COMPUTATIONAL FLUID DYNAMIC MODELING OF A SECONDARY LEAD REVERBERATORY FURNACE

by

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ABSTRACT

Over half of lead production worldwide comes from secondary sources. The main secondary source of lead is lead-acid batteries. Currently, over 99% of all lead based batteries in North America are recycled, amounting to 1.7 million short tons of lead annually. Secondary lead battery scrap is recycled through a combination of physical concentration, hydrometallurgical and pyrometallurgical processes. A common type of furnace used for the pyrometallurgical steps in this process is a directly fired reverberatory furnace. In the directly fired reverberatory furnace, the burden (the solid feed material) is heated through direct contact with the burner flame as well as through radiant heat transfer from the walls and combustion gases. The impingement of the flame on the burden can facilitate large amounts of heat transfer, leading to greater melting and production rates, but can also cause areas of high velocity turbulent flow and local high temperature zones within the furnace’s refractory lining. These phenomena can lead to excessive erosion and thermal stresses thereby prematurely shortening the lifetime of the refractory lining. Understanding the cause of refractory wear is critical to many operations as the rate of refractory wear will directly affect the length of refractory lifetime and the productivity of the furnace. Therefore, obtaining velocity and temperature distributions within the furnace under different conditions was the focus of this project with the goal of identifying and minimizing high wear zones while maintaining the smelting rate.

A computational fluid dynamic (CFD) model has been developed to accomplish the project’s goals by calculating the temperature distribution, velocity profile and overall heat transfer within the furnace. The preliminary portion of the project focused on model development and validation. Once a base case simulation was validated using data from an operational lead reverberatory furnace, predicted areas of high refractory wear were identified through the calculation of the temperature and velocity distributions within the furnace. The average burden surface temperature was also evaluated as this parameter was used as a measure of smelting rate. The CFD model was used to assess whether the predicted areas of high refractory wear could be minimized by various operational changes to the burden geometry and burner alignment. The results showed that the amount and location of the burner flame impingement was sensitive to changes in both burden geometry and burner alignment and greatly affected the overall flow patterns and heat transfer within the furnace. The results also indicated that there could be a tradeoff between smelting rate and refractory lifetime. As a final step, a semi-empirical wear function was constructed in attempt to evaluate the combined influence of temperature and velocity on the predicted areas of high wear within the furnace refractory.
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MATHEMATICAL CONVENTION & SYMBOLS

The mathematical conventions throughout the document are Cartesian coordinates, bolded variables denote vectors and bolded capitalized variables denote tensors. Complex partial differential equations are written in Cartesian tensor form where the subscripts 1, 2, and 3 denote x, y and z, respectively. Italicized letters within the text denote symbols or variables. Below is a list of the symbols used consistently throughout document.

**General:**
- A: area
- c: speed of sound
- CFL: flow courant number
- \( C_p \): constant pressure specific heat
- \( D_H \): hydraulic diameter
- \( E_a \): activation energy
- g: acceleration due to gravity
- h, H: specific enthalpy and total enthalpy
- I: turbulent intensity
- k: turbulent kinetic energy
- \( k \): thermal conductivity
- ṁ: mass flow rate
- Ma: Mach number
- MW: molecular weight
- P: pressure
- \( \dot{Q} \): volumetric flow rate
- q, Q: heat transfer per area and total heat transfer
- R: gas constant
- \( R_u \): Universal gas constant
- Re: Reynolds number
- t: time
- v: velocity
- V: volume
- Y: mass fraction

**Greek Letters:**
- \( \gamma \): ratio of specific heats
- \( \varepsilon \): emissivity
- \( \varepsilon \): turbulent kinetic energy dissipation rate
- \( \eta \): furnace efficiency
- \( \mu \): dynamic viscosity
- \( \rho \): density
- \( \sigma \): normal stress
- \( \sigma \): Stefan-Boltzmann constant
- \( \tau \): shear stress
- \( \phi \): generic flow field variable
- \( \omega \): turbulent kinetic energy specific dissipation rate
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CHAPTER 1
INTRODUCTION

Lead is a relatively soft metal with a bluish-white luster, a high density and a low melting point. Modern lead mines produce about three million metric tons of lead annually, which supplies only about half of the lead used worldwide. The other half is produced from secondary sources [1]. The main secondary source of lead is the lead-acid battery. Pure lead is used for the production of oxide pastes within the battery while alloyed lead is used to construct the battery grids, terminals and bridges. Over 99% of all battery lead in North America is recycled annually [2].

Although the details of the lead-acid battery recycling process can vary from one processing plant to the next, the general sequence of unit processes remains fairly consistent. The batteries are first drained of acid and the outer casing is removed by hand or crushing. A series of physical and chemical separation techniques are then performed to produce a lead concentrate. The lead bearing material is then smelted with coke and other fluxes in either a rotary furnace, a reverberatory furnace, a blast furnace, or a combination thereof. The smelting process is followed by a refining process in which unwanted impurities are removed from the lead through preferential oxidation. The final lead product is then sent to casting operations [3].

Over a third of the North American lead smelters use a reverberatory furnace. The reverberatory furnace in these plants is always used in combination with a blast furnace [4]. The reverberatory furnace is a type of furnace in which the material under treatment is heated indirectly by means of the combustion gases and radiant heat rather than directly by the burner flame. The reverberatory furnace design dates back to the 19th century and has found uses in the copper, lead and aluminum industries [5]. However, the definition of the reverberatory furnace has broadened over the years and in many cases the same terminology is also used to describe directly fired furnaces where the flame is in contact with the charge or burden (terms used to describe the material that is being fed to the furnace). Modern secondary lead processing plants typically use a direct style reverberatory furnace [6]. The impingement of the flame on the burden can facilitate large amounts of heat transfer, leading to greater production rates, but can also cause areas of high-velocity turbulent flow and high-temperature zones on the refractory lining. These phenomena can lead to excessive erosion and thermal stress, thereby prematurely shortening the lifetime of the refractory. Understanding the mechanisms of refractory wear is critical to many operations as the rate of refractory wear will directly affect the length of refractory lifetime and productivity of the furnace.

The mechanisms of refractory wear in lead processing furnaces fall under three main categories: chemical, thermal and mechanical. Chemical corrosion of the refractory typically occurs below the slag line. At this location, the slag and metal phases are in direct contact with the refractory lining. Above the slag line, in the combustion gas zone, the refractory is more susceptible to thermally and/or mechanically
caused wear than chemical corrosion. The refractory wear below the slag line is typically more continuous and even, whereas refractory wear in the combustion gas space is more acute and concentrated.

The complex transport phenomena that cause wear within secondary lead reverberatory furnaces cannot be fully understood without some form of modeling. Due to the complex nature of the equations that describe the transport phenomena within the furnace, Computational Fluid Dynamics (CFD) was chosen as the method to model these distributions rather than any analytical methods. Computational Fluid Dynamics is a branch of fluid mechanics that uses numerical methods and algorithms for multiphase fluid analysis for both reacting and non-reacting flows and can include complexities which couple thermodynamics, heat transfer, turbulence, and chemical reactions. CFD is based on the Navier-Stokes equations which describe how velocity, pressure, temperature and density of a moving fluid are all related. CFD gives an insight into flow patterns that are difficult, expensive or impossible to study using traditional experimental techniques. Obtaining the velocity and temperature distributions within the furnace, which could be produced through the use of CFD, was necessary to detect the areas of high thermal and mechanical wear in the combustion gas zone.

The scope of this research was to develop a CFD model to generate data that could be used to find ways to increase the lifetime of the reverberatory furnace refractory in the combustion gas zone while maintaining or increasing the smelting rate. A large portion of the project focused on model development as the model could only be used as a predictive tool if it was able to accurately describe the physics occurring within the furnace. Once the model was validated using data from an operational lead reverberatory furnace, areas of high potential for thermal and mechanical refractory wear were identified through the calculation of the temperature and velocity distributions within the furnace. The CFD model was then used to assess whether these areas could be minimized by various physical and operational changes.
CHAPTER 2
A REVIEW OF SECONDARY LEAD PRODUCTION AND USES

A literature survey pertaining to production of primary and secondary lead metal was conducted to provide the researcher with proper background information. This chapter details a summary of the literature findings. The information gained from the literature survey provided valuable knowledge that was useful for designing and validating the CFD model.

2.1 Lead Production and Uses

Lead is a soft, gray, lustrous metal with a high density and low melting point. Lead has been extracted and used in various applications for over 6000 years [1]. The common ores of lead are the sulfide mineral galena (PbS) and its oxidized products, cerussite (PbCO$_3$) and anglesite (PbSO$_4$) [7]. The standard method for the production of lead from primary sources is to first roast the sulfide ore to yield lead oxide. The oxide is then reduced with carbon in a blast furnace. The products from the lead blast furnace are lead bullion which will typically contain impurities such as antimony, tin, arsenic and copper and a slag phase that contains complex silicates rich in iron, calcium and sodium. The formation of a matte, a molten metal sulfide phase, and speiss, a liquid phase rich in antimony or arsenic where cobalt and nickel collect, is also possible within the blast furnace depending on the composition of the feed [5]. Although lead concentrates from mining sources are still produced, there are currently no primary lead smelters in operation within the United States. There are several secondary lead smelters. Secondary lead plants typically utilize different types of furnaces and operations than the primary production plants. These operations are discussed in detail later in this chapter [4].

Over the past 40 years, greater awareness about the negative health effects of lead on human health has resulted in many countries banning numerous lead products, such as leaded fuel, paints and pipes [8]. Despite the hazards to human health, lead is still used in various industrial applications. Currently, the main use for lead is in the production of lead-acid batteries, which accounts for approximately 80 percent of the metal’s use. Lead alloys are also used to produce some bullets and metal solders. Although pure lead is very reactive, some lead compounds such as lead oxide can be very stable, making them suitable as constituents in corrosion resistant coatings for iron and steel. These lead coatings are used to protect ship hulls as well as underwater power and communication cables. Lead metal is used for radiation protection as well [2].

Table 2.1 lists the locations, furnace types and nominal capacities of the North American lead processing plants. In 2015, the total North American lead production capacity was estimated to be 2,090,000 short tons. About 86% or 1,800,000 short tons of the total production capacity came from secondary sources with the remaining 14% or 290,000 short tons produced from primary sources.
Currently, over 99% of all lead based batteries in North America are recycled, resulting in around 95% of secondary lead being derived from this source. The remaining 5% of secondary lead came from copper-based cable, solder scrap, leaded glass, contaminated soil, manufacturing scrap, residue, ash and dust. [4].

Table 2.1: North American Lead Smelting Capacities as of 2015 [4]

<table>
<thead>
<tr>
<th>Country</th>
<th>Company</th>
<th>Location</th>
<th>Furnace Type</th>
<th>Primary (short tons)</th>
<th>Secondary (short tons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Canada</td>
<td>Cominco</td>
<td>Trail, BC</td>
<td>Kivcet</td>
<td>90,0000</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Xstrata</td>
<td>Belledune, NB</td>
<td>Blast</td>
<td>80,0000</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Nova Pb</td>
<td>Montreal, QC</td>
<td>Long Rotary</td>
<td>-</td>
<td>80,000</td>
</tr>
<tr>
<td></td>
<td>Tonnoll</td>
<td>Toronto, Ontario</td>
<td>Rotary</td>
<td>-</td>
<td>45,000</td>
</tr>
<tr>
<td>Mexico</td>
<td>Penoles</td>
<td>Terreon</td>
<td>Blast</td>
<td>120,0000</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>JCI</td>
<td>Cienega de Flores, NL</td>
<td>Rotary</td>
<td>-</td>
<td>125,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Garcia, NL</td>
<td>Rotary</td>
<td>-</td>
<td>135,000</td>
</tr>
<tr>
<td></td>
<td>M3</td>
<td>Roynosa</td>
<td>Rotary</td>
<td>-</td>
<td>30,000</td>
</tr>
<tr>
<td></td>
<td>Omega</td>
<td>Planta Dr</td>
<td>Rotary</td>
<td>-</td>
<td>25,000</td>
</tr>
<tr>
<td></td>
<td>Pipsa</td>
<td>Garcia, NL</td>
<td>Rotary</td>
<td>-</td>
<td>25,000</td>
</tr>
<tr>
<td></td>
<td>Riasa</td>
<td>St. Caterina, NL</td>
<td>Rotary</td>
<td>-</td>
<td>35,000</td>
</tr>
<tr>
<td>USA</td>
<td>BRC</td>
<td>Arecibo, PR</td>
<td>Rotary</td>
<td>-</td>
<td>18,000</td>
</tr>
<tr>
<td></td>
<td>Doe Run</td>
<td>Boss, MO</td>
<td>Reverb / Blast</td>
<td>-</td>
<td>140,000</td>
</tr>
<tr>
<td></td>
<td>East Penn</td>
<td>Lyons, PA</td>
<td>Reverb / Blast</td>
<td>-</td>
<td>100,000</td>
</tr>
<tr>
<td></td>
<td>Exide</td>
<td>Forrest City, MO</td>
<td>Blast</td>
<td>-</td>
<td>35,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Muncic, IN</td>
<td>Reverb / Blast</td>
<td>-</td>
<td>90,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Vernon, CA</td>
<td>Reverb / Blast</td>
<td>-</td>
<td>95,000</td>
</tr>
<tr>
<td></td>
<td>JCI</td>
<td>Florence, SC</td>
<td>Rotary</td>
<td>-</td>
<td>120,000</td>
</tr>
<tr>
<td></td>
<td>Gopher</td>
<td>Eagan, MN</td>
<td>Reverb / Blast</td>
<td>-</td>
<td>130,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Tampa, FL</td>
<td>Reverb / Blast</td>
<td>-</td>
<td>110,000</td>
</tr>
<tr>
<td></td>
<td>RSR</td>
<td>City of Industry, CA</td>
<td>Reverb / Elec</td>
<td>-</td>
<td>120,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Indianapolis, IN</td>
<td>Reverb/ Elec</td>
<td>-</td>
<td>120,000</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Middletown, NY</td>
<td>Reverb / Blast</td>
<td>-</td>
<td>120,000</td>
</tr>
<tr>
<td></td>
<td>Sanders</td>
<td>Troy, AL</td>
<td>Blast</td>
<td>-</td>
<td>100,000</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td>290,000</td>
<td>1,798,000</td>
</tr>
</tbody>
</table>
2.1.1 Lead Acid Battery

Figure 2.1 shows a schematic of a typical lead acid battery. Lead acid batteries are ideal for all types of vehicles because of their large power-to-weight ratio, which allows them to supply the high surge currents required by automobile engine starters [9]. Various advances in lead acid battery technology have also made them viable as power storage cells at emergency power stations for hospitals and computer servers. They are also used as storage cells for renewable energy sources, such as wind turbines and solar cells [10].

![Schematic of a typical lead acid battery](image)

The major components of the lead acid battery are the sulfuric acid electrolyte, the positive and negative lead plates, metallic and oxide lead grid parts and posts, the plastic battery casing and the silica separators [4]. Table 2.2 gives a breakdown of these battery components by weight.

<table>
<thead>
<tr>
<th>Description</th>
<th>Weight (lbs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Battery paste</td>
<td>14</td>
</tr>
<tr>
<td>Battery grids &amp; posts</td>
<td>9</td>
</tr>
<tr>
<td>Casing</td>
<td>2</td>
</tr>
<tr>
<td>Separators</td>
<td>1</td>
</tr>
<tr>
<td>Sulfuric acid</td>
<td>10</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>36</strong></td>
</tr>
</tbody>
</table>
The plastic casing is usually made from polyethylene but can also be constructed from alternative co-polymers, various metals or a synthetic rubber [11]. Before use, the positive electrode plate typically consists of pure lead dioxide paste that is supported on a metallic grid. The spent battery paste is much more complex and not only contains lead dioxide but also lead oxide, lead sulfate and a small amount of metallic lead. The negative electrode plate consists of a grid of metallic lead alloy containing various elemental additives [12]. Alloying elements are used in the construction of the battery grids in order to improve strength and increase corrosion resistance as well as reduce overpotential and internal resistances [13]. The plates are immersed in a liquid electrolyte consisting of 35% sulfuric acid and 65% water. The electrolyte facilitates the chemical reactions that enable the storage and discharge of electrical energy and permit the passage of electrons that provide the current flow. The terminal posts used to connect the battery to the car are also made of metallic lead [4]. Table 2.3 shows a chemical breakdown of the major compounds in the spent battery grid and paste after physical concentration operations have occurred.

Table 2.3: Typical U.S. Lead Acid Battery Grid and Paste Analyses After Physical Concentration Operations have been Performed [4]

<table>
<thead>
<tr>
<th>Component</th>
<th>Grid (%)</th>
<th>Paste (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb</td>
<td>90</td>
<td>1 – 5</td>
</tr>
<tr>
<td>PbOx</td>
<td>1</td>
<td>20 – 25</td>
</tr>
<tr>
<td>PbSO₄</td>
<td>1</td>
<td>55 – 60</td>
</tr>
<tr>
<td>Sb</td>
<td>0.6</td>
<td>0.2</td>
</tr>
<tr>
<td>Sn</td>
<td>0.4</td>
<td>&lt; 0.1</td>
</tr>
<tr>
<td>As</td>
<td>0.1</td>
<td>&lt; 0.1</td>
</tr>
<tr>
<td>Organics</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Moisture</td>
<td>3 – 8</td>
<td>8 – 20</td>
</tr>
<tr>
<td>Silica</td>
<td>-</td>
<td>2</td>
</tr>
<tr>
<td>Carbon</td>
<td>-</td>
<td>2</td>
</tr>
</tbody>
</table>

2.1.2 Lead Acid Battery Recycling Processes

Figure 2.2 shows a schematic of the general process used for the recycling of lead acid batteries. Most secondary lead battery scraps are recycled through a combination of physical concentration, hydrometallurgical and pyrometallurgical processes [4], [11], [12], [14]–[16]. The first step in the process is to break the battery casing and drain the spent electrolyte. Various lead processing facilities handle the spent sulfuric acid electrolyte in different ways, such as recover it as a saleable product or use it to make pH adjustments for other unit processes within the plant. The drained batteries are then shredded. The most common equipment used for the shredding of the batteries are hammer mills. The
shredded material undergoes a series of separation and concentration steps in which three major material fractions emerge: battery casings, battery paste and a metallic fraction.

The battery casing fraction mainly consists of polypropylene which is typically either sold or further processed on site into pellets by extrusion for use in injection molding. In most cases, the battery paste fraction which is a mixture of lead sulfate, oxidized lead and metallic lead or alloy, will be subjected to a sulfur removal stage using caustic or soda ash leach solutions. The reaction of lead sulfate with either soda ash or caustic proceeds by the following reactions [4]:

\[
PbSO_4 + Na_2CO_3 \rightarrow PbCO_3 + Na_2SO_4
\]

\[
PbSO_4 + NaOH \rightarrow PbO + Na_2SO_4 + H_2O
\]

Battery paste that has been leached in soda ash solutions has reportedly lowered the sulfur content from 5% to less than 0.5%. The use of caustic or soda ash leach tanks for early sulfur removal has become
popular as it greatly minimizes SO$_2$ emissions and matte generation during subsequent smelting operations. After the sulfur removal stage, the battery paste is dried and fed into a series of pyrometallurgical furnaces along with the metallic fraction. The refractory lining in these pyrometallurgical furnaces is subjected to significant wear and must be replaced on a regular basis [17]. Magnesia-chromite refractory are the preferred material for refractorylinings in the secondary lead industries due to their high corrosion and erosion resistance [18], [19].

In the United States, the most typical furnace setup used to produce secondary lead is a combination of a reverberatory and blast furnace. The feed material is first processed in the reverberatory furnace which has a neutral to slightly reducing atmosphere and is typically continuously tapped and co-current. The feed material is mixed with coke or coal to aid in reduction and other fluxes (i.e silica sand) to promote slag formation. The carbon input will reduce the lead according to [4]:

$$2\text{PbO} + C (s) \rightarrow 2\text{Pb} + \text{CO}_2 (g)$$

Some of the lead is also reduced with less noble metal impurities present in the feed like antimony, arsenic and tin. These reduction reactions proceed according to [4]:

$$\text{PbO} + \text{Sn} \rightarrow \text{Pb} + \text{SnO}.$$  

$$3\text{PbO} + 2\text{Sb} \rightarrow 3\text{Pb} + 2\text{Sb}_2\text{O}_3$$  

$$3\text{PbO} + 2\text{As} \rightarrow 3\text{Pb} + 2\text{As}_2\text{O}_3$$

The outputs from this furnace are a “soft” or impurity free lead bullion and a slag rich in impurities as well as lead oxide.

The slag from the reverberatory furnace is then processed in the blast furnace to recover the lead content. In contrast to the reverberatory furnace, the blast furnace is not continuously tapped and operates in a counter-current fashion. This furnace has a much more reducing atmosphere than the reverberatory furnace to ensure that the maximum amount of lead is recovered from the reverberatory furnace slag. The blast furnace can be fluxed with iron which will also help reduce the lead oxide according to [15]:

$$\text{PbO} + \text{Fe} \rightarrow \text{Pb} + \text{FeO}$$

The reducing atmosphere of the blast furnace produces a “hard” or impurity containing lead and a slag with little lead content. This slag is disposed of after processing. The typical slag system in both the reverberatory and blast furnace is a mixture of FeO, SiO$_2$, CaO and Na$_2$O which can be highly corrosive. The Na$_2$O is introduced from the upstream de-sulfurization process and the rest of the slag constituents are flux additions to the feed material. The “soft” and “hard” lead from the furnaces both undergo various refining operations and are then cast as salable products [3].
2.2 Causes of Refractory wear in secondary lead processing furnaces

Understanding the mechanisms of wear in lead processing furnaces has been a focus of several studies [17], [19]–[23] in recent years as the rate of refractory wear will directly affect the length of refractory lifetime and productivity of the furnaces. The mechanisms of wear in lead processing furnaces using magnesia-chromite refractory fall under three main categories: chemical, thermal and mechanical [17]. Table 2.4 lists various mechanisms of wear that fall under these three categories.

<table>
<thead>
<tr>
<th>Type</th>
<th>Mechanism</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical</td>
<td>Acidic slag attack &amp; infiltration</td>
<td>Dissolution reaction occurring at the immediate refractory hot face within the refractory microstructure causing intergranular corrosion and weakening of refractory microstructure</td>
</tr>
<tr>
<td>Chemical</td>
<td>Forsterite Bursting</td>
<td>Formation of forsterite ($\text{Mg}_2\text{SiO}_4$) causes a volume expansion resulting in the destruction of refractory structure due to structural spalling</td>
</tr>
<tr>
<td>Chemical</td>
<td>Sulfur Corrosion</td>
<td>Penetration of $\text{SO}_2$ into the refractory causes formation of $\text{SO}_3$ which reacts with $\text{MgO}$ to form $\text{MgSO}_4$ and results in degeneration of the refractory microstructure</td>
</tr>
<tr>
<td>Chemical</td>
<td>Iron oxide attack</td>
<td>High iron oxide results in degeneration of refractory microstructure due to the formation of Mg-Fe oxide</td>
</tr>
<tr>
<td>Chemical</td>
<td>High Na$_2$O supply</td>
<td>Alkali oxides (i.e., Na$_2$O) enhance oxidation of Cr$^{+3}$ to Cr$^{+6}$ in magnesia-chromite refractory. Cr$^{+6}$ can react with soda and deposit sodium bearing chromates or chromium salts on the refractory surface furthering degeneration of the refractory</td>
</tr>
<tr>
<td>Chemical</td>
<td>Hydration</td>
<td>MgO reacts with H$_2$O to form brucite (Mg(OH)$_2$) causing expansion in the refractory resulting in cracks</td>
</tr>
<tr>
<td>Thermal</td>
<td>Temperature Levels</td>
<td>Areas of hot spots within the furnace / overheating</td>
</tr>
<tr>
<td>Thermal</td>
<td>Thermal shock</td>
<td>Thermal fluctuations caused by disruptions and by irregularities in furnace operation or improper heat up procedures can cause stresses in the refractories</td>
</tr>
<tr>
<td>Thermal</td>
<td>Noncorrosive metal infiltration</td>
<td>Causes densification of the refractory resulting in area of differing thermal expansion coefficients which can cause high internal stresses</td>
</tr>
<tr>
<td>Mechanical</td>
<td>Erosion</td>
<td>Wear of refractory due to interaction with high velocity dust-laden combustion gas and/or low viscosity slag</td>
</tr>
</tbody>
</table>
The wear of these types of refractory can be continuous (corrosion or erosion) or discontinuous (cracking or spalling) [21]. Chemical attack through the interaction of the refractory with the slag and other feed components has been cited as the main factor affecting refractory damage in secondary lead furnaces. Temperature and turbulence are cited as being lesser but still important factors of wear. Although, in many cases, refractory wear can be caused by a combination of chemical, thermal and mechanical mechanisms. For example, weakened microstructures due to slag attack and metal infiltration can make refractory more susceptible to continuous wear by hot erosion [19].

Table 2.5 lists the locations of the wear mechanisms specifically experienced in reverberatory furnaces used to process lead. High wear areas are reported to occur on the roof above the furnace charge and on the side wall across from the charge or burden. Wear in these types of furnaces has also been reported at the opening of the flue. Roof wear is typically very significant in reverberatory furnaces due to the impingement of the burner flame on the furnace burden which can cause hot flows to be directed at the roof. The roof of the reverberatory furnace typically experiences wear due to mainly thermal and some chemical mechanisms whereas the side wall wear has been contributed to all three types of mechanisms [17].

Table 2.5: Typical Locations of Wear Mechanisms within Reverberatory Furnaces used in Lead Processing [17]

<table>
<thead>
<tr>
<th>Type</th>
<th>Mechanism</th>
<th>Roof</th>
<th>Wall</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical</td>
<td>Acidic slag attack &amp; infiltration</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Sulfur Corrosion</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Iron oxide attack</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td></td>
<td>High Na$_2$O supply</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Hydration</td>
<td>+</td>
<td>±</td>
</tr>
<tr>
<td>Thermal</td>
<td>Temperature Levels</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Thermal Shock</td>
<td></td>
<td>+</td>
</tr>
<tr>
<td></td>
<td>Noncorrosive metal infiltration</td>
<td>±</td>
<td>+</td>
</tr>
<tr>
<td>Mechanical</td>
<td>Erosion</td>
<td></td>
<td>+</td>
</tr>
</tbody>
</table>

+ Standard phenomenon
± Possible phenomenon
CHAPTER 3
BACKGROUND THEORY FOR COMPUTATIONAL FLUID DYNAMIC MODELING

This chapter details background theory for computational fluid dynamic (CFD) modeling. The following sections focus on the mathematical principles behind CFD modeling as well as the various sub-models used for the simulation of metallurgical furnaces. Also included in this chapter is a literature review of the CFD modeling studies done on reverberatory, rotary, and blast furnaces. The information gained from the background theory was used for the setup and evaluation of the CFD model.

3.1 Introduction to CFD

Computational Fluid Dynamics is a branch of fluid mechanics that uses numerical methods and algorithms for multiphase fluid analysis for both reacting and non-reacting flows and can include complexities which couple thermodynamics, heat transfer, turbulence, and chemical reactions. Figure 3.1 illustrates that CFD can be thought of as a combination of three different disciplines: fluid dynamics, computer science and mathematics. All of these disciplines are needed to develop an accurate and representative CFD model. These models can be used for predictive purposes to test different scenarios that may be too risky or expensive to try in existing operations, to test how processes will scale up, to simulate the consequences of potentially dangerous conditions and to control and optimize existing processes [24].

Figure 3.1 The different disciplines involved in the development of computational fluid dynamics [24].
CFD modeling is based on the fundamental governing equations of fluid dynamics which are the conservation of mass, conservation of momentum and conservation of energy. The conservation of a certain fluid property means that its total variation inside an arbitrary volume can be expressed as the net amount of the quantity being transported across the boundary, of any internal forces and sources and of external forces acting on the volume. As such, CFD is typically constructed on the basis of finite control volumes or an arbitrary finite region of the flow which is bounded by a closed surface and fixed in space [25]. The governing equations are complex partial differential equations (PDE) that are very difficult or impossible to solve analytically. Therefore, the first step in obtaining a computational solution of the control volume or computational domain is to convert the PDEs and corresponding boundary and initial conditions into a system of discrete algebraic equations that can be solved using various boundary and initial numerical methods. This process is known as discretization. Discretization is mainly accomplished through a few different common methods, namely the finite-difference method (FDM), finite-volume method (FVM) and the finite-element method (FEM). The FDM, FVM and FEM are all considered to be local methods as they can be identified in terms of discrete nodal unknowns. Although these methods are utilized in the majority of CFD codes, there are other methods that are used to discretize the governing equations. Spectral methods are becoming more common for solving CFD problems. Unlike the FDM, FVM and FEM, spectral methods are global methods where the computation at any given point depends not only on the information at the neighboring points, but also on the information from the entire domain [24].

Currently, almost all commercial CFD software utilizes the FVM for discretization. In the FVM, the governing equations are discretized by dividing the computational domain into a finite number of elementary control volumes. The network of these finite control volumes is called the grid or mesh. Solutions for the governing equations are then approximated in each mesh element or cell. The FVM starts by integrating the governing equations over the volume of each cell. The Gauss theorem is then applied to transform the volume integrals into surface integrals. These terms are evaluated as fluxes at the surfaces of each finite volume which are then transformed into discrete integrals and integrated numerically [26], [27]. The FVM approximations for first and second order partial differentials are described mathematically by [24]:

\[
\frac{\partial \phi}{\partial x_1} \cdot \frac{1}{\Delta V} \int \frac{\partial \phi}{\partial x_1} \, dV = \frac{1}{\Delta V} \int \phi \, dA_i \approx \frac{1}{\Delta V} \sum_{n=1}^{N} \phi_n A_{n_i} \tag{3.1a}
\]

\[
\frac{\partial^2 \phi}{\partial x_1^2} \cdot \frac{1}{\Delta V} \int \frac{\partial^2 \phi}{\partial x_1^2} \, dV = \frac{1}{\Delta V} \int \frac{\partial \phi}{\partial x_1} \, dA_i \approx \frac{1}{\Delta V} \sum_{n=1}^{N} \left( \frac{\partial \phi}{\partial x_{1_i}} \right)_n A_{n_i} \tag{3.1b}
\]
where \( \phi \) is a generic flow field variable and \( N \) represents the number of bonding surfaces on an elemental volume.

The FVM is advantageous for CFD problems for two main reasons. The first advantage to the FVM is that its mathematical formulation mirrors the physics and the conservation principles it models. The second advantage is that this method can accommodate both structured and unstructured meshes whereas the FDM can only be used with structured grids. In structured grids, each grid point can be identified by a set of three indices. In contrast, points in unstructured grids have no ordering and neighboring cells or grid points cannot be directly identified by their indexes. Figure 3.2 shows examples of 2D structured and unstructured meshes. Unstructured grids offer greater flexibility for handling complex geometries [24], [26].

![Control Volume](image1)

(a) Structured Mesh

![Control Volume](image2)

(b) Unstructured Mesh

Figure 3.2 Examples of 2D (a) structured and (b) unstructured meshes [24].

The solution techniques used to solve a CFD problem are iterative processes that successively improve the solution until the criteria for convergence are reached. Convergence of a numerical process is when the solution of the system of algebraic equations used to approximate PDEs approached the true solution of the PDEs. During the numerical procedure, imbalances (errors) of the discretized PDEs occur which are called residuals. The three general conditions that must be satisfied to ensure the CFD solution has converged are:

1) The residual values have reduced to an acceptable value
2) Iterative convergence has been achieved
3) Mesh independence has been achieved
The acceptable value for normalized residuals for most flow variables is $10^{-3}$ which indicates a 0.01% error. It is also recommended that the residual values drop three orders of magnitude. Stricter convergence consideration is typically required for the energy and species residuals. For most situations, the energy residual must reach a value of $10^{-6}$ and the species residual must reach a value of $10^{-5}$ for convergence to be achieved. Iterative convergence means that the parameters of interest (e.g. temperature, pressure, velocity) in the model have reached a steady value and do not change with additional numerical iterations. Mesh independence is achieved when the parameters of interest in the model no longer change with additional mesh refinement (i.e. reducing the cell size) [28].

The following sections detail the governing equations solved in each cell. Descriptions and transport equations of the different sub-models used to simulate metallurgical furnaces have also been described. The forms of the equations presented and the descriptions of the particular sub-models are specific to ANSYS Fluent 17.0 [29] commercial CFD software which was used in this research.

### 3.2 Navier-Stokes Equations

The Navier-Stokes equations describe the physics of fluid flow and are the fundamental basis for CFD modeling. These equations are derived from two governing equations of fluid dynamics, the continuity equation and the momentum equation [30], [31]. The continuity equation states that mass is conserved and for a finite control volume is mathematically described by the following equation [28]:

$$\frac{\partial \rho}{\partial t} + \nabla (\rho \mathbf{v}) = 0$$

The momentum equation is a form of Newton’s second law and states that the rate of change of momentum equals the sum of the forces acting on the fluid. Both body forces and surface forces are included in the momentum force balance. The resulting momentum equations for a finite volume are [28]:

$$\frac{D(\rho \mathbf{v}_1)}{Dt} = \frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \tau_{21}}{\partial x_2} + \frac{\partial \tau_{31}}{\partial x_3} + \sum F_{1\text{body forces}}$$

$$\frac{D(\rho \mathbf{v}_2)}{Dt} = \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \tau_{21}}{\partial x_1} + \frac{\partial \tau_{32}}{\partial x_3} + \sum F_{2\text{body forces}}$$

$$\frac{D(\rho \mathbf{v}_3)}{Dt} = \frac{\partial \sigma_{33}}{\partial x_3} + \frac{\partial \tau_{13}}{\partial x_1} + \frac{\partial \tau_{32}}{\partial x_2} + \sum F_{3\text{body forces}}$$

where $\frac{D}{Dt}$ is the substantial derivative, $\sigma$ is the normal stress due to pressure, $P$, and $\tau$ is the viscous or shear stress component.
Figure 3.3 shows a schematic of the normal and shear stresses acting on a finite fluid volume.

Figure 3.3 Schematic of the (a) normal and (b) shear stresses acting on a finite fluid volume [25].

For a Newtonian fluid where viscosity is constant, the normal stresses can be defined as [28]:

\[
\sigma_{11} = -P + 2\mu \frac{\partial v_1}{\partial x_1} \tag{3.4a}
\]
\[
\sigma_{22} = -P + 2\mu \frac{\partial v_2}{\partial x_2} \tag{3.4b}
\]
\[
\sigma_{33} = -P + 2\mu \frac{\partial v_3}{\partial x_3} \tag{3.4c}
\]

and the viscous or shear stresses can be defined as [28]:

\[
\tau_{12} = \tau_{21} = \mu \left( \frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1} \right) \tag{3.5a}
\]
\[
\tau_{23} = \tau_{32} = \mu \left( \frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_2} \right) \tag{3.5b}
\]
\[
\tau_{13} = \tau_{31} = \mu \left( \frac{\partial v_3}{\partial x_1} + \frac{\partial v_1}{\partial x_3} \right) \tag{3.5c}
\]

where \( \mu \) is the dynamic viscosity. The normal and viscous stresses as defined in Equations 3.4 and 3.5 can be substituted into Equations 3.3 and simplified by using the continuity equation for incompressible flow where density remains constant. These substitutions yield the following vector form of the Navier-Stokes equation for incompressible, Newtonian fluids [27]:
\[
\rho \frac{Dv}{Dt} = -\nabla p + \mu \nabla^2 v + \rho g
\]  

(3.6)

This form of the Navier-Stokes equation is easily recognized as a form of Newton’s second law where density (\(\rho\)) times acceleration (\(\frac{Dv}{Dt}\)) equals the sum of forces, i.e. pressure force (\(-\nabla P\)), viscous force (\(\mu \nabla^2 v\)) and gravity or body force (\(\rho g\)). If the fluid is compressible and/or non-Newtonian, the general vector form of the Navier-Stokes must be used and is written as [27]:

\[
\frac{\partial (\rho v)}{\partial t} = -[\nabla \cdot (\rho v v)] - \nabla P - [\nabla \cdot T] + \rho g
\]

(3.7)

where \(\rho v v\) is the dyadic product of \(\rho v\) and \(v\). Due to the complex nature of the Navier-Stokes equations, analytical solutions range from difficult to practically impossible. Therefore, the most common way to make use of the Navier-Stokes equations is through computational modeling.

The existence of turbulence also adds complexity to the Navier-Stokes equation. In turbulent flow, the motion of the fluid particles is irregular and all flow properties vary in a random and chaotic way. Turbulent flow is characterized by large Reynolds numbers (\(Re\)) or high inertia to viscous forces. The flow is laminar when \(Re < 2300\), transitional when \(2300 < Re < 4000\) and turbulent when \(Re > 4000\) [31]. In principle, turbulent flow can be modeled by the Navier-Stokes equations, but it is not feasible in most situations to resolve the wide range of scales in time and space by Direct Numerical Simulation (DNS). For this reason, the Reynolds Averaged Naiver-Stokes (RANS) equations were developed. The RANS equations are time averaged governing equations in which all instantaneous fluctuations in the flow field are eliminated and a smooth variation of the averaged velocity and pressure fields can be obtained. The RANS equations have the same general form as the instantaneous Navier-Stokes equation with the velocities and other flow field variables now representing time-averaged values. Therefore, the generic flow field variable, \(\phi\), can be represented as [32]:

\[
\phi_t = \bar{\phi}_t + \phi'_t
\]

(3.8)

where \(\bar{\phi}_t\) and \(\phi'_t\) are the mean and fluctuating components of the variable, respectively. Although this averaging process reduces overall complexity, additional unknown terms called Reynolds stresses or fluxes are introduced into the transport equations that need to be described by a suitable turbulence model [33].

### 3.3 Turbulence Models

Various turbulence sub-models based on the RANS equations are available within ANSYS Fluent. Fluent also provides sub-models based on Scale-Resolving Simulations (SRS) methods which
partially resolve the full turbulent spectrum in the flow domain. For this reason, the SRS models are substantially more computationally expensive than RANS simulations. In most cases, RANS turbulence models offer the most economic approach for computing complex turbulent industrial flow [34]. The most commonly used RANS models are the k-ε and the k-ω models in their different forms. Both models are two equations models that allow for the determination of both a turbulent length and time scale by solving two separate transport equations [32], [35]. The following transport equations are written in Cartesian tensor form with \(i = 1,2,3\)

3.3.1 The k-ε model

The standard k-ε model is based on the transport equations for the turbulent kinetic energy (\(k\)) and its rate of dissipation (\(\varepsilon\)). The k-ε models are very robust and can be used to describe a wide range of turbulent flows with reasonable accuracy. Two variants of the standard k-ε model are available within Fluent: the RNG k-ε model and the realizable k-ε model. These variants were developed to better handle different flow applications. All three models have very similar forms with transport equations for \(k\) and \(\varepsilon\).

The main differences between the models related to the method of calculating turbulent viscosity and the turbulent Prandtl number governing the turbulent diffusion of \(k\) and \(\varepsilon\) as well as the generation and destruction terms in the \(\varepsilon\) equation. The major weakness of these models is their insensitivity to adverse pressure gradients and boundary layer separation which can lead to optimistic design evaluations for flows that separate from smooth surfaces [33].

The transport equations for the k-ε model are [32]:

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho k v_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \mu_t \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \tag{3.9}
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon v_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_3 \varepsilon G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \tag{3.10}
\]

where \(\mu_t\) is the turbulence viscosity defined as [32]:

\[
\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} \tag{3.11}
\]

and \(G_k\) represents the generation of turbulence kinetic energy due to mean velocity gradient and \(G_b\) is the generation of turbulence kinetic energy due to buoyancy. \(Y_M\) represents the contribution of the fluctuating dilation in compressible turbulence to the overall dissipation rate. The theory on how to calculate these parameters can be found in the ANSYS Fluent Theory Guide [32]. \(C_{1\varepsilon}, C_{2\varepsilon}, C_{\mu}, \sigma_\varepsilon\) and \(\sigma_\varepsilon\) are all empirical
model constants. The default values for these constants have been determined from experiments on fundamental turbulent flows. $S_k$ and $S_\epsilon$ are user-defined source terms [32], [33].

3.3.2 The $k-\omega$ model

The standard $k-\omega$ model is based on the transport equations for the turbulent kinetic energy ($k$) and the specific dissipation rate ($\omega$). The $k-\omega$ turbulence model offers some advantages over the $k-\epsilon$ model. The most significant advantage is the model’s ability to predict adverse pressure gradients due to boundary layer flows and separation. The downside to this model is that the solution can be sensitive to the freestream values of $k$ and $\omega$. For this reason, a variant of the $k-\omega$ model was developed called the shear-stress transport (SST) $k-\omega$ model. Both models have very similar forms, but the SST $k-\omega$ was designed to avoid the freestream sensitivity of the standard $k-\omega$ model by combining elements of the $\omega$-equation and the $\epsilon$-equation [33].

The transport equations for the standard $k-\omega$ model are: [32]

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho k v_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \Gamma_k \frac{\partial k}{\partial x_i} \right) + G_k - Y_k + S_k \tag{3.12}
\]

\[
\frac{\partial (\rho \omega)}{\partial t} + \frac{\partial (\rho \omega v_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \Gamma_\omega \frac{\partial \omega}{\partial x_i} \right) + G_\omega - Y_\omega + S_\omega \tag{3.13}
\]

where $\Gamma_k$ and $\Gamma_\omega$ represent the effective diffusivity of $k$ and $\omega$. $G_k$ and $G_\omega$ denote the generation of the turbulence kinetic energy due to mean velocity gradients and the generation of $\omega$, respectively. $Y_k$ and $Y_\omega$ represent the dissipation of $k$ and $\omega$ due to turbulence. $S_k$ and $S_\omega$ are user-defined source terms. The theory on how Fluent calculates these specific parameters can be found in the ANSYS Fluent Theory Guide [32].

3.4 The Energy Equation

The third governing equation on which CFD is fundamentally based is the energy equation. The energy equation is derived from the first law of thermodynamics which states that the rate of change of energy equals the sum of the rate of heat addition to the fluid and the rate of work done on or by the fluid [24]. Fluent includes physical models for all three modes of heat transfer: conduction, convection and radiation. These modes of heat transfer are described by the following area heat flux equations [36]:

\[
q_{\text{cond}} = -k \nabla T \tag{3.14}
\]

\[
q_{\text{conv}} = h(T_s - T_\infty) \tag{3.15}
\]

\[
q_{\text{rad}} = \varepsilon \sigma (T_{\text{max}}^4 - T_{\text{min}}^4) \tag{3.16}
\]
where \( q \) is the heat flux, \( k \) is the thermal conductivity, \( h \) is the heat transfer coefficient, \( \varepsilon \) is the emissivity and \( \sigma \) is the Stefan-Boltzmann constant. \( T_s \) and \( T_\infty \) are the surface and fluid temperatures, respectively.

 Fluent will solve a variation of the energy equation depending on the heat transfer methods the user has selected. The general form of the energy equations is [32]:

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho (\rho E + p)) = \nabla \cdot \left( k_{\text{eff}} \nabla T - \sum_j h_j J_j + (T_{\text{eff}} \cdot \mathbf{v}) \right) + S_h
\]  

(3.17)

where \( k_{\text{eff}} \) is the effective conductivity defined as [32]:

\[
k_{\text{eff}} = k + k_t
\]

(3.18)

and \( k_t \) is the turbulent thermal conductivity, \( J_j \) is the diffusion flux of species \( j \), \( T_{\text{eff}} \) is the effective shear stress and \( S_h \) is a source term used to capture heat of a chemical reaction and any other volumetric heat source the user defines. Conductive and convective heat transfer modes are explicitly solved by a variation of the energy equation whereas radiation heat transfer is taken into account through the selection of different sub-models. Therefore, \( S_h \) will also include radiation source terms when a radiation model is being used [33]. \( E \) in Equation 3.16 is the total energy per unit mass and is defined as [32]:

\[
E = h - \frac{p}{\rho} + \frac{v^2}{2}
\]

(3.19)

where \( h \) is the sensible enthalpy defined as [32]:

\[
h = \sum_j Y_j h_j
\]

(3.20)

\( Y_j \) is the mass fraction of species \( j \) and \( h_j \) in both Equations 3.13 and 3.16 is defined as [32]:

\[
h_j = \int_{T_{\text{ref}}}^{T} C_{p,j} \, dT
\]

(3.21)

### 3.4.1 Radiation Models

Radiation is the emission of thermal energy through electromagnetic waves from the surface of an object. Radiation models should be considered when the radiant heat flux is large compared to the heat transfer rate due to convection or conduction. This typically occurs when the absolute temperatures rather than temperature gradients are large as radiative heat flux has a fourth order dependency on absolute temperature as described in Equation 3.16 [36]. The radiative transfer equation (RTE) used to model radiation describes the intensity of a beam of radiation when it travels, how it loses energy through
absorption, how it redistributes radiation through scattering and gains energy through emission. The form of the RTE used by the Fluent radiation sub-models is [32]:

\[
\frac{dl(r,s)}{ds} + (a + \sigma_s)l(r,s) = an^2 \frac{\sigma T^4}{4\pi} \int_0^{4\pi} l(r, s') \Phi(s \cdot s') d\Omega'
\]

(3.21)

where

- \( r \) = position vector
- \( s \) = direction vector
- \( s' \) = scattering direction vector
- \( s \) = path length
- \( a \) = absorption coefficient
- \( n \) = refractive coefficient
- \( \sigma_s \) = scattering coefficient
- \( \sigma \) = Stefan-Boltzmann constant
- \( I \) = radiation intensity which depends on position \( (r) \) and direction \( (s) \)
- \( T \) = local temperature
- \( \Phi \) = phase function
- \( \Omega' \) = solid angle

Five sub-models for radiation are built into ANSYS Fluent. The five models are the Discrete Transfer radiation model (DTRM), the P-1 Radiation model, the Rosseland radiation model, the Surface-to-Surface (S2S) radiation model and Discrete Ordinate (DO) radiation model. The DTRM is based on the assumption that the radiation leaving a surface element in a certain range of solid angles can be approximated by a single ray. It is a relatively simple approach and its accuracy can be increased by increasing the number of rays. However, solving a problem with a large number of rays can become computationally demanding. The P-1 mode is based on the expansion of the radiation intensity \( (I) \) into an orthogonal series of spherical harmonics. This model works well for combustion applications where the optical thickness is large. The Rosseland radiation model is derived from the P-1 model but is only valid when the medium is optically thick. The S2S radiation model is typically used for modeling radiative transfer in an enclosure of gray-diffuse surfaces without participating media. The main assumption in this model is that any absorption, emission or scattering of radiation can be ignored. This model requires the calculation of view factors, which are geometric functions used to account for the dependence of radiative energy exchange as a function of the size, separation distance and orientation of the surfaces within the enclosure [36]. The DO model solves the RTE for a finite number of discrete solid angles. The DO model is valid in the entire range of optical thicknesses which means it can be used to model a wide...
variety of problems ranging from surface to surface radiation to participating radiation in combustion. One notable advantage of the P-1 and DO radiation models is that they can be used when a mixture material is modeled. In these models, radiative properties are computed based on the volume fraction averaging of the radiative properties of the individual phases. Addition theory and information on transport equations for the specific models can be found in ANSYS Fluent Theory Guide [32].

3.5 Combustion Modeling

ANSYS Fluent includes many different built-in reaction sub-models to simulate the combustion reactions typically experienced in metallurgical furnaces. Reactions for which the kinetics cannot be practically described by Arrhenius rate style kinetics are not standard in Fluent. Other styles of kinetics can be added through user defined source terms. The three different types of combustion that can be modeled in Fluent are premixed, partially premixed and non-premixed [32], [33]. In premixed combustion, the fuel and oxidizer are mixed at the molecular level prior to ignition making the reaction kinetically limited rather than diffusion limited. In non-premixed combustion, the fuel and oxidizer enter the reaction zone in distinct streams and is considered to be a mixing problem with infinitely fast chemistry. Partially premixed combustion is an intermediate between premixed and non-premixed combustion [37].

Built in sub-models based on finite-rate chemistry governed by the Arrhenius equation can be used to simulate the three types of combustion within Fluent. These are not dedicated combustion models but rather species transport / chemical reaction models. The four available sub-models of this type are: (1) finite-rate chemistry, (2) finite-rate/eddy-dissipation, (3) eddy-dissipation and (4) eddy-dissipation concept (EMC) models. The eddy-dissipation model (EDM) and the finite-rate chemistry model (FRC) are used to simulate fast and slow reactions, respectively, when compared to rate of mixing of reactants due to turbulent flows. The FRC model uses molecular kinetics to calculate the reaction rates whereas the EDM calculates the mean reaction rate based on the turbulent mixing rate with the assumption that the chemical reactions occur much faster than turbulence can mix reactants and heat into the reaction region. The finite rate/eddy dissipation model is a hybrid of the FRC and EDM models. In this model, the kinetic rate is calculated in addition to the mixing rate predicted by the eddy-dissipation model. The slowest reaction rate is the one that is used. If turbulence is low, mixing will be slow and thereby limit the reaction rate. On the other hand, if turbulence is high, but the kinetic rate is low, the reaction will be kinetically limited. Partially premixed flames can also be modeled using the finite-rate/eddy-dissipation model. The EMC model is an extension of the EDM model where detailed chemical mechanisms are incorporated into turbulent reacting flows which is very computationally expensive [32], [33].
Fluent also has dedicated combustion models for premixed, partially premixed and non-premixed combustion problems. Premixed combustion is much more difficult to model than non-premixed combustion. The difficulty arises because premixed combustion occurs as a thin, propagating flame that is stretched and contorted by turbulence. Therefore, the essence of the premixed combustion model is to capture the turbulent flame speed which is influenced by both the laminar flame speed and the turbulence. The premixed combustion model uses either the C-equation or the G-equation for the basis of the calculation. The C-equation method tracks the flame front by evaluating the progression of the reaction from unburnt to burnt species. The G-equation method tracks the flame-front through the transport equations governing the unsteady evolution of a propagating flame interface [32].

The dedicated non-premixed combustion model was developed to simulate turbulent diffusion flames with fast chemistry where the reaction rate is limited by mixing. For this type of combustion, this approach offers benefits over the eddy-dissipation model as it allows for intermediate species prediction, dissociation effects and rigorous turbulence-chemistry coupling without solving a large number of species transport equations. The non-premixed combustion model solves for the mixture fraction, which is a conserved scalar and is defined as the elemental mass fraction that originated from the fuel stream. In this model, a PDF table is calculated prior to the calculation which is used during the calculation of the reacting flow. The PDF table is a chemistry look-up table containing mean values of species fractions, density and temperature as a function of mean mixture fraction, mixture variance, enthalpy and scalar dissipation [32].

### 3.6 CFD Modeling of Select Metallurgical Furnaces

In many primary and secondary metal industries, CFD modeling has played an increasingly important role as a cost-effective tool for evaluating and improving industrial processes. In recent years, economic and environmental drivers have greatly pushed for the use of CFD to model many types of metallurgical furnaces [36]. This can be challenging though, as metallurgical processing involves various chemical reactions and transport phenomena that take place within a moving media at high temperatures and in the presence of phase transformations. These processes are also intrinsically multi-phase which further increases model complexity [37]. CFD models of metallurgical furnaces have greatly benefited from continuous improvements in the physics and sub-models available in commercial CFD packages. The advancements in commercial CFD packages have provided new mathematical power to more accurately describe turbulence, general gas flow and other transport phenomena within industrial furnaces. This has allowed modern, commercially available computational software to produce high-quality numerical models that are capable of providing detailed and reliable descriptions of the complex processes that are characteristic of the operation of industrial metallurgical furnaces [40].
The secondary aluminum industry has become a major user of CFD and has implemented this technique to analyze and improve the aluminum melting processes [40–52]. There has been an increase in the utilization of CFD modeling in the steel industry for various metallurgical studies of blast furnaces as well [54]. Improvements in production, energy efficiency and furnace operation optimization are the main areas of focus in the literature related to CFD modeling of industrial metallurgical furnaces. Furnace efficiency is typically described by [6]:

$$\eta = \frac{Q_p}{Q_s}$$  \hspace{1cm} (3.22)

where $\eta$ is the furnace efficiency, $Q_p$ is the heat embedded in the final product and $Q_s$ is the heat supplied by combustion. This parameter has been of particular interest to many researchers as it directly affects the cost to produce metal [55]. The following sections describe recent CFD studies on reverberatory, blast and rotary furnaces presented in literature.

### 3.6.1 Reverberatory Furnaces

A traditional reverberatory furnace, often called a reverb, is a type of furnace in which the material under treatment is heated indirectly by means of the combustion gases and radiant heat rather than directly by the burner flame. Its design dates back to the 19th century and has found uses in the copper, lead and aluminum metallurgical industries [7]. This type of furnace is typically only used when neutral or slightly reducing conditions are required for a reduction or for a re-melting process. These furnaces are shaped in a rectangular manner with an arched roof to allow the combustion product of the fuel to be reflected or ‘reverberated’ from the furnace roof to the charge. The long, wide hearth also allows for good phase separation in processes where multiple phases exist. The feed is usually charged through an opening in the roof or the end wall of the furnace. Metal is withdrawn from the furnace through a hole in the side wall and if present, slag typically exits through a notch in the opposite wall [5], [3].

The term “reverberatory furnace” has broadened over the years and has been used to describe direct fire furnaces where the flame is in contact with the charge or burden. As the difference between strictly defined reverberatory furnaces and direct fired hearth furnaces are often down to burner alignment alone, it is difficult to make the distinction to where one starts and the other ends [6]. Figure 3.4 shows both a schematic of (a) a traditional and (b) a direct fire style reverberatory furnace. The CFD studies found in literature only have modeled the modern direct fire style reverberatory furnace [40–49], [51], [52], [56].
Despite the long history of reverberatory furnace use, there still only exists a relatively small body of research pertaining to these types of furnaces. CFD investigations of reverberatory furnaces in recent years have mainly been done in relation to secondary aluminum processing [40 – 49], [51], [52]. The secondary aluminum industry uses reverberatory furnaces for the re-melting of aluminum scrap with varying compositions [59]. Two different types of reverberatory furnaces are used for this application: sidewell and direct charge. Sidewell furnaces have been used for the melting of light scrap for several decades and were originally designed to eliminate the direct interaction between the combustion gases and solid scrap which minimizes the melt loss and dross generation [60], [61]. Sidewell reverberatory
furnaces are fitted with a well separated from the main furnace hearth by a refractory wall with an opening which allows molten metal to flow from the furnace hearth to the sidewell. The solid metal scrap is charged into the sidewell and melts which means that only two phases need to be modeled within the furnace hearth: molten metal and the combustion gases [39], [59]. Figure 3.5 shows a simplified top down cross section of a sidewell furnace where the sidewell is separated into a charge and pump well. The direct charged reverberatory furnaces do not have sidewells and the metal scrap is charged directly into the furnace hearth where it is exposed to the open flames. Figure 3.4a is an example of a direct charge furnace. Three phases are present in the hearth of the direct charge reverberatory furnace: molten metal, solid metal charge and combustion gases. Although the presence of the third phase makes the direct charge furnaces more difficult to model than the sidewell furnaces, there have been many more CFD studies performed on direct charge rather than sidewell reverberatory furnaces [40 – 49], [51], [52], [56]. The main areas of focus in these studies are burner type and location, applicability of various sub-models, evaluation of new furnace designs and the use of lab scale furnaces in conjunction with CFD modeling.

![Cross section of a simple sidewell furnace with a charge and pump well](image)

**Figure 3.5** Cross section of a simple sidewell furnace with a charge and pump well [39].

### 3.6.1.1 Burner Type and Location

The influence of burner type and location has been an area of focus for CFD modeling of direct fired reverberatory furnaces over the past several years. Baukal *et al.* [39] reports a study done to model a sidewell reverberatory furnace used to produce aluminum at the Roth Bros Corporation using ANSYS Fluent. The main propose of the study was to evaluate the use of three different burner types: air/fuel (AF), air-oxy/fuel (AOF) and oxy/fuel (OF). The model was designed to solve both laminar and turbulent
flow conditions for the separate phases simultaneously; the combustion gases were solved under turbulent flow conditions while the flow of the aluminum bath was considered laminar. The CFD model showed the advantages and disadvantages for each firing mode. For example, a model comparison of the three firing modes showed that the specified firing rate was not high enough to melt the aluminum at the desired rate of production with the AF burner. On the other hand, the AOF and OF burners could melt the aluminum at the desired production rate under the specified firing rate and therefore consumed less natural gas per unit aluminum produced. Other parameters were investigated for the three burner types such as refractory temperature profiles as well as conditions that contributed to overheating and oxidation of the melt surface.

Furu et al. [43] also studied the impact of different burner types for the melting of aluminum using CFD. This study focused on comparing a newly developed low temperature oxy-fuel (LTOF) burner against a conventional cold air-fuel burner in a pilot scale direct fire furnace. Oxy-fuel combustion technology has been used in the aluminum industry in the past, but high temperature burners of this nature result in high dross formation and furnace wear due to hot spots in refractory linings. The newly developed LTOF burners claimed to have minimized these problems while still maintaining the advantages of oxy-fuel combustion such as reduced heat lost in the flue gas and greater radiation heat transfer [41], [62]. The CFD model was developed using ANSYS Fluent. The realizable k-ε model was used to model turbulence. Heat conduction into the materials, convection at the gas-solid interface and radiation modeled by the DO method were all included in the model as well. Combustion was modeled by the Eddy Dissipation method using a 2-step reaction for propane and air. The main purpose of the CFD simulations was to reproduce measured furnace temperatures and to identify the heat transfer mechanisms created by the burners.

Table 3.1 lists the four different conditions considered and some of the results obtained from lab experiments. The furnace temperature corresponds to the average temperature taken at sixteen different locations within the furnace wall. The CFD model was validated by these measurements. The heating time denotes the time it took to heat an aluminum sample with dimensions of 85 x 85 x 40 mm that was placed in the furnace from 100 to 600 °C. Several conclusions were drawn from this study. Both the experiments and CFD simulations showed that the flame created by the LTOF burner was more spread out which resulted in a more uniform temperature throughout the furnace. The CFD simulations showed that radiation was the dominate form of heat transfer into the aluminum samples. The two burner styles resulted in similar convective heat flux into the sample, but the LTOF burner had a much higher radiative heat flux into the sample due to the absent of nitrogen, thereby facilitating shorter heating times with lower power input.
Table 3.1: Description and Results of the Four Different Firing Conditions Modeled in the Study Performed by Furu et al. [43]

<table>
<thead>
<tr>
<th>Case</th>
<th>Burner Type</th>
<th>Burner Power</th>
<th>Cooling</th>
<th>Furnace T</th>
<th>Heating Time</th>
<th>Average Heat Flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>Units</td>
<td>(kW)</td>
<td>(kW)</td>
<td>(°C)</td>
<td>(s)</td>
<td>(kW / m²)</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>Air-fuel</td>
<td>311</td>
<td>23</td>
<td>1131</td>
<td>688</td>
<td>79</td>
</tr>
<tr>
<td>2</td>
<td>Air-fuel</td>
<td>308</td>
<td>64</td>
<td>1016</td>
<td>766</td>
<td>71</td>
</tr>
<tr>
<td>3</td>
<td>LTOF</td>
<td>257</td>
<td>66</td>
<td>1142</td>
<td>497</td>
<td>109</td>
</tr>
<tr>
<td>4</td>
<td>LTOF</td>
<td>257</td>
<td>133</td>
<td>1008</td>
<td>675</td>
<td>84</td>
</tr>
</tbody>
</table>

Buchholz et al. [49] constructed a CFD model based on an aluminum reverberatory furnace equipped with 1.0 and 2.5 MW cold air-fuel burners using ANSYS Fluent to analyze the impact of burner location and type. The study focused on understanding what factors dominated heat transfer and evaluated the impact of varied burner positions on energy utilization. The model utilized the RNG version of the $k-\varepsilon$ turbulence model and the Eddy Dissipation combustion model. Radiation was modeled by the DO method and a latent heat term was included in the heat transport equation by a user defined function to account for the heat of fusion of the feed. The authors stated that a major limitation to the model was that the metal shape could not change during the melting process. Due to this limitation, two different metal arrangements were considered, one in which the metal was modeled as a melt pool spread at the bottom of the furnace and the other in which the metal is arranged as an ingot assembly with gaps. Figure 3.6 shows a schematic of the two different metal configurations investigated. The CFD analysis was performed for both metal configurations.

Figure 3.6 The two metal configurations considered in the CFD study by Buchholz et al. where (a) is the melt pool configuration and (b) is the ingot configuration [49].
Once the calculation for the baseline condition of the furnace was performed, several modifications to the burner positions as well as the use of OF burners were investigated. Simulations were performed to find the burner configuration that allowed for the longest combustion gas residence time relative to a baseline condition. Table 3.2 lists the furnace configurations that were investigated.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Description</th>
<th>Metal Geometry</th>
<th>Burner Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Original Furnace</td>
<td>Flat</td>
<td>AF</td>
</tr>
<tr>
<td>B</td>
<td>Original Furnace</td>
<td>Ingot</td>
<td>AF</td>
</tr>
<tr>
<td>C</td>
<td>Burners shifted to flue side</td>
<td>Flat</td>
<td>AF</td>
</tr>
<tr>
<td>D</td>
<td>Burners shifted to flue side, 2.5 and 1.0 MW burners exchanged positions &amp; were adjusted to be parallel to flue axis</td>
<td>Flat</td>
<td>AF</td>
</tr>
<tr>
<td>E</td>
<td>Burners shifted to flue side, 2.5 and 1.0 MW burners exchanged positions &amp; were adjusted to be parallel to flue axis</td>
<td>Ingot</td>
<td>AF</td>
</tr>
<tr>
<td>F</td>
<td>Original Furnace</td>
<td>Flat</td>
<td>OF</td>
</tr>
</tbody>
</table>

Figure 3.7 shows results for total heat flow into the metal and average gas residence time for the different furnace configurations investigated.

The authors concluded from the results of the CFD model that the heat transfer inside the furnace for both metal configurations was dominated by radiation effects and that changing the burner positions had very little effect on the gas residence times and energy utilization. The model showed that the heat transfer
into the ingot stack was larger than into the melt pool configuration and that much higher heat transfer efficiencies were achieved when oxy-fuel burners were used when compared against the cold air burners.

Hongie et al. [56] also constructed a CFD model using ANSYS Fluent to assess the fluid flow, heat transfer and combustion process in a reverberatory furnace used for the production of secondary copper as a function burner type and installation location. The authors indicated that it was extremely difficult to measure the operating parameters of the secondary copper reverberatory furnace which led to little understanding of the transport phenomena within the furnace. Therefore, the operation and control of the furnace was solely based on experience which resulted in high energy losses and poor quality copper. CFD modeling was identified as the most effective technology for analyzing and optimizing the furnace. The model was validated through a comparison of measured and calculated values. Table 3.3 and Table 3.4 shows a comparison of the measured and calculated temperature and chemical species mass fraction data. The measured and predicted values were in very close agreement and the authors concluded that the model was reliable.

Table 3.3: Comparison between Measured and Calculated Temperatures from the Study Performed by Hongie et al. [56]

<table>
<thead>
<tr>
<th>Location</th>
<th>Measured (K)</th>
<th>Calculated (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outside of furnace wall</td>
<td>378</td>
<td>381</td>
</tr>
<tr>
<td>Roof</td>
<td>423</td>
<td>425</td>
</tr>
<tr>
<td>Gas Outlet</td>
<td>1553</td>
<td>1562</td>
</tr>
</tbody>
</table>

Table 3.4: Comparison between Measured and Calculated Mass Fraction at the Outlet of the Flue from the Study Performed by Hongie et al. [56]

<table>
<thead>
<tr>
<th>Species</th>
<th>Measured (%)</th>
<th>Calculated (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>0.14</td>
<td>0.15</td>
</tr>
<tr>
<td>H₂O</td>
<td>15.15</td>
<td>15.69</td>
</tr>
<tr>
<td>O₂</td>
<td>1.60</td>
<td>1.80</td>
</tr>
</tbody>
</table>

The model showed that the flame region was very short and was mainly located along the roof of the furnace. This proved disadvantageous for two reasons: (1) the charge was located at the bottom of the furnace which resulted in poor heat transfer between the flame and the charge material and (2) the flame region was too close to the roof which caused the refractory material to overheat and dramatically decreased roof lifetime. The burners were changed from DC burners to rotary burners and were angled into the furnace at 45 degrees. The model showed that the change in burner type and location enhanced mixing in the furnace and lowered the maximum gas temperature. The authors reported a decrease in fuel
consumption, pollutant emissions and copper loss due to the CFD model investigation and subsequent change in burner configuration. The consumption of coal and charcoal per furnace decreased from 17 to 13 tons and 6 to 2 tons, respectively. The loss ratio of copper decreased from 5% to 3% and the smelting time per furnace was cut down from 23 to 13 hours due to the increase in furnace efficiency.

3.6.1.2 Sub-model Investigations in Reverberatory Furnace Simulations

The impact of different sub-models used to simulate the phenomena within reverberatory furnaces is not well documented in literature. A notable study done with this focus was performed by Furu et al. [44]. The researchers used the same aluminum reverberatory furnace that was modeled in Buchholz et al. [49] to investigate the influence of various turbulence and combustion models on the overall transient numerical solution. The turbulence models investigated in this study were the standard k-ε, RNG k-ε, k-ω and SST k-ω. The researchers found that the k-ε and the RNG k-ε models showed rapid temperature fluctuations in the furnace with time for the transient calculations and explained that the reason for the fluctuations might be due to the flow regions with large pressure gradients and insufficient boundary layer treatment. On the other hand, the k-ω and SST k-ω model showed much smoother changes in chamber temperature. Combustion models using Finite-rate / Eddy Dissipation, Eddy Dissipation and Eddy Dissipation concept were all solved and compared in this study as well. The researchers found that there was a major difference between the Eddy Dissipation Concept model and the other two models evaluated and concluded that the combustion was not only limited by mixing rate but also by chemical kinetics.

3.6.1.3 Evaluation of New Furnace Designs

Performance of newly designed reverberatory furnaces have also been tested using CFD modeling. Baukal et al. [39] describe a study done by RBSC, an aluminum smelting company, on a newly designed sidewell reverberatory furnace with 50% more aluminum bath surface to accommodate a scheduled increase in plant production. CFD modeling was used to assess if the new furnace would handle the scheduled production increase and what burner angles should be used to maximize efficiency. Two models were built using ANSYS Fluent, one to evaluate the existing furnace and the other to evaluate the newly designed larger furnace. The combustion reactions were solved using a mixture fraction approach. The model showed that the new furnace would be able to handle the scheduled production increase and predicted the firing rates needed for the production increase. The model also showed that the burner orientation played a significant role in the optimization of the furnace. The best burner configuration was reported to be downward at a 10° angle toward the melt surface with the side burners inclined toward the center of the furnace hearth. A comparison between the thermal efficiencies
of the new and existing furnace showed that the new furnace had about a 4% lower efficiency than the existing furnace.

Arutyunov et al. [40] reported modeling the combustion within a specially designed reverberatory furnace with a roll-out hearth using the computational software package called PHOENICS [63]. The reverberatory furnace was equipped with a radiant vortex injector (RVI) used for the secondary combustion of products. The nature of RVI added complexity to the model due to the addition of other high-speed gas streams and turbulence. The standard $k$-$\varepsilon$ model was used to model turbulence and radiative heat transfer was modeled by the differential method. The authors concluded that the CFD model was successful in calculating distributions of velocities, pressures, temperatures and concentrations of components of the mixture within the furnace. The model was also used to determine the configuration of the combustion zone and provided information to evaluate the ejection capacity of the RVI.

### 3.6.1.4 CFD with Lab Scale Furnaces

In recent years, there have also been CFD studies performed in conjunction with the construction and utilization of laboratory scale reverberatory furnaces used to test new technologies. The U.S. Department of Energy’s Albany Research Center (ARC) along with Secat, Inc. designed and built a lab scale reverberatory furnace for experimentation and validation of CFD models involving new and emerging technologies related to the secondary aluminum industry [45 – 47]. Figure 3.8 shows a schematic and picture of the experimental furnace. The overall goal of the experimental reverberatory furnace coupled with CFD modeling was to aid in the production of secondary aluminum by studying ways to optimize the re-melt process, increase furnace efficiency and decrease emissions [64].

The experimental reverberatory furnace had a nominal holding capacity of 2000 lbs and was outfitted with two burners anti-symmetrically located on adjacent walls with a total burner firing capacity of 1.6 MMBtu/hr. It was equipped with an advanced data acquisition system that monitored specified process variables such as gas temperature, composition and velocity at several points in the furnace and in the flue. Furnace wall temperature measurements were recorded at several locations as well. The experimental furnace also was designed to be modular in nature so that the roof height could be adjusted to change the combustion space volume.

The combustion space of Albany’s Research Center experimental reverberatory furnace was modeled using an Argonne National Lab (ANL) developed CFD software called ICOMFLO [65]. Measurements taken from experimental studies that were used to evaluate the impact of total power input, varying combustion space volumes and individual burner firing rate were used to validate the CFD model. The purpose of the validated CFD model was to accurately estimate optimal burner location and angles, flue size and location, insulation material and firing rates prior to a furnace redesign or update. One study
[46] done in conjunction with the U.S. Department of Energy’s Albany Research Center experimental furnace used flue temperature measurements as a function of power input as a means for validation. Figure 3.9 shows the results of this validation method. The validated CFD model in this study was used to better understand the temperature distribution within the furnace as well as combustion species fractions.

![Figure 3.8](image1.png)  A picture and schematic of the U.S. Department of Energy’s Albany Research Center experimental reverberatory furnace [48].

![Figure 3.9](image2.png)  Measured and calculated flue temperature as a function of input power for the U.S. Department of Energy’s Albany Research Center experimental reverberatory furnace [46].

In another study [47], parameters such as temperature and gas composition were used for model validation. Table 3.5 shows the calculated and measured values of flue temperature and gas composition for this simulation.
Table 3.5: Measured and Computed Values for the U.S. Department of Energy’s Albany Research Center Experimental Reverberatory Furnace [47]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Measured</th>
<th>Predicted by CFD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flue T (°F)</td>
<td>1100</td>
<td>1080</td>
</tr>
<tr>
<td>CO in Flue (ppm)</td>
<td>8.43</td>
<td>10</td>
</tr>
<tr>
<td>O₂ in Flue (%)</td>
<td>6.86</td>
<td>5.5</td>
</tr>
<tr>
<td>N₂ (%)</td>
<td>86.6</td>
<td>85.2</td>
</tr>
<tr>
<td>CO₂ (%)</td>
<td>9</td>
<td>11</td>
</tr>
</tbody>
</table>

The authors concluded that the calculated and measured values for this simulation were within reasonable agreement and that CFD model could be used to help determine ways to improve furnace efficiency. Parameters studied through the CFD model were vertical injection angle of the burners and fuel loading between the two burners. Figure 3.10a shows the results from the burner angle injection study. The peak value of heat transferred into the melt was achieved at a downward injection angle of 10 degrees. The authors concluded that this downward angle counteracted the buoyant lift of the flame and kept the flames parallel to the load, thereby maximizing radiant heat transfer. Figure 3.10b shows the impact of fuel loading between the two burners. A value of one indicated that all the fuel entered through the front burner while the other was effectively shut off. The opposite situation occurred at a value of zero. This study showed that splitting the fuel between the two burners nearly minimized the heat transfer to the melt and that greater heat transfer was achieved at a larger fraction of gas through the front burner.

![Figure 3.10](image-url)  
**Figure 3.10** Amount of heat transferred to the melt in the study performed by Golchert *et al.* as a function of (a) vertical injection angle and (b) fraction of gas through the front burner [47].
The flame-burden interaction during the re-melting of aluminum ingots was also investigated using the experimental reverberatory furnace [48]. Figure 3.11 shows the furnace and burden geometry used in this study. The CFD simulation resolved the flow as well as the thermal and chemical composition fields. From these fields, flame behavior and heat transfer characteristics were found. The CFD model showed that the burden configuration tested in this study was not high enough to cause an obstruction to the flame, which resulted in direct flame impingement on the opposite wall, creating a hot spot. However, the simulation also showed that the flame impingement on the opposite wall created desirable gas recirculation, which increased the residence time of the combustion gases within the furnace. The findings from the experimental furnace and CFD investigation continue to inform on new and improved designs for reverberatory furnaces used in the secondary aluminum industry.

Kumar et al. [45] also performed studies using a lab scale experimental furnace coupled CFD modeling. The CFD modeling was done using ANSYS Fluent. The focus of the studies was to investigate the convective and radiative heat fluxes for aluminum melting furnaces. Figure 3.12 shows a picture and a schematic of the experimental furnace used in this study. The experimental furnace was a rectangular box with a raised step toward the middle of the furnace. The raised step was made from water-cooled calorimetric plates that had heat flux sensor sockets drilled into them. Heat flux sensors were inserted into the sockets and were also water-cooled during testing. The plates were covered with ¼” of Fiberfrax material which eliminated direct exposure to the flame. This design was chosen to simulate the effect of flame impingement on the corner of a solid charge, which is a commonly encountered phenomenon in metallurgical operations. Various geometric features of the physical furnace were simplified for the CFD model. For example, detailed burner modeling was not performed and the outer furnace walls were
replaced with equivalent thermal resistances. The turbulence model used for this study was the standard k-ε model and the premixed flame was simulated using the Eddy-Dissipation model. The DO model was used to model radiation heat transport.

Figure 3.12 A (a) picture and (b) schematic of the experimental furnace used in the study by Kumar et al. [42]

Figure 3.13 compares the measured and calculated furnace crown temperature as a function of furnace length. These data were used for model validation.

Figure 3.13 Comparison of measured and calculated furnace crown temperature found in the study by Kumar et al. [45].

The CFD model predictions were found to be in good agreement from a qualitative standpoint. The measured and calculated results had similar profiles, but the CFD model overpredicted the maximum crown temperature by about 10 – 12%. The authors explained that this discrepancy could be due to the use of an overall effective heat transfer coefficient to model the wall heat transfer external to the furnace. The use of the effective heat transfer coefficient assumed uniform refractory thickness and
does not account for the presence of viewing ports and other inclusions in the walls of the experimental furnace. The authors concluded that the computational costs involved in including all the details of the furnace geometry did not justify the minor loss in accuracy by ignoring them. Calculated and measured heat flux values were also compared for validation. The calculated peak heat flux value in the furnace was 224 kW/m$^2$ which agreed very well with the measured value of 226 kW/m$^2$. The validated model resolved the flow, thermal and chemical composition fields within the furnace, which were used to evaluate the flame behavior and quantify convective and radiative heat fluxes.

3.6.2 Blast Furnace

A blast furnace is a metallurgical shaft furnace generally used for the smelting of primary or secondary iron, lead, copper and zinc [3]. Blast furnace processing is counter-current, and typically used when a high reduction potential is required. Ironmaking blast furnaces, as shown in Figure 3.14, are the primary focus of CFD studies found in literature. The ironmaking blast furnace consists of several different regions namely the throat, stack, belly, bosh and the hearth. The alternating layers of coke and iron ore-containing burden are charged in the throat region at the top of the furnace. Preheated air and/or fuel is injected into tuyères at the base of the furnace shaft. Combustion takes place at the base of the furnace as the preheated air and in some cases fuel reacts with coke in the charge material which produces carbon dioxide. The carbon dioxide then reacts with the remaining coke to form carbon monoxide, the principle reductant in this type of furnace. Reduction reactions start in the stack and are completed in the belly and bosh region of the furnace as the charge material moves downward and reacts with the carbon monoxide rich combustion gases that are flowing upward. The metal and slag settle in the hearth where the two phases remain separate from each other with the slag floating on top of the denser iron. The highest temperatures in the iron blast furnace are achieved in the hearth immediately in front of the tuyères. The local temperature in this area is around 3700 °F. Outside the combustion zone, the temperatures decrease steeply. In normal practice, the slag is tapped at 2550 to 2730 °F while the average tapped metal temperature is about 125 °F lower due to the thermal losses through the hearth [66].

Various zones exist within the regions of the blast furnace. The cohesive zone is the area within the stack where the ore starts to soften and melt. Below the cohesive zone is the active coke zone. This zone is sometimes called the dripping zone because it is an area within the furnace where liquid iron and slag flow through a layer of solid coke. The raceway is a large cavity within the furnace created by the high velocity gas from the tuyères and the consumption of coke. In the center of the furnace hearth, there is an area called a deadman or the coke bed, which a stable pile of porous coke [54], [66]. The deadman is composed of coke particles and during the tapping process, the hot metal flows through and around the dead man to the taphole. The rate and the nature of the hot metal flow and the composition of
the hot metal (carbon unsaturated or saturated) is determined by the interaction between the hot metal and the deadman. The deadman may either sit on the bottom of the hearth or float partly or completely in the liquid bath if the buoyancy force of the liquids is sufficient to lift the dead man. A partly floating deadman sits on the central hearth bottom and gives rise to an annular coke free zone at the hearth edges, which offers little flow resistance when the hearth is drained [66].

Figure 3.14 Schematic of an iron making blast furnace showing the furnace zones [54].

CFD is usually used to model different portions of the blast furnace rather than the entire blast furnace all at once. The main blast furnace regions modeled with CFD are the hearth, the shaft and the tuyère s. The following sections detail the blast furnace CFD models found in literature.

3.6.2.1 Modeling of Blast Furnace Hearth

CFD Modeling of the blast furnace hearth has been of particular interest for many years [66 – 87]. Understanding the transport phenomena in the hearth has become very important as the campaign life of an ironmaking blast furnace is mainly determined by the wear of the hearth refractory [89]. Erosion of the hearth lining is significantly affected by the hot metal flow patterns and heat transfer through the refractory which are both dependent on the furnace operating conditions. The CFD studies in literature related to the modeling of the blast furnace hearth focus on finding ways to increase refractory lifetime by: (1) evaluating shear stress on the hearth wall as a function of various furnace parameters, (2) understanding liquid iron flow and heat transfer within the hearth and (3) prediction of the hearth inner profiles.
1) Shear Stress on Hearth Wall

Liquid iron flow and the resulting shear stress on the inner hearth wall as a function taphole depth and angle as well as deadman state have been studied with CFD [66 – 69]. These studies all reported the use of ANSYS Fluent. Dash et al. [68], [69] were able to suggest an optimum taphole depth and angle to minimize refactory erosion on the basis of the shear stress analysis on different vertical levels of the hearth sidewall. The computational domain for this model was constructed using an operational blast furnace hearth with a floating deadman configuration. Table 3.6 shows the variation of maximum non-dimensional stress as a function of taphole angle and number of computational cells as this parameter was also used to check for grid independence. The simulations showed that there was an optimum length and angle for which the shear stress on the hearth wall was at a minimum and that grid independence could be achieved.

Table 3.6: Results from a study performed by Dash et al. showing the variation of maximum non-dimensional stress as a function of taphole angle with a floating deadman [68]

<table>
<thead>
<tr>
<th>Taphole Angle</th>
<th>Cells</th>
<th>Maximum non-dimensional stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>-10°</td>
<td>75400</td>
<td>352</td>
</tr>
<tr>
<td></td>
<td>140600</td>
<td>358</td>
</tr>
<tr>
<td></td>
<td>250750</td>
<td>360</td>
</tr>
<tr>
<td>0°</td>
<td>72670</td>
<td>256</td>
</tr>
<tr>
<td></td>
<td>135680</td>
<td>259</td>
</tr>
<tr>
<td></td>
<td>242760</td>
<td>260</td>
</tr>
<tr>
<td>15°</td>
<td>74670</td>
<td>42</td>
</tr>
<tr>
<td></td>
<td>145690</td>
<td>46</td>
</tr>
<tr>
<td></td>
<td>250700</td>
<td>47</td>
</tr>
<tr>
<td>30°</td>
<td>76800</td>
<td>270</td>
</tr>
<tr>
<td></td>
<td>148600</td>
<td>274</td>
</tr>
<tr>
<td></td>
<td>256800</td>
<td>275</td>
</tr>
</tbody>
</table>

Cheng et al. [67] developed a similar study in which the impact of taphole length on hearth wall shear stress was also investigated. Figure 3.15 shows the results for this study. Figure 3.15a shows a schematic of the hearth bottom and the definition of theta. Figure 3.15b shows the hearth wall shear stress as a function of taphole length and theta. The simulations from this study showed that an increase in taphole length resulted in a decrease in maximum shear stress. An increase in taphole length was also shown to shift the location of the peak shear stress values away from the taphole location.

Shao et al. [70] investigated the shear stress on the refractory wall as a function of three different deadman states. Figure 3.16 shows a result of this investigation. The simulations showed that the deadman state played an important role in the development of flow and erosion conditions within the
A high shear stress zone appeared in the interior of the hearth bottom for the sitting deadman configuration. The authors concluded that the fully floating deadman state relieved some of the shear stress in the hearth as the stress was distributed more uniformly for this condition.

Figure 3.15  Result from the study done by Cheng et al. [67] showing a (a) schematic of the hearth bottom with theta defined and (b) the calculated wall shear stress as a function of taphole length and theta at a vertical height of 5.933 m with the blast furnace hearth.

Figure 3.16  Results from the study performed by Shao et al. [70] showing contours of shear stress on the hearth bottom as a function of different deadman states.
2) Liquid Flow and Heat Transfer Through Hearth

Shibata et al. [71] developed a three-dimensional CFD model to evaluate the iron flow and temperature fields within the blast furnace hearth as a function of different types of coke free zones. The model was developed using a code called STREAM [90]. Figure 3.17a shows a schematic of the four coke free spaces evaluated. This study found that the shape of the coke free space significantly affected the molten iron flow and heat transfer within the hearth. Case A had the most significant circumferential flows which resulted in areas of high heat loads within the refractory. The velocity of the molten iron near the bottom of the hearth decreased with an increase in the free space thickness. Figure 3.17b shows the velocity vectors for Case A.

Figure 3.17 Schematics from the study performed by Shibata et al. [71] showing (a) the four coke zones investigated and (b) resulting velocity vectors calculated for Case A.

Panjkovic [72] developed a CFD model using ANSYS-CFX to address natural convection heat transfer and fluid flow through the deadman within the blast furnace hearth. The model was validated using plant data and was able to predict fluid flow and temperature distributions in the liquid iron as well as the temperature profiles in the refractory within reasonable accuracy. The authors concluded that the standard k-ε model was not appropriate for modeling turbulence within the hearth. The turbulent viscosity for liquid metal flow in a packed bed of coke was instead estimated using a simple algebraic turbulence model which was solved numerically. The derivation of the model was outlined in the study [72]. This treatment of turbulence was later adopted and improved by Guo et al. [72 – 77].

Guo et al. [72 – 77] performed many CFD studies using ANSYS – CFX on the blast furnace hearth. One model [73] investigated the gas-slag interaction within the hearth and its effect on the slag
drainage. The gas flow and pressure distributions on the liquid surface in the lower zone of the furnace were analyzed in this study with special interest on the gas flow near the raceway and its effect on the liquid surface. These parameters were examined because large variations in the liquid surface pressure could result in poor slag drainage. The variables considered were liquid level, location and shape of the cohesive zone and deadman properties. The simulation results showed that the gas flow was sensitive to the assumed deadman structure as well as the location of the cohesive zone relative to the tuyère raceway. It was also found that the gas flow created a non-uniform pressure distribution over the slag surface, thereby causing the surface to deform. Figure 3.18 shows the pressure distribution on the slag surface as a function of three different liquid levels within the blast furnace hearth. Higher liquid levels resulted in areas of localized high pressure directly under the tuyère, but as the liquid levels decreased, the pressure regions become interconnected and spread out. The pressure difference between the various regions dropped as the liquid level in the hearth decreased. The study also showed that the amount of slag residual was influenced by the taphole location, slag surface level and shape of the coke free zone.

![Figure 3.18](image)

**Figure 3.18** Contours of the pressure distribution on the slag surface for hearth liquid levels of (a) 0.75 m, (b) 1 m and (c) 2 m below the tuyère center level generated in a study performed by Guo et al. [73].

Other models [74], [75] were developed to examine the liquid iron flow and coupled refractory-liquid heat transfer in the hearth. The effects of several factors were investigated such as two versus three dimensional regimes, fluid buoyancy versus constant density as well as different shapes and positions of the coke free layer in the hearth. The model predicted flow patterns and temperature profiles within the hearth. The results showed that natural convection was very significant and controlled the overall flow patterns of the molten iron phase which resulted in two distinct iron flow regions for all the deadman
configurations investigated. Figure 3.19 shows these two regions, one moving and one stagnant, in the molten iron phase for a fully sitting deadman configuration.

![Figure 3.19](image)

Figure 3.19 Results obtained in studies performed by Guo et al. [74], [75] showing the moving and stagnant flow regions within the blast furnace hearth with a sitting deadman through (a) velocity vector and (b) streamline plots.

Guo et al. [76], [77] and other authors [79] have also developed models to study Ti(C,N) formation due to titania addition in the blast furnace. The addition of titanium-rich materials to the blast furnace has been implemented as a way to extend the lifetime of the hearth refractory through the formation of a wear resistance coating on the hearth wall [80]. The coating is a solidified metal matrix in which loose Ti(C,N) crystal particles are present. The crystals are made of titanium nitride (TiN) and titanium carbide (TiC) [78]. The influence of hearth geometry and temperature were investigated in these models. The studies by Guo et al. [76], [77] found that low temperature was essential for the formation of Ti(C,N) particles, but also that the flow behavior of the liquids and solids within the hearth greatly the affected amount of solid Ti(C,N) buildup.

Post et al. [81], [82] developed a CFD model of the deadman using ANSYS – CFX that was coupled with a special porosity and population balance model that was used to understand the hot metal flow in this region of the blast furnace. The porosity model was used to evaluate the local porosity and the population model was used to keep track of the local particle size [91], [92]. The coke-bed in the hearth consists of coke particles that exhibit a particle size distribution in regards to both space and time. This leads to non-uniform porosity in the hearth which causes the flow of molten metal through the coke-bed to be irregular and further increases the erosion rate. A dissolution model was also developed and used in conjunction with the CFD model. The CFD process model, dissolution model and porosity model were all used together to evaluate the specific hot metal flow behavior in the hearth as a function of coke type used. Each scenario resulted in different hearth wall refractory erosion behavior.

Huang et al. [83] and Chang et al. [84] also investigated the influence of the deadman porosity on the hot metal flow, heat transfer and erosion rate of the refractory hearth in one of China Steel
Corporation’s operational blast furnaces. The models were developed using ANSYS Fluent. Huang et al. [83] first developed a CFD model for the blast furnace hearth to evaluate the flow patterns and heat transfer for different deadman heights during the tapping process. Figure 3.20 shows the resulting flow patterns of liquid iron through the deadman during the tapping process for the two deadman states evaluated: (1) floating deadman and (2) sitting deadman with a gutter coke-free space. The simulations showed that the hot metal tended to travel to the hearth bottom before it reached the taphole for the floating deadman configuration. The authors concluded that this flow pattern enhanced heat transfer into the deadman and the renewal of deadman coke by dissolving carbon into the hot metal which made the floating deadman easier to keep active and unclogged than the sitting deadman.

![Figure 3.20](image_url)  
Figure 3.20 Schematic of (a) the sitting deadman with gutter coke-free space configuration and (b) the resulting streamlines of the hot metal with different deadman types evaluated in the study performed by Huang et al. [83].

Chang et al. [84] then examined the impact of the deadman porosity on liquid metal flow and resulting erosion. The calculated velocity, temperature and carbon concentration at each node was used to determine the erosion rate, \( \dot{m}_c \) (units = kg/m\(^2\)s) of the carbon refractory within the blast furnace hearth by:

\[
\dot{m}_c = K \rho (C_s - C)
\]

where \( K \) was the mass convection coefficient, \( \rho \) was the density of carbon, \( C_s \) was the concentration of the carbon at the surface and \( C \) was the concentration of the carbon in the bulk. This method assumes that erosion is only caused by carbon dissolution. The study evaluated three different deadman heights as well as three different deadman porosity distributions which are described in Table 3.7. Figure 3.21 shows the contours of the erosion rates for the different cases evaluated in this study.

It was concluded that different deadman heights caused erosion within the hearth to occur at different locations and to varying extents. The porosity of the coke-bed was also shown to significantly
impact the erosion rate. Uniform porosity within the deadman was shown to lower the erosion rate. This meant that an optimal deadman height and porosity could be found in which erosion rate was minimized.

Table 3.7: Description of Porosity Cases Evaluated in the Study by Chang et al. [84]

<table>
<thead>
<tr>
<th>Case</th>
<th>Porosity Distribution Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cylindrical zone starting from center of hearth with a radius of 2.5 m with a porosity of 0.1; all other zones have a porosity of 0.35</td>
</tr>
<tr>
<td>2</td>
<td>All zones have a porosity of 0.35</td>
</tr>
<tr>
<td>3</td>
<td>Cylindrical zone starting from center of hearth with a radius of 2.5 m with a porosity of 0.35; all other zones have a porosity of 0.7</td>
</tr>
</tbody>
</table>

Figure 3.21 Calculated erosion rates in the study done by Chang et al. [84] for both floating deadman configurations (a) 10 (b) 30 and (c) 50 cm above the hearth floor as well as porosity distributions within the dead man for (d) case 1 (e) case 2 and (f) case 3.
3) Prediction of Hearth Inner Profile

A group of researchers studied many aspects of the internal conditions within the blast furnace hearth including the inner profile of the refractory [84 – 86]. In one study by Zhou et al. [86], a model of the blast furnace hearth was developed that integrated both a 3-D CFD model and a 1-D heat transfer model. The principle of this methodology was to use a 3-D CFD model to predict the hot face temperatures within the hearth based on an assumed inner hearth profile. These calculated temperatures, measured refractory temperatures and material properties were then used in a 1-D heat transfer model to revise the assumed inner profile and thereby predict the hot face position. Based on this methodology, the authors estimated and analyzed the erosion of the hearth as well as changes in the inner profile of the hearth over time due to refractory wear and skull (metal crust) formation for a real blast furnace in operation. The model provided real time monitoring of the hearth refractory thickness and inner profile which allowed for adjustments in operating conditions to reduce erosion and extend refractory life. Figure 3.22 shows an example of one of the predicted inner profiles of the hearth after a period of operation obtained from the developed process model.

![Figure 3.22: Predicted inner profile of the hearth at a vertical plane through the taphole found by the integrated 3-D CFD model and 1-D heat transfer model developed Zhang et al. [85].](image)

3.6.2.2 Modeling of Blast Furnace Shaft

Several studies have been performed where CFD has been coupled with the Discrete Element Method (DEM) to simulate the ironmaking blast furnace shaft [92 – 97]. DEM is applied to describe each individual ore and coke particle within the layered burden. This approach can reveal details about gas and particle movement within the hearth, but it is computationally expensive because the blast furnace is a dense moving bed and a transient simulation is needed for a DEM model. CFD-DEM coupled studies are not a focus of this review and only purely CFD studies of the blast furnace hearth have been summarized.

Fu et al. [98 – 100] developed a CFD model to simulate the multiphase reacting flow within the blast furnace shaft. The simulation was conducted using an in-house code developed through the
FORTRAN [102] language. The gas flow dynamics, burden movement, chemical reactions, heat and mass transfer between the gas phase and burden phase are all included in the model. The layered structure of the burden is important for furnace operation as the permeability differs significantly between the coke and ore layers and different reactions take place in each type of layer. The computational grid was divided into four types of cells depending on the material present in the region. The four types of cells were denoted as “coke cells”, “ore cells”, “free space cells” and “interface cells”. Figure 3.23 shows schematics of these four types of cells.

The conservation equations for both the gas and solid phases were solved in each cell. Various source terms were prescribed to the different types of cells to account for the effect of the layered structure of the furnace burden from both a thermal and chemical standpoint. Several steady state cases with different burden structures were modeled to evaluate the effect of the layered structure on gas composition, pressure drop through the furnace and coke rate. As an example of the results obtained in this study, Figure 3.24 shows the volume fractions of the major gas species within the blast furnace shaft. These results were used to better understand the phenomena occurring within the blast furnace shaft and thereby how to improve the furnace operations.

3.6.2.3 Modeling of Blast Furnace Shaft

Gas injection into the blast furnace tuyère s is another process that has been modeled with the aid of CFD. Hellberg et al. [103] used CFD to investigate the effect of using two different types of reducing gases, coke oven gas and basic oxygen furnace gas, in the blast furnace. The authors also used the CFD model to investigate other parameters such as the effect of the number of injection lances in the tuyère and tuyère angle. The chemical reactions within the combustion zone were modeled using the Extended Simple Chemically Reaction System (ESCRS) which is a combustion model for gases available with the
CFD software PHOENICS [63]. The results from the CFD model were presented as properties such as temperature, velocity and composition data at the end of the tuyère. The authors concluded from the developed process model that the coke oven gas produced higher temperatures at the tuyère when compared to the basic oxygen furnace gas and that a tuyère with two injection lances provided better combustion conditions.

Figure 3.24 Volume fractions of (a) CO, (b) CO$_2$, (c) H$_2$ and (d) H$_2$O gas species present within the blast furnace shaft studied by Fu et al. [100].

Pulverized coal injection (PCI) through the blast furnace tuyère s has also been investigated using CFD [103 – 111]. PCI is one of the most important recent technologies in blast furnace ironmaking and is widely used to reduce coke consumption and CO$_2$ emissions [113]. The University of New South Wales and BlueScope Steel research corporation partnered to develop three CFD models of pulverized coal injection in the blast furnace. Figure 3.25 shows a schematic of the PCI process in the lower part of the blast furnace. The CFD models investigated the phenomena relating to pulverized coke injection for three different computational domains. The first model simulated the flow and combustion in a tuyère and raceway according to a pilot-scale test reactor. The second and third models both simulated the lance, tuyère and raceway of an actual blast furnace in operation. The difference between the second and third models was that the third model also included a portion of the coke bed in the computational domain. Each model was developed for a different purpose.

The combustion of coal was simulated as a four-step process in each model: (1) preheating; (2) de-volatilization of raw coal modeled using the two-competing model; (3) gaseous combustion modeled using the eddy-dissipation model and (4) the oxidation and gasification of residual char modeled using the Gibbs model. The results of the CFD analysis were compared and the applicability of each model was
characterized. Model 1 was developed for validation purposes and fundamental analysis of the PCI process. Model 2 was developed to test different lance / tuyère designs and model 3 was used to study in-furnace phenomena as a result of PCI. It was concluded that all the models described the PCI process qualitatively but only model 3 was reliable for qualitatively simulating the in-furnace phenomena of the PCI process as it was more sensitive to changes in operational conditions. Model 3 was able to accurately predict gas composition, distribution and temperature within the raceway which are all parameters that dictate furnace stability in practice. Figure 3.26 shows the results of this analysis.

Figure 3.25 Schematic of PCI in the lower part of a blast furnace [114].

Figure 3.26 Main simulations results for the third PCI model developed by Shen et al. [107] showing (a) the gas mass fractions as a function of the distance from the lance tip and (b) the temperature distribution within the centerline of the raceway plane.
3.6.3 Rotary Furnace

Rotary furnaces are used for many different applications in process metallurgy. This type of furnace is cylindrical in shape and rotates slowly around its longitudinal axis. The feed is introduced in one end and the product can be discharged out either sides of the furnace. Figure 3.27 shows a general schematic of a rotary furnace. Within a rotary furnace, heat can be transferred to the charge by direct radiation from the flame and/or reflected radiation from the furnace lining as well as convection from the furnace lining [5]. Rotary furnaces are very robust and can handle feed of variable size which is one reason why they are used in the metal recycling industries where the particle size of the charge can be varied. This type of furnaces can also run in batch rather than continuous mode, giving flexibilities in plant operations. Limited CFD studies have been performed on rotary furnaces used in metallurgical applications. One reason for this could be because the modeling of rotary furnaces can be very challenging due to the need to simulate the movement of the charge bed as well as the heat and mass transfer within it [115].

Figure 3.27 Schematic of a rotary furnace [39].

In recent years, several notable studies have been presented by Zhou et al. [50 – 52] on the use of CFD for modeling secondary aluminum scraps in a rotary furnace. The CFD model in these studies was developed to aid in the optimization of aluminum scrap melting by finding ways to reduce energy, reduce metal loss, improve the operation of the furnace and decrease environmental impacts. The authors noted that there were challenges modeling this process not only due to the high temperatures, complex chemical reactions involved and the rotating movement of the furnace, but also because of the highly complex post-consumer scrap feed that contained various types of aluminum and different particle size distributions. Modeling the melting of the aluminum feed within the furnace was also challenging because of the
presence of a molten salt layer in the furnace that is typically added in the secondary processing of aluminum to help minimize oxidation. The molten salt layer causes the formation of a salt skull around the aluminum scrap which acts as insulation and affects the rate of melting. To aid in the development of an accurate process model, several experiments were performed in a laboratory tube furnace using Thermal Gravity Analysis (TGA) to investigate the melting kinetics of the varying feed in the presence of molten salt [116]. The data obtained from this study was used to generate a user defined sub-model within the ANSYS-CFX platform. The melting sub-model was coupled with the overall process model to solve for melting information such as the fraction of liquid and solid in the melt [51]. Figure 3.28 shows the melting curve obtained from the CFD simulation where the fraction of the solids remaining was plotted against the heating time. It should be noted that the solids consisted of both the aluminum scrap as well as the salt charge. The investigators also developed a scrap-burn off sub-model to describe the energy generated due to the metal oxidation during the melting process as a function of scrap type and quality.

![Figure 3.28 Melting curve of the solid in the scrap-salt zone of the rotary furnace modeled by Zhou et al. [52].](image)

The overall process model consisted of two regions, a gas region with combustive turbulent flow as well as radiative heat transfer in the upper part of the furnace and a multiphase region in which there was a solid-liquid mixture of salt and aluminum metal in the lower part of the furnace. Figure 3.29 shows the temperature distribution in the lower multi-phase portion of the rotary furnace. Figure 3.30 shows the resolved temperature distribution of the combustion gases in the upper portion of the rotary furnace [51]. The authors concluded many things from the CFD process model such as the influence of the scrap size and shape as well as the salt to metal scrap ratio on the overall transport phenomena in the furnace. One of the main conclusions drawn from this analysis was that the insulation from both the salt shell that
formed on the scrap particles as well as the top salt layer significantly affected heat transfer to the aluminum. Therefore, it was suggested that a lower salt to scrap ratio would improve aluminum melting within the rotary furnace [53].

Figure 3.29  Temperature distribution after 3000 seconds on the wall of the scrap-salt zone of the rotary furnace modeled by Zhou et al. [51].

Figure 3.30  Temperature distribution after 4800 seconds in the combustion air zone of the rotary furnace modeled by Zhou et al. [51].
CHAPTER 4
MODEL DEVELOPMENT

This chapter outlines the development of the CFD model used for this research. Included in this discussion are details about the computational domain, boundary conditions, sub-models and the solver settings used in the model. The validation procedure and the convergence criteria that were used are also discussed. The last component in this chapter is a model sensitivity analysis which provides justification for the different model parameters chosen for the overall CFD model.

4.1 Methods
The 3-D model of the computational domain representing the reverberatory furnace was created using SolidWorks 2015 [117]. ANSYS Fluent 17.0 [29] was used for the CFD modeling. Utilizing a commercial code for this project significantly cut down on development time. ANSYS Fluent is a relatively adjustable code that includes several built in sub-models for turbulence, combustion and radiation. The user can also input various user defined functions for boundary conditions and has control over numerical solver settings.

4.2 Computational Domain
Figure 4.1 shows a cross sectional schematic of the general layout for a common reverberatory furnace. The reverberatory furnace modeled in this research was a continuously tapped furnace used to process lead containing battery scrap combined with coke or coal and other fluxes. Solid lead bearing material or the burden was fed into the end wall on the burner side of the furnace. The shape of the furnace burden can vary depending on feed composition and smelting rates. The feed can also be very heterogeneous which can cause the surface characteristics of the burden to vary as well [3], [57].

Figure 4.1 Cross sectional schematic of the general layout for common reverberatory furnaces. (orientation: side view)
Most of the melting and smelting reactions occur in the front half of the furnace and separation of the resulting metal and slag layers occur in the back half of the furnace. The combustion gases reside above the slag layer and exit through the flue [4]. The computational domain in the CFD model consisted of only the combustion gas space above the slag line as well as the gas space inside of a portion of the burners.

4.2.1 Combustion Gas Space

Only the combustion gas space was considered in the CFD model as the main goal of the project was to determine the temperature distribution and other flow parameters on the refractory hot face above the slag line. Modeling the slag layer, metal layer and/or the refractory in the furnace would have added significant complexity to the model while providing little benefit to the specified goal. These portions of the furnace can be incorporated into the model for future work if the purpose of the model changes and additional information about these areas of the furnace are needed.

Figure 4.2 shows a representative schematic (not to scale) of the 3-D model of the combustion gas space used for the computational domain. The full-scale geometry was used for the CFD model. The computational domain also included the gas space inside a portion of the side and end burners. The burner geometry used is further described in section 4.2.3.

![Figure 4.2 Representative schematic (not to scale) of computational domain used in the CFD model. (orientation: isometric view)](image)

The bottom surface of the computational domain denoted the gas-slag interface and a small section of the flue was included at the outlet of the domain. The burden geometry shape was directly cut out of the
combustion gas space geometry starting at the gas-slag interface. The feature left a raised void in the gas-slag interface which was used to represent the solid furnace burden.

4.2.2 Burden Geometry

Burden geometry was loosely constructed based on photographs taken of the inside of an operational secondary lead reverberatory furnace. Figure 4.3 shows a schematic of the burden geometry used for the base case simulation. The burden shape within these types of furnaces can vary significantly from one day to the next as the feed composition and rate can change. Therefore, the burden geometry used for the base case simulation was first estimated based on the photographs provided and then modified to meet certain validation criteria. The surface characteristics of the burden, such as roughness, were also variable since the feed could be very heterogeneous. Fluent allowed for a roughness coefficient and height to be applied at the gas-slag interface boundary. Several different values of the roughness coefficient and height were tried with little to no change in the overall numerical solution. Therefore, the burden was modeled as a smooth surface since accurate information about the surface features were unknown and changing.

![Base Case](image)

Figure 4.3 Shape of furnace burden cutout for the base case simulation showing the (a) top down view and (b) side view.
The burden geometry was constructed based on three different dimensions: total length \( (x_t) \), the width in front of the side burners \( (y_t) \) and the height in front of the side burners \( (z_t) \). These dimensions were used as they were easy to change in the 3-D model and could theoretically be adjusted in an active furnace through operational changes or some form of physical manipulation. For the base case simulation, \( x_t \) was 50% of the furnace length (not including the flue), \( y_t \) was 90% of the furnace width and \( z_t \) was 28% of the combustion gas space height.

### 4.2.3 Burners

The burners used in the model were commercially available American Combustion PyreTron II air/oxygen/fuel burners [118]. Figure 4.4 shows an isometric view of the burners. Combustion in these burners is completed in two stages. The two-stage combustion process creates three zones within the flame, namely the fuel rich combustion zone, the fuel lean combustion zone and the final combustion zone. Oxygen, natural gas and air or oxygen-enriched air are all used in this burner technology. A portion of the burner geometry was included in the computational domain.

![Figure 4.4 Isometric view of the commercially available American Combustion PyreTron II air/oxygen/fuel burners used in the CFD model [118]. (orientation: isometric view)](image)

Figure 4.5 shows a cross section of the burner and the combustion zones present in the flame. In the first stage of combustion, the fuel is partially mixed with a less than stoichiometric amount of oxygen inside the central portion of the flame creating the fuel rich combustion zone. In this zone, there is a fuel rich core in which the fuel is partially combusted and pyrolyzed. The pyrolysis process in the flame core creates a cloud of micro particles of carbon and hydrocarbon radicals that are very hot and have high
emissivities due to the absence of nitrogen. The cloud of carbon particles and hydrocarbon radicals is luminous and greatly enhances radiative heat transfer. In the second stage of combustion, the remaining unreacted fuel combusts with the air or oxygen-enriched air, creating the fuel lean and final combustion zones. High gas velocities occur in these zones which can enhance convective heat transfer [118].

Figure 4.6 shows a cross sectional schematic of the burner. The section of the gas space from the diffusion plate forward was included in the computational domain. The diffusion plate is a metal plate with rings of circular openings. These circular openings are the gas flow inlets and were represented as surface entities on the exposed surface of the burner geometry included in the computational domain.

Figure 4.5 Cross sectional schematic of the commercially available American Combustion PyreTron II air/oxygen/fuel burners showing the three different combustion zones within the flame [118]. (orientation: side view)

Figure 4.6 Cross sectional schematic of the commercially available American Combustion PyreTron II air/oxygen/fuel burners showing the geometry included in the CFD model [118]. (orientation: side view)
All four burners were pointed down at the gas-slag interface and in towards the furnace centerline at a certain angle. Figure 4.7 shows a description of the inward and downward angles. The angles of the burners caused the flame to come in direct contact or impinge the furnace burden. The impingement of the flame on the burden can facilitate large amounts of heat transfer, leading to greater melting and production rates, but can also cause areas of high velocity turbulent flow and hotspots within the refractory lining [42].

![Diagram of burners angles](image)

Figure 4.7 Description of the (a) inward angles for the end and side burners (orientation: top view), (b) downward angle for the end burners (orientation: side view) and (c) downward angle for the side burners (orientation: front view) used in the model.

### 4.2.4 Mesh Information

Table 4.1 shows general mesh details for the base case geometry.

<table>
<thead>
<tr>
<th>Mesh Details</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td># of Elements</td>
<td>5,059,265</td>
</tr>
<tr>
<td># of Nodes</td>
<td>1,181,425</td>
</tr>
<tr>
<td>Relevance Value</td>
<td>100</td>
</tr>
<tr>
<td>Size Function</td>
<td>Proximity &amp; Curvature</td>
</tr>
<tr>
<td>Max Face Size</td>
<td>1.2 in</td>
</tr>
<tr>
<td>Max Tet Size</td>
<td>2.2 in</td>
</tr>
<tr>
<td>Growth Rate</td>
<td>1.1</td>
</tr>
<tr>
<td># of Inflation Layers</td>
<td>5</td>
</tr>
</tbody>
</table>
An unstructured mesh consisting of about five million elements was used. This size of mesh was chosen because it produced a grid independent solution (see section 4.7.3). The five million elements resulted in a very dense mesh which took between eight and ten hours to obtain a numerical solution. Figure 4.8 demonstrates the mesh density by showing top down view of the meshed computational domain with a close-up section of the front half of the roof.

Figure 4.8  Top down view of the meshed computational domain showing a close-up section of the front half of the roof. (orientation: top view)
The quality of the mesh is important to consider for CFD problems as bad quality mesh can cause convergence difficulties and inaccurate solutions. The ANSYS meshing software calculates various mesh metrics that can be used to assess quality. The three main metrics used to assess mesh quality in this research were element quality, orthogonal quality and skewness. The element quality metric provided a composite quality metric that ranges from zero to one. For 3-D elements, this metric is based on the volume to square root of the cube of the sum of the square of the edge lengths where a value of one indicates a perfect cube or square and a value of zero indicates the element has zero or negative volume. This metric is mathematically defined by [32]:

\[
\text{Element Quality} = c \left[ \frac{\text{volume}}{\sqrt{\sum (\text{Edge Length})^2}} \right]^3
\]  \hspace{1cm} (4.1)

where \( c \) is a constant equal to different values for different element spaces. Element quality values close to one are ideal. Orthogonal quality also ranges from zero to one and is computed using the face normal vector, the vector from the cell centroid to the centroid of each of the adjacent cells, and the vector from the cell centroid to each of the faces. Non-orthogonal meshes create large jumps in adjacent cell volumes which can introduce numerical errors when calculating the flux between cells. Values close to one indicate good orthogonal quality. Skewness is a measure of how close a face or cell is to ideal (i.e. equilateral or equiangular). This metric ranges from zero to one as well and values close to zero are ideal [32]. The best practice is to keep the minimum orthogonal quality greater than 0.1 and maximum skewness less than 0.95. Figure 4.10 shows the spectrum of values for both the orthogonal quality and the skewness mesh metric [119].
Figure 4.10  Mesh metric spectrum for (a) orthogonal quality and (b) skewness.

Table 4.2 shows the minimum, maximum and average values for the mesh metrics reviewed for the base case simulation. The minimum element and orthogonal quality value of 0.13 was above 0.1, but was still in the bad element range on the spectrum. The maximum skewness value of 0.87 was well below the recommended maximum of 0.95 and within the acceptable range on the spectrum. The mesh quality was significantly improved when inflation layers were not included. Although the prism layers adversely affected the mesh quality, they were necessary for obtaining a stable solution. A higher quality mesh without inflation layers was tried, but the numerical solution did not reach residual or iterative convergence. Any increase in the number of inflation layers beyond five decreased the mesh quality to unacceptable levels.

Table 4.2: Minimum, Maximum and Average Values for Various Mesh Quality Metrics

<table>
<thead>
<tr>
<th>Mesh Metric</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Element Quality</td>
<td>0.13</td>
<td>1</td>
<td>0.77</td>
</tr>
<tr>
<td>Orthogonal Quality</td>
<td>0.13</td>
<td>0.99</td>
<td>0.87</td>
</tr>
<tr>
<td>Skewness</td>
<td>4.6 x 10^{-6}</td>
<td>0.87</td>
<td>0.22</td>
</tr>
</tbody>
</table>

Figure 4.11 - Figure 4.13 show the distribution of the metrics for both the tetrahedron and prism elements. The element quality distribution was bimodal with the prism layers centered around a lower value than the tetrahedron elements. The distribution of the element and orthogonal quality values shows that very few cells were at the lower, bad element region on the spectrum.
Figure 4.11  
Distribution of the element quality mesh metric among both tetrahedron and prism elements.

Figure 4.12  
Distribution of the orthogonal quality mesh metric among both tetrahedron and prism elements.
4.3 Boundary Conditions

The following sections describe the boundary conditions used in the CFD model. The gas inlets, the flue and the refractory walls were the main boundaries in the model. Some of the boundary conditions were based on measurements and others were estimated or calculated.

4.3.1 Flow Boundary Conditions

The mass flow rates for oxygen, natural gas and enriched air at the inlets and static pressure at the outlet was used to define the flow boundary conditions. Gas temperatures based on measurements at the inlets and outlet were also specified. The actual flow rates and pressures used in the model will not be provided to protect the project’s industrial sponsor. The mass flow rates, $\dot{m}$, were calculated by [31]:

$$\dot{m} = \frac{\dot{Q}}{\rho}$$  \hspace{1cm} (4.2)

where $\dot{Q}$ was a provided measured volumetric flow rate and $\rho$ was the calculated density of the gas at the point of measurement. The volumetric flow rate was measured in the gas lines before the entrance to the burners. The density for each gas was calculated using the ideal gas law [31]:

$$\rho = \frac{P \ast MW}{R_{u} \ast T}$$  \hspace{1cm} (4.3)
where $P$ is the pressure, $MW$ is the molecular weight of the gas, $R_u$ is the universal gas constant and $T$ is the temperature. The pressure in each gas line was a measured value whereas the temperature of the gas in the lines at the point of the volumetric flow measurement was estimated based on measured ambient and gas line skin temperatures. The estimate of temperature added some uncertainty to the calculated mass flow value. Mass flow was used instead of velocities because it is a conserved quantity. This meant that the mass flow values calculated at the point of volumetric flow measurements could be directly applied downstream at the boundary of the computational domain. The pressure at the outlet was a measured quantity.

Estimates of velocities and pressures through the burners at the boundary of the computational domain were calculated using the continuity and Bernoulli’s equation for incompressible, subsonic flow. Flow of a gas may be considered incompressible provided that the Mach number ($Ma$) is less than about 0.3 [31]. The Mach number is the ratio of the fluid speed to the speed of sound in the fluid and can be defined as [31]:

$$Ma = \frac{v}{c} \quad (4.4)$$

The speed of sound in the fluid, $c$, is equal to [31]:

$$c = \sqrt{\gamma RT} \quad (4.5)$$

where $\gamma$ is ratio of specific heats, $R$ is the individual gas constant and $T$ is the temperature of the fluid. The incompressible assumption was made because the Mach number for each gas stream was calculated to be less than 0.3 at the entrance to the burners. Conditions within the burners were unknown so it is possible that the Mach number could have changed as the flow entered the burner. The flow boundary conditions could be improved by modeling the full burner or obtaining pressure, temperature and velocity measurements within the burners. These calculations also assumed insignificant frictional losses.

The calculated pressures were specified at the inlets along with the mass flow rate and the velocities were used to determine the turbulence quantities at the inlets. Specification of turbulence quantities is required by Fluent anytime flow enters the domain at an inlet when a turbulence model is used. The set of turbulence parameters used in this CFD model was the turbulence intensity, $I$, and hydraulic diameter, $D_H$. Velocities in the gas lines before the burners were first obtained by dividing the measured volumetric flow rate by the area of the pipe. Velocities within the burners were then calculated from the continuity equation. The form of the continuity equation used to find velocities within the burners was:

$$A_1 v_1 = A_2 v_2 \quad (4.6)$$
where \( A \) is the cross-sectional area, \( v \) is velocity and the subscripts 1 and 2 denote the upstream and downstream locations, respectively. Both burner dimensions and gas line cross sectional areas were known which allowed for the calculation of velocity within the burner based on an area change. Pressures within the burners were calculated based on the following form of Bernoulli’s equation [31]:

\[
\Delta P = \frac{1}{2} \rho (v_1^2 - v_2^2)
\]  

(4.7)

The calculated velocities were used to determine the turbulence intensity at each inlet by [33]:

\[
I = 0.16(Re_{D_H})^{\frac{1}{8}}
\]  

(4.8)

\( Re_{D_H} \) denotes the Reynolds number based on the hydraulic diameter and was calculated by [31]:

\[
Re_{D_H} = \frac{\rho v D_H}{\mu}
\]  

(4.9)

where \( v \) is the calculated velocity, \( D_H \) is the hydraulic diameter and \( \mu \) is the dynamic viscosity. The diameter of the circular openings in the diffusion plate used for gas inlets was taken as the hydraulic diameter.

### 4.3.2 Wall Boundary Conditions

The actual refractory layers were not included in the 3-D geometry used in the CFD model. Instead, the refractory walls were modeled as thermal resistances. For this strategy, wall thickness, material and outer wall temperature were specified. Literature values for wall roughness coefficients and heights were also input at each wall boundary condition. Outer wall temperatures were measured in several locations along the length of the operational reverberatory furnace used for this study. The measured temperatures were then averaged for the different walls. The averaged values were applied as part of the wall boundary condition. The thermal and physical properties of the walls were specified based on three different types of commercially available refractories typically used in lead processing furnaces. Different refractory properties were applied to different walls boundaries in the models. Table 4.3 show the chemical composition and thermal conductivities of the refractory materials used in the model. The thermal conductivity of the different refractory materials was taken at 2000 °F.

The gas-slag interface was considered a wall in the model as well. The gas-slag interface wall was set to be an adiabatic surface in which no heat flux occurred through it. This was because a heat sink was defined just above gas-slag interface surface to account for the heat flux into it due to smelting, melting and super heat (see section 4.6.2). The roughness coefficient and height were left at the default values for this surface.
Table 4.3: Thermal Conductivity of the Refractory Used in the CFD Model at 2000 °F [120]

<table>
<thead>
<tr>
<th>Refractory Type</th>
<th>Thermal Conductivity at 2000 °F (w/mk)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refractory 1</td>
<td>2.9</td>
</tr>
<tr>
<td>Refractory 2</td>
<td>3.6</td>
</tr>
<tr>
<td>Refractory 3</td>
<td>3.4</td>
</tr>
</tbody>
</table>

4.3.3 Symmetry Boundary Condition

A symmetry boundary condition was used in the construction of the CFD model. Figure 4.14 shows a schematic displaying where the symmetry boundary condition was applied in the 3-D geometry. Symmetry boundary conditions are used when the physical geometry of interest as well as the expected pattern of the flow and thermal solutions have mirror symmetry [32]. Fluent assumes a zero flux of all quantities across a symmetry boundary so it is important that the actual domain has no mass or heat transfer across the defined plane of symmetry. Fluent also assumes that the shear stress is zero at a symmetry boundary which means that a slip condition is applied at the symmetry plane when used in viscous flow calculations [33].

The locations of the temperature and velocity measurements provided for validation (see section 4.6.1) were used to assess whether a symmetry boundary condition could be applied along the centerline of the furnace. Two simulations were run, one which utilized the full computational domain and one in which a symmetry boundary condition was applied along the furnace centerline. Adiabatic conditions in which no heat was lost through the furnace walls or gas-slag interface was used for this evaluation.

Table 4.4 shows the calculated temperatures and velocity at the validation points for both simulations. The percent difference value was calculated by:

\[
\% \text{ Difference} = \frac{(T_{\text{Full Domain}} - T_{\text{Symmetry}})}{T_{\text{Full Domain}}} \quad \text{or} \quad \frac{(v_{\text{Full Domain}} - v_{\text{Symmetry}})}{v}
\]

(4.10)

Both simulations calculated very similar temperatures and velocity at the location of validation points provided. All the percent differences were within the relative standard deviation (RSD) values of the validation points as well (see section 4.6.1). Running the symmetry boundary condition cut the computational time down from eight to ten hours to two to four hours. Therefore, the slight loss in model accuracy was traded off for a dramatic decrease in computational time.
Table 4.4: Comparison of the Temperature and Velocity Measurements at the Provided Validation Locations for the Full Domain versus Centerline Symmetry Simulations

<table>
<thead>
<tr>
<th>Location</th>
<th>Units</th>
<th>Full</th>
<th>Symmetry</th>
<th>Absolute Difference</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>OP A</td>
<td>°F</td>
<td>3870</td>
<td>3872</td>
<td>-2</td>
<td>-0.1%</td>
</tr>
<tr>
<td>OP B</td>
<td>°F</td>
<td>3857</td>
<td>3857</td>
<td>0</td>
<td>0.0%</td>
</tr>
<tr>
<td>OP C</td>
<td>°F</td>
<td>3868</td>
<td>3872</td>
<td>-4</td>
<td>-0.1%</td>
</tr>
<tr>
<td>SH A</td>
<td>°F</td>
<td>3795</td>
<td>3784</td>
<td>11</td>
<td>0.3%</td>
</tr>
<tr>
<td>SH B</td>
<td>°F</td>
<td>3774</td>
<td>3784</td>
<td>-10</td>
<td>-0.3%</td>
</tr>
<tr>
<td>SH C</td>
<td>°F</td>
<td>3899</td>
<td>3892</td>
<td>7</td>
<td>0.2%</td>
</tr>
<tr>
<td>Flue T1</td>
<td>m/s</td>
<td>3783</td>
<td>3778</td>
<td>5</td>
<td>0.1%</td>
</tr>
<tr>
<td>Flue T2</td>
<td>m/s</td>
<td>3775</td>
<td>3781</td>
<td>-6</td>
<td>-0.2%</td>
</tr>
</tbody>
</table>

4.4 Sub-Models

Turbulence and combustion sub-models were used to construct the overall CFD model. A radiation sub-model was not used in the CFD model. See section 4.8.3 for justification on the omission of a radiation sub-model. The Reynolds number within the furnace was calculated to ensure the flow was turbulent. Table 4.5 shows the calculated Reynolds number at three locations within the furnace. The Reynolds number decreased with an increase in furnace length, but was still well above the turbulent threshold, which is a value of 4000 for internal flows [31]. Therefore, the flow was modeled as turbulent.
throughout the furnace. The turbulence model selected was the standard k-ω model. See section 0 for turbulence sub-model sensitivity analysis.

<table>
<thead>
<tr>
<th>% of Total Furnace Length</th>
<th>Reynolds #</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>160,728</td>
</tr>
<tr>
<td>50</td>
<td>93,765</td>
</tr>
<tr>
<td>90</td>
<td>88,803</td>
</tr>
</tbody>
</table>

The combustion sub-model used was Fluent’s dedicated model for non-premixed combustion which utilized a PDF lookup table. This model was used as it most closely mirrored the actual physical system of combustion in which the three gas streams, oxygen, natural gas and enriched air, exited the burners in distinct streams, mixed and then combusted. The oxygen was defined as a secondary oxidizer stream. The composition of these gas streams was input as mole fractions. Both the inlet diffusion and compressibility effects options were selected. The inlet diffusion option allowed for diffusion flux of the mixture fraction at the inlet. The compressibility effects option was selected to allow for a change in density of the gases based on the inlet temperature and pressure as the pressures within each gas line and the furnace were all different [33]. The furnace was modeled as a non-adiabatic system under equilibrium conditions. The equilibrium chemistry option was selected as the residence time within the furnace was estimated to be on the order of seconds rather than milliseconds.

The stream rich flammability option was used as well. In this approach, Fluent will compute the composition at the rich limit specified using equilibrium. For mixture fractions above this limit, Fluent will suspend the equilibrium chemistry calculation and will compute the composition based on mixing, but not burning, of the fuel. This increases the efficiency of the PDF calculation by bypassing the complex equilibrium calculations in the fuel-rich region [32]. The stream rich flammability limit for both the fuel and the secondary stream was calculated as 20% greater the stoichiometric mixture fraction. The PDF table was calculated for twenty different chemical species.

### 4.5 Solver Settings

There are two different types of solvers available in Fluent, pressure-based and density based. The difference between these solvers is the order in which the flow variables are solved. There are three algorithms based on these solver methods available in Fluent: pressure-based segregated solver, pressure-based coupled solver (PBCS) and density-based coupled solver (DBCS). Figure 4.15 shows a schematic of the way in which these three algorithms solve the governing equations.
In the segregated algorithm, the governing equations are solved sequentially, segregated from one another, while in the PBCS and DBCS algorithms, the mass and momentum equations are solved simultaneously. The DBCS also solves the energy and species equations with the mass and momentum equations. The DBCS is typically used when there is a strong interdependence between density, energy, momentum, and/or species which occurs in combusting flows, but the non-premixed combustion model is only available with the pressure-based solver. Therefore, the PBCS was selected for this model. The PBCS was chosen over the segregated algorithm as it has significantly better convergence speed.

All the solvers within Fluent require an initial guess for the solution flow field. This process is called solution initialization [121]. It is important to provide a good initial solution that will allow a final solution to be attained. The standard initialization method was used where the initial guess was computed from the air inlet on the end burners. This method was used as the air flow parameters were the most understood boundary condition.

The discretization scheme chosen for the gradients, pressure and all other parameters were the least squares based, PREssure STaggering Option (PRESTO!) and first-order upwind, respectively. The PRESTO! scheme is recommended for highly complex reacting flows with steep pressure gradients [33].
In general, first-order discretization yields better convergence than second-order schemes, but can also produce less accurate results [32]. See section 4.8.1 for a comparison of solutions obtained from first and second order discretization schemes.

The default under-relaxation values ($\alpha$) were used except for the density and body forces parameters which were set at 0.2 and 0.8, respectively. The under-relaxation factors control the advancement of the transport variable during the iteration process. Decreasing the under-relaxation value will decrease the allowed change in the variable from one iteration to the next. The default under-relaxation values for density and body forces were adjusted because they were too aggressive for the complex reacting flows [32]. The flow courant number (CFL) was set to be 50. The flow courant number is used to stabilize the convergence behavior of the solution when the PBCS is used for time independent or steady state flows. This number is related to the specified under-relaxation factors by [33]:

$$\text{CFL} = \frac{\alpha}{1 - \alpha}$$

4.6 Validation

Validation of the model was achieved through both quantitative and qualitative means. Validation was first assessed by comparing measured temperatures at different points in an operational industrial furnace to temperatures calculated by the model. The second means of validation was achieved by comparing simulated end burner flames dimensions to the measured end burner flame dimensions. The last test of validation was a comparison of the expected areas of high refractory wear in the model to areas of high refractory wear reported in literature.

4.6.1 Online Furnace Measurements

Temperature and velocity measurements from inside an operational industrial reverberatory furnace were provided for model validation. Figure 4.16 shows the locations of the temperature and velocity measurements. Temperature measurements were taken at three different locations inside of the furnace through both an observation port near the front of the furnace as well as through the slag hole near the back of the furnace. The thermocouple used to take the measurements was bent at a 45° angle and inserted through both openings. Two temperature measurements were taken parallel to the furnace floor on either side of the openings and one measurement was taken perpendicular to the furnace floor. These measurements were taken one foot from the refractory hot face. Two temperature measurements were also taken through the flue port at one and two feet in towards the furnace centerline from the refractory hot face, denoted as Flue 1 and Flue 2, respectively. Flue velocity was also measured through
the flue port one and half feet in towards the furnace centerline from the refractory hot face using a pitot static tube.

![Diagram showing observation ports and flue port](image)

**Figure 4.16** Locations of temperature and velocity measurements. *(orientation: side view)*

Two temperature measurements were taken at each location. A sample standard deviation and RSD was then calculated for each set of data. The RSD of each data set was calculated to be between 0.1 – 6%. Several pressure readings from the pitot static tube were recorded over the course of a thirty second measurement period. The standard deviation of the pressure readings was used to calculate the overall RSD of the calculated velocity. The RSD of the flue velocity measurement was calculated to be 23%.

### 4.6.2 Placement of Heat Sink

Table 4.6 and Table 4.7 list the heat of reaction for the smelting reactions and the latent heat values for the melting reactions considered for the heat sink calculation.

**Table 4.6: List of Smelting Reactions Considered in the Calculation of the Heat Sink Term [122], [123]**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>ΔH_{rxn @100°F} (kJ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbCO$_3$ = PbO + CO$_2$ (g)</td>
<td>87.5</td>
</tr>
<tr>
<td>PbSO$_4$ + 2C = PbS + 2CO$_2$ (g)</td>
<td>36.7</td>
</tr>
<tr>
<td>Pb(OH)$_2$ = PbO + H$_2$O (g)</td>
<td>55.7</td>
</tr>
<tr>
<td>2PbO + PbS = 3Pb + SO$_2$ (g)</td>
<td>238.5</td>
</tr>
<tr>
<td>2PbO + C = 2Pb + CO$_2$ (g)</td>
<td>42.5</td>
</tr>
</tbody>
</table>
A user-defined volumetric heat sink term (W/m$^3$) was included in the CFD model to account for the melting and smelting reactions that occur within the furnace as well as the super heating of the lead and slag phases. The estimate of the heat sink value was calculated based on a set of smelting and melting reactions that take place within typical lead processing reverberatory furnaces.

The latent heat values were taken at the temperature of the specified phase change. The main smelting reactions were all endothermic and the heat of reaction at 100 °F was used as this was the temperature at which the feed material entered the furnace. The energy content needed to super heat the lead and slag phases was determined by breaking these two phases into their major individual constituents and calculating the heat capacity for each one. The slag and the lead phases were assumed to be super-heated to the temperature at which they exited the furnace. These exit temperatures were measured. The consumption of heat from the smelting, melting and super heating occurring within the furnace was simulated by sinking the estimated heat needed for these reactions into a volume of cells just above the gas-slag interface. The volume of cells used as the location of the heat sink was created by separating a layer of cells one inch above the gas-slag interface into a new cell zone.

<table>
<thead>
<tr>
<th>Phase Transformation</th>
<th>Latent Heat (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pb = Pb (l)</td>
<td>4.8</td>
</tr>
<tr>
<td>PbO = PbO (l)</td>
<td>25.4</td>
</tr>
<tr>
<td>Na$_2$SO$_4$ = Na$_2$SO$_4$ (l)</td>
<td>19.5</td>
</tr>
<tr>
<td>PbS = PbS (l)</td>
<td>48.9</td>
</tr>
<tr>
<td>Cd = Cd (l)</td>
<td>6.2</td>
</tr>
<tr>
<td>Cd (l) = Cd (g)</td>
<td>111.9</td>
</tr>
<tr>
<td>H$_2$O (l) = H$_2$O (g)</td>
<td>44.2</td>
</tr>
</tbody>
</table>

Figure 4.17 shows the different heat sink configurations evaluated. In Heat Sink A, only one new cell zone was created an inch above the gas-slag interface and the heat content was sunk evenly down the length of the furnace. In Heat Sink B, C and D, two new cell zones were created above the gas-slag interface and different percentages of the heat content were sunk in the front and back half of the furnace. In Heat Sink E, three new cell zones were created where the new cell zone in the front half of the furnace was split in half. The heat content was distributed in different amounts into each of the three zones.
Table 4.8 shows the percent difference between the calculated and measured values at the validation points for the different heat sink configurations evaluated. The percent difference value was calculated by:

\[
\text{% Difference} = \frac{(T_{\text{measured}} - T_{\text{calculated}})}{T_{\text{measured}}} \quad \text{or} \quad \frac{(v_{\text{measured}} - v_{\text{calculated}})}{v_{\text{measured}}} \quad (4.10)
\]

The positive values indicate an over prediction and the negative values indicate an under prediction of the measured values. In the adiabatic simulation, no heat was lost through wall boundaries or a heat sink. The wall loss only simulation just took the heat loss through refractory walls into account.

The heat sink configuration that was chosen as the setup for the base case simulation was Heat Sink D as that simulation most closely predicted the measured temperatures and velocity. This
configuration physically made sense as well because the majority of the smelting and melting reactions are assumed to occur in the front half of the furnace. All the calculated temperatures overpredicted the measured temperatures. This could be because dust, which can be quite significant in these furnaces, was not modeled. If the dust phase was included in the model, some of the heat content in the gas phase would have been absorbed by the dust phase, thereby making the gas temperatures cooler.

Table 4.8: Percent Difference between the Calculated and Measured Values at the Validation Points for the Different Heat Sink Configurations Evaluated

<table>
<thead>
<tr>
<th>Heat Lost Configuration</th>
<th>% Difference between calculated and measured value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Observation Port Temperature</td>
</tr>
<tr>
<td></td>
<td>A</td>
</tr>
<tr>
<td>Adiabatic</td>
<td>63</td>
</tr>
<tr>
<td>Wall Loss Only</td>
<td>57</td>
</tr>
<tr>
<td>Heat Sink A</td>
<td>13</td>
</tr>
<tr>
<td>Heat Sink B</td>
<td>8</td>
</tr>
<tr>
<td>Heat Sink C</td>
<td>4</td>
</tr>
<tr>
<td>Heat Sink D</td>
<td>1</td>
</tr>
<tr>
<td>Heat Sink E</td>
<td>1</td>
</tr>
</tbody>
</table>

The trends in the calculated parameters were also evaluated in this stage of the validation procedure to make sure that they matched the measured trends and physically made sense. The absolute temperatures calculated in the model were highest in the front half of the furnace by the burners and lowest in the flue which was the measured trend as well. Figure 4.18 shows temperature and velocity contours on the flue plane where the validation points were measured. These contours were used to check the temperature and velocity trends within the flue. The temperature contour shows that the temperature gradually increases from the refractory hot face towards the flue centerline which was the trend in the measured temperature values. The velocity contour shows slow velocities at refractory boundaries where a boundary layer would be expected.

Although not all the calculated parameters at the validation locations were within the RSD of the measured values, it was concluded that this stage of validation was satisfied because of the variability of the furnace burden. The dimensions and other characteristics of the furnace burden can vary dramatically. A change in burden shape can significantly impact the calculated parameters at the validation locations (see section 5.2). Therefore, the exact burden shape would have to be known and
perfectly modeled to exactly match the validation temperatures and velocity. Obtaining the exact burden dimensions was not possible with the means of measurement available.

Figure 4.18 The (a) temperature and (b) velocity contours on the flue plane where the validation temperatures and velocity were measured. (orientation: front view)

4.6.3 Flame Characteristics

The final step in the validation process was to examine how well the CFD model predicted the flame characteristics. The burners modeled in the CFD simulations could produce very different looking flame depending on the gas flow rates used. Figure 4.19 shows the flame from the modeled burner running at slightly rich and rich conditions. In the slightly rich flame, the inner premixed flame was very well defined and the luminous, blackbody radiation zone was smaller than what was observed in the rich flame. Flame dimensions from the modeled burners were measured by the project’s industrial sponsors.

The slightly rich flow conditions were used for the validation procedure. Only the flame produced by the end burners were evaluated. A computational domain in which the burners pointed straight into the furnace, rather than at a downward and inward angle, was used for this evaluation because the flame dimensions were measured under similar conditions. Flame length was calculated based on temperature profiles. Figure 4.20 plots the normalized temperature down the centerline of the flame against the normalized flame length. The normalized temperature was calculated by dividing all the absolute temperatures by the maximum flame temperature. The normalized length was calculated as a percentage of the total modeled flame length. The location of the maximum temperature was taken as the end of the inner premixed flame. After this maximum, the flame temperature decreases slightly and then plateaued. The plateau in temperature indicated the end of the outer diffusion flame. Just outside of the flame, there was a heat transfer region where the temperature drops off dramatically and then leveled out.
into the ambient furnace temperature. The flame width was also calculated using temperature profiles. Figure 4.21a shows the temperature contour plot through the end burner centerline plane. The percentage values marked on the contour plot are the normalized lengths at which the temperature is plotted across the flame in Figure 4.21b. The maximum width was found to occur at 40% of the total flame length which was about where the inner premixed flame ended.

![Temperature Contour Plot](image)

Figure 4.21a shows the temperature contour plot through the end burner centerline plane. The percentage values marked on the contour plot are the normalized lengths at which the temperature is plotted across the flame in Figure 4.21b. The maximum width was found to occur at 40% of the total flame length which was about where the inner premixed flame ended.

![Flames](image)

Figure 4.19 Pictures of the flames produced by the modeled burners running at (a) slightly rich and (b) rich conditions.

Figure 4.22 shows a contour plot of the normalized CO₂ mass fraction along the end burner centerline plane. The CO₂ mass fraction along the end burner centerline was evaluated to assess the validity of using temperature to estimate the flame length and width. The CO₂ mass fraction contour plot shows a negative of the flame. This is expected as CO₂ is a product of the global methane combustion reaction described by:

\[
\text{CH}_4 + a(O_2 + xN_2) = b\text{CO}_2 + c\text{H}_2\text{O} + x\text{N}_2
\]

where \(a\), \(x\), \(b\) and \(c\) are all reaction coefficients which can vary based on the air to fuel ratio and gas composition. The calculated flame length based on the temperature data was the same as the length calculated based on the CO₂ mass fraction. This conclusion provided evidence that temperature data produced a good estimate of the flame dimensions. Species mass fractions were not used to estimate the flame dimensions as a first order solver was used and it is recommended that species data be calculated with second or third order solvers.
Figure 4.20 Normalized temperature as a function of normalized end burner flame length showing the different regions of the flame.

Figure 4.21 Data used in the calculation of end burner flame width showing the (a) temperature contour plot at the end burner centerline (orientation: top view) and (b) the plot of normalized temperature as a function of normalized flame width at different lengths along the flame.
Figure 4.22  Contour plot of normalized CO₂ mass fraction along the end burner centerline.

*(orientation: top view)*

Table 4.9 shows the difference in flame lengths and width as a function of changes in normalized mass flow rates. The normalized mass flow rates were calculated as a percentage of the base case values. All three mass flow rates for the different gas streams were either increased or decreased by the percent of base case value listed. The flame lengths and width are shown as a percentage of the measured dimensions. For the base case simulation (a normalized mass flow rate of 0%), the length of the inner premixed flame and the maximum width of the flame were almost exactly predicted by the model whereas the outer diffusion flame length was slightly overpredicted by the model. Four other mass flow rate conditions were run to assess the sensitivity of the flame dimensions with a change in mass flow rate. This analysis was performed as there was some uncertainty associated with the mass flow rate calculation. The analysis showed that the flame dimensions can vary slightly with changes in mass flow rates.

Table 4.9: Difference in Flame Lengths and Width as a Function of Changes in Mass Flow Conditions

<table>
<thead>
<tr>
<th>Normalized Mass Flow Rate (% of Base Case Value)</th>
<th>Inner Premixed Flame Length (% of measured value)</th>
<th>Outer Diffusion Flame Length (% of measured value)</th>
<th>Maximum Flame Width (% of measured value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20%</td>
<td>86</td>
<td>95</td>
<td>80</td>
</tr>
<tr>
<td>-10%</td>
<td>91</td>
<td>103</td>
<td>92</td>
</tr>
<tr>
<td>0%</td>
<td>101</td>
<td>112</td>
<td>101</td>
</tr>
<tr>
<td>+10%</td>
<td>108</td>
<td>117</td>
<td>112</td>
</tr>
<tr>
<td>+20%</td>
<td>114</td>
<td>120</td>
<td>117</td>
</tr>
</tbody>
</table>
The last flame characteristic evaluated in this stage of validation was the effect of side burner flame impingement on the furnace burden. Figure 4.23 shows a picture of test work performed using the American Combustion PyreTron II air/oxygen/fuel burner to evaluate the effect of direct flame contact with the furnace burden. A stack of lead blocks was used to represent the furnace burden. The test work setup mirrored the side burner angles and location within the operational furnace. The impingement of the flame on the lead blocks caused flow separation and recirculation at the point of impact. The lower recirculation zone rotated in a counter-clockwise fashion while the upper recirculation zone rotated in a clockwise fashion.

Figure 4.23 Picture of test work performed showing the effect of flame impingement on a stack of lead blocks used to represent the furnace burden.

Velocity vector plots from the base case simulation results were generated to assess whether the model predicted the same flow separation and recirculation phenomena shown in the test work. Figure 4.24 (see page 80) shows a velocity vector plot at the point of side burner flame impingement on the modeled furnace burden. Both a clockwise (CW) recirculation zone above the flame and a counterclockwise (CCW) recirculation zone below the flame are seen in the velocity vector plot. This result was used as another measure of validation for the model.

4.6.4 General Wear Patterns

The final step in the validation process was to qualitatively assess general areas of high wear within the furnace. Figure 4.25 shows the main areas of wear reported in a typical reverberatory furnace used to process lead battery scrap. The schematic only shows wear on the refractory in the combustion space volume. High wear areas are reported to occur on the roof above the furnace charge, at the opening
to the flue and next to side burners. The cause of the observed wear phenomena can generally be subdivided into chemical, thermal and mechanical stresses. These can appear as a single stress factor, but more commonly, a combination of these stresses occurs and adversely affect the furnace refractory. The two parameters used to assess areas of high refractory wear within the CFD model were temperature and wall shear stress. Hot spots within the refractory lining can cause thermal stresses that significantly reduce the refractory’s hot strength [5]. This reduction in strength can cause the refractory to be more susceptible to other mechanisms of wear such as erosion or chemical corrosion [17]. Wall shear stress was used as a measure of erosion experienced by the refractory. Many CFD studies in literature on the blast furnace hearth use wall shear stress to assess areas of high refractory wear [66 – 69]. Experimental work has also been performed which showed that flow induced shear stresses can cause erosive damage to the walls of refractory lined furnaces [124], [125].

Figure 4.24 Velocity vector plot at the point of side burner flame impingement on the furnace burden showing the clockwise and counter-clockwise recirculation zones. (orientation: front view)
Figure 4.26 - Figure 4.28 show temperature and wall shear stress contour plots for the base case simulation. Boxed areas on these contour plots indicated hot spots or areas of concentrated wall shear stress. The temperatures and wall shear stresses in these plots are normalized as a percentage of the average value of the parameter in the area of interest. Figure 4.26 shows the resulting contour plots for the front half of the furnace roof where the high areas of wear are expected. The temperature contour plot shows a hot spot which extends from the middle of this portion of roof up to the furnace centerline. The wall shear stress plot shows an area of concentrated wall shear stress at the furnace centerline which extends backwards towards the middle of the front of the roof. The boxed areas in these contour plots overlap meaning that the model predicts an area where both temperature and wall shear stress on the roof are high. Therefore, it would be expected that the overlapping area would experience high wear. The hot spots and high wall shear stress occur in this area of the furnace refractory because the end burner flames impinge on the furnace burden which causes flow and heat to be redirected towards the roof.

Figure 4.25 Schematic of computational domain showing the locations of high refractory wear areas [17]. (orientation: isometric view)

Figure 4.27 shows temperature and wall shear stress contour plots for the front half of the furnace side wall. These contour plots show an overlapping area of high temperature and wall shear stress just below and to the right of the side burner opening. This high wear location would also be expected as the side burner flames directly contact the furnace burden. This contact causes flow separation and recirculation (see section 4.6.3) which would direct flow and heat to the side wall.
Lastly, Figure 4.28 shows temperature and wall shear stress contour plots for the flue wall. Again, there is an overlapping area of high temperatures and concentrated wall shear stress right below the flue opening which would suggest that this is an area of high wear as well. This area of high wear occurs because all the hot combustion gases are abruptly funneled into the flue opening causing heat and flow to be directed at the flue edges. Informal discussions with operators of secondary lead reverberatory furnaces indicate that the locations on the roof, side wall and flue are common areas of high wear.

Figure 4.26 Contour plots of normalized (a) temperature and (b) wall shear stress on the front half of the furnace roof. (orientation: top view)

Figure 4.27 Contour plots of normalized (a) temperature and (b) wall shear stress on a portion of the furnace side wall. The white square represents the side burner block. (orientation: side view)
4.7 Convergence

In general, CFD problems involve groups of nonlinear PDEs that are solved by iterative processes that successively improve a solution until a level of ‘convergence’ is reached. Convergence means that the numerical solution has reached a limit for a specified degree of accuracy. Model convergence was assessed in three different ways: (1) residual values, (2) iterative convergence and (3) mesh independence. All three of these methods are important in concluding whether the solution has reached an overall level of convergence.

4.7.1 Residual Values

Residuals are errors of the discretized PDEs that occur during the numerical solution procedure. They measure the extent of imbalances arising from the discretized PDEs and terminate the numerical process once a specified tolerance has been reached [24]. For convergence to be achieved, the residual values must diminish as the numerical process progresses. Residual values are calculated for all the transport variables included in the model [32].

Figure 4.29 shows a plot of the scaled residual values versus iteration number for the base case simulation. Scaled residuals are a measure of the relative rather than the absolute imbalance in the transport variable of interest. Scaled residuals are displayed by default in Fluent as they are a more appropriate indicator of convergence for most problems [33]. Generally, a decrease of scaled residual values by three orders of magnitude during the iteration process indicates residual convergence. Most of the time, this means that the residual value drops below $10^{-3}$. Although, stricter residual tolerance is recommended for the energy transport variable. For best practice, it is suggested that the scaled energy
residual reach $10^{-6}$[24]. All the scaled residuals for transport variables in each simulation performed in this research decreased at least three orders of magnitude except for the scaled energy residual which decreased to a value of $10^{-6}$.

4.7.2 Iterative Convergence

Iterative convergence is achieved when specified quantities of interest plateau and do not change from one iteration to the next [24]. Three quantities of interest were evaluated for iterative convergence: (1) mass flow on the pressure outlet (flue boundary), (2) maximum temperature within the computational domain and (3) the average velocity on the pressure outlet. Temperature and velocity parameters were chosen to be monitored because these variables were used for validation which means that it was important that they remain unchanged after a certain number of iterations for the solution to be considered converged. Figure 4.30 (see page 85 shows the plots of the three quantities monitored for iterative convergence as a function of iteration number. The monitored quantities were normalized as a percentage of their steady value achieved. All the quantities monitored leveled out before residual convergence was reached.

4.7.3 Mesh Independence

The last convergence criteria evaluated in this study was mesh independence. Mesh independence is met when the numerical solution no longer changes with an increase in the number of
cells [24]. Adiabatic conditions in which no heat was lost through the walls or the gas-slag interface was used in the simulations for the mesh independence study. The temperature and velocity measurements taken at the validation locations (see section 4.6.1) were evaluated for the different mesh densities assessed. Figure 4.31 shows the results of this analysis.

Figure 4.30 Assessment of iterative convergence showing normalized (a) mass flow rate on the pressure outlet, (b) maximum temperature in the domain and (c) average velocity on the pressure outlet as a function of iteration number.
The calculated temperatures and velocity at the validation locations all level out between 2.5 and 3 million cells. This trend was true for all the computational domains with the different burden shapes evaluated (see Appendix A). Therefore, a 2.5 million cell mesh was used for all the simulations reported in this research.
4.8 Model Sensitivity Analysis

Various assumptions were made in the construction of the CFD model which all had the potential to affect the numerical solution. The following sections provide justification for the three main assumptions made in the CFD model. The first was the use of a 1st order solver, the second was the choice of the standard k-ω turbulence model and the third was the omission of a radiation sub-model.

4.8.1 Solver Settings

The main solver setting evaluated was the order of the solution. The numerical solution for the base case simulation was obtained using a first order upwind discretization scheme. In the first order upwind scheme, quantities at the cell faces are determined by assuming that cell-center values of any transport variable represent a cell-average value and hold throughout the entire cell, i.e. the face quantities are identical to the cell quantities. In contrast, the second-order upwind scheme computes the quantities at the cell faces using a multidimensional linear reconstruction approach. In this approach, greater accuracy is achieved at the cell faces through a Taylor series expansion of the cell-centered solution about the cell centroid [27].

The base case simulation was run using the 2nd order discretization scheme to understand the sensitivity of the order of solution on the numerical results. Table 4.10 shows the normalized 2nd order solution results at the validation points.

<table>
<thead>
<tr>
<th>Validation Location</th>
<th>% of 1st Order Solution Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>OP A</td>
<td>110</td>
</tr>
<tr>
<td>OP B</td>
<td>104</td>
</tr>
<tr>
<td>OP C</td>
<td>106</td>
</tr>
<tr>
<td>SH A</td>
<td>100</td>
</tr>
<tr>
<td>SH B</td>
<td>100</td>
</tr>
<tr>
<td>SH C</td>
<td>102</td>
</tr>
<tr>
<td>Flue 1</td>
<td>99</td>
</tr>
<tr>
<td>Flue 2</td>
<td>100</td>
</tr>
<tr>
<td>Flue Velocity Point</td>
<td>100.4</td>
</tr>
</tbody>
</table>

The results are normalized as a percentage of the first order solution results. The quantities produced at the validation points using the 1st and 2nd order solutions are very similar. The largest difference in the
results was 10% at OP A. Table 4.11 shows the normalized 2nd order results for maximum and average of temperature and wall shear stress on the roof and sidewall. There was some variability between the magnitudes of these parameters calculated using the 1st versus the 2nd order solver scheme.

Table 4.11: Normalized 2nd Order Results for Maximum and Average Values of Temperature and Wall Shear Stress on the Roof and Sidewall

<table>
<thead>
<tr>
<th>Parameter</th>
<th>% of 1st Order Solution Value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Maximum</td>
</tr>
<tr>
<td>Roof Temperature</td>
<td>101.1</td>
</tr>
<tr>
<td>Roof Wall Shear Stress</td>
<td>115.3</td>
</tr>
<tr>
<td>Side Wall Temperature</td>
<td>107.7</td>
</tr>
<tr>
<td>Side Wall Shear Stress</td>
<td>86.9</td>
</tr>
</tbody>
</table>

Figure 4.32 - Figure 4.34 show a comparison of the contour plots at the main areas under investigation for this research generated through 1st and 2nd order solution schemes. The temperature, velocity and wall shear stress values used to construct these plots were all normalized as a percentage of the average 1st order solution value of each parameter at the location under evaluation. The contour plots in these figures are all reasonably similar between the 1st and 2nd order solutions. The key areas assessed as high wear locations are boxed in red and appear in the same location for both the 1st and 2nd order solutions. The plots show that the magnitudes of the parameters investigated vary slightly between the different solution schemes. The 1st order solution scheme was concluded to be sufficient for the model as the 2nd order solution did not provide any additional information and was more computationally expensive. The purpose of the model was to assess relative changes in the high wear locations not to resolve the absolute magnitudes of the variables of interest. Therefore, matching the magnitudes of the temperature and wall shear stress at the locations evaluated was not as critical as matching the key areas of high wear.

It was more difficult to reach residual convergence with the 2nd order solution as well. The energy residual in the 2nd order solution did not quite reach 10^{-6} but did drop three orders of magnitude. Higher grid resolution would most likely be needed to improve the residual convergence behavior, but would also increase the computational time. The 2nd order solution ran for four to five hours before satisfying all of the convergence criteria whereas the 1st order solution only ran between two and three hours before achieving convergence. There was also some uncertainty in various boundary conditions applied in the model which meant that increasing the solution accuracy would not increase the overall accuracy of the model.
Figure 4.32  Comparison of 1\textsuperscript{st} versus 2\textsuperscript{nd} order solutions of flue (a) temperature and (b) velocity at the plane of the flue validation points.  \textit{(orientation: front view)}

Figure 4.33  Comparison of 1\textsuperscript{st} versus 2\textsuperscript{nd} order solutions of roof (a) temperature and (b) wall shear stress.  \textit{(orientation: top view)}
Figure 4.34 Comparison of 1st versus 2nd order solutions of side wall (a) temperature and (b) wall shear stress. The white square represents the side burner block. (orientation: side view)

4.8.2 Turbulence Sub-Models

In the beginning of the modeling process, it was unknown what turbulence model would be sufficient for simulating the flow within the furnace. Therefore, four different turbulence sub-models were investigated for use in the CFD model. Two k-ε models, the standard and realizable, were evaluated first. Figure 4.35 and Figure 4.36 show the residuals generated for the base case simulation when the standard and realizable k-ε turbulence models were used. Both simulations that utilized the k-ε models did not achieve residual convergence as the epsilon residual did not drop three orders of magnitude. More refined inflation layers that better resolve the boundary layer would probably have had to be used in the mesh to reach residual convergence using a k-ε turbulence model. The smaller inflation layers severely decreased the mesh quality though. For this reason, it was concluded that the k-ε models were not appropriate for resolving flow characteristics.

The standard k-ω and k-ω SST models were evaluated next. Both simulations using the different models satisfied all criteria for convergence. Table 4.12 shows the percent difference between the calculated and measured value at the validation points for both simulations. The simulation using the standard k-ω model more closely predicted the values at the majority of the validation points.

Figure 4.37 - Figure 4.39 show a comparison of the contour plots at the areas of interest for the simulations using the standard k-ω and k-ω SST turbulence models. The parameters of interest are normalized as a percentage of the average standard k – ω solution value at the location evaluated. Although the magnitudes of the different variables vary slightly between the two simulations, all the
contour plots show the same key features of high wear in the same locations. The simulation using the standard k-ω turbulence model also converged in less time and the residuals were reduced to a greater extent than in the simulation which utilized the k-ω SST turbulence model. For these reasons, the standard k-ω was selected for use in the model.

Figure 4.35  Plot of residual values as a function of the number of iterations for the base case simulation run with the k-ε turbulence model.

Figure 4.36  Plot of residual values as a function of the number of iterations for the base case simulation run with the k-ε realizable turbulence model.
Table 4.12: Percent Difference between the Calculated and Measured Value at the Validation Points for the Base Case Simulation using the k – ω and k – ω SST Turbulence Models

<table>
<thead>
<tr>
<th>Validation Point</th>
<th>% Difference between calculated and measured value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>k – ω</td>
</tr>
<tr>
<td>OP A</td>
<td>1</td>
</tr>
<tr>
<td>OP B</td>
<td>3</td>
</tr>
<tr>
<td>OP C</td>
<td>6</td>
</tr>
<tr>
<td>SH A</td>
<td>5</td>
</tr>
<tr>
<td>SH B</td>
<td>2</td>
</tr>
<tr>
<td>SH C</td>
<td>4</td>
</tr>
<tr>
<td>Flue 1</td>
<td>3</td>
</tr>
<tr>
<td>Flue 2</td>
<td>4</td>
</tr>
<tr>
<td>Flue Velocity Point</td>
<td>20</td>
</tr>
</tbody>
</table>

Figure 4.37 Comparison of contour plots of flue (a) temperature and (b) velocity at the plane of the flue validation points obtained from simulations using the standard k-ω and k-ω SST turbulence models. (orientation: front view)
Figure 4.38 Comparison of contour plots of roof (a) temperature and (b) wall shear stress obtained from simulations using the standard k-ω and k-ω SST turbulence models. (orientation: top view)

Figure 4.39 Comparison of contour plots of side wall (a) temperature and (b) wall shear stress obtained from simulations using the standard k-ω and k-ω SST turbulence models. The white square represents the side burner block. (orientation: side view)

4.8.3 Radiation

A radiation sub-model was not included at this stage due to the lack of boundary and material conditions required to successfully implement the radiation models without introducing additional inaccuracies to the numerical solution. The feed and refractory material properties needed for the
radiation calculation were unknown. The P-1 and DO models are typically used in the modeling combustion applications. In both models, an emissivity value needs to be defined at the wall boundary conditions. The emissivity value of the refractory could be estimated based on information found in literature, but the emissivity value for the furnace burden surface would have been more difficult to define. This is because the furnace burden is a heterogeneous mixture of several different constituents. Even if the emissivity of all the constituents were known, they would need to be averaged and applied to the surface in a way that was physically representative of the actual burden. The material properties and distribution of dust particles within the gases was also not well understood. The dust particles in the gases could greatly affect the radiative heat transfer within the furnace. Applying inaccurate material properties at the wrong boundary conditions could cause the radiation sub-model to produce more error in the numerical solution.

The measurements at the validation points and trends within the furnace could be predicted within reasonable accuracy without the inclusion of a radiation sub-model. Literature also reports convection rather than radiation as being a major cause of stresses within furnace refractory. Therefore, the addition of a radiation sub-model would have provided limited, if any, additional information that could be used to assess relative changes within the furnace.
CHAPTER 5
SIMULATION RESULTS: EFFECT OF FURNACE BURDEN GEOMETRY

The developed CFD model of the secondary lead reverberatory furnace was first used to assess the influence of burden geometry on the overall numerical solution as well as the areas of high wear. The following chapter details the findings from this study. The front half of the roof and side wall are the main areas of interest that were evaluated.

5.1 Evaluated Burden Geometries

Figure 5.1 shows a schematic of the base case burden geometry. The burden shape was defined by three dimensions, \( x_1, y_1 \) and \( z_1 \) (see section 4.2.2). Three variations of the base case geometry were constructed by changing one of these three dimensions. Figure 5.2 shows the three other burden shapes evaluated. These burden geometries were investigated because similar shapes could theoretically be achieved in an active furnace through operational changes or some form of physical manipulation. The dimensions for these burden shapes were changed in the following ways: \( z_2 \) was 50% greater than \( z_1 \), \( x_2 \) was 20% less than \( x_1 \) and \( y_2 \) was 10% less than \( y_1 \). The labels in the top right-hand corner of the figures denote the name of each burden geometry and are used to identify the geometries throughout the chapter.

Figure 5.1   Schematic of the base case burden geometry showing a (a) top down and (b) side view.
Figure 5.2  Schematic of the four addition burden geometries evaluated which were identified as the (a) tall burden, (b) short burden and (c) narrow burden where \( z_2 \) was 50% greater than \( z_1 \), \( x_2 \) was 20% less than \( x_1 \) and \( y_2 \) was 10% less than \( y_1 \).

It should be noted that the volume of the cell zones created above the gas-slag interface varied between the different burden geometries. This occurred because the surface area of the burdens changed for the different shapes studied. The variation in surface areas also slightly changed the mesh between the different computational domains. Table 5.1 shows the normalized cell zone volumes as a percentage of the base case value for the different burden geometries. Cell zone 1 was created above the burden in the front half of the furnace and cell zone 2 was created above the gas-slag interface in the back half of the furnace. Due to this variation in cell zone volume, the total heat flow (W) into these zones was kept constant rather than the volumetric heat flow (W/m\(^3\)).
Table 5.1: Average Burden Surface Temperature Normalized as a Percentage of the Base Case Value for the Different Burden Geometries Evaluated

<table>
<thead>
<tr>
<th>Burden Geometry</th>
<th>Cell Zone 1 (% of Base Case Value)</th>
<th>Cell Zone 2 (% of Base Case Value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tall Burden</td>
<td>106</td>
<td>97</td>
</tr>
<tr>
<td>Short Burden</td>
<td>98</td>
<td>97</td>
</tr>
<tr>
<td>Narrow Burden</td>
<td>93</td>
<td>92</td>
</tr>
</tbody>
</table>

5.2 Calculated Values at Validated Points

The parameters at the validation points were calculated for all the burden geometries investigated. Table 5.2 shows the percent difference between the calculated and measured values at the validation locations for the simulations with the different burden geometries (see section 4.6.1).

Table 5.2: Difference between the Calculated and Measured Values at the Validation Points for all the Burden Geometries Evaluated

<table>
<thead>
<tr>
<th>Burden Geometry</th>
<th>Observation Port Temperature</th>
<th>Slag Hole Temperature</th>
<th>Flue Temperature</th>
<th>Flue Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
<td>C</td>
<td>A</td>
</tr>
<tr>
<td>Base Case</td>
<td>1</td>
<td>3</td>
<td>6</td>
<td>5</td>
</tr>
<tr>
<td>Tall Burden</td>
<td>-10</td>
<td>11</td>
<td>19</td>
<td>6</td>
</tr>
<tr>
<td>Short Burden</td>
<td>2</td>
<td>-1</td>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>Narrow Burden</td>
<td>-18</td>
<td>-13</td>
<td>-9</td>
<td>5</td>
</tr>
</tbody>
</table>

The base case geometry was used for the validation of the model and therefore has the smallest difference between the calculated and measured values. In most cases, the most significant differences between the calculated and measured values occurred at the observation port locations. The slag hole and flue temperatures were all overpredicted by about the same amount for all the burden geometries evaluated. The larger sensitivity in temperature near the observation port was because the flow in the front half of the furnace would be most affected by a change in burden shape whereas the flow in the back half of the furnace would be less affected by this change. These results were generated to show that the burden shape used in the computational domain had the potential to significantly affect the parameters calculated at the validation locations. Therefore, it is important to document the dimensions of the burden when furnace measurements are made so that the model can be properly validated.
5.3 Burden Surface Temperature

The burden surface temperature was used as a measure of smelting rate. Furnace efficiency could not be calculated because of the way the model was constructed. The model was setup to sink the same amount of total heat (W) into the cell zones created above the gas-slag interface regardless of burden shape. This assumption might not be physically accurate though as different burden shapes would most likely facilitate different amounts of heat flow into the surface of the burden due to varying amounts of flame impingement and surface areas. Figure 5.3 shows contour plots of the CO\textsubscript{2} mass fraction from the side burner flame, demonstrating different degrees of the side burner flame impingement on the different burden geometries studied. The differing amount and location of the flame impingement on the burden not only caused changes in smelting rate but also flow patterns and heat transfer within the furnace. These trends are discussed later in the chapter.

![Figure 5.3 Contour plots of CO\textsubscript{2} mass fraction along the centerline plane of the side burner the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. (orientation: normal to plane)](image)

Furnace efficiency could be measured if the actual burden and the reactions that occur within it were included in the model. The effect of flame impingement and surface area can be seen from the equation for total convective heat flow (W) which is:
\[ Q_{\text{conv}} = hA(T_s - T_\infty) \]  

(5.1)

where \( h \) is the heat transfer coefficient, \( A \) is the surface area, \( T_s \) is the surface temperature and \( T_\infty \) is the ambient temperature. A larger amount of flame impingement would increase the surface temperature of the burden and thereby increase the amount of heat flow into the feed material. Larger burden surface areas would also increase the heat flow to the burden. See Appendix B for further discussion on the sensitivity of the results for the heat sink values used.

Table 5.3 shows the average burden surface temperatures normalized as a percentage of the base case value for all the burden geometries evaluated. The average burden surface temperature was the highest for the tall burden and lowest for the narrow burden. Therefore, based on burden surface temperatures, it would be expected that the greatest total heat flow to the burden would occur for the tall burden geometry and the lowest total heat flow to the burden would occur for the narrow burden geometry. The order of the average burden surface temperatures occurs because the tall burden experienced the largest degree of flame impingement and the flat burden experienced the least amount of flame impingement.

<table>
<thead>
<tr>
<th>Burden Geometry</th>
<th>Average Burden Surface Temperature (% of Base Case Value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tall Burden</td>
<td>107</td>
</tr>
<tr>
<td>Short Burden</td>
<td>94</td>
</tr>
<tr>
<td>Narrow Burden</td>
<td>91</td>
</tr>
</tbody>
</table>

5.4 Furnace Roof Results

The front half of the furnace roof was the first high wear location within the furnace to be evaluated. The temperature and wall shear stress values in this location were compared for the different burden geometries. The following sections detail the results of the simulations.

5.4.1 Comparison of Roof Temperature

Figure 5.4 shows bar graphs that display the maximum roof temperature and a measure of the roof area that was affected by high temperatures. Both parameters were normalized as a percentage of the base case value. The affected area was defined as the total area on the roof where the temperature was greater than 90% of maximum roof temperature for the base case simulation. The dashed lines on the bar
graphs represent 100% of the base case value. Therefore, values above the dashed line were greater than the base case result and values below the dashed line were less than the base case result. The maximum roof temperature for the tall burden geometry was 7% greater than the base case whereas the narrow burden geometry produced slightly lower maximum roof temperature than the base case. The short burden had the same maximum roof temperature as the base case with a slightly larger affected area. The affected roof area was 50% greater and 75% less than the base case for the tall and narrow burdens, respectively.

Figure 5.4 The (a) maximum roof temperature and (b) temperature affected roof area normalized as percentages of the base case value for all the burden geometries evaluated.

Figure 5.5 shows contour plots of the temperature affected area on the roof for each of the burden geometries studied. These plots visually depict the difference in roof area affected by high temperatures for each burden shape. The maximum temperature for each case all roughly occur in the same location on the front half of the roof. These contour plots visually confirm that the largest temperature affected roof area occurred for the tall burden and the smallest temperature affected roof area occurred for the narrow burden. The base case and short burden geometry produced roughly the same shape and sized temperature affected roof area.

Figure 5.6 shows contour plots of the roof temperatures normalized as a percent of the average base case roof temperature for all simulations. These plots visually depict the difference in temperature magnitudes between each case since they are all normalized to the same value. The roof in the tall burden simulation experienced the highest temperatures. The roof in the narrow burden simulation experienced the lowest temperatures. The tall burden resulted in a hotter, more concentrated zone on the roof whereas
the narrow burden resulted in a more even roof temperature distribution. Again, the roof temperature distribution for the short burden was very similar to that of the base case simulation.

![Temperature Affected Area](image)

Figure 5.5 Contour plots of the temperature affected roof area for the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. *(orientation: top view)*

The roof temperature trends for these simulations can be explained through the use of Figure 5.7 and Figure 5.8. Figure 5.7 shows the velocity vectors along the end burner centerline for the different burden geometries studied and Figure 5.8 shows contour plots of temperatures along the end burner centerline for all the different burden geometries. The velocity vector plots show that the impingement of the end burner flame on the furnace burner caused the flow to be reflected towards the roof. The impingement also caused flow separation and recirculation. A counter-clockwise (CCW) recirculation zone above the end burner flame was observed for all the burden geometries. A recirculation zone was also observed below the end burner flame for the tall burden geometry. The locations of the recirculation zones and area of flow redirection caused different amounts of heat to be directed at the furnace roof. The tall burden resulted in a recirculation zone above the end burner that was much closer to the roof than was
observed for the other burden simulations, thereby causing hotter roof temperatures when compared to the
rest of the simulations. The temperature contour plots also show that the tall burden resulted in a greater
degree of end burner flame impingement closer to the roof, which caused hotter gases to be redirected at
the roof. The recirculation zones above the end burner for the base case and short burden were in the
same location and both geometries had similar degrees of end burner flame impingement. The
recirculation zone above the end burner for the narrow burden simulation occurred a little below the
location observed in the base case simulation, which caused the roof temperatures to be lower than the
base case simulation. The narrow burden also had less direct contact with the end burner flame, resulting
in less redirection of heat at the furnace roof.

![Figure 5.6](image)

**Figure 5.6** Contour plots of roof temperatures for the (a) base case, (b) tall, (c) short and (d) narrow geometries normalized as a percentage of average base case roof temperature value. *(orientation: top view)*
Figure 5.7  Velocity vectors along the end burner centerline for the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. (orientation: side view)
Figure 5.8 Contour plots of the temperatures along end burner centerline for the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. 
(orientation: side view)
5.4.2 Comparison of Roof Wall Shear Stress

Figure 5.9 shows bar graphs that display the maximum roof wall shear stress and a measure of the roof area that was affected by high shear stress values. Both parameters were normalized as a percentage of the base case value. The affected area was defined as the total area on the roof where the wall shear stress was greater than 90% of maximum roof wall shear stress for the base case simulation. The dashed lines on the bar graphs represent 100% of the base case value. The tall and the narrow burdens resulted in slightly lower maximum roof wall shear stress values when compared to the base case maximum. The short burden produced a slightly larger maximum roof wall shear stress value. The size of the wall shear stress affected areas for the tall and narrow burden were only 3.7% and 4.7% of the base case value. The short burden resulted in a 63% increase in wall shear stress affected area when compared to the base case.

![Bar Graphs](image)

Figure 5.9 The (a) maximum roof wall shear stress and (b) wall shear stress affected roof area normalized as percentages of the base case values for all the burden geometries evaluated.

Figure 5.10 shows contour plots of the wall shear stress affected area on the roof for each of the burden geometries studied. These plots visually depict the difference in roof area affected by high wall shear stress values for each burden shape. The maximum wall shear stress for each case occurs in roughly the same location on the front half of the roof. The area affected by high wall shear stress was very small and occurred at the centerline of the furnace for all the simulations. The small size of the base case wall shear stress affected area caused the changes in the affected area results for the other burden geometries to be amplified. The base case affected area was 0.46% of the total roof area. Although the wall shear stress affected area for the short burden may have been 63% greater than the base case value, it was still a very small percentage of the total roof area, i.e. 0.75%.
Figure 5.11 shows contour plots of the roof wall shear stress normalized as a percentage of the average base case roof wall shear stress for all simulations. These plots visually depict the difference in wall shear stress magnitudes between each case since they are all normalized to the same value. The wall shear stress values on the roof in the narrow burden simulation were the lowest and the most evenly distributed. The other simulations produced reasonably similar contours with the roof from short burden simulation experiencing the highest magnitude of wall shear stress.

The trends for the roof wall shear stress can be explained with Figure 5.12. Figure 5.12 shows a side view of the velocity vectors on the symmetry plane in the furnace. Fluent calculates wall shear stress as a function of the normal velocity gradient at the wall as:

$$\tau_w = \mu \frac{\partial v_i}{\partial x_i}$$  \hspace{1cm} (5.2)

where $\mu$ is viscosity. Therefore, higher velocities near the roof would result in a larger wall shear stress.
The velocity vectors show that the impingement of the end burners caused flow redirection to happen in the same location along the length of the burden for each simulation. The short burden resulted in a higher concentration of faster velocity vectors to be redirected at the furnace roof when compared to the base case simulation. This occurred because of the burden shape. The base case, short and narrow burdens were all modeled with a small divot about half way down the total burden length. For both the base case and narrow burden geometries, the end burner impinged before the divot on the inclined portion of the burden which caused the gases to slow down. The divot was shifted back further towards the end wall for the short burden. This caused the end burner to impinge after the divot on a declined rather than an inclined portion of the burden, resulting in less drag and higher redirected velocities than the base case and narrow burden. The tall burden resulted in slower velocity vectors to be redirected at the roof. A larger portion of the end burner flame came in contact with the tall burden which resulted in a greater drag force and slowed the velocity of the redirected gases.

Figure 5.11 Contour plots of roof wall shear stress for the (a) base case, (b) tall, (c) short and (d) narrow geometries normalized as a percentage of average base case roof wall shear stress value. (orientation: top view)
Figure 5.12  Velocity vectors along symmetry plane for the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. (*orientation: side view*)
5.5 Furnace Side Wall Results

The furnace side wall was the second area of high wear that was evaluated. Only the front half of the side wall was evaluated as that was the reported location of high wear. Both temperature and wall shear stress at this location were compared for the different burden geometries studied. The following sections detail the results of the simulations.

5.5.3 Comparison of Side Wall Temperatures

Figure 5.13 shows bar graphs that display the maximum roof temperature and a measure of the roof area that was affected by high temperatures. Both parameters were normalized as a percentage of the base case value. The affected area was defined as the total area on the side wall where the temperature was greater than 90% of maximum side wall temperature for the base case simulation. The dashed lines on the bar graphs represent 100% of the base case value. The maximum side wall temperatures for each simulation were all very similar. The maximum temperature was 6% greater and 8% less than the base case simulation for the tall and narrow burden, respectively. The short burden produced the same maximum side wall temperature as the base case. There was a significant difference in the size of the side wall area affected by temperature for the different burden geometries simulated though. The tall burden produced a 341% increase in the temperature affected area whereas the short and narrow burdens resulted in a 42% and 100% reduction in the temperature affected area compared to the base case.

Figure 5.13 The (a) maximum side wall temperature and (b) temperature affected side wall area normalized as percentages of the base case values for all the burden geometries evaluated.
Figure 5.14 shows contour plots of the temperature affected area on the side wall for each of the burden geometries studied. These plots visually depict the difference in roof area affected by high temperatures for each burden shape. The affected area for the tall burden encompassed most of the side wall area to the right of the side burner opening. The base case and short burden geometries resulted in affected areas both above and below the side burner opening. There was no affected area for the narrow burden simulation.

Figure 5.15 shows contour plots of the side wall temperatures normalized as a percent of the average base case side wall temperature for all simulations. These plots visually depict the difference in temperature magnitudes between each case since they are all normalized to the same value. The side wall from the tall burden simulation experienced the highest temperatures whereas the sidewall from the narrow burden simulation experienced the lowest temperatures.

These trends were a consequence of the amount of side burner flame impingement on the burden. Figure 5.16 (see page 111) shows contour plots of temperature along the centerline plane of the side burner. The tall burden had the largest degree of side burner flame impingement on the burden, which caused the most flow separation and recirculation on the side wall as well as the roof. On the other hand,
the narrow burden geometry experienced very little side burner flame impingement which caused less recirculation on the side wall.

![Normalized Temperature](image)

<table>
<thead>
<tr>
<th>Normalized Temperature (%) of Average Base Case Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Color Scale" /></td>
</tr>
</tbody>
</table>

Figure 5.15 Contour plots of side wall temperatures for the (a) base case, (b) tall, (c) short and (d) narrow geometries normalized as a percentage of average base case side wall temperature value. The white square represents the side burner block. *(orientation: side view)*

5.5.4 Comparison of Side Wall Shear Stress

Figure 5.17 (see page 112) shows bar graphs that display the maximum side wall shear stress and a measure of the side wall area that was affected by high shear stress values. Both parameters were normalized as a percentage of the base case value. The affected area was defined as the total area on the side wall where the wall shear stress was greater than 90% of maximum side wall shear stress for the base case simulation. The dashed lines on the bar graphs represent 100% of the base case value. The side wall from the tall burden simulation experienced a significant increase in the maximum wall shear stress and wall shear stress affected area on the side wall when compared to the base case. The maximum wall shear stress decreased from the base case value for the short and narrow burden simulations. The short and narrow burden geometries also resulted in a 100% decrease in the wall shear stress affected area.

Figure 5.18 (see page 114) shows contour plots of the temperature affected area on the roof for each of the burden geometries studied. These plots visually depict the difference in side wall area
affected by high wall shear stress for each burden shape. The maximum wall shear stress on the side wall for the base case and tall burden simulations occurred below and to the right of the side burner opening. Again, there was no wall shear stress affected area for the short and narrow burden simulations.

Figure 5.16 Contour plots of temperature along the centerline plane of the side burner the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. 
(orientation: front view)

Figure 5.19 (see page 115) shows contour plots of the wall shear stress on the side wall normalized as a percent of the average base case side wall shear stress for all simulations. These plots visually depict the difference in wall shear stress magnitudes between each case since they are all normalized to the same value. The side wall from the tall burden simulation experienced the largest magnitude of wall shear stress. The side wall from the narrow burden simulation experienced wall shear stress values that were significantly less than the base case average. The wall shear stress trends can again be explained by the amount of side burner flame impingement on the burden.
Figure 5.20 (see page 116) shows contour plots of velocity along the centerline plane of the side burner for the different burden geometries studied. In the case of the tall burden, the side burner flame impingement on the burden occurred closer to the side wall and to a greater extent than the other cases. This resulted in the recirculation of higher velocity gases on the side wall, thereby causing higher shear stress values. In the case of the narrow burden, the side burner flame impingement on the burden was further from the side wall and to a lesser degree than all the other cases which resulted in less and slower recirculation of gases on the side wall.

![Figure 5.20](image)

Figure 5.17 The (a) maximum side wall shear stress and (b) wall shear stress affected side wall area normalized as percentages of the base case values for all the burden geometries evaluated.

5.6 Summary of Burden Geometry Study

Three different variations from the base case burden geometry were evaluated. The front half of the side wall and roof were the two main locations within the furnace that were studied. These two locations were chosen because they are the main locations of acute wear within lead processing reverberatory furnaces [17]. Both temperature and wall shear stress at these locations were compared as a function of burden geometry to assess high wear locations. The amount and location of the end and side burner flame impingement greatly affected the flow patterns and heat transfer within the furnace. The tall burden geometry resulted in a larger and more intense hot spot on the furnace roof as well as a greater amount of flow recirculation on the side wall which significantly enhanced the side wall shear stress affected area. The narrow burden geometry caused a significant reduction in the area affected by high temperatures and wall shear stress. This result was most likely caused by the decrease in side burden
flame impingement. The length of the burden was shown to be insignificant in most cases, except for the roof wall shear stress. The results from these simulations indicate that operating the furnace with a tall burden will increase refractory wear whereas running with a narrower burden could help minimize wear. Running the furnace with a taller burden may enhance the smelting rate though due to greater flame impingement and burden surface area, which could lead to higher smelting rates. More information on the smelting rate as a function of burden height and temperature would need to be known to fully understand this effect. Ultimately, these results seem to indicate that there is a tradeoff between smelting rate and refractory wear. Additional information on the burden chemistry and heat absorption as well as the specific relationship between different wear mechanisms would need to be obtained before the model could be used to fully optimize the furnace.

Figure 5.18 Contour plots of the wall shear stress affected side wall area for the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. The white square represents the side burner block. (orientation: side view)
Figure 5.19 Contour plots of side wall shear stress for the (a) base case, (b) tall, (c) short and (d) narrow geometries normalized as a percentage of average base case side wall shear stress value. The white square represents the side burner block. (orientation: side view)
Figure 5.20  Contour plots of velocity along the centerline plane of the side burner for the (a) base case, (b) tall burden, (c) short burden and (d) narrow burden geometries. (orientation: front view)
CHAPTER 6
SIMULATION RESULTS: EFFECT OF BURNER ALIGNMENT

The developed CFD model of the secondary lead reverberatory furnace was also used to assess the influence of burner alignment on the areas of high wear. The following chapter details the findings from this study. The front half of the roof and the portion of the side wall by the side burners were the main areas of interest that were evaluated.

6.1 Burner Alignment Simulations

Sixteen different burner alignment configurations were simulated. The base case burden geometry was used for all of the different burner alignment configurations tested. The first eight configurations adjusted only the side burner position and focal point. Figure 6.1 shows a schematic of the three different side burner positions evaluated. The $S_{\text{Forward}}$ position was the base case position. The burner block was moved back towards the end wall by a distance of $x$ and $2x$ for the $S_{\text{Middle}}$ and $S_{\text{Back}}$ positions, respectively.

![Figure 6.1 Schematic of the side burner positions evaluated. (orientation: top view)](image)

The focal point of the side burners was adjusted as well. Figure 6.2 shows a schematic of the three focal points evaluated in the study.

![Figure 6.2 Schematic of the side burner focal points evaluated. (orientation: top view)](image)
Both inward and downward angles of the side burners were adjusted to obtain the various focal points. The side burner focal points fell on the furnace centerline because the model was constructed using a symmetry boundary condition. $F_{S, \text{Forward}}$ was the base case focal point. $F_{S, \text{Middle}}$ and $F_{S, \text{Back}}$ were the focal points obtained when the burner block was moved to positions $S_{\text{Middle}}$ and $S_{\text{Back}}$, respectively, without any adjustments in the burner angles. Table 6.1 shows the different combinations of the side burner position and focal point that were simulated.

<table>
<thead>
<tr>
<th>Simulation Number</th>
<th>Side Burner Position</th>
<th>Side Burner Focal Point</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – Base Case</td>
<td>$S_{\text{Forward}}$</td>
<td>$F_{S, \text{Forward}}$</td>
</tr>
<tr>
<td>2</td>
<td>$S_{\text{Middle}}$</td>
<td>$F_{S, \text{Middle}}$</td>
</tr>
<tr>
<td>3</td>
<td>$S_{\text{Back}}$</td>
<td>$F_{S, \text{Back}}$</td>
</tr>
<tr>
<td>4</td>
<td>$S_{\text{Middle}}$</td>
<td>$F_{S, \text{Forward}}$</td>
</tr>
<tr>
<td>5</td>
<td>$S_{\text{Middle}}$</td>
<td>$F_{S, \text{Middle}}$</td>
</tr>
<tr>
<td>6</td>
<td>$S_{\text{Back}}$</td>
<td>$F_{S, \text{Back}}$</td>
</tr>
<tr>
<td>7</td>
<td>$S_{\text{Middle}}$</td>
<td>$F_{S, \text{Forward}}$</td>
</tr>
<tr>
<td>8</td>
<td>$S_{\text{Back}}$</td>
<td>$F_{S, \text{Middle}}$</td>
</tr>
<tr>
<td>9</td>
<td>$S_{\text{Back}}$</td>
<td>$F_{S, \text{Back}}$</td>
</tr>
</tbody>
</table>

The second eight configurations adjusted the end burner position and focal point. Figure 6.3 shows a schematic of the three different end burner positions evaluated. The $E_{\text{Outside}}$ position was the base case position. The $E_{\text{Middle}}$ and $E_{\text{Inside}}$ positions moved the burner block in towards the furnace centerline by a distance of $y$ and $2y$, respectively.

Figure 6.3 Schematic of the three different side burner positions evaluated. *(orientation: top view)*
Figure 6.4 shows a schematic of the three different downward angle focal points evaluated in the study. $F_{E, Middle}$ was the base case downward angle focal point. $F_{E, Top}$ and $F_{E, Bottom}$ were obtained by shifting the end burner downward angle so that the focal point was a distance of $z$ below and above the base case focal point. The end burner inward angle focal point was maintained at the same location for all the simulations. Again, the focal points for the end burners fell on the furnace centerline because the model was constructed using a symmetry boundary condition. Table 6.2 shows the different combinations of the end burner position and focal point that were simulated.

![Figure 6.4 Schematic of the end burner downward angle focal point adjustments. (orientation: side view)](image)

Table 6.2: List of the Eight Simulated End Burner Alignment Configurations

<table>
<thead>
<tr>
<th>Simulation Number</th>
<th>End Burner Position</th>
<th>Downward Angle Focal Point</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>$E_{Outside}$</td>
<td>$F_{E, Bottom}$</td>
</tr>
<tr>
<td>11</td>
<td>$E_{Outside}$</td>
<td>$F_{E, Top}$</td>
</tr>
<tr>
<td>12</td>
<td>$E_{Middle}$</td>
<td>$F_{E, Middle}$</td>
</tr>
<tr>
<td>13</td>
<td>$E_{Middle}$</td>
<td>$F_{E, Bottom}$</td>
</tr>
<tr>
<td>14</td>
<td>$E_{Middle}$</td>
<td>$F_{E, Top}$</td>
</tr>
<tr>
<td>15</td>
<td>$E_{Bottom}$</td>
<td>$F_{E, Middle}$</td>
</tr>
<tr>
<td>16</td>
<td>$E_{Bottom}$</td>
<td>$F_{E, Bottom}$</td>
</tr>
<tr>
<td>17</td>
<td>$E_{Bottom}$</td>
<td>$F_{E, Top}$</td>
</tr>
</tbody>
</table>

6.2 Burden Surface Temperatures

The average burden surface temperature was used as a measure of smelting rate (see section 5.3). Table 6.3 lists the average and maximum burden surface temperatures for the different burner configurations evaluated. Both parameters were normalized as a percentage of the base case value. The adjustments in side burner configuration resulted in a decrease in the average burden surface temperature.
whereas adjustments in the end burner configuration resulted in the same or an increase in the average burden surface temperature.

The lowest average burner temperature occurred in simulation 7 where the side burner was shifted to position $S_{\text{back}}$ and the focal point to $F_{s, \text{Forward}}$. Figure 5.3 shows contour plots of the CO$_2$ mass fraction along the centerline plane of the side burner for the base case and simulation 7. The CO$_2$ mass fraction was used to identify the flame as it is a product of the combustion reactions. Therefore, higher concentrations of CO$_2$ occur outside of the flame and lower concentrations occur inside the flame. The side burner flame had a greater degree of direct contact in the base case than in simulation 3. The side burner in simulation 3 had the largest inward angle and shallowest downward angle out of all the configurations investigated. This configuration led to the least side burner flame impingement which resulted in the lowest average burden temperature.

### Table 6.3: Average and Maximum Burden Surface Temperatures for the Different Burner Configurations Evaluated

<table>
<thead>
<tr>
<th>SIM #</th>
<th>Burner Adjusted</th>
<th>Block Position</th>
<th>Focal Point</th>
<th>Ave. Burden Surface Temperature (% of Base Case Value)</th>
<th>Max Burden Surface Temperature (% of Base Case Value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Side Burner</td>
<td>$S_{\text{Forward}}$</td>
<td>$F_{s, \text{Forward}}$</td>
<td>100.0</td>
<td>100.0</td>
</tr>
<tr>
<td>2</td>
<td>Side Burner</td>
<td>$S_{\text{Forward}}$</td>
<td>$F_{s, \text{Middle}}$</td>
<td>96.5</td>
<td>94.4</td>
</tr>
<tr>
<td>3</td>
<td>Side Burner</td>
<td>$S_{\text{Forward}}$</td>
<td>$F_{s, \text{Back}}$</td>
<td>96.4</td>
<td>95.7</td>
</tr>
<tr>
<td>4</td>
<td>Side Burner</td>
<td>$S_{\text{Middle}}$</td>
<td>$F_{s, \text{Forward}}$</td>
<td>99.6</td>
<td>101.1</td>
</tr>
<tr>
<td>5</td>
<td>Side Burner</td>
<td>$S_{\text{Middle}}$</td>
<td>$F_{s, \text{Middle}}$</td>
<td>95.6</td>
<td>98.1</td>
</tr>
<tr>
<td>6</td>
<td>Side Burner</td>
<td>$S_{\text{Middle}}$</td>
<td>$F_{s, \text{Back}}$</td>
<td>95.8</td>
<td>94.4</td>
</tr>
<tr>
<td>7</td>
<td>Side Burner</td>
<td>$S_{\text{Back}}$</td>
<td>$F_{s, \text{Forward}}$</td>
<td>92.0</td>
<td>93.9</td>
</tr>
<tr>
<td>8</td>
<td>Side Burner</td>
<td>$S_{\text{Back}}$</td>
<td>$F_{s, \text{Middle}}$</td>
<td>92.5</td>
<td>94.3</td>
</tr>
<tr>
<td>9</td>
<td>Side Burner</td>
<td>$S_{\text{Back}}$</td>
<td>$F_{s, \text{Back}}$</td>
<td>95.5</td>
<td>96.4</td>
</tr>
<tr>
<td>10</td>
<td>End Burner</td>
<td>$E_{\text{Outside}}$</td>
<td>$F_{e, \text{Bottom}}$</td>
<td>101.5</td>
<td>101.4</td>
</tr>
<tr>
<td>11</td>
<td>End Burner</td>
<td>$E_{\text{Outside}}$</td>
<td>$F_{e, \text{Top}}$</td>
<td>101.8</td>
<td>100.0</td>
</tr>
<tr>
<td>12</td>
<td>End Burner</td>
<td>$E_{\text{Middle}}$</td>
<td>$F_{e, \text{Middle}}$</td>
<td>101.4</td>
<td>100.0</td>
</tr>
<tr>
<td>13</td>
<td>End Burner</td>
<td>$E_{\text{Middle}}$</td>
<td>$F_{e, \text{Bottom}}$</td>
<td>101.2</td>
<td>102.3</td>
</tr>
<tr>
<td>14</td>
<td>End Burner</td>
<td>$E_{\text{Middle}}$</td>
<td>$F_{e, \text{Top}}$</td>
<td>102.3</td>
<td>97.2</td>
</tr>
<tr>
<td>15</td>
<td>End Burner</td>
<td>$E_{\text{Inside}}$</td>
<td>$F_{e, \text{Middle}}$</td>
<td>101.3</td>
<td>96.6</td>
</tr>
<tr>
<td>16</td>
<td>End Burner</td>
<td>$E_{\text{Inside}}$</td>
<td>$F_{e, \text{Bottom}}$</td>
<td>101.2</td>
<td>102.0</td>
</tr>
<tr>
<td>17</td>
<td>End Burner</td>
<td>$E_{\text{Inside}}$</td>
<td>$F_{e, \text{Top}}$</td>
<td>100.0</td>
<td>97.1</td>
</tr>
</tbody>
</table>

The highest average burner surface temperature occurred in simulation 14 where the end burner was shifted in toward the furnace centerline to position $E_{\text{Middle}}$ and the downward angle focal point was
shifted up above the base case position to $F_{E, Top}$. This end burner configuration resulted in the highest average burden surface temperature, even though the end burner flame impingement was not as direct because the flame contacted the burden over a larger surface area.

![CO$_2$ Mass Fraction Contour Plots](image)

Figure 6.5  Contour plots of CO$_2$ mass fraction along the centerline plane of the side burner the (a) base case and (b) simulation 3 which shifted the side burner back to position $S_{Back}$ and the focal point to $F_{x, Back}$. *(orientation: normal to plane)*

6.3 Furnace Roof

The front half of the furnace roof was the first high wear location within the furnace to be evaluated in this portion of the research. The temperature and wall shear stress values in this location were compared for the different burner configurations evaluated. The following sections detail the results of the simulations.

6.3.1 Comparison of Roof Temperatures

Table 6.4 shows the maximum roof temperature and the temperature affected roof area. Both parameters were normalized as a percentage of the base case value. The affected area was defined as the total area on the roof where the temperature was greater than 90% of maximum roof temperature for the base case simulation. The side burner configurations simulated resulted in a decrease in the maximum roof temperature whereas the end burner configurations simulated resulted in higher roof maximum temperatures when compared to the base case simulation.

Figure 6.6 shows the temperature affected roof area as a function of the burner block position and focal point. Figure 6.6a shows the trends in the data for the side burner configurations evaluated and Figure 6.6b shows the trends in the data for the end burner configurations evaluated. The side burner

120
block position significantly changed the temperature affected roof area in the simulations that adjusted side burner alignment. The high temperature areas on the roof dramatically decreased as the burner block was moved back towards the end wall. The side burner focal point did not impact the calculated affected area as much as the burner block position. The burner block position also greatly impacted the calculated temperature affected roof area in the simulations that adjusted end burner alignment. The middle end burner block position resulted in the largest temperature affected roof areas and the outside end burner block position resulted in the smallest temperature affected roof areas. Similar to the simulations that adjusted side burner configurations, the downward angle focal point did not impact the results as much at the end burner block position.

Table 6.4: The maximum roof temperature and temperature affected roof area normalized as percentages of the base case value for the burner alignment simulations

<table>
<thead>
<tr>
<th>SIM #</th>
<th>Burner Adjusted</th>
<th>Block Position</th>
<th>Focal Point</th>
<th>Temperature Affected Roof Area (% of Base Case Value)</th>
<th>Maximum Roof Temperature (% of Base Case Value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Side Burner</td>
<td>S Forward</td>
<td>FS, Forward</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td>Side Burner</td>
<td>S Forward</td>
<td>FS, Middle</td>
<td>95</td>
<td>97</td>
</tr>
<tr>
<td>3</td>
<td>Side Burner</td>
<td>S Forward</td>
<td>FS, Back</td>
<td>91</td>
<td>97</td>
</tr>
<tr>
<td>4</td>
<td>Side Burner</td>
<td>S Middle</td>
<td>FS, Forward</td>
<td>88</td>
<td>99</td>
</tr>
<tr>
<td>5</td>
<td>Side Burner</td>
<td>S Middle</td>
<td>FS, Middle</td>
<td>87</td>
<td>98</td>
</tr>
<tr>
<td>6</td>
<td>Side Burner</td>
<td>S Middle</td>
<td>FS, Back</td>
<td>87</td>
<td>97</td>
</tr>
<tr>
<td>7</td>
<td>Side Burner</td>
<td>S Back</td>
<td>FS, Forward</td>
<td>&lt;1</td>
<td>90</td>
</tr>
<tr>
<td>8</td>
<td>Side Burner</td>
<td>S Back</td>
<td>FS, Middle</td>
<td>1</td>
<td>92</td>
</tr>
<tr>
<td>9</td>
<td>Side Burner</td>
<td>S Back</td>
<td>FS, Back</td>
<td>3</td>
<td>94</td>
</tr>
<tr>
<td>10</td>
<td>End Burner</td>
<td>E Outside</td>
<td>FE, Bottom</td>
<td>105</td>
<td>101</td>
</tr>
<tr>
<td>11</td>
<td>End Burner</td>
<td>E Outside</td>
<td>FE, Top</td>
<td>115</td>
<td>101</td>
</tr>
<tr>
<td>12</td>
<td>End Burner</td>
<td>E Middle</td>
<td>FE, Middle</td>
<td>135</td>
<td>104</td>
</tr>
<tr>
<td>13</td>
<td>End Burner</td>
<td>E Middle</td>
<td>FE, Bottom</td>
<td>129</td>
<td>103</td>
</tr>
<tr>
<td>14</td>
<td>End Burner</td>
<td>E Middle</td>
<td>FE, Top</td>
<td>136</td>
<td>103</td>
</tr>
<tr>
<td>15</td>
<td>End Burner</td>
<td>E Inside</td>
<td>FE, Middle</td>
<td>128</td>
<td>104</td>
</tr>
<tr>
<td>16</td>
<td>End Burner</td>
<td>E Inside</td>
<td>FE, Bottom</td>
<td>134</td>
<td>105</td>
</tr>
<tr>
<td>17</td>
<td>End Burner</td>
<td>E Inside</td>
<td>FE, Top</td>
<td>130</td>
<td>105</td>
</tr>
</tbody>
</table>
Figure 6.7 shows contours of the temperature affected roof area for the base case, simulation 7 and simulation 14. Contours for simulation 7 and 14 are presented because these simulations produced the lowest and highest temperature affected roof area, respectively. Simulation 7 resulted in the lowest average burden surface temperature, but also the lowest temperature affected roof area. Simulation 14 produced the highest burden surface temperature, but also the largest temperature affected roof area. The location of the affected roof area in simulation 14 also slightly shifted back towards the end wall.

Figure 6.6 Temperature affected roof area as a function of burner block position and focal point for changes in the (a) side burner and (b) end burner.

Figure 6.8 shows contour plots of the roof temperatures normalized as a percent of the average base case roof temperature for the base case, simulation 7 and simulation 14. These plots visually depict the difference in temperature magnitudes between each case since they are all normalized to the same value. Simulation 7 resulted in lower and more even distributed temperatures on the roof. The roof in simulation 14 experienced hotter temperatures than the base case. Again, area of maximum roof temperatures in simulation 14 were shifted towards the end wall.

The roof temperature trends for these simulations can be explained through the use of Figure 6.9 which shows velocity vectors along the end burner centerline. The side burner alignment in simulation 7 influenced the recirculation zone above the end burner flame. This recirculation zone was not as well defined as the one in the base case simulation and was further away from the roof. The end burner alignment in simulation 14 also influenced the recirculation zone above the end burner. The recirculation zone was shifted towards the end wall which caused the same shift in the location of the high roof
temperatures. The end burner downward angle focal point was at the top position in simulation 14 resulting in the end burner flame closer to the roof, which may have caused the increase in the maximum roof temperature and temperature affected roof area.

Figure 6.7 Contour plots of the temperature affected roof area for the (a) base case, (b) simulation 7 and (c) simulation 14 which had the highest average burden surface temperature. (orientation: top view)
Figure 6.8  Contour plots of roof temperatures normalized as a percentage of the average base case roof temperature for (a) base case, (b) simulation 7 and (c) simulation 14 burden surface temperature. (*orientation: top view*)
Figure 6.9 Velocity vectors along the end burner centerline for the (a) base case, (b) simulation 7 and (c) simulation 14. (orientation: side view)
6.3.2 Comparison of Roof Wall Shear Stress

Table 6.5 shows the maximum roof wall shear stress and the wall shear stress affected roof area. Both parameters were normalized as a percentage of the base case value. The affected area was defined as the total area on the roof where the temperature was greater than 90% of maximum roof temperature for the base case simulation. The maximum roof wall shear stress stayed the same as or decreased from the base case value for all the burner alignment configurations tested. This is because all the burner configurations tested either caused slower velocities to be directed at the roof or less direct redirection of flow at the roof when compared to the base case.

Table 6.5: The maximum roof wall shear stress and wall shear stress affected roof area normalized as percentages of the base case value for all the burner alignment configurations

<table>
<thead>
<tr>
<th>SIM #</th>
<th>Burner Adjusted</th>
<th>Block Position</th>
<th>Focal Point</th>
<th>Wall Shear Stress Affected Roof Area (% of Base Case Value)</th>
<th>Maximum Roof Wall Shear Stress (% of Base Case Value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Side</td>
<td>S</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Forward</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td>S</td>
<td>S&lt;sub&gt;S&lt;/sub&gt;, Middle</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Middle</td>
<td>69</td>
<td>98</td>
</tr>
<tr>
<td>3</td>
<td>S</td>
<td>S&lt;sub&gt;S&lt;/sub&gt;, Back</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Back</td>
<td>0</td>
<td>79</td>
</tr>
<tr>
<td>4</td>
<td>Side</td>
<td>S&lt;sub&gt;Middle&lt;/sub&gt;</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Forward</td>
<td>5</td>
<td>95</td>
</tr>
<tr>
<td>5</td>
<td>S</td>
<td>S&lt;sub&gt;Middle&lt;/sub&gt;</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Middle</td>
<td>1</td>
<td>90</td>
</tr>
<tr>
<td>6</td>
<td>S</td>
<td>S&lt;sub&gt;Middle&lt;/sub&gt;</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Back</td>
<td>0</td>
<td>82</td>
</tr>
<tr>
<td>7</td>
<td>S</td>
<td>S&lt;sub&gt;Back&lt;/sub&gt;</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Forward</td>
<td>0</td>
<td>72</td>
</tr>
<tr>
<td>8</td>
<td>S</td>
<td>S&lt;sub&gt;Back&lt;/sub&gt;</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Middle</td>
<td>0</td>
<td>73</td>
</tr>
<tr>
<td>9</td>
<td>S</td>
<td>S&lt;sub&gt;Back&lt;/sub&gt;</td>
<td>F&lt;sub&gt;S&lt;/sub&gt;, Back</td>
<td>0</td>
<td>63</td>
</tr>
<tr>
<td>10</td>
<td>E</td>
<td>E&lt;sub&gt;Outside&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Bottom</td>
<td>180</td>
<td>100</td>
</tr>
<tr>
<td>11</td>
<td>E</td>
<td>E&lt;sub&gt;Outside&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Top</td>
<td>39</td>
<td>94</td>
</tr>
<tr>
<td>12</td>
<td>E</td>
<td>E&lt;sub&gt;Middle&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Middle</td>
<td>164</td>
<td>96</td>
</tr>
<tr>
<td>13</td>
<td>E</td>
<td>E&lt;sub&gt;Middle&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Bottom</td>
<td>173</td>
<td>96</td>
</tr>
<tr>
<td>14</td>
<td>E</td>
<td>E&lt;sub&gt;Middle&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Top</td>
<td>12</td>
<td>94</td>
</tr>
<tr>
<td>15</td>
<td>E</td>
<td>E&lt;sub&gt;Inside&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Middle</td>
<td>171</td>
<td>90</td>
</tr>
<tr>
<td>16</td>
<td>E</td>
<td>E&lt;sub&gt;Inside&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Bottom</td>
<td>304</td>
<td>98</td>
</tr>
<tr>
<td>17</td>
<td>E</td>
<td>E&lt;sub&gt;Inside&lt;/sub&gt;</td>
<td>F&lt;sub&gt;E&lt;/sub&gt;, Top</td>
<td>87</td>
<td>92</td>
</tr>
</tbody>
</table>

Figure 6.10 shows the wall shear stress affected roof area as a function of the burner block position and focal point. Figure 6.10a shows the trends in the data for the side burner configurations evaluated and Figure 6.10b shows the trends in the data for the end burner configurations evaluated. The side burner block position significantly influenced the wall shear stress affected roof area. As the side burner block was moved towards the end wall, the wall shear stress affected roof area decreased. The
furthest back side block position produced a value of zero wall shear stress affected roof area regardless of burner focal point. Both the end burner block position and downward angle focal point influenced the wall shear stress affected roof area. As the end burner block was moved in towards the furnace centerline, the wall shear stress affected roof area increased. The affected roof area also increased as the downward angle focal point was moved down toward the gas-slag interface.

Figure 6.10 Wall shear stress affected roof area as a function of burner block position and focal point for changes in the (a) side burner and (b) end burner.

Figure 6.11 shows contours of the wall shear stress affected roof area for the base case, simulation 7 and simulation 16. Contours for simulation 16 are presented because this simulation produced the highest wall shear stress affected roof area. Several simulations produced the minimum wall shear stress affected roof area at a value of zero. The contours for simulation 7 are presented as this simulation produced both the minimum wall shear stress affected roof area and the average burden surface temperature. The wall shear stress affected roof area for simulation 16 was much larger and shifted towards the end wall when compared to the base case simulation.

Figure 6.12 shows contour plots of the roof temperatures normalized as a percent of the average base case roof temperature for the base case, simulation 7 and simulation 16. These plots visually depict the difference in temperature magnitudes between each case since they are all normalized to the same value. Simulation 7 produced a much lower and more even wall shear stress distribution on the roof. On the other hand, simulation 16 produced a higher and more concentrated area of shear stress on the roof.
Figure 6.13 shows velocity vectors along the symmetry plane for the base case, simulation 7 and simulation 16. These show the relative magnitudes and angles of the redirected flow to the roof which was influenced by both the end and the side burners. Simulation 7 had the shallowest angle of flow redirection whereas simulation 16 had the steepest angle of flow redirection. All the simulation in which the end burner downward angle focal point was shifted to the bottom position had the steep angle of flow redirection. The highest velocity vectors along the symmetry plane occurred in the base case, which caused a highest maximum wall shear stress on the roof. The angle of the flow redirection towards the roof and the relative velocities of the redirected gases caused the differences in wall shear stress affected area.

Figure 6.11 Contour plots of the wall shear stress affected roof area for the (a) base case, (b) simulation 7 and (c) simulation 16. (orientation: top view)
Figure 6.12 Contour plots of roof wall shear stress for the (a) base case, (b) simulation 7 and (c) simulation 16 normalized as a percentage of average base case roof wall shear stress value. (orientation: top view)
Figure 6.13 Velocity vectors along symmetry plane for the (a) base case, (b) simulation 7 and (c) simulation 16. (orientation: side view)
6.4 Furnace Side Wall

The furnace side wall was the second area of high wear that was evaluated in the burner alignment study. Only the front half of the side wall was evaluated as that was the reported location of high wear. Both temperature and wall shear stress at this location were compared for the different burner configurations evaluated. The following sections detail the results of the simulations.

6.4.3 Comparison of Side Wall Temperatures

Table 6.6 shows the maximum roof temperature and the temperature affected side wall area. Both parameters were normalized as a percentage of the base case value. The affected area was defined as the total area on the side wall where the temperature was greater than 90% of maximum side wall temperature for the base case simulation. The maximum side wall temperatures were both less and greater than the base case value for the simulations that adjusted the side burners. The maximum temperature was always greater than the base case value for the simulations that adjusted the end burners.

Table 6.6: The Maximum Side Wall Temperature and Temperature Affected Side Wall Area Normalized as Percentages of the Base Case Value for all the Burner Alignment Configurations

<table>
<thead>
<tr>
<th>SIM #</th>
<th>Burner Adjusted</th>
<th>Block Position</th>
<th>Focal Point</th>
<th>Temperature Affected Side Wall Area (% of Base Case Value)</th>
<th>Maximum Side Wall Temperature (% of Base Case Value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Side Burner</td>
<td>SForward</td>
<td>FS, Forward</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td>FS, Middle</td>
<td>54</td>
<td>98</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td>FS, Back</td>
<td>28</td>
<td>98</td>
</tr>
<tr>
<td>4</td>
<td>Side Burner</td>
<td>SMiddle</td>
<td>FS, Forward</td>
<td>45</td>
<td>109</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td></td>
<td>FS, Middle</td>
<td>32</td>
<td>98</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td></td>
<td>FS, Back</td>
<td>25</td>
<td>98</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>SBack</td>
<td>FS, Forward</td>
<td>7</td>
<td>115</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
<td>FS, Middle</td>
<td>1</td>
<td>97</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td></td>
<td>FS, Back</td>
<td>0</td>
<td>89</td>
</tr>
<tr>
<td>10</td>
<td>End Burner</td>
<td>EOutside</td>
<td>FE, Bottom</td>
<td>118</td>
<td>101</td>
</tr>
<tr>
<td>11</td>
<td></td>
<td></td>
<td>FE, Top</td>
<td>121</td>
<td>102</td>
</tr>
<tr>
<td>12</td>
<td>End Burner</td>
<td>EMiddle</td>
<td>FE, Middle</td>
<td>163</td>
<td>102</td>
</tr>
<tr>
<td>13</td>
<td></td>
<td></td>
<td>FE, Bottom</td>
<td>155</td>
<td>102</td>
</tr>
<tr>
<td>14</td>
<td></td>
<td></td>
<td>FE, Top</td>
<td>160</td>
<td>104</td>
</tr>
<tr>
<td>15</td>
<td></td>
<td>EInside</td>
<td>FE, Middle</td>
<td>183</td>
<td>105</td>
</tr>
<tr>
<td>16</td>
<td></td>
<td></td>
<td>FE, Bottom</td>
<td>190</td>
<td>104</td>
</tr>
<tr>
<td>17</td>
<td></td>
<td></td>
<td>FE, Top</td>
<td>191</td>
<td>104</td>
</tr>
</tbody>
</table>
Figure 6.14 shows the temperature affected side wall area as a function of the burner block position and focal point. Figure 6.14a shows the trends in the data for the side burner configurations evaluated and Figure 6.14b shows the trends in the data for the end burner configurations evaluated. For changes in side burner configuration, both the burner block position and the focal point impacted the temperature affected side wall area. The temperature affected side wall area decreased as the side burner block moved further towards the end wall and as the focal point moved from the forward to the back position. The end burner downward angle focal point did not influence the temperature affected side wall area as much at the end burner block position. As the end burner block moved in towards the furnace centerline, the temperature affected side wall area increased.

Figure 6.14a (a) Side Burner Focal Point

Figure 6.14b (b) End Burner Downward Focal Point

Figure 6.14 shows temperature affected side wall area as a function of burner block position and focal point for changes in the (a) side burner and (b) end burner.

Figure 6.15 shows contours of the temperature affected roof area for the base case, simulation 9 and simulation 17. Contours for simulation 9 and 17 are presented because these simulations produced the lowest and the highest temperature affected side wall area. The temperature affected side wall area was 0% of the base case for simulation 9. Simulation 17 produced a much larger temperature affected side wall area above and to the right of the side burner opening.

Figure 6.16 shows contour plots of the side wall temperatures normalized as a percent of the average base case roof temperature for the base case, simulation 9 and simulation 17. These plots visually depict the difference in temperature magnitudes between each case since they are all normalized to the same value. The temperature contours show that simulation 9 produced a lower and more even
temperature distribution on the side wall. The side wall in simulation 17 had experienced significantly hotter temperatures than the base case above and to the right of the side burner opening.

Figure 6.15 Contour plots of the temperature affected side wall area for the (a) base case, (b) simulation 9 and (c) simulation 17. The white square represents the side burner block. (*orientation: side view*)

Figure 6.16 Contour plots of side wall temperatures for the (a) base case, (b) simulation 9 and (c) simulation 17 normalized as a percentage of average base case side wall temperature value. The white square represents the side burner block. (*orientation: side view*)
The trends in this data can be explained through the use of Figure 6.17. Figure 6.17 presents contour plots of temperature along the centerline plane of the side burners for the base case, simulation 9 and simulation 17. The position of the side burner in simulation 9 caused less direct flame impingement on the burden which resulted in a decrease of flow separation and recirculation on the furnace side wall. On the other hand, the position of the end burners in simulation 17 caused a greater amount of heat to be recirculated on the furnace side wall.

![Normalized Temperature](image)

(a)

![Base Case](image)

(b)

![EXP 9 - Low](image)

(b)

![EXP 17 - High](image)

(c)

Figure 6.17 Contour plots of temperature along the centerline plane of the side burner the (a) base case, (b) simulation 9 and (c) simulation 17. (orientation: normal to plane)

6.4.4 Comparison of Side Wall Shear Stress

Table 6.7 shows the maximum side wall shear stress and the wall shear stress affected side wall area. The affected area was defined as the total area on the side wall where the wall shear stress was
greater than 90% of maximum side wall shear stress for the base case simulation. The maximum side wall shear stress values for both sets of simulations were both less and greater than the base case value.

Table 6.7: The Maximum Side Wall Shear Stress and Wall Shear Stress Affected Side Wall Area Normalized as Percentages of the Base Case Value for all the Burner Alignment Configurations

<table>
<thead>
<tr>
<th>SIM #</th>
<th>Burner Adjusted</th>
<th>Block Position</th>
<th>Focal Point</th>
<th>Temperature Affected Side Wall Area (% of Base Case Value)</th>
<th>Maximum Side Wall Temperature (% of Base Case Value)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>S</td>
<td>SForward</td>
<td>FS, Forward</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td>S</td>
<td>SForward</td>
<td>FS, Middle</td>
<td>9</td>
<td>93</td>
</tr>
<tr>
<td>3</td>
<td>S</td>
<td>SForward</td>
<td>FS, Back</td>
<td>0</td>
<td>85</td>
</tr>
<tr>
<td>4</td>
<td>Side Burner</td>
<td>SMiddle</td>
<td>FS, Forward</td>
<td>53</td>
<td>98</td>
</tr>
<tr>
<td>5</td>
<td>Side Burner</td>
<td>SMiddle</td>
<td>FS, Middle</td>
<td>10</td>
<td>91</td>
</tr>
<tr>
<td>6</td>
<td>Side Burner</td>
<td>SMiddle</td>
<td>FS, Back</td>
<td>0</td>
<td>80</td>
</tr>
<tr>
<td>7</td>
<td>S</td>
<td>SBack</td>
<td>FS, Forward</td>
<td>256</td>
<td>219</td>
</tr>
<tr>
<td>8</td>
<td>S</td>
<td>SBack</td>
<td>FS, Middle</td>
<td>0</td>
<td>87</td>
</tr>
<tr>
<td>9</td>
<td>S</td>
<td>SBack</td>
<td>FS, Back</td>
<td>0</td>
<td>87</td>
</tr>
<tr>
<td>10</td>
<td>E</td>
<td>EOutside</td>
<td>FE, Bottom</td>
<td>95</td>
<td>109</td>
</tr>
<tr>
<td>11</td>
<td>E</td>
<td>EOutside</td>
<td>FE, Top</td>
<td>48</td>
<td>97</td>
</tr>
<tr>
<td>12</td>
<td>End Burner</td>
<td>EMiddle</td>
<td>FE, Middle</td>
<td>79</td>
<td>102</td>
</tr>
<tr>
<td>13</td>
<td>End Burner</td>
<td>EMiddle</td>
<td>FE, Bottom</td>
<td>59</td>
<td>99</td>
</tr>
<tr>
<td>14</td>
<td>End Burner</td>
<td>EMiddle</td>
<td>FE, Top</td>
<td>73</td>
<td>99</td>
</tr>
<tr>
<td>15</td>
<td>E</td>
<td>EInside</td>
<td>FE, Middle</td>
<td>79</td>
<td>106</td>
</tr>
<tr>
<td>16</td>
<td>E</td>
<td>EInside</td>
<td>FE, Bottom</td>
<td>0</td>
<td>89</td>
</tr>
<tr>
<td>17</td>
<td>E</td>
<td>EInside</td>
<td>FE, Top</td>
<td>54</td>
<td>98</td>
</tr>
</tbody>
</table>

Figure 6.18 shows the wall shear stress affected side wall area as a function of the burner block position and focal point. Figure 6.18a shows the trends in the data for the side burner configurations evaluated and Figure 6.18b shows the trends in the data for the end burner configurations evaluated. The main trend for the simulations that adjusted side burner alignment was that the side wall shear stress affected area decreased as the focal point was moved from the forward to the back position. The forward focal point allowed for more recirculation of flow than the back focal point. The trend in the simulations that adjusted end burner alignment was not as clear. The side wall shear affected area decreased for the end burner middle and inside block positions.

Figure 6.19 (see page 137) shows contours of the wall shear stress affected side wall area for the base case, simulation 16 and simulation 7. Figure 6.20 (see page 138) shows contour plots of the roof temperatures normalized as a percent of the average base case roof temperature for the base case,
simulation 16 and simulation 7. These plots visually depict the difference in temperature magnitudes between each case since they are all normalized to the same value. The contours for simulation 7 were evaluated because this simulation had the largest wall shear stress affected side wall area and maximum side wall shear stress. Simulation 16 was chosen to evaluate the low range of side wall shear stress affected area. The side burner inward angle had to be increased the greatest in simulation 7 to meet the forward focal point position. This caused the side burner flame to impact the inside edge of the burner block. The side view of the side wall shown in Figure 6.19 and Figure 6.20 did not capture this area of the burner block.

Figure 6.21 (see page 138) shows an isometric view of the side burner block where the maximum side wall shear stress area occurred. If the side burner configuration were to be used, the burner block dimensions would need to be adjusted to eliminate the flame contact. The area of maximum wall shear stress occurred in the same location for all the other burner configurations evaluated, i.e. below and to the right of the side burner opening.

![Figure 6.18](image)

**Figure 6.18** Wall shear stress affected side wall area as a function of burner block position and focal point for changes in the (a) side burner and (b) end burner.

### 6.5 Summary of Burner Alignment Study

Sixteen different burner alignment configurations were evaluated and compared to the base case burden geometry. The first eight simulations altered the side burner alignment and the second eight altered the end burner alignment. The front half of the side wall and roof were the two main locations
within the furnace that were studied. These two locations were chosen because they are the main locations of acute wear within lead processing reverberatory furnace [17]. Both temperature and wall shear stress at these locations were compared as a function of burner alignment to assess high wear locations. Similar to the burden geometry simulations, the amount and location of the end and side burner flame impingement greatly affected the flow patterns and heat transfer within the furnace. Moving the side burners towards the end wall greatly reduced the temperature and the wall shear stress affected area on both the roof and side wall. Shifting the side burners back also decreased the average burden surface temperature which could negatively impact the smelting rate. Moving the end burners towards the furnace centerline increased the average burden surface temperature while decreasing the wall shear stress affected areas on the roof and the side wall. The simulations in which the end burner downward angle focal point was in the top position had the smallest wall shear stress affected areas on the roof and side wall among the simulations in which only the end burner was adjusted. The inward shift of the end burner block increased the temperature affected areas on the roof and side wall though. Again, these results seem to indicate that there could be a tradeoff smelting rate and refractory wear. More information on the relationship between temperature and wall shear stress that causes high wear will need to be known before the burner alignment could be fully optimized.

Figure 6.19  Contour plots of the wall shear stress affected side wall area for the (a) base case, (b) simulation 16 and (c) simulation 9. The white square represents the side burner block. (orientation: side view)
Figure 6.20 Contour plots of side wall shear stress for the (a) base case, (b) simulation 16 and (c) simulation 7 normalized as a percentage of average base case side wall shear stress value. The white square represents the side burner block. (orientation: side view)

Figure 6.21 Isometric view of the side burner block in simulation 9 showing contours of (a) wall shear stress affected area and (b) wall shear stress normalized as a percentage of the average side wall shear stress for the base case. (orientation: isometric view)
CHAPTER 7
DISCUSSION

This research focused on investigating the impact of burden geometry and burner configuration on the thermal and momentum stresses on the refractory surfaces along with burden surface temperatures; which could be used to provide insight into wear patterns and productivity of lead reverberatory furnaces. The thermal and momentum stresses were evaluated through the development of a 3D CFD model coupled with combustion chemistry. The model was used to study the temperature and wall shear stress contours on the roof and side wall as a function of burden geometry and burner alignment. The following sections discuss and summarize the results of the simulations presented in Chapter 5 and 6 as well as preliminary economics and recommendations for future work.

7.1 Results summary and analysis

A CFD model was developed and validated based on an industrially operated secondary lead reverberatory furnace. The computational domain consisted of the combustion gas space which included two end burners and two side burners. The model was run using mass flow inlets for the burner gas streams as well as a symmetry boundary condition. The addition of the symmetry boundary condition significantly decreased the computational time while maintaining acceptable accuracy. A volumetric heat sink term was applied to the group of cells just above the gas-slag interface to account for the heat loss due to the smelting and melting reactions as well as super heating of the burden material. This method was calibrated based on the base case simulation and therefore caused some loss in accuracy when other burden geometries and burner alignment configurations that had different degrees of flame impingement were modeled (see Appendix C). Modeling the actual chemical reactions that occur within the burden could help minimize these inaccuracies, but could also be very computationally expensive. Another way to account for the smelting and melting reactions would be to specify a volumetric absorption coefficient at the gas-slag interface rather than a certain amount of heat flux. This method would allow different amounts of heat to be transferred into the burden when the degree of flame impingement and burden surface area are modified. Therefore, once the absorption coefficient was calibrated for the base case, a more direct comparison of various burden geometries and burner alignments could be evaluated. The use of different sub-models was evaluated as well. The standard k-ω turbulence model and the non-premixed combustion model were used. The model was shown to predict measured temperatures and velocities in the furnace, the burner flame dimensions and the general refractory wear patterns within an acceptable accuracy range. Better understanding of the variability in the validation measurements and burden dimensions will help improve upon the overall accuracy of the model.
The validated model was first used to assess the influence of burden geometry on the flow patterns and heat transfer within the furnace. In theory, burden geometry could be altered through operational changes by modifying the feed rate or inlet location/orientation. Both the tall and narrow burden caused the most significant changes in the flow patterns and heat transfer within the furnace. Operating the furnace with a tall burden resulted in a large increase in the temperature and wall shear stress affected areas on the side wall. The tall burden also resulted in a hotter and larger zone of roof refractory. On the other hand, the narrow burden caused a substantial decrease in the temperature and wall shear stress affected areas on both the roof and the side wall. There was a tradeoff associated with these burden geometries. The tall burden had the hottest average burden surface as a consequence of the increased burden and flame interaction whereas the narrow burden had the lowest average burden surface temperature. This may indicate that the smelting rate would be faster in a furnace with a tall burden versus a narrow burden. Therefore, one suggestion would be to maintain the volume of the tall burden while employing a mechanism to guide the feed away from the side walls, thereby creating the desired narrow burden shape.

Burner alignment was the second parameter investigated in these simulation studies. The burner alignment is a physical change that could be made to the furnace to aid in optimization. Sixteen different burner alignment configurations were examined. The first eight altered the side burner alignment and the last eight altered the end burner alignment. The results showed several trends. Moving the side burners towards the end wall greatly reduced the temperature and wall shear stress affected area on both the roof and side wall, but also decreased the average burden surface temperature. Shifting the end burners in towards the furnace centerline increased the average burden surface temperature and decreased the wall shear stress affected areas on the roof and the side wall. Although, the inward shift of the end burner block increased the temperature affected areas on the roof and side wall. The simulations in which the end burner downward angle focal point was in the top position had the smallest wall shear stress affected areas on the roof and side wall and the largest temperature affected zones on the roof. The burner alignment from simulation 4 would be suggested if minimizing wear while maintaining smelting rate is the goal. The burner alignment in this simulation shifted the side burner block towards the end wall to position $S_{Middle}$ and the focal point to $F_{S, Forward}$. This alignment resulted in lower temperature and wall shear stress affected areas on both the roof and end wall when compared to the base case simulation. The maximum temperature and wall shear stress on the roof and side wall were also slightly lower than the base case values. The average burden surface temperature for this simulation was only marginally lower than the base case simulation, i.e. 99.6%.

The trends from the burden geometry and the burner alignment simulations point to a tradeoff between refractory lifetime and smelting rate. More information on how the burden height and surface
temperature impact the smelting rate as well as the relationship between the parameters that cause high refractory wear is needed to fully optimize the link between refractory lifetime and smelting rate. One way to improve the predictive power of the CFD model would be to perform simulations on the furnace refractory material to gain a better understanding of the relationship between the parameters that cause high areas of refractory wear. Literature reports that refractory wear in lead processing furnaces can be caused or worsened through the combination of chemical, thermal and mechanical mechanisms [17], i.e. a mixture of temperature and wall shear stress. Therefore, developing an empirical or semi-empirical correlation between temperature and wall shear stress that was able to predict areas of high refractory wear could add greater accuracy to the CFD model when being used to evaluate operational and physical changes that would result in a reduction of refractory wear. One group of researchers reported using this approach when constructing a CFD model used to assess carbon brick wear within the blast furnace hearth [125]. Refractory wear rate coefficients were calculated based on wear tests performed using a rotating disk apparatus. The wear rate coefficient, \( \dot{w} \), calculated and evaluated using the data generated by the model was:

\[
\dot{w} = k_e \left( \frac{\tau}{\tau_0} \right)^\frac{1}{3}
\]

where \( k_e \) was the effective mass transfer parameter, \( \tau \) was the wall shear stress at the iron – refractory interface and \( \tau_0 \) was the reference wall shear stress based on the rotating disk simulation. The wear rate coefficient was used to predict changes in the high wear areas within the refractory hearth as a function of operational changes.

Several different wear functions could be constructed to estimate the relationship of temperature and wall shear stress that influences refractory wear, but actual furnace wear patterns and/or simulational work would be needed to verify the expression. Other variables found to influence wear could also be added to the developed function. Two example wear functions, Wear Function 1 and Wear Function 2, were established to examine how different relationships between temperature and wall shear stress could affect predicted areas of high wear. Wear Function 1 and Wear Function 2 are based on conjecture and further investigation into an appropriate wear function could be performed as part of future work. The numerical solutions from the burden geometry study were used to construct contour plots of the two example wear functions on the roof and side wall. These contour plots were used to evaluate the differences between the two wear functions. The first function investigated was:

\[
\text{Wear Function 1} = \text{Temperature} \times \text{Wall Shear Stress}
\]

This function was constructed under the assumption that both parameters influence the refractory wear equally. Figure 7.1 and Figure 7.2 (see page 160 and 161) show contour plots of Wear Function 1
for the furnace roof and side wall burden geometry simulations. The contour plots were very similar to the ones shown in Figure 5.11 and Figure 5.19, which were the contour plots of the wall shear stress normalized as a percentage of the average base case wall shear stress value. Therefore, refractory wear would occur in about the same locations where high shear stress was predicted if large values of Wear Function 1 was used to assess the likelihood of wear. This occurred because the range for the wall shear stress values was much larger than the range for the temperature values. The large wall shear stress values were also concentrated in small locations on the roof and side wall and were not as evenly distributed as the temperature values.

Figure 7.1 Contour plots of Wear Function 1 on the roof for the (a) base case, (b) tall, (c) short and (d) narrow burden geometries. (orientation: top view)
The second function investigated was:

\[
\text{Wear Function 2} = A e^{-\frac{E_a}{(R \times \text{Temperature})}} \times (\text{Wall Shear Stress})^{\frac{1}{2}}
\]  

(7.3)

where \(A\) was the pre-exponential factor, \(E_a\) was the activation energy and \(R\) was the universal gas constant. The pre-exponential factor was defined as one and the activation energy was estimated to be \(40 \text{ KJ mol}^{-1}\). Activation energies greater than \(40 \text{ KJ mol}^{-1}\) indicate chemically controlled reactions [126].

Therefore, the construction of this function assumed that the influence of temperature scaled as a chemically controlled reaction based on the Arrhenius equation. The influence of wall shear stress was decreased by raising it to the one-half power. Figure 7.3 and Figure 7.4 show contour plots of the Wear Function 2 for the furnace roof and side wall for each burden case.

![Wear Function 1](image)

![Wear Function 2](image)

Figure 7.2 Contour plots of Wear Function 1 on the side wall for the (a) base case, (b) tall, (c) short and (d) narrow burden geometries. The white square represents the side burner block. 

(orientation: side view)

The shape and location of the high wear areas were slightly different for Wear Function 2 compared to Wear Function 1. This function weighted the influence of temperature greater than the influence of wall shear stress which resulted in predicted high wear areas that were more of an intermediate between the two parameters. Therefore, the high wear locations on the roof moved towards the furnace end wall and high roof temperatures occurred more in the center of the front half of the roof.
whereas high shear stress values occurred at the furnace centerline. The high wear locations also grew larger because the high temperature locations typically encompassed a larger area than the high shear stress locations. Using Wear Function 2 did not affect the predicted locations of high wear on the side wall as much. This was because the areas of high temperature and wall shear stress roughly occurred in the same location and to the same extent on the side wall for all the burden geometries evaluated.

![Wear Function 2 Contour Plots](image)

Figure 7.3 Contour plots of Wear Function 2 on the roof for the (a) base case, (b) tall, (c) short and (d) narrow burden geometries. (orientation: top view)

Figure 7.5 and Figure 7.6 show the average Wear Function 2 value in the high wear zones on the roof and side wall as a function of average burden surface temperature for the burden geometry and burner simulations. Again, the conclusions drawn from these plots are only valid if Wear Function 2 is an accurate predictor of high wear areas within the furnace refractory. Wear Function 2 was used for this analysis as informal conversations with reverberatory furnace operators suggested that this function predicted more accurate locations of high refractory wear. The high wear zone was the area on the roof or
side wall where the wear function values were greater than 90% of maximum wear function value for each individual case. This definition was constructed to determine the average wear function value in the simulated high wear zones. All the plots show a trend between the average wear and the average burden surface temperature, i.e. increased average burden surface temperature results in higher values for the wear function. The trend lines and associated \(R^2\) value are included on the plots. Points above the trend line are not ideal as they correspond to conditions in which higher wear than the trend predicted would occur for a given average burden surface temperature. Points below the line would indicate conditions at which lower wear than the trend predicted occurred for a given average burden surface temperature. The simulations with the three lowest burden surface temperatures were omitted from Figure 7.6b as they produced extremely high average wear function values in the high wear zones due to flame contact with the edge of the burner block as shown in Figure 6.21. These simulations should be rerun with altered burner block geometry.

![Contour plots of Wear Function 2 on the side wall for different burden geometries.](image)

Figure 7.4 Contour plots of Wear Function 2 on the side wall for the (a) base case, (b) tall, (c) short and (d) narrow burden geometries. The white square represents the side burner block. (orientation: side view)

The average wear function value on the side wall was more sensitive to changes in the average burden surface temperature than the average wear function value on the roof. This implies that if the average burden surface temperature is increased to push lead throughout, the side wall would become the main area of concern. The tall burden produced in the highest average burden surface temperature which
resulted in the highest average wear function value in the high wear zones on both the roof and the side wall. The points for the tall burden fall below or on the trend line though, which could indicate that this condition results in the same relative refractory wear for increased lead throughput. The simulations that manipulated the end burners all produced higher wear function values than the base case whereas the simulations that manipulated the side burners all produced lower wear function values than the base case on the roof and the side wall. A preliminary economic analysis was performed to assess which simulation produced the most advantageous combination of average wear function and average burden surface temperature.

Figure 7.5 The average wear function 2 value in the high wear zone on the (a) roof and (b) the side wall as a function of the average burden surface temperature for the burden geometry simulations.

7.2 Preliminary economic analysis

The wear function was used to construct a preliminary economic analysis. This analysis is very simple and does not account for the time value of money or the cost of refractory material, which was assumed to be insignificant. It is presented to show how the data calculated from the CFD model could be used to assess the economic consequence of potential operational and physical changes. Table 7.1 lists the process assumptions made for this analysis. These data were estimated from literature [4] and taken from informal discussions with operators of secondary lead reverberatory furnaces.
The average wear function 2 in the high wear zone on the (a) roof and (b) the side wall as a function of the average burden surface temperature for the burner alignment simulations.

Table 7.1: Process Assumptions for the Economic Analysis

<table>
<thead>
<tr>
<th>Process Assumptions – Base Case Situation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Production (short tons/year)</td>
</tr>
<tr>
<td>Refractory Lifetime (months)</td>
</tr>
<tr>
<td>Rebrick downtime duration (days)</td>
</tr>
<tr>
<td>Uptime (days/year)</td>
</tr>
<tr>
<td>Starting Brick Thickness (in)</td>
</tr>
<tr>
<td>Ending Brick Thickness (in)</td>
</tr>
<tr>
<td>Market Price of Lead ($/short ton)</td>
</tr>
<tr>
<td>Point of Refractory Failure</td>
</tr>
</tbody>
</table>

The relationship between lead production and average burden surface temperature for this analysis was assumed to be:

\[ \text{Lead Production} = \alpha \times T_{\text{Burden}} \]

(7.4)
where $\alpha$ is a constant with units of $\text{short tons/year} \ast ^\circ\text{F}$. The relationship between wear rate and the wear function for this analysis was assumed to be:

$$\text{wear rate} = c \ast \text{wear function}^2$$  \hspace{2cm} (7.5)

where $c$ is a constant with units of $\text{in}^{0.5} \ast \text{s} \ast \text{kg}^{0.5} \ast \text{month}^{-1}$. Both $\alpha$ and $c$ were calibrated based on the base case simulation and process assumptions. These two relationships were based on conjecture and are purely preliminary estimates. More test work will need to be done to fully understand these relationships.

Table 7.2 and Table 7.3 show the preliminary economics of the different simulations evaluated. The wear rate was calculated by equation 7.5. The roof was assumed to be the point of failure for this evaluation. Therefore, average wear function in the high wear zone on the roof was used. The refractory lifetime and uptime per year were direct consequences of the wear rate. The lead production was calculated using equation 7.4 where the average burden surface temperature was determined from the CFD model. The total revenue for the base case was calculated using the market price of lead and the change in revenue for each simulation is based off that value.

The results from this analysis show that the simulations with the highest burden surface temperatures from both sets of results, i.e. the tall burden and simulation 14, resulted in the greatest economic benefit. This may seem counter intuitive as both these simulations also produced the large indicators of high wear. The revenue from the higher production of lead outweighed the cost of the additional downtime for refractory repair. Therefore, optimization of the furnace may result in a marginally shorter refractory lifetime with a large increase in lead production. Again, these conclusions are only valid if the assumed wear function, wear rate and lead production equations are accurate. Developing accurate equations for these parameters and using them in conjunction with a CFD model would result in a very powerful optimization tool for reverberatory furnaces.

Table 7.2: Preliminary Economic Analysis for the Burden Geometry Simulations when the Roof is the Point of Refractory Failure.

<table>
<thead>
<tr>
<th>Burden Shape</th>
<th>Wear Rate (in/month)</th>
<th>Refractory Lifetime (months)</th>
<th>Uptime (days/year)</th>
<th>Lead Production (short tons/day)</th>
<th>Lead Production (short tons/year)</th>
<th>Change in Revenue</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>1.42</td>
<td>12</td>
<td>351.0</td>
<td>284.9</td>
<td>100000</td>
<td>$-$</td>
</tr>
<tr>
<td>Tall</td>
<td>1.49</td>
<td>11.4</td>
<td>350.3</td>
<td>323.1</td>
<td>113167</td>
<td>$30,442,188</td>
</tr>
<tr>
<td>Short</td>
<td>1.26</td>
<td>13.5</td>
<td>352.6</td>
<td>282.7</td>
<td>99664</td>
<td>$(775,355)</td>
</tr>
<tr>
<td>Narrow</td>
<td>1.17</td>
<td>14.6</td>
<td>353.5</td>
<td>273.1</td>
<td>96546</td>
<td>$(7,983,618)</td>
</tr>
</tbody>
</table>
Table 7.3: Preliminary Economic Analysis for the Burden Alignment Simulations when the Roof is the Point of Refractory Failure.

<table>
<thead>
<tr>
<th>SIM #</th>
<th>Wear Rate (in/month)</th>
<th>Refractory Lifetime (months)</th>
<th>Uptime (days/year)</th>
<th>Lead Production (short tons/day)</th>
<th>Lead Production (short tons/year)</th>
<th>Change in Revenue</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.83</td>
<td>6</td>
<td>351.0</td>
<td>284.9</td>
<td>100000</td>
<td>$-</td>
</tr>
<tr>
<td>2</td>
<td>1.42</td>
<td>11.9</td>
<td>350.9</td>
<td>274.8</td>
<td>96435</td>
<td>$(8,241,390)</td>
</tr>
<tr>
<td>3</td>
<td>1.22</td>
<td>14.0</td>
<td>353.0</td>
<td>274.7</td>
<td>96946</td>
<td>$(7,061,659)</td>
</tr>
<tr>
<td>4</td>
<td>1.29</td>
<td>13.2</td>
<td>352.3</td>
<td>283.8</td>
<td>99980</td>
<td>$(45,813)</td>
</tr>
<tr>
<td>5</td>
<td>1.28</td>
<td>13.3</td>
<td>352.4</td>
<td>272.3</td>
<td>95958</td>
<td>$(9,345,074)</td>
</tr>
<tr>
<td>6</td>
<td>1.21</td>
<td>14.0</td>
<td>353.0</td>
<td>273.0</td>
<td>96378</td>
<td>$(8,373,873)</td>
</tr>
<tr>
<td>7</td>
<td>0.95</td>
<td>17.8</td>
<td>355.6</td>
<td>262.2</td>
<td>93237</td>
<td>$(15,635,597)</td>
</tr>
<tr>
<td>8</td>
<td>1.01</td>
<td>16.8</td>
<td>355.0</td>
<td>263.6</td>
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<td>11.9</td>
<td>350.9</td>
<td>284.5</td>
<td>99835</td>
<td>$(380,351)</td>
</tr>
</tbody>
</table>

### 7.3 Future work

- Obtain additional temperature, velocity and pressure measurements within burners to confirm or correct flow boundary conditions. Modeling the full burner could accomplish this as well.
- Obtain better understanding of the variability in the validation measurements and burden dimensions to help improve upon the overall accuracy of the model.
- Alter heat sink treatment to be more accurate when adjusting various parameters such as burden geometries and burner alignment. This could be accomplished through modeling the full chemistry of the smelting and melting reactions or by applying an absorption coefficient to the burden surface area. The absorption coefficient could be estimated from the base case simulation or determined experimentally.
- Develop a wear function based on experimentation that could be used to predict areas of high wear within the furnace as a function of all significant variables.
• Explore the significance of a radiation sub-model on the overall numerical solution.
• Include dust particles in the model
• Add a chemical corrosion mechanism of refractory wear to the model
CHAPTER 8
CONCLUSIONS

The goal of this research was to identify and minimize refractory wear zones caused by excess thermal and mechanical stresses that occur within secondary lead reverberatory furnaces. Maintaining or increasing the average burden surface temperature (used as a measure of the smelting rate) was a secondary goal. Decreasing areas of high thermal and mechanical stresses on the refractory within these types of furnaces is important to the economics of many operations at the rate of refractory wear will directly affect the length of refractory lifetime and the productivity of the furnace. The project’s goal was accomplished through the development of a 3D Computational Fluid Dynamic (CFD) model coupled with combustion chemistry. The CFD model allowed the complex transport phenomena that cause wear within secondary lead reverberatory furnaces to be predicted and evaluated how changes made to the furnace affected the temperature and wall shear stress distributions. The main conclusions of the present work are as follows:

- The developed CFD model successfully predicted temperature and velocity measurements, flame dimensions and general wear patterns based on an operational lead reverberatory furnace with reasonable accuracy.

- The burden geometry significantly affected the temperature and wall shear stress distributions on the roof and side wall refractory. The tall burden caused a more intense and concentrated hot spot on the furnace roof as well as increased the flow recirculation on the furnace side wall. The narrow burden resulted in a decrease in the thermal and mechanical wear indicators both on the roof and on the side wall.

- The burner alignment also significantly affected the temperature and wall shear stress distributions on the roof and side wall refractory. Altering the side burner configuration had a greater impact on the wear indicators than altering the end burner configuration. In general, moving the side burners towards the end wall decreased the thermal and mechanical wear indicators on the roof and side wall.

- Changes in both burden geometry and burner alignment altered the amount and location of the end and side burner flame impingement on the furnace burden. Varying degrees in flame impingement is what caused differences in the wear indicators on the roof and side wall as well as the average burden surface temperature which was used as a measure of smelting rate.

- A semi-empirical wear function was developed that combined the influence of temperature and wall shear stress on the areas of high refractory wear within the furnace. This evaluation showed that simulations that resulted in a higher average wear function of the roof and side wall also had a hotter average burden surface temperature. These results may indicate that there is a tradeoff between smelting rate and refractory lifetime.
REFERENCES


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APPENDIX A
MESH REFINEMENT STUDY

Below are plots of the mesh refinement studies performed for the three additional burden geometries evaluated. The calculated temperatures and velocity at the validation locations all level out between 2.5 and 3 million cells.

Figure A.1 Calculated temperatures at the validation points through the (a) observation port, (b) slag hole, (c) flue port and (d) calculated velocity through the flue port as a function of number of cells for the taller burden geometry.
Figure A.2 Calculated temperatures at the validation points through the (a) observation port, (b) slag hole, (c) flue port and (d) calculated velocity through the flue port as a function of number of cells for the shorter burden geometry.
Figure A.3 Calculated temperatures at the validation points through the (a) observation port, (b) slag hole, (c) flue port and (d) calculated velocity through the flue port as a function of number of cells for the narrow burden geometry.
APPENDIX B
DISCUSSION ON THE FURNACE HEAT SINK

The value for the heat sink included in the model to account for melting, smelting and superheat was estimated based on average feed rates and fine-tuned for the base case burden geometry. The total heat flow (W) into the burden remained constant regardless of burden geometry. As discussed in section 5.3, the value of the heat content sunk into the burden would be dependent on both the burden surface area and temperature. The burden geometries with the largest flame surface area in contact with the burden had the highest burden surface temperature. Therefore, for the burden geometry simulations, it would be expected that taller burden would have a larger heat sink term and that the short and narrow burdens would have a smaller heat sink term than the base case simulation. Maintaining a constant total heat flow into the heat sink would then lead to over predictions of temperatures for the tall burden geometry and under predictions of temperature for the short and narrow burden geometries. It was important to understand the effect of the heat sink value as various conclusions were drawn based on roof and side wall temperatures.

The sensitivity of the results to the value of the total heat flow sunk into the burden was evaluated using the tall burden geometry. Two additional simulations were run; one in which the total heat flow into the heat sink was increased by 5% and the other in which the total heat flow into the heat sink was increased by 10%. An increase in 5% corresponds to the amount of heat flow that would have been sunk into the burden if the volumetric (W/m$^3$) heat flow was held constant rather than the total heat flow as the heat sink volume for the tall burden was slightly larger than the base case.

Figure C.1 shows contour plots of roof temperatures for the tall burden geometry normalized as percentages of the average base case roof temperature for the three different heat sink conditions. The area of maximum temperature decreased as the total heat flow into the burden was increased. Table C.1 shows a comparison of average and maximum roof parameters for the different heat sink conditions normalized as a percentage of the base case value. Table C.2 shows a comparison of average and maximum side wall parameters for the different heat sink conditions normalized as a percentage of the base case value. Ideally, all the heat sink conditions would produce very similar results, indicating that the variables investigated were not sensitive to the heat sink value. The average and maximum wall shear stress values were not sensitive to changes in total heat flow into the heat sink. The roof and side wall temperatures were more sensitive to changes in the heat sink value. The changes in temperatures did not scale linearly with changes in the heat sink value though. A 10% increase in the heat sink value caused the average and maximum temperature on the roof to decrease by only 2%. The average and maximum side wall temperatures both decreased by 6% for a 10% increase in the heat sink value.
Table B.1: Comparison of Average and Maximum Roof Parameters for the Different Heat Sink Conditions Normalized as a Percentage of the Base Case Value

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Original</th>
<th>5% Increase</th>
<th>10% Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Temperature</td>
<td>101</td>
<td>99</td>
<td>98</td>
</tr>
<tr>
<td>Maximum Temperature</td>
<td>107</td>
<td>106</td>
<td>105</td>
</tr>
<tr>
<td>Average Wall Shear Stress</td>
<td>105</td>
<td>105</td>
<td>105</td>
</tr>
<tr>
<td>Maximum Wall Shear Stress</td>
<td>93</td>
<td>93</td>
<td>93</td>
</tr>
</tbody>
</table>

Table B.2: Comparison of Average and Maximum Side Wall Parameters for the Different Heat Sink Conditions Normalized as a Percentage of the Base Case Value

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Original</th>
<th>5% Increase</th>
<th>10% Increase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Temperature</td>
<td>106</td>
<td>103</td>
<td>100</td>
</tr>
<tr>
<td>Maximum Temperature</td>
<td>106</td>
<td>103</td>
<td>100</td>
</tr>
<tr>
<td>Average Wall Shear Stress</td>
<td>146</td>
<td>146</td>
<td>146</td>
</tr>
<tr>
<td>Maximum Wall Shear Stress</td>
<td>146</td>
<td>147</td>
<td>147</td>
</tr>
</tbody>
</table>

Figure B.1 Comparison of roof temperature contours for different heat sink values. 
(orientation: top view)
APPENDIX C
DISCUSSION ON FLAT BURDEN GEOMETRY

An additional burden geometry was evaluated in which the gas-interface was left unaltered. Figure C.1 shows a schematic of the burden geometry. The results for the flat geometry were not presented in the main body of the thesis because this was a case in which the heat sink assumption become very inaccurate. Figure C.2 shows a contour plot of the CO\textsubscript{2} mass fraction along the side burner centerline. Figure C.3 shows a contour plot of the temperature along the end burner centerline. Both plots show that the end and side burner flames had very little contact with the burden surface. The lack of flame impingement on the burden surface would lead to lower total heat flow into the burden. Therefore, it would be expected that the model underpredicted temperatures in the main part of the furnace and on the refractory walls because the total heat flow into the burden was kept constant for all simulations. The average burden surface temperature for this simulation was 88% of the base case value.

![Figure C.1 Schematic of the flat burden geometry. (orientation: side view)](image1)

![Figure C.2 Contour plots of CO\textsubscript{2} mass fraction along the centerline plane of the side burner the flat burden geometry. (orientation: normal to plane)](image2)

Temperature was the main parameter affected by the heat sink assumption. The flow characteristics were not as sensitive to the way the heat sink was defined. Figure D.3 and Figure D.4 show the contour plots of the roof and side wall shear stress normalized as a percentage of the average
base case wall shear stress values. These plots visually depict the difference in wall shear stress magnitudes between each case since they are all normalized to the same value.

![Normalized Temperature](image)

Figure C.3 Contour plots of the temperatures along end burner centerline for the flat burden geometry. *(orientation: side view)*

![Normalized Wall Shear Stress](image)

Figure C.4 Contour plots of wall shear stress on the (a) roof *(orientation: top view)* and (b) side wall *(orientation: side view)* normalized as a percentage of the average base case value for flat burden geometry.

The wall shear stress on the side wall and roof was lower and much more even distribution. The maximum wall shear stress on the roof and side wall were 74% and 48% of the maximum in the base case simulation, respectively. This burden geometry could be useful to consider if the goal was to minimize refractory wear, but the average burden surface temperature was much lower than the base case which
would surely decrease the smelting rate. A flat burden would also mean that less material could be fed into the furnace at any given time.
APPENDIX D

FLUENT

Saving residuals for post processing and exporting addition solution parameters into CFD post were two tasks in Fluent that allowed for the post processing of data which was important in the model setup stage of this research. The steps for completing each one of these commands are presented below for reference.

**Saving Residuals**

Use the Text User Interface (TUI)

Step 1: Activate export with TUI command: `/plot/residuals-set/plot-to-file` as shown in Figure D.1

Step 2: Plot the residuals with TUI command: `/plot/residuals` as shown in Figure D.1

The file will be saved in the simulation directory.

![Console]

1. `/plot/residuals-set/plot-to-file filename [""] example1`
2. `/plot/residuals`
   - Plot continuity residuals? [yes]
   - Plot x-velocity residuals? [yes]
   - Plot y-velocity residuals? [yes]
   - Plot z-velocity residuals? [yes]
   - Plot energy residuals? [yes]
   - Plot k residuals? [yes]
   - Plot omega residuals? [yes]
   - Plot fmean residuals? [yes]
   - Plot fmean2 residuals? [yes]
   - Plot fvar residuals? [yes]
   - Plot fvar2 residuals? [yes]

Figure D.1  TUI commands used to save residuals for post processing

**Exporting Additional Solution Parameters**

Step 1: Go into the run calculation window

Step 2: Click of the “Data File Quantities” button

Step 3: Select desired additional quantities to be imported into CFD post

A picture of steps 1 through 3 are shown in Figure D.2.
Figure D.2  Steps for exporting additional solution parameters into CFD post.