady-state system. In a steady-state system the temperature field in a material is independent of the heat capacity. Furthermore, in a steady-state, two-phase system, the latent heat of melting does not contribute to the temperature field; thus, the closer the model is to a steady-state the less bearing the EHC parameters have on the solution.

Once the model has reached a pseudo-steady-state the only transient behavior is the eddies in the fluid disturbing the melting front. It is possible that the instabilities introduced by the eddies are overwhelmed by the overall steady-state behavior of the model; and,
Figure 4.13. Modified Total Temperature RSS as a function of the latent heat of melting location relative to the melting temperature.

Figure 4.14. Cold Wall RSS as a function of the latent heat of melting location relative to the melting temperature.
Figure 4.15. Melting Front RSS as a function of the latent heat of melting location relative to the melting temperature.

Figure 4.16. Average RSS as a function of the latent heat of melting location relative to the melting temperature.
thus, whether or not the system is accounting for the latent heat of melting becomes irrelevant. Evidence of this effect is observed in the time required for the model to reach pseudo-steady-state. Models with the more narrow EHC transition zones, tend to take much longer to reach pseudo-steady-state while models with large transition zones settle faster. The difference in settling times makes it clear that the EHC zone plays a significant role in the accuracy of models under a transient situations.

To show that the EHC location is a critical modeling parameter for transient conditions a transient study is preformed using the same transient boundary conditions as the \( dT_{C_p} \) study above. In this study the transition zone width \( (dT_{C_p}) \) is set back to 0.6 K and transition zone location is increased from 1 K to 10 K in increments of 3 K. Values of \( dT_{\nu} \) greater then 10 K are out of the range of the experimental boundary conditions. Figures 4.17 and 4.18 show the melting front locations for the high and mid/low temperature probe elevations respectively.

Figure 4.17 shows that the melting front location near the top of the numerical model is relatively consistent for increasing \( dT_{\nu} \), while Figure 4.18 shows that the melting front location becomes unstable once \( dT_{\nu} \) is larger then 1 K. The stability observed in the melting front near the top of the model is likely caused by the large temperature gradient in the solid

![Figure 4.17](image-url)
in this region. The horizontal distance between the melting front and the step in the heat capacity decreases with increasing temperature gradients, thus it is expected that width of $dT_{nu}$ does not affect the melting front near the top as much as it does elsewhere. The width of the buffer zone is a key modeling parameter for transient conditions, although as the temperature gradient near the melting front increases the buffer zone width becomes less important than a narrow transition zone. In this particular study, a narrow transition zone is necessary to stabilize the location of the melting front preventing the front from being eroded by eddies in the liquid region.

4.3. Maximum Allowable Time Step

The default maximum time step was initially set to automatic in COMSOL. The non-linearities introduced by the EHC method tended to cause problems for the COMSOL solvers when the maximum time step was automatically determined. In automatic mode, COMSOL starts with extremely small time steps (hundredths of a second). If the model does not change significantly the program takes a larger step on the next iteration. COMSOL continues to increase the time step of each iteration until it satisfies its time stepping error routine. At this point COMSOL stops increasing the time step. At each iteration COMSOL
runs time stepping error routine and decides whether to increase, maintain, or decrease the
time step. Under normal circumstances this feature allows COMSOL to self regulate time
stepping and optimize the time it takes it to run models. Unfortunately, the automatic
time stepping often causes the formation of singularities in the EHC models. It is not clear
why taking too large a time step causes instabilities in COMSOL's solvers, but this was
a significant source of frustration in this project. Figure 4.19 shows the formation of a
singularity in a model. To solve this problem automatic time stepping was replaced by the
following process:

1. Set up a test model to run for 2000 seconds, and have COMSOL update a
temperature plot at each iteration of the solver,

2. set the maximum allowed time step to a relatively large value (5 seconds),

3. tune the model and watch for the formation of singularities at the melting front during
the first 50 seconds of the run,

4. if a singularity occurs decrease the time step by half and rerun the model, then

5. repeat the previous step until singularities no longer form at the melting front.

During the mesh resolution sweeps performed for the mesh resolution study a loose
correlation between mesh refinement and the maximum allowable time step was observed.
Table 4.2 shows the maximum allowable time steps for various mesh resolutions. The
observation that higher mesh resolutions require smaller time steps parallels the other studies
in this work which show that the discontinuities in the material properties makes the model
unstable.

<table>
<thead>
<tr>
<th>Mesh Resolution</th>
<th>Maximum Allowable Time Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>1.25 s</td>
</tr>
<tr>
<td>Normal</td>
<td>0.625 s</td>
</tr>
<tr>
<td>Fine</td>
<td>0.625 s</td>
</tr>
<tr>
<td>Finer</td>
<td>0.625 s</td>
</tr>
<tr>
<td>Extra Fine</td>
<td>0.3125 s</td>
</tr>
<tr>
<td>Extremely Fine</td>
<td>0.3125 s</td>
</tr>
</tbody>
</table>
Figure 4.19. The formation of a singularity in the validation model caused by too large of a time step.

4.4. Jump in Dynamic Viscosity

The magnitude of the step function in the temperature dependent dynamic viscosity is another important modeling parameter used to simulate the solid region and control the minimum threshold at which a fluid will behave as a solid. Previous models used a temperature dependent dynamic viscosity which transitioned from $2.41 \times 10^{-3} \text{ Pa} \cdot \text{s}$, for regions above the melting temperature, to $10^7 \text{ Pa} \cdot \text{s}$ for regions below the melting
temperature. In this study the viscosity for material below the melting temperature is varied logarithmically from $10 \text{ Pa} \cdot \text{s}$ to $10^7 \text{ Pa} \cdot \text{s}$. The resulting models are compared using the RSS error metrics. Figures 4.20-4.23 show the results of this study.

Modeling cases with a solid dynamic viscosity greater than $1000 \text{ Pa} \cdot \text{s}$ result in good RSS values. Although the model with a solid dynamic viscosity of $1000 \text{ Pa} \cdot \text{s}$ agrees with the higher solid dynamic viscosity cases for the Modified Total Temperature RSS, the Melting Front RSS, and the Average RSS (Figures 4.20, 4.22, and 4.23 respectively), the melting front began to creep slightly into the liquid region. The slightly higher Cold Wall RSS in Figure 4.21 for a solid dynamic viscosity of $1000 \text{ Pa} \cdot \text{s}$ may be a manifestation of the slight melting front creep. Once the solid dynamic viscosity is lower than $1000 \text{ Pa} \cdot \text{s}$ all of the metrics clearly indicate that the model is diverging from the experimental results. A minimum of $10,000 \text{ Pa} \cdot \text{s}$ is recommended as a guideline for using a high dynamic viscosity to simulate a solid.
Figure 4.20. The Modified Total Temperature RSS as the pseudo material definition of the solid’s dynamic viscosity is varied from 1 to $10^7$ Pa · s.

Figure 4.21. The Cold Wall RSS as the pseudo material definition of the solid’s dynamic viscosity is varied from 1 to $10^7$ Pa · s.
Figure 4.22. The Melting Front RSS as the pseudo material definition of the solid’s dynamic viscosity is varied from $1$ to $10^7$ Pa $\cdot$ s.

Figure 4.23. The average RSS as the pseudo material definition of the solid’s dynamic viscosity is varied from $1$ to $10^7$ Pa $\cdot$ s.
CHAPTER 5
SUMMARY AND CONCLUSIONS

The present research studies the Effective Heat Capacity (EHC) method applied to the numerical simulation of the interface between a solid and a naturally convecting pool of liquid heavy metal. A pseudo-material with discontinuous temperature dependent material properties near the melting temperature simulates the melting front between a solid and a naturally convecting pool of liquid heavy metal. The pseudo-material implements the EHC method with a high heat capacity transition zone near the melting temperature. The pseudo-material also uses a step in the dynamic viscosity at the melting temperature to simulate the solid region. The non-linearities introduced by the EHC method, and the stiff nature of numerical models of a melting front under the influence of natural convection, make this modeling technique difficult to implement.

Root Sum of the Squares (RSS) based metrics are employed to quantify how close numerical results are to experimental data. Four RSS metrics, that rely on temperature probes placed in the numerical model at the same locations as the temperature probes in the experiment, quantify how accurately the numerical model is reproducing experimental results. The Total Temperature RSS considers all of the temperature probes and is used for the second set of experimental data only. The Modified Total Temperature RSS considers a select set of the temperature probes and is used with only the first set of experimental data. The Cold Wall RSS considers the temperature probes closest to the cold wall. The Melting Front RSS considers the location of the melting front found by linear extrapolation based on the temperature probes located in the solid. The Average RSS is the mean of all the metrics.

The cold wall temperature and hot wall heat flux were not given in the literature for the validation model. A two parameter sweep of the boundary conditions resulted in a family of models in the range of the two available sets of pseudo-steady-state experimental data. The minimum Average RSS points in each parametric sweep are plotted versus the sweep parameters. Fitting third order polynomial functions to the plots extracts the relationship between the hot wall heat flux and the cold wall temperature. Solving the polynomial functions for their minimum values yields the best case boundary conditions for each set of experimental data. The time averaged temperature probe readings from the best case numerical models are in close agreement with experimental data.

The boundary conditions that best match the first set of data are 590.4 K for the cold wall temperature, and 11195.8 W/m² for the hot wall heat flux. With these boundary conditions the Modified Total Temperature RSS is 1.07 K, the Cold Wall RSS is 0.25 K,
the Melting Front RSS is 0.36 cm, and the Average RSS is 0.56. A cold wall temperature of 589.4 K and a hot wall heat flux of 11525.7 W/m² results in a Total Temperature RSS is 1.05 K, a Cold Wall RSS is 0.43 K, a Melting Front RSS is 0.60 cm, and an Average RSS is 0.69 when compared with the second set of data.

The key modeling parameters for the EHC modeling approach were studied parametrically to understand the limitations of the EHC method and to provide guidelines for future use of the EHC method in an FEA environment. Specifically, the mesh refinement, the transition zone width and location, the maximum allowable time step, and the dynamic viscosity of the solid were varied with the boundary conditions that best fit the experimental data.

The number of mesh elements varied from 2184 to $2.02 \times 10^5$. The error metrics indicate that an extra fine mesh with a maximum element size of $1.24 \times 10^{-3}$ m² is necessary for the model to produce accurate results. Temperature and velocity field plots indicate that the fluid is on the verge of turbulence. Since the full blown Navier-Stokes equation is used in this modeling approach, a high mesh refinement is necessary to capture the fine scale fluid fluctuations associated with turbulent flow. The behavior of the fluid affects the shape and location of the phase change boundary and ultimately the behavior of the entire model.

Studies of the width and location of the EHC transition zone demonstrate that the accuracy of pseudo-steady-state models is not effected by the EHC zone. The error metrics remained relatively unchanged when transition zone width is varied from 0.5 K to 100 K. The error metrics also remain unchanged when the transition zone location relative to the melting temperature is varied from 0.5 K to 16 K. The size and position of the EHC zone affects the settling times of the models, indicating that these metrics impact the transient behavior of the model.

The width of the EHC transition zone plays a critical role in the behavior of the model under transient conditions. Models with transition zone widths of 0.6 K and 4.8 K have delayed transition times between states, similar to experiments preformed by Szekely and Chhabra. Models with extremely wide, or nonexistent, transition zones have a more instantaneous response to transient boundary conditions; thus, it is necessary to use narrow transition zone widths for transient modeling.

Manual tuning of the maximum allowable time step in COMSOL is necessary to avoid singularities at the melting front. Large time steps tend to cause more singularities while smaller time steps lead to increased run times. Higher mesh resolution models tend to require smaller time stepping.

The value of the solid region’s dynamic viscosity varied from 10 Pa·s to $1 \times 10^7$ Pa·s.
The transition from solid to liquid behavior begins around 1000 Pa · s thus a minimum of 10,000 Pa · s is recommended as a guideline for choosing a pseudo-solid, dynamic viscosity.
CHAPTER 6
RECOMMENDATIONS FOR FUTURE RESEARCHERS

This work is the result of a tremendous amount of trial, error, and help from the COMSOL support team. Implementation of the Effective Heat Capacity (EHC) method in COMSOL for studying a melting front under the influence of natural convection is made difficult by several obstacles. The non-linearities introduced by the EHC method often cause issues for the COMSOL solver routines. For example, the turbulent flow Reynolds Averaged Navier-Stokes (RANS) model does not allow for step functions in the dynamic viscosity definitions, limiting this work to the laminar flow module with the full blown Navier-Stokes equation. Since the experiment was performed near the onset of turbulence, a fine mesh resolution is necessary to accurately account for fine fluid structures. Additionally, the stiff nature of a numerical model of a melting front under the influence of natural convection requires small time steps. Previous studies on the behavior of a melting front under the influence of natural convection have very long run times resulting in computationally expensive numerical models. Furthermore, large models in COMSOL are very prone to execution issues.

The original goal of this project was to model the start-up of a lead cooled reactor from a cold solid state. The limitations encountered in this work have made it clear that such an endeavor would require extreme computational resources if COMSOL is the modeling platform. It is the author’s opinion that other modeling programs and approaches should be explored for use with models that are more sophisticated than the validation model used in this work.

The lack of a good liquid metal phase change benchmark model in the existing literature is disappointing. The resolution of the experimental data used in this work was too coarse to fully verify some of the effects observed in the numerical models. It is possible that the experiment had a wavy melting front like that of the numerical model but lacked the resolution to observe it. The experiment was reported to have a more steady temperature field in the liquid than the one observed in the numerical model. There may have been some thermal capacitance in the temperature probes that resulted in a time averaged reading without fluctuations. The two-dimensional representation of the model may not be adequate to fully account for mixing in the fluid. A three-dimensional model of this system would be interesting although it would be extremely computationally expensive.
REFERENCES


Li, N., “Lead-alloy coolant technology and materials - technology readiness level evaluation,”


76
APPENDIX A - THERMOPHYSICAL PROPERTIES OF LEAD BISMUTH EUTECTIC AND LEAD
**A.1 Thermophysical Properties of Lead Bismuth Eutectic** (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007b)

<table>
<thead>
<tr>
<th>Property</th>
<th>Correlation</th>
<th>Units</th>
<th>Tem Range</th>
<th>Error±</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting temperature</td>
<td>$T_m = 397.7$</td>
<td>K</td>
<td>n/a</td>
<td>0.6</td>
</tr>
<tr>
<td>Latent heat of melting</td>
<td>$Q_m = 38.6$</td>
<td>kJ/kg</td>
<td>n/a</td>
<td>0.2</td>
</tr>
<tr>
<td>Boiling temperature</td>
<td>$T_{boil} = 1943$</td>
<td>K</td>
<td>n/a</td>
<td>10</td>
</tr>
<tr>
<td>Latent heat of boiling</td>
<td>$Q_{boil} = 854$</td>
<td>kJ/kg</td>
<td>n/a</td>
<td>2.0</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho(T) = 11096 - 1.3236 \times T$</td>
<td>kg/m$^3$</td>
<td>403-1300</td>
<td>0.8%</td>
</tr>
<tr>
<td>Isobaric specific heat</td>
<td>$C_p(T) = 159 - 2.72 \times 10^{-2} \times T + 7.12 \times 10^{-6} \times T^2$</td>
<td>J/kg/K</td>
<td>430-605</td>
<td>5%</td>
</tr>
<tr>
<td>Dynamic viscosity</td>
<td>$\nu(T) = 4.94 \times 10^{-4} \times e^{754.1/T}$</td>
<td>Pa · s</td>
<td>5%</td>
<td></td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$\lambda(T) = 3.61 + 1.517 \times 10^{-2} \times T - 1.741 \times 10^{-6} \times T^2$</td>
<td>W/m/K</td>
<td>403-1100</td>
<td>5%</td>
</tr>
</tbody>
</table>
### A.2 Thermophysical Properties of Lead (Organisation for Economic Co-operation and Development - Nuclear Energy Agency, 2007b)

<table>
<thead>
<tr>
<th>Property</th>
<th>Correlation</th>
<th>Units</th>
<th>Temp. Range</th>
<th>Error ±</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting temperature</td>
<td>$T_m = 600.6$</td>
<td>K</td>
<td>n/a</td>
<td>0.1</td>
</tr>
<tr>
<td>Latent heat of melting</td>
<td>$Q_m = 23.8$</td>
<td>kJ/kg</td>
<td>n/a</td>
<td>0.7</td>
</tr>
<tr>
<td>Boiling temperature</td>
<td>$T_{boil} = 2016$</td>
<td>K</td>
<td>n/a</td>
<td>10</td>
</tr>
<tr>
<td>Latent heat of boiling</td>
<td>$Q_{boil} = 858.2$</td>
<td>kJ/kg</td>
<td>n/a</td>
<td>1.9</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho(T) = 11367 - 1.1944 \times T$</td>
<td>kg/m$^3$</td>
<td>601-1900</td>
<td>0.7%</td>
</tr>
<tr>
<td>Isobaric specific heat</td>
<td>$C_p(T) = 175.1 - 4.961 \times 10^{-2} \times T + 1.985 \times 10^{-5} \times T^2$ $-2.099 \times 10^{-9} \times T^3 - 1.524 \times 10^6 \times T^{-2}$</td>
<td>J/kg/K</td>
<td>601-1300</td>
<td>7%</td>
</tr>
<tr>
<td>Dynamic viscosity</td>
<td>$\nu(T) = 4.55 \times 10^{-4} \times e^{1069/T}$</td>
<td>Pa·s</td>
<td>601-1470</td>
<td>4%</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$\lambda(T) = 9.2 + 0.011 \times T$</td>
<td>W/m/K</td>
<td>601-1300</td>
<td>10%</td>
</tr>
</tbody>
</table>