Numerical Modelling of a Rotary Cement Kiln with External Shell Cooling Fans

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A thesis submitted in partial fulfillment of the requirements for the Master of Engineering Science degree in Mechanical and Materials Engineering
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Abstract

This thesis describes the process taken for the computational analysis of convective heat transfer from multiple large jets impinging on a large cylinder, and a one-dimensional model of chemistry and heat transfer within a rotary cement kiln. A correlation describing the forced convection effect of these jets was determined and was integrated into the one-dimensional model to represent the effect of large kiln shell cooling fans impinging on the shell of a rotary cement kiln. Formulations from previously developed one-dimensional models were combined together to form the model outlined in this thesis. Modifications were made to the chemistry formulation, thermal resistance through the kiln, and the inclusion of the effects of forced convection on the kiln shell. It was concluded that the correlation developed was accurate within an interval of ±26%, while the one-dimensional model represented temperature profiles and species mass fractions reasonably well. Furthermore, the inclusion of forced convection in the kiln resistance model resulted in a decrease in shell temperature when compared to the case of only free convection.

Keywords

Impinging Jet, Convection, CFD, Rotary Kiln, Numerical Modelling, Cement, Kiln Shell Cooling, Heat Transfer
Co-Authorship Statement

All papers were drafted by Christopher Csernyei and revised under the supervision of Dr. A.G. Straatman.
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## Nomenclature

- $A_{rgb}$: Radiation area internal gas to bulk bed [m]
- $A_{rgw}$: Radiation area internal gas to internal wall [m]
- $A_{rwb}$: Radiation area internal wall to bed [m]
- $A_{cgb}$: Convection area internal gas to bulk bed [m]
- $A_{cgw}$: Convection area internal gas to internal wall [m]
- $A_{cwb}$: Convection area internal wall to bed [m]
- $A_{segment}$: Area of bed segment [m]
- $A_{sh}$: Area of steel shell [m]
- $A_j$: Pre-exponential factor for $j^{th}$ reaction [1/s]
- $A_i$: Initial value of $\text{Al}_2\text{O}_3$ at input
- $C_{p_b}$: Specific heat of bulk bed [J/kgK]
- $C_{Tmax}$: Maximum coating thickness [m]
- $d$: Jet diameter [m]
- $D_e$: Hydraulic diameter of kiln [m]
- $D$: Diameter of kiln, diameter of cylinder [m]
- $E_j$: Activation energy for $j^{th}$ reaction [J/mol]
- $F_i$: Initial value of $\text{Fe}_2\text{O}_3$ at input
- $\Delta H_{\text{CaCO}_3}$: Heat of reaction $\text{CaCO}_3$ [J/kg]
- $\Delta H_{\text{C2S}}$: Heat of reaction C2S [J/kg]
- $\Delta H_{\text{C3S}}$: Heat of reaction C3S [J/kg]
- $\Delta H_{\text{C3A}}$: Heat of reaction C3A [J/kg]
- $\Delta H_{\text{C4AF}}$: Heat of reaction C4AF [J/kg]
- $h_{ave}$: Average heat transfer coefficient [W/m$^2$K]
- $h_{cgb}$: Convective heat transfer coefficient freeboard gas to bulk bed [W/m$^2$K]
- $h_{cgw}$: Convective heat transfer coefficient freeboard gas to internal wall [W/m$^2$K]
- $h_{cwb}$: Coefficient for conduction from wall to bed [W/m$^2$K]
- $h_{csh}$: Convective heat transfer coefficient from shell to atmosphere [W/m$^2$K]
- $k$: Turbulent kinetic energy, [m$^2$/s$^2$]
- $k_f$: Thermal conductivity of fluid [W/mK]
- $k_g$: Thermal conductivity of freeboard gas [W/mK]
- $k_b$: Thermal conductivity of bulk bed [W/mK]
- $k_a$: Thermal conductivity of air [W/mK]
- $k_1$: Reaction rate $\text{CaCO}_3$ [1/s]
- $k_2$: Reaction rate C2S [1/s]
- $k_3$: Reaction rate C3S [1/s]
- $k_4$: Reaction rate C3A [1/s]
- $k_5$: Reaction rate C4AF [1/s]
- $L_{fus}$: Latent heat of fustion [J/kg]
- $L_{gcl}$: Chord length of bed segment [m]
- $\dot{m}_{\text{CO}_2}$: Mass flow rate of $\text{CO}_2$ [kg/s]
- $\dot{m}_{\text{CaCO}_3}$: Mass flow rate of $\text{CaCO}_3$ [kg/s]
- $M_n$: Molar mass of $n^{th}$ species [kg/kmol]
- $N_{U_{ave}}$: Average Nusselt number for forced convection from cylinder
- $Pr$: Prandtl number
\( Q_{rgb} \)  Radiation heat transfer gas to bulk bed [W/m]
\( Q_{rgw} \)  Radiation heat transfer gas to internal wall [W/m]
\( Q_{rwb} \)  Radiation heat transfer internal wall to bed [W/m]
\( Q_{cgb} \)  Convection heat transfer gas to bulk bed [W/m]
\( Q_{cgw} \)  Convection heat transfer gas to internal wall [W/m]
\( Q_{cwb} \)  Conduction heat transfer internal wall to bed [W/m]
\( Q' \)  Heat gained by bed due to heat transfer [W/m]
\( q_c \)  Heat generated by chemical reactions [W/m³]
\( Q_{coat} \)  Heat transfer through coating [W/m]
\( Q_{ref} \)  Heat transfer through refractory [W/m]
\( Q_{stl} \)  Heat transfer through steel shell [W/m]
\( Q_{conv-shell} \)  Heat transfer from shell by convection [W/m]
\( Q_{rad-shell} \)  Heat transfer from shell by radiation [W/m]
\( Ra_D \)  Rayleigh number
\( Re_d \)  Jet Reynolds number
\( Re_D \)  Axial Reynolds number, cylinder Reynolds number
\( Re_w \)  Angular Reynolds number
\( R_g \)  Universal gas constant [J/molK]
\( R \)  Internal radius of kiln [m]
\( Si \)  Initial value of SiO₂ at input
\( S_{CO2} \)  Source term for heat release from CO₂ [W/m]
\( T_g \)  Freeboard gas temperature [K]
\( T_b \)  Bulk bed temperature [K]
\( T_w \)  Internal wall temperature [K]
\( T_0 \)  Temperature of atmosphere [K]
\( T_{sh} \)  Temperature of steel shell [K]
\( u_g \)  Airspeed of freeboard gas [m/s]
\( V_J \)  Airspeed of fluid at jet exit [m/s]
\( v_b \)  Velocity of bulk bed [m/s]
\( y^+ \)  Non-dimensional wall distance
\( Y_n \)  Mass fraction of nᵗʰ species
\( Y_{fus} \)  Fusion fraction
\( d/D \)  Ratio of jet diameter to cylinder diameter
\( y/d \)  Jet-to-cylinder spacing
\( z/d \)  Jet-to-jet spacing
\( x/d \)  Jet offset from centerline

Greek characters:
\( \alpha_b \)  Bulk bed thermal diffusivity [m²/s]
\( \alpha_g \)  Absorptivity of freeboard gas
\( \beta \)  Angle of repose [rad]
\( \varepsilon \)  Turbulent dissipation rate [m²/s²]
\( \varepsilon_{sh} \)  Emissivity of steel shell
\( \varepsilon_g \)  Emissivity of freeboard gas
\( \varepsilon_b \)  Emissivity of bulk bed
\( \varepsilon_w \) Emissivity of internal wall
\( \Gamma \) angle of fill of kiln [rad]
\( \mu_g \) Dynamic viscosity of freeboard gas [s/m\(^2\)]
\( \eta \) Degree of solid fill
\( \omega \) Rotational speed of kiln [rad/s]
\( \Omega \) view factor for radiation
\( \rho_g \) Density of freeboard gas [kg/m\(^3\)]
\( \rho_s \) Density of solids [kg/m\(^3\)]
\( \sigma \) Stefan-Boltzmann constant
\( \nu_g \) Kinematic viscosity of freeboard gas [m\(^2\)/s]
\( \nu \) Kinematic viscosity of fluid at jet exit [m\(^2\)/s]

Species:
- \( CaCO_3 \)
- \( SiO_2 \)
- \( CaO \)
- \( Fe_2O_3 \)
- \( Al_2O_3 \)
- \( C_2S \)
- \( C_3S \)
- \( C_3A \)
- \( C_4AF \)
Chapter 1

1 Introduction

Throughout history, civilizations have utilized many different binding substances to join materials together for the purpose of construction. The usage of gypsum and lime as a mortar dates back to the Egyptians, whereas the first recorded use of cement and concrete can be dated back to the Roman Empire [1]. Originating from the word *opus caementicium*, cement is a fine grey powder that when mixed with other solid additives and water, and then left to harden, it becomes concrete. Concrete is one of the most predominant construction materials used around the world [2]. Currently Canada is home to 16 cement plants which produce upwards of approximately 14.3 million tonnes per year, of which 5 million tonnes is exported to the United States [3]. Fig. 1.1 shows a breakdown of the locations of each cement plant and their respective distribution centers across Canada.

![Locations of Canadian Cement Plants and Distribution Centers](image)

**Figure 1.1: Locations of Canadian Cement Plants and Distribution Centers [4]**
The breakdown of the number of plants and their respective production values can be seen in Table 1.1.

Table 1.1: Breakdown of tonnes of cement produced in Canada by location [3]

<table>
<thead>
<tr>
<th>Location</th>
<th>Number of Plants</th>
<th>Millions of Tonnes Produced</th>
<th>% of Total Canadian production</th>
</tr>
</thead>
<tbody>
<tr>
<td>British Columbia</td>
<td>3</td>
<td>2.2</td>
<td>16</td>
</tr>
<tr>
<td>Alberta</td>
<td>2</td>
<td>1.9</td>
<td>14</td>
</tr>
<tr>
<td>Ontario</td>
<td>7</td>
<td>6.6</td>
<td>48</td>
</tr>
<tr>
<td>Quebec</td>
<td>3</td>
<td>2.7</td>
<td>20</td>
</tr>
<tr>
<td>Nova Scotia</td>
<td>1</td>
<td>0.4</td>
<td>2</td>
</tr>
</tbody>
</table>

According to the 2012 Environmental Performance Report performed by the Cement Association of Canada, production of cement in 2010 required approximately 3 GJ per tonne cement (86%) of thermal energy consumption, and 0.5 GJ per tonne cement (14%) of electrical energy input (see Fig. 1.2) [5]. According to Statistics Canada, the cement manufacturing industry is one of the top six consumers of energy in Canada requiring approximately 3.2% of the total energy demand for all manufacturing industries in 2010 [6]. As a significant consumer of energy within Canada, it is important to understand how this energy is being utilized within the cement industry, and how its usage can be improved.

Figure 1.2: Overall thermal and electrical energy consumption for cement production in Canada. [5]
1.1 The Rotary Cement Kiln

Although the mixing of cement is a relatively simple process, the manufacturing of cement is complex and arduous. In Canada, the cement manufacturing process begins and ends on the same site. Fig. 1.3 shows a schematic of the manufacturing process from start to finish.

Figure 1.3: Schematic of typical cement manufacturing process. [2]

Beginning at the quarry, raw material typically comprised of limestone (CaCO$_3$), alumina (Al$_2$O$_3$), iron (Fe$_2$O$_3$), silica (SiO$_2$), and small traces of other minerals are harvested. This raw material is transported to storage hoppers where it is then transported to a raw mill that dries and grinds the material into smaller pieces. The raw material then passes through a primary baghouse and into homogenizing silos where the constituents are filtered into their proper quantities, depending on the required cement type. From there, the raw material travels through a pre-heater where it is heated up to around 700°C - 900°C causing initial calcination to occur before entering the kiln. Inside the kiln, the formation of cement “clinker” (tiny balls of cement) occurs due to a series of simultaneously occurring chemical reactions. The clinker is then cooled as it exits the kiln, and moves on to the finishing mill where it is crushed to fine powder, stored, and then packaged for distribution. Of all the processes occurring within the cement plant, the largest consumer of thermal energy is the rotary cement kiln.
Formation of cement clinker is a complex chemical process that requires numerous chemical reactions occurring simultaneously with each requiring a separate thermodynamic requirement [7]. These reactions have been simplified to a series of five different reactions [8] that describe the development of the primary mineral constituents within cement clinker: dicalcium silicate, C2S (Belite), tricalcium silicate, C3S (Alite), tricalcium aluminate, C3A, and tetracalcium aluminoferrite, C4AF. The main mineral in all of these compounds is calcium oxide, CaO, which is formed from the highly endothermic initial reaction, the decomposition of limestone, CaCO3, into CaO and carbon dioxide:

\[
\begin{align*}
\text{CaCO}_3 & \rightarrow \text{CaO} + \text{CO}_2 \\
2\text{CaO} + \text{SiO}_2 & \rightarrow \text{C}_2\text{S} \\
\text{C}_2\text{S} + \text{CaO} & \rightarrow \text{C}_3\text{S} \\
3\text{CaO} + \text{Al}_2\text{O}_3 & \rightarrow \text{C}_3\text{A} \\
4\text{CaO} + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 & \rightarrow \text{C}_4\text{AF}
\end{align*}
\]

There exists two types of rotary cement kilns: wet and dry types. Wet kilns are typically longer (200m) than their dry counterparts (50 – 100m) in order to account for the full evaporation of the water. Utilizing a slurry mixture of upwards of 40% water, the primary benefit to utilizing a wet rotary kiln is the due to the reason that blending the raw materials as a slurry is more convenient and suitable for achieving a proper blend of input constituents. On the other hand, dry-type rotary kilns are more thermally efficient and more common in industry. With improved techniques for the blending of raw materials prior to entering the kiln, the use of water as a substrate to improve the blend is no longer required. Furthermore, dry kilns typically utilize some form of precalciner which when coupled with the low quantity of water in the mixture and the improved thermal efficiency, allows for a shorter kiln length.

At a length of 50 – 100 m and a diameter of 3 – 6 m, rotary kilns are usually tilted at an angle of 2 – 5° to the horizontal, and rotate slowly at a speed of 1 – 5 rpm, causing the raw material to be gravity driven as it travels towards the discharge end [9]. The kiln is comprised of a steel outer shell lined with refractory brick material on the inside. The steel shell acts as a strong and rigid outer support, while the refractory brick helps to enhance the thermal resistance on the inside, protecting the steel shell and allowing for more heat
to remain inside of the kiln. Refractory material must be both thermally and chemically stable as it is required to withstand extremely high temperatures, and its composition cannot interfere with the composition of the clinker formation. A single type of brick is not used throughout the entire length of the kiln, but rather multiple different types of bricks are used in different regions of the kiln. This is due to the fact that there exists typically four major regions within a kiln in which different chemical reactions and temperatures occur. As described by Peray [10] the four regions in a kiln are (see Fig. 1.4):

- **Preheating/Drying**: Temperature of the raw material increases to approximately 900°C (1173K) where calcination can begin, and any excess moisture is evaporated.
- **Calcining/Decomposition**: Calcination occurs in this region, indicating that the limestone, CaCO₃, will decompose into calcium oxide (free lime), CaO and carbon dioxide.
- **Burning/Clinkerizing**: This is the hottest region of the kiln where temperatures can reach above 1260°C (1533K) and the solid components begin to liquefy. Coating formation of on the refractory material occurs.
- **Cooling**: The size of the cooling region is dependent on the location of the flame. Liquid material begins to solidify into clinker and ends up being discharged into the grate cooler where rapid cooling occurs.

![Figure 1.4: Schematic of regions within a rotary cement kiln](image-url)
In the event where a precalciner exists before the feed inlet of the kiln, the preheating/drying region is much shorter and in some cases, almost non-existent. This is because temperature of the material has already reached the stage where calcination can begin before it enters the kiln.

Coating formation in the burning region of the kiln is an important aspect of improving the refractory lifetime. As the raw materials liquefy, solid-liquid and solid-solid reactions occur simultaneously in the burning region. Some of this liquid solidifies over the refractory brick creating a coating layer. Since this coating is formed in the region where the flame is located, temperatures within the kiln can reach upwards of 2000°C in the gas phase, and >1450°C in the bed phase. This coating layer significantly reduces the amount of heat that is transferred through the kiln shell into the environment. External from the kiln, a series of vertical and angled fans impinge on the kiln in the vicinity of the burning region. Ranging in diameter from 0.762 – 1.524m (30 – 60”), these fans utilize electrical energy to cool the outer shell of the kiln and promote coating formation within the kiln.

It comes as no surprise then that the production of clinker is the most intensive thermal energy operation within the entire cement production process. Typically 90% of the total thermal energy is consumed in the rotary cement kiln [11]. Atamaca [11] and Kabir [12] reported that 30 – 40% of the output heat from a cement plant is the result of clinker production, and 50 – 60% of the input energy is from the combustion of fuel. A case study of a dry-type cement plant performed by Engin and Vedat [13] reported that approximately 40% of the input energy required for the process was lost as: hot flue gas (19.15%); cooler stack gas (5.61%), and through the kiln shell wall (15.11%). Of these three sources, the energy of the hot flue gas is not considered a total loss as it is typically used to pre-heat the raw material before it enters the kiln, and to dry the raw material before it is transported to the main baghouse. The cooler stack gas is a low-quality, inconsistent source of heat which is difficult to reclaim. The heat lost through the kiln shell wall is typically completely lost to the surrounding environment. As this represents a major source of energy waste, this thesis seeks to understand the quantity and quality of this energy such that it may be considered for conversion or reuse.
In order to better understand the thermal energy within the kiln, and lost from the kiln shell, researchers have developed one-dimensional mathematical models. Through the utilization of principles of thermodynamics, heat transfer, and chemistry, these models have proven to be sufficient in predicting the thermal and chemical processes that occur within a rotary kiln.

1.2 Literature Review

This literature review will look at the formulation of previous one-dimensional mathematical models of rotary cement kilns. There are two primary components to the formation of a mathematical model of a rotary kiln, a thermal side focusing on classical methods of heat transfer prediction, and a chemistry side that focuses on the implementation of the five chemical reactions listed previously. The first section of this review focuses on development of relationships characterizing the forms of heat transfer within a rotary kiln, and the second section discusses previous existing models and the influence of chemistry in each model.

1.2.1 Classical Forms of Heat Transfer

Due to the complexity and scale of rotary kilns, full scale experimental results are costly and impractical. Measured data from operating cement plants although available at times, is subject to confidentiality and inherent limitations. This data is restricted to the precise operating parameters that occurred at that time, and more often than not, a majority of these parameters can only be estimated within a certain degree of accuracy. It is due to these reasons that research on the continued understanding of rotary kilns is not only slow, but heavily focuses on small scale experiments and numerical models.

Rotary cement kilns are highly complex machines that exist for the sole purpose of cement clinker production. As the heart and soul of the cement manufacturing industry, rotary kilns incorporate a combination of convection, radiation, and conduction to achieve their purpose. Fig. 1.5 shows the three distinct phases within the kiln where heat transfer occurs:
1. Bulk bed phase
2. Freeboard gas phase
3. Wall phase

![Diagram of heat transfer and phases within a rotary cement kiln.](image)

**Figure 1.5: Types of heat transfer and phases within a rotary cement kiln.**

Beginning with convection inside of the kiln, initial work was performed by Tscheng and Watkinson [14] regarding convection between the gas and wall, and gas and bed inside of a rotary kiln. Originating from Tscheng’s PhD thesis [15], an experimental observation of convection within a rotary kiln was completed, and a correlation for convection between the phases was derived. Experiments were performed in a 2.5 m long, 0.19 m inner diameter pilot kiln wherein Ottawa sand entered at one end and preheated air entered through the other end. Modifications to operating parameters such as kiln inclination angle, particle size and throughput of solids were deemed to be insignificant on the effects of heat transfer. Correlations of Nusselt number for heat transfer between the gas and bed, and gas and internal wall were developed; these correlations were influenced by Reynolds number (1600 – 7800), Rotational Reynolds number (20 - 800), and the amount of solids fill inside the cylinder.

The effect of radiation within the kiln was studied by Hottel and Sarofim. Publishing a book on their work, “Radiative Transfer” [16] outlines the effects of radiation between the gas and bed, as well as between the gas and internal wall. These relationships are analogous to one-zone models of radiation, where any variation in circumferential temperature...
gradients are neglected. Further investigation into the effects of radiation and a comparison between a one-zone model and a four-zone model was performed by Gorog et al. in a series of papers [17,18]. The first focuses solely on the effect of a non-gray freeboard gas assumption within a rotary kiln through the evaluation of radiative exchange integrals by numerical methods. The authors seek to develop a relationship describing the emissive characteristics of the freeboard gas based on the work of Hottel and Sarofim [16]. In their comparison between non-gray freeboard gas and gray freeboard gas models, it was concluded that an error of less than 20% was achievable when the internal wall and bulk bed emissivites were greater than 0.8. Their second study developed a mathematical model that can approximate the temperature field in the internal kiln wall. Employing relationships provided by Tscheng and Watkinson [14] and neglecting the effects of chemistry, a simplified analog describing heat flows within a rotary kiln was established. It was also determined that utilization of a one-zone method when compared to a four-zone method resulted in an error of less than 10% in regards to radiant energy incident on the exposed kiln wall inside of the kiln.

Based on the works listed above, there exists little variation between the convective and radiative components of heat transfer within a rotary kiln. The prediction of conduction through the kiln wall is straightforward as it travels through individual layers; however, determining the appropriate thermal conductivities and sizes of the layers is more complicated. These issues arise with the inclusion of a refractory layer and coating layer. A majority of models consider a constant refractory thickness and thermal conductivity [9, 19-25], while variations in coating thickness are approximated more thoroughly. Refractory material typically changes in different areas of the kiln, breaks down and shrinks as the process progresses. Material is also deposited on top of the brick in small quantities, and mortar exists between the bricks. Estimation of a single thickness and conductivity for refractory material comes with error; as mentioned previously, this cannot be avoided the majority of the time as real time refractory information is near impossible to achieve without the assistance of a partner organization that would be willing to shut down their operation in order for measurements to be taken. If scanned kiln shell temperature data is available, the thermal conductivity of the refractory material and any
unknown thermal resistances through the shell are better suited as a calibration parameter in one-dimensional models.

Convection from the kiln shell into the environment is another parameter that has not yet been fully defined. Existing models utilize a natural convection heat transfer coefficient over the length of the kiln to describe convection from the kiln shell. As stated previously, kiln shell cooling fans are utilized to cool the kiln shell in the burning zone and to help facilitate coating formation inside. With the exception of the numerical model developed by Mastorakos [22], the presence of these fans and their impact on convective heat transfer from the kiln shell has never been mentioned in these existing models. Mastorakos [22] mentions that these fans are utilized in the cement industry and includes their presence by the inclusion of a singular value for convective heat transfer. To the author’s knowledge, the origin of this value was unidentifiable; however, it is likely that it was derived from using the well-known correlation for external flow over a cylinder found in most heat transfer textbooks.

1.2.2 Clinker Chemistry

The second component in the development of an appropriate numerical model for heat transfer within a rotary cement kiln involves the incorporation of clinker chemistry. The rotary kiln is essentially a large chemical reactor. Raw material enters at one end and, in response to heating at very high temperatures, various solid-solid and solid-liquid reactions occur resulting in clinker, which is the building block for cement. Each stage has its own thermodynamic requirements for the reaction to initiate. According to a review in the book “Thermodynamics of Silicates” by Babushkin et al. [7], there exist approximately >20 chemical reactions that describe the formation of cement clinker. Depending on the type of cement, such as the creation of Portland cement, certain additional reactions can also be present. Due to the complex nature of these equations, it has been determined that the total set of equations can be simplified to five equations that describe the development of the four main constituents found in cement clinker, and the decomposition of limestone into calcium oxide. Additional components such as C\textsubscript{12}A\textsubscript{7}, C\textsubscript{2}AS, CS, C\textsubscript{3}S\textsubscript{2}, CS\textsubscript{2}, CF, and C\textsubscript{2}F are usually present at the output of the kiln, although their quantities are so small that they can be neglected [9,19,20,22].
Characterizing these five equations in a numerical model requires appropriate assumptions to achieve accurate chemistry kinetics. The first reaction, the decomposition of limestone (\(\text{CaCO}_3\)) into calcium oxide (\(\text{CaO}\)) and carbon dioxide (\(\text{CO}_2\)) is generally well understood. The highly referenced study of Watkinson and Brimacombe [26] performed in 1991 focuses on the variation of operating conditions to better understand limestone calcination in rotary kilns. An experimental study was performed in a pilot-scale rotary kiln in order to determine the influence that limestone type, feed rate, rotational speed, inclination angle, and particle size has on calcination and heat flow within a rotary kiln [26]. In contrast to this calcination reaction, the remaining four reactions have not been extensively studied, and information regarding variations of diffusion coefficients as a response to the temperatures and conditions present within a kiln is almost non-existent [9,19]. As a result, a pseudo-homogenous characterization of these reactions is utilized [9,19,20,22].

Determining appropriate chemistry kinetics for each reaction requires certain assumptions; the most predominant ones are that a steady state, steady plug flow process is occurring [11]. Boateng [27] presented an extensive review on the transport phenomenon and transport processes occurring within a rotary kiln. He proposes a relationship based on Froude number to characterize the transverse motion of the bed material inside of the kiln. Typical rotational speeds and kiln dimensions result in a rolling characteristic for bed motion, which is representative of plug flow within a rotating cylinder. Furthermore, with the fact that there is only one entrance and one exit, the general equation for mass balance in a plug flow chemical reactor allows for reaction rates of these species to be based on Arrhenius’ law. Following the trends of other models [9,19,20,22,24,25], the heats of reactions, specific heats of formation, latent heat of solid material, activation energies, and pre-exponential factors remain constant as the species progress axially through the kiln.

The major differences between how the clinker chemistry is implemented in each model lies within the formulation of the reaction rates, activation energies, and pre-exponential factors used. Since the calcination reaction is the most well understood reaction, typical values for chemistry kinetics for use with Arrhenius’ law are readily available. Issues arise with the other four chemical reactions. A model developed by Mastorakos [22] and adapted by Mujumdar [9,19] utilizes pre-exponential factors and activation energies chosen by trial
and error in order to achieve appropriate output mass fractions of each species. These models also do not include temperature range limitations for certain reactions, which reduces the models predictive capabilities [28]. Comparing this model to the work of Spang [20] and later Darabi [28], drastically different kinetic constants were used.

Until the chemistry kinetics of the four additional chemical reactions are better understood, modelling clinker chemistry in a one-dimensional numerical model is restricted to an assortment of assumptions and appropriate approximations.

1.2.3 Existing Models

The use of one-dimensional models to characterize the operating parameters, temperature profiles, clinker formation, and energy consumption are useful in improving the design, operation, and understanding of rotary kilns. Many one-dimensional models exist for the purpose of improving the understanding of energy use within a rotary kiln. With each new model that is developed, formulations and techniques are adapted from previous versions, and new modifications are made. Numerical modelling of rotary kilns is a collective process of ideas and techniques. There has yet to be a single, universal model that has been developed for use in both a research and commercial setting due to the complexities that exist within rotary kiln modelling, and the variations in chemistry and heat transfer formulations.

Mujumdar [9] proposes that there exists two spectrums of one-dimensional models. The first type acts essentially as a two-point boundary value problem in which the freeboard gas profile and bulk bed profile inlet conditions are known [9]. From these the temperature profiles for the bulk bed and freeboard gas, and species mass fractions are solved numerically. Mujumdar argues that use of a one-dimensional model to compute the freeboard gas profile is questionable due to the complex three-dimensional nature of flow that is generated from a burner. The second type incorporates experimental or coupled three-dimensional CFD models of the burners in order to generate a more accurate representation of the freeboard gas profile. Out of the existing models reviewed, the work of Mujumdar [19], Spang [20], Li [21], Martins [24], and Sadighi [25] fall under Type 1, while Mujumdar [9], Mastorakos [22], Barr [23], and Darabi [28] fall under Type 2.
The oldest model reviewed, developed in 1972 by Spang [20] is a dynamic model that is qualitatively capable of predicting the temperature profiles of the freeboard gas, bulk bed, and internal wall, as well as the species compositions of each product as they progressed along the kiln. Some key features which make Spang’s model unique to many others reviewed is that it does not operate at a steady state. Spang developed formulations for the freeboard gas and bulk bed temperature profiles as functions of axial distance. His formulations for species mass fractions, and wall temperature are functions of time. The transient response to temperature profiles and mass fractions after the flame inside of the kiln was turned off was observed. Although qualitatively capable of predicting trends within the kiln, Spang’s model overestimates the peak heat transfer in the burning region (~2250°C) and does not include features such as coating formation, mass transfer during the decomposition of limestone, and a shell temperature profile.

Originating as a PhD thesis [23] and adapted to a series of papers, Barr et al. [29] first performed experiments on a pilot-scale rotary kiln. The authors developed a one-dimensional model for the calcination region in an attempt to describe trends observed in the experiments. Using different feed materials such as limestone, sand, and petroleum coke, their model was able to reasonably predict temperature profiles of the bed and inner kiln wall.

The first CFD coupled model reviewed was developed in 1999 by Mastorakos et al. [22] for a coal-fired rotary cement kiln. The commercially available FLOW-3D – RAD-3D package to calculate heat transfer from the flame, and coupled with both an axial and radial formulation for temperature distribution in the wall. The temperature profile for the bed was solved in one-dimension. The authors also generated a method of determining the presence of the melt within the kiln based on the latent heat of fusion indicating when liquid was forming. This model predicts both temperature profile and species mass fractions quite reasonably; however, their model requires the use of chemistry kinetics based on trial and error as well as an estimate of thermal conductivity of the refractory and forced convection heat transfer coefficient on the outside shell. Temperature range restrictions are also not present indicating that certain reactions may have occurred earlier than they would in
actuality, especially with estimates made on the chemistry kinetics influencing the proper species outputs.

In 2004 Martins et al. [24] developed a model focusing on the calcination of limestone within a rotary kiln. Utilizing equations developed by Hottel and Sarofim [16] and Tscheng and Watkinson [13], their work was able to closely replicate the work of Watkinson and Brimacombe [26]. Providing further credence to the radiative and convective correlations that were developed by those works. This model utilized a linearization of the heat balance through the kiln wall and was solved by the use of a Picard iteration scheme and relaxation formula.

Li et al. [21] developed a one-dimensional model in 2005 focusing on the calcination region and the different methods of calculating the conductive heat transfer between the bed and the wall. They were able to closely compare the freeboard gas, bulk bed, and wall temperature profiles to the experimental data of Barr et al. [23]. Convection inside of the kiln was based on Tscheng and Watkinson [13] while the one-zone radiation method developed by Gorog et al. [18] was used for internal radiation. As a result, Li et al. were successful in developing a formulation for conduction between the bed and wall based on the penetration theory that is often seen in the case of fluidized beds and fixed beds.

Two models were developed by Mujumdar et al. [9,19] in 2006. The first is a Type 2 model that incorporates an area-weighted average data set for the freeboard gas determined from a previous CFD model of the burner. Utilizing the same formulation for convective and radiative heat transfer both inside the kiln and outside that is used in Martins et al. [24] and the same chemistry kinetics used in Mastorakos et al. [22] variations in the model come when determining the axial distribution of the bed along the length of the kiln, the calcination reaction, and melt formation. As opposed to other models, Mujumdar does not assume that the bed height stays constant, but rather it changes due to mass transfer from the solid to the gas during the calcination reaction. This influences the cross-sectional area of the bed and velocity of the material as it travels through the kiln. Mujumdar also incorporates a shrinking core model to more closely predict the calcination reaction. Limestone does not decompose instantaneously but rather in segments as the outer layer of
a particle continually decreases as material decomposes; this is similar to the devolatization of coal during combustion. Lastly, using the liquidus and solidus temperatures to determine when all mass is liquid and when the first drop of liquid is formed, a ratio using the bed temperature was determined in order to predict the amount of melt formed in the kiln. This melt fraction alongside a different latent heat of fusion as seen in Mastorakos et al. [22] and mass flow rate of the bed acted as the formulation for coating in the burning region. Mujumdar also included the effect of dust entrained in the freeboard gas which would affect the properties of the gas, such as emissivity and thermal conductivity. The second model developed was a Type 1 model that incorporated a second set of PDE’s that also describe the combustion of coal. This was used to predict the freeboard gas temperature profile as opposed to the area-weighted average approach from the first model. Additionally, the second model incorporated an analysis of putting a secondary shell around the kiln shell with a gap to allow for air to pass through it in an attempt to reclaim energy. Both models reasonably predicted temperature profiles and species mass fractions along the axial length of the kiln.

A second one-dimensional model coupled with CFD was developed for a thesis by Darabi [28] in 2007. This model was a combination of the fusion fraction formulation seen in Mastorakos [22] as well as the species mass fractions formulation seen in Spang [20]. Utilizing these two formulations, temperature restrictions as to when certain reactions would occur were incorporated as well as closure equations describing the mass transfer from the solid bed to the gas. Coupled with a previously developed in-house CFD model for the kiln wall and burner, Darabi sought to determine the effect of tire burning as an alternate fuel within a rotary kiln. Like the previous models before it, Darabi’s model was able to reasonable predict the temperature profiles, species mass fractions, and NOx emissions as the result of tire burning.

The most recent model reviewed was developed by Sadighi et al. [25] in 2011. Borrowing the freeboard gas, bed temperature, and species mass fraction formulation from Spang [20], Sadighi utilized a formulation for flame length from a separate work performed by Gorog et al. [30] in order to calculate flame length and heat released from combustion.
Furthermore, using scanned shell temperature data, the internal temperature profiles were generated, and the thickness of the coating generated on the inside was estimated.

1.3 Objectives and Scope

After an extensive review of the previous one-dimensional models that exist, it is quite apparent that there exists a collection of different models that utilize different formulations for both heat transfer and clinker chemistry, and all are capable of reasonably predicting trends within a rotary cement kiln. It is also apparent that through each model developed, a small modification or technique is added to improve upon the existing methods that have already been developed. By observing previous models, certain areas of improvement become recognizable.

A largely overlooked subject is that of convective heat transfer from the kiln shell. In each previous model reviewed, the convective heat transfer is typically assumed to be due to natural convection. Although this is suitable for specific kilns, those that include the effect of external shell cooling fans would not be able to use this assumption. Furthermore, utilizing a one-dimensional model in an attempt to quantify energy both internally and externally, an accurate estimation of the forced convection effects of shell cooling fans should be included.

CFD analysis is already being coupled with one-dimensional models of rotary kilns in the form of accurate flame and burner modelling. The spirit of utilizing CFD to analyze a previously overlooked component of one-dimensional models is the driving motivation behind this work.

Through a CFD analysis of external fans impinging on a large cylinder in order to mimic the effect of these shell cooling fans, a correlation to predict forced convection heat transfer is sought. Furthermore, testing the effects of this correlation requires the implementation of it in a one-dimensional model. Therefore, it is also necessary to implement a functioning one-dimensional model of a rotary cement kiln to accommodate the results of the CFD study to improve the prediction of shell temperature, and in turn allow for a more accurate estimation of energy lost from the kiln shell in future models.
1.4 Outline of Thesis

A brief overview of the contents of this thesis are as follows:

- **Chapter 2:**

  A Computational Fluid Dynamics study of the forced convection heat transfer from the outside of the cement kiln is presented. This study develops the geometric and numerical formulations and present results for several conditions observed specifically in the cement production industry.

- **Chapter 3:**

  A one-dimensional numerical model is presented, which includes implementation of the forced convection heat transfer correlation developed in Chapter 2. A comparison of the shell temperature profile assuming full natural convection, and including forced convection against scanned shell temperature data is performed.

- **Chapter 4:**

  A brief synopsis of the work performed along with contributions made in the areas of impinging jets and one-dimensional rotary kiln modelling. Future recommendations and areas of improvement are also identified.

1.5 References


From url
http://www.cement.ca/images/content/2012EnvironmentalPerformanceReport.pdf

http://www5.statcan.gc.ca/cansim/a05?lang=eng&id=1280016#F16


Chapter 2

2 Forced Convective Heat Transfer on a Horizontal Circular Cylinder due to Multiple Impinging Circular Jets*

A computational study is undertaken to investigate convective heat transfer on a horizontal cylinder due to a bank of vertically oriented circular jets. The importance of this study stems from the real-world application of convective cooling of rotary cement kilns by the use of large axial fans. A computational model is developed which considers one spatially-periodic section of the domain, and solutions of the conservation equations combined with an appropriate two-equation turbulence model are obtained using the commercial software ANSYS Fluent™. The computational model is validated by a comparison to previous studies of a single circular jet impinging on a cylinder. A parametric study is presented which considers the impact on average heat transfer due to: jet-to-cylinder spacing ($y/d$), axial jet spacing ($z/d$), jet-to-cylinder diameter ratio ($d/D$), jet offset from the axial centerline ($x/d$), and jet Reynolds number. Results of the parametric study show that for jet-to-cylinder ratios of $d/D \geq 0.23$, that movement away from the cylinder axis, increased axial spacing and lateral offset all lead to degradation of heat transfer from the cylinder. For $d/D = 0.15$, similar degradation occurs, but in part of the parametric space studied, increased distance from the cylinder and lateral offset leads to enhancements of the heat transfer. The complete set of results is presented as a correlation wherein the influence of all parameters studied are included as power-law corrections to the average Nusselt number.

2.1 Introduction

Convective cooling of large cylinders by banks of fans has many applications in the process industry. A pertinent example is in the cement industry where large (4-5m in diameter and 50-100 m in length) rotary kilns are utilized for the production of cement clinker. A

*The following is from a version of a manuscript submitted for review with the journal Applied Thermal Engineering.
schematic showing the layout of a typical rotary cement kiln is given in Fig. 2.1. Tilted at an angle of 2 - 5° with respect to horizontal, and operating at a slow rotational speed of approximately 1 – 5 rpm, the raw feed (typically limestone, silica, aluminum and iron oxide [1]) travels through the cylindrical kiln due to gravity/tumbling. The kiln itself is comprised of a steel shell for strength and rigidity, lined on the inner surface with refractory brick to enhance the thermal resistance, and isolate the steel shell from the high temperature process taking place inside. Raw feed enters the kiln at one end, and fuel (petroleum coke), which is combusted in a burner located approximately 1 m into the kiln, enters at the opposite end. Near the burner, the temperature of the exhaust gases can reach upwards of 2200 K, and the reacting raw material can reach as high as 1900 K. The solids begin to melt in this region allowing for the required solid-liquid reactions to occur. As this liquid mixture re-solidifies, tiny balls referred to as clinker are formed, as well as a thin coating layer adjacent to the inner refractory wall of the kiln. This process is essential to the formation of clinker, and requires significant heat removal through the kiln wall to occur. To facilitate heat transfer through the kiln wall, banks of large kiln shell cooling fans are often used in the burning region of the kiln.

Positioning of the cooling fans requires consideration of the process occurring in the kiln, and the path that the heat takes to reach the outer wall of the kiln. Fig. 2.2 shows that the particle bed inside the kiln is skewed to one side, due to the slow rotation of the kiln, and that the particle bed is in contact with the only 10-15% of the refractory material at a time. While this produces a local hot-spot on the inner refractory surface, this hot spot is in continuous motion due to the rotation of the kiln. Furthermore, because the refractory brick is typically 10-20 cm thick and is bonded to a thick steel outer shell, the exposed surface of the kiln is nearly isothermal. Despite this fact, many production facilities offset the fans so that they are directed more closely at the tumbling particle bed, which may or may not enhance the overall heat transfer from the kiln. The purpose of this study is to consider a bank of impinging fans directed at the kiln wall at different distances from the kiln shell, different axial separation, and different lateral offsets from the kiln centerline to quantify the convective heat transfer and specifically, to understand the degradation/enhancement in heat transfer associated with offsetting the fans away from the cylinder axis. In the interest of generality, the kiln in this study is considered to be a horizontal cylinder and
rotation is ignored; as mentioned above, the slow rotation only serves to make the outer surface more nearly isothermal, which is the heating condition used in this study. While there have been many studies that have considered convective heat transfer due to impinging jets and banks of jets, they have been predominantly focused on impingement on a flat plate. The most notable of these are the works of Martin [2], Jambunathan et al. [3], and Zuckerman and Lior [4]. Far fewer investigations of jet impingement on a circular cylinder exist in open literature, especially for cases where the jet to cylinder diameter is large.

![Schematic of a Rotary Cement Kiln.](image)

**Figure 2.1: Schematic of a Rotary Cement Kiln.**

Several studies involving impingement on a cylinder relate to impingement from slotted jets that are oriented with the axis of the cylinder. Olsson et al. [5] studied the effect of a single slot jet impinging on a single cylinder for operational parameters such as jet-to-cylinder distance, and cylinder curvature for jet Reynolds numbers (based on jet exit
velocity and slot width) ranging from 23,000 – 100,000. It was concluded that average and stagnation Nusselt numbers increase with increasing jet Reynolds number and surface curvature; however, the effect of jet-to-cylinder spacing was not found to be significant. Another study by Olsson et al. [6] considered multiple slotted jets impinging on multiple cylinders for the same range of parameters as in [5], but including the non-dimensional effect of distance between the jets. Here, they observed that variation of the distance between jets and the opening of the jets were important when trying to achieve higher rates of heat transfer. Jeng et al. [7] studied the effect of a lateral impinging slotted air jet on a rotating cylinder for jet Reynolds numbers in the range 655 – 60,237 and for a range of rotational Reynolds numbers from 0 – 7,899. They showed that the average Nusselt number increases as the rotational Reynolds number increases and that this effect is reduced for higher jet Reynolds numbers. Another study involving a single slotted jet along the length of a free cylinder was conducted by McDaniel and Webb [8], where it was shown that an optimal nozzle-to-cylinder spacing exists where maximum heat transfer occurs. Gori and Bossi [9,10] also investigated experimentally the effect of slot width to cylinder separation distance for a fixed cylinder diameter ($D$) and slot to cylinder spacing ($H$), within ratios of $H/D$ ranging from 2 to 10 for cylinder Reynolds number, $Re_D$, between 4,000 and 20,000. This study also considered the effect of slot width ($S$) through the dimensionless ratio of cylinder diameter over slot width, $D/S$, at values of 1, 2, and 4, and found that the maximum

Figure 2.2: Cross-section of Rotary Cement Kiln.
Nusselt number occurs at $H/D = 8$ [10]. Sparrow and Alhomoud [11] provide a comprehensive study on the effect of Sherwood number when offsetting a single slot jet from the axis of the cylinder that it is impinging upon. The study showed that offsetting the jet decreased the Sherwood number, and that the effect was greatest for small slot-to-cylinder separation distances. Furthermore, the results were sensitive to modification of the slot width, especially as the offset was increased.

The effect of an array of slotted jets impinging on a cylinder has been investigated experimentally by Nada [12], where a comparison is drawn between a single slot jet aligned with the cylinder axis and multiple slot jets aligned orthogonal to the cylinder axis. Similar to previous studies, the effect of jet-to-jet spacing and jet-to-cylinder spacing was examined. Again, it was found that there exists an optimal region of $H/S$ where the average Nusselt number reached a maximum. Zuckerman and Lior [13] considered different turbulence models in their numerical study of convective heat transfer from a circular cylinder. Their simulations study the effect of 2 to 8 slot jets positioned equally-spaced radially around a cylinder for a range of operating parameters and jet Reynolds number from 5,000 to 80,000. The so-called “fountain flow” shape generated from the secondary region of impingement between two adjacent jets was shown to greatly increase the heat transfer from the cylinder. A correlation was proposed to characterize the heat transfer from the cylinder for 2 – 8 slot jets equally spaced radially around the cylinder.

Existing research on convective heat transfer due to circular impinging jets on a cylinder primarily focuses on single, small circular jets impinging directly on the axis of the cylinder. To this end, Tawfek [14] conducted an experimental investigation of a single circular jet impinging on an isothermally heated brass cylinder. Three different jet diameters and various jet-to-cylinder separation distances were studied for $Re_j$ ranging from 3,800 to 40,000. The highest heat transfer was observed at the region of impingement. They also observed that as the jet-to-cylinder spacing increased, stagnation heat transfer rate decreased. Turbulent flow and convective heat transfer over a curved surface was examined by Lee et al. [15]. The jet potential core length was observed to range from $3.1d – 4.2d$ for the range of jet Reynolds numbers from 11,000 – 50,000. The stagnation Nusselt number was reported to vary with increasing jet-to-cylinder spacing ($L/d$) reaching a
maximum between \( L/d = 6 – 8 \). Wang et al. [16] studied three different cylinder-to-jet diameter ratios, \( D/D_j = 0.5, 2.0, \) and \( 5.0 \) for a fixed jet diameter \( D_j \), and a jet Reynolds number of 20,000. They concluded that ratios of \( D/D_j \geq 2.0 \) follow similar local heat transfer characteristics for circular jets impinging on a flat plate. A study performed by Sparrow et al. [17] used a naphthalene sublimation technique to quantify heat transfer from a cylinder in the area of impingement. Correlations for stagnation point Nusselt and Sherwood numbers were derived from experiments conducted in the range of \( Re_j \) from 4,000 to 25,000 and non-dimensional jet-to-cylinder spacing \( H/d \) from 5 to 15 for three different jet diameters. Peak heat transfer was determined to exist as the jet-to-cylinder spacing decreased, and as the jet diameter decreased. A detailed experimental and computational approach to turbulent impingement of a single cylinder for parameters of jet-to-cylinder spacing from 4 – 16, and the ratio of jet diameter over cylinder diameter, \( d/D \), from 0.11 – 0.25 for \( Re_j \) from 10,000 to 25,000 was performed by Singh et al. [18]. Various different turbulence models were tested for the numerical model. From this study it was concluded that stagnation Nusselt number increases consistently as jet-to-cylinder spacing decreases. It was also determined that outside of the region of impingement, modifications to jet-to-cylinder spacing and \( d/D \) do not have an impact on heat transfer. Furthermore, regardless of the turbulence model used, stagnation Nusselt number was over-estimated. Lastly, Dong et al. [19] conducted a study on a row of three cylindrical butane/air flame jets impinging on a flat plate. Through the modification of jet-to-jet and jet-to-cylinder spacing for values of (2, 5) and (2.6, 5, 7), respectively, they concluded that as the jet-to-cylinder spacing increased, the area-averaged heat flux also increased. Additionally, heat transfer was shown to increase to a peak value before decreasing again with the increase of jet-to-jet spacing.
To the knowledge of the authors, no studies exist in the literature that consider banks of highly turbulent circular jets of large jet-to-cylinder diameter ratio impinging on a circular cylinder at different axial and lateral offsets. The unique nature of this phenomenon within an industrial application is the driving motivation of this study. In this respect, the question that will be answered is whether there is a jet position relative to the cylinder axis that yields optimal heat transfer, or conversely, how much degradation/enhancement in heat transfer is occurring when the bank of jets is not (or cannot) be positioned directly under the cylinder axis. Moreover, is there a jet-to-cylinder distance (in close range) that produces maximum heat transfer? This study presents numerical simulations over a range of jet-to-cylinder ratios, jet-to-cylinder distances, and axial and lateral offsets to specifically determine the convective heat transfer performance of the system. Parameters have been

Figure 2.3: Geometric model of horizontal cylinder and vertical jet bank. (a) Isometric view, (b) side view and (c) front view.
selected based on those relevant to the cement production industry where such configurations are realized. Validation of the numerical model is done by comparing to the work of previous studies on single impinging jets. A correlation is provided that characterizes the forced convective heat transfer for the entire parametric space considered in terms of relevant dimensionless quantities.

![Figure 2.3: A schematic of the horizontal cylinder geometry with the bank of vertical jets considered in this study is shown in Fig. 2.3.](image)

**Figure 2.3: A schematic of the horizontal cylinder geometry with the bank of vertical jets considered in this study is shown in Fig. 2.3.**

**Figure 2.4: Geometry for computational domain as extracted from Fig. 2.3a.**

### 2.2 Problem Formulation

A schematic of the horizontal cylinder geometry with the bank of vertical jets considered in this study is shown in Fig. 2.3. While the dimensions of the cylinder and jet are scaled out in the presentation of results, rotary kilns typically have a diameter in the range 4-5 m and a length in the range 50-100 m, and these sizes require consideration for determination of a relevant Reynolds number range. The cylinder shown in Fig. 2.3 is assumed to have a large length-to-diameter ($L/D$) aspect ratio and the bank of vertical jets is evenly spaced. By these assumptions, only a single repeating segment of the geometry is required in the simulations. The symmetry planes shown in Fig. 2.3 reduce the geometry substantially by cutting through the centerline of a vertical jet, and the center-plane between two vertical jets. This serves to reduce the grid size and simulation run time by an enormous amount and was done for all simulations. The computational domain for the reduced segment is shown in Fig. 2.4. The model is shown to have an inner cylinder wall, which is assumed
isothermal, a circular far-field boundary, which is discussed further in the model validation, and a semi-circular jet inlet, which represents the vertical jet bank. Using this model, the jet spacing \((z/d)\) is varied by changing the width between symmetry planes; the jet position relative to the cylinder \((y/d)\) is changed by adjusting the length of the vertical inlet region; and the jet offset \((x/d)\) is adjusted by moving the position of the vertical inlet region away from the axial centerline.

The horizontal cylinder diameter was fixed at a diameter of \(D = 4.8\) m. The non-dimensional jet to cylinder diameter was varied across \(d/D = 0.15, 0.23,\) and \(0.31\) by varying the jet diameter, \(d\). The jet-to-cylinder spacing, \(y/d\), was varied from \(0.21 - 2.14\), by considering physical dimensions of \(y = 0.305\) m – 1.524 m. Each case was then simulated for the same jet-to-jet spacings, \(z/d\), which ranged from 1.21 to 3.41. Finally, in terms of jet offset, the vertical jet ranged from being positioned directly beneath the axial centerline of the horizontal cylinder \(x/d = 0\), to being offset to the point where the outer edge of the jet was aligned with the edge of the horizontal cylinder. Since the jet diameter varied in this study, jets with a smaller diameter had higher offset values when positioned at their maximum offset, which is given as:

\[
\left(\frac{x}{d}\right)_{\text{max}} = \frac{(D - d)}{2d}
\]

2.3 Mathematical Formulation

ANSYS Fluent\textsuperscript{TM} 13.0 was used to solve the governing equations for mass, momentum, turbulence and energy. The governing equations are as given in the ANSYS Fluent Theory Guide [20]:

Conservation of mass:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m
\]

Conservation of momentum:

\[
\frac{\partial \left(\rho \vec{v}\right)}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\vec{\tau}) + \rho \vec{g} + \vec{F}
\]
Conservation of energy:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = \nabla \cdot \left( k_{\text{eff}} \nabla T - \sum_j h_j \vec{j}_j + (\tau_{\text{eff}} \cdot \vec{v}) \right) + S_h \quad (2.4)$$

where the stress tensor in the momentum equation is defined as:

$$\tau_{\text{eff}} = \mu \left[ (\nabla \vec{v} + (\nabla \vec{v})^T) - \frac{2}{3} \nabla \cdot \vec{v} I \right] \quad (2.5)$$

Since all cases considered are fully-turbulent, selection of a turbulence model is also necessary. To this end, the industry-standard, $k-\varepsilon$ turbulence model was used with standard wall functions. While the use of other turbulence closures was considered, the scale of the problem and the well-established nature of the standard $k-\varepsilon$ closure model made it a suitable choice for this study. Furthermore, Zuckerman [13] showed that while there exists a tendency for all turbulence models to over-predict the heat transfer in stagnation region, the standard $k-\varepsilon$ model is at the lower end of this spectrum with errors in predicted Nusselt numbers of less than 22%. It is also noted that in the work of Singh et al. that for small jet-to-cylinder spacings ($h/d \leq 4$) there is little variation between the different turbulence models that were studied [18]. Since the largest jet-to-cylinder spacing used in this study is 2.1, it was concluded that a standard $k-\varepsilon$ turbulence model would be sufficient. Furthermore, the study of different turbulence models has been done by numerous other authors and is outside the scope of this study. The transport equations for the standard $k-\varepsilon$ closure used herein are [21]:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m$^3$)</td>
<td>1.225</td>
</tr>
<tr>
<td>Specific Heat (J/kg·K)</td>
<td>1006.43</td>
</tr>
<tr>
<td>Thermal Conductivity (W/m·K)</td>
<td>0.0242</td>
</tr>
<tr>
<td>Kinematic Viscosity (kg/m·s)</td>
<td>1.7894e-05</td>
</tr>
</tbody>
</table>

Table 2.1: Thermophysical properties of air at 298.15 K.
Turbulent Kinetic Energy:

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

Dissipation rate:

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_\varepsilon \frac{\varepsilon}{k} (G_k + C_3 \varepsilon G_b) - C_2 \varepsilon \rho \frac{\varepsilon^2}{k} + S_\varepsilon
\]

where the turbulent eddy viscosity is computed as:

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

turbulence production is:

\[
G_k = \mu_t S^2
\]

and the body force term is:

\[
G_b = \beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i}
\]

with:

\[
S \equiv \sqrt{2 S_{ij} S_{ij}}
\]

\[
\beta = -\frac{1}{\rho} \frac{\partial (\rho T)}{\partial T}
\]
The body force term $G_b$ is turned off by default in the turbulence dissipation rate equation. Due to the high flow from the jets, inclusion of this term when solving for turbulence dissipation rate did not influence the results.

2.4 Computational Model

The second-order upwind differencing scheme available in ANSYS Fluent™ 13.0 was used to model advection in all transport equations. Standard wall-functions were used to bridge the sharp hydrodynamic and thermal boundary layers at all solid surfaces. In this manner, the grid was developed such that $y^+ \geq 30$ for as much as possible of the cylinder surface. The simulation time averaged between 15 - 20 hours per case using a 4-core Intel Core i7-3820 3.60 GHz CPU with 16 GB of RAM running Windows 7 Professional. Multiple cases were also run on the Shared Hierarchical Academic Research Computing Network (SHARCNET) when the grid was larger than 2,000,000 cells. The working fluid was air and properties were evaluated at a reference temperature of 298.15 K. Thermophysical properties for air are given in Table 2.1.

Figure 2.5: Views of surface meshes generated for computational domain; the lower image is a close-up of the inlet jet region.
The model geometry shown in Fig. 2.4 was designed and modified using SolidWorks\textsuperscript{TM} 2013 where it was then exported as a PARASOLID\textsuperscript{TM} file and imported into ANSYS ICEM\textsuperscript{TM} for mesh generation. Fig. 2.5 shows the geometry and surface meshes on the segment shown in Fig. 2.4. The computational domain was discretized using tetrahedral cells wherein a fine mesh size was used at the cylinder surface and in the vicinity of the jet exit to accommodate the sharp velocity and temperature gradients that were expected in the impingement and entrainment regions. A grid utilizing prism elements on the cylinder surface transitioning to tetrahedral elements was also tested for one configuration. In a comparison between the mesh utilizing a prism layer to the mesh with only tetrahedral elements, a difference of less than 0.5% in heat transfer was observed. As a result, meshes utilizing only tetrahedral elements were used due to the reduced time required to generate a mesh for each geometric condition. Even with the pure tetrahedral meshes, there was no difficulty in maintaining a fine grid spacing at the cylinder wall to be in the proper range of \( y^+ \). A grid independence study, described in detail below, was performed to ensure accuracy of the computational results to within 5\% based on overall heat flux from the cylinder.

Boundary conditions were imposed on all external faces of the computational domain, as shown in Fig. 2.6. Flow at the jet inlet was set using a velocity inlet condition, with a uniform velocity. The jet velocity condition was based on an area weighted average of measured outlet velocities from jets utilized at a cement production facility. The fans used at the facility were comprised of long (8m) cylindrical ducts with fans drawing in air at their base. The air passed across the electric fan motor and through straighteners before exiting at the outlet, which is the location where the vertical jet velocity is imposed, as seen in Fig. 2.6. Measurements across the outlet of the fan revealed a flat “Mexican-hat” profile, which the authors felt would be most generally implemented in the computational model as a uniform plug flow. Velocity values of order 10 m/s were measured; this value was also modified to accommodate a suitable range of Reynolds numbers. The turbulence intensity at the velocity inlet was set to a high value to accommodate the large diameter of the jets and distance from the fan to the jet outlet; assignment of the proper value is considered below in the model verification. The cylinder wall was set as a stationary, no-slip, impermeable wall with a constant temperature of 473K for all cases; the temperature is
based on the target average shell temperature for a typical cement kiln. In terms of the stationary assumption, we refer back to the work of Jeng et al. [7], who reported that the effect of rotational Reynolds number on convective heat transfer decreases as jet Reynolds number increases. Since the present cases consider a high jet Reynolds number, and the rotational speed of the cylinder is small in practice, the effect of rotation on heat transfer should be negligible. As a test, simulations were performed for one case at rotational speeds of 1.5 and 3 rpm, which is a typical rotational speed for a cement kiln. Heat flux results were predicted to within 1% of the results of a stationary cylinder, corroborating the assumption that the effect of rotation on heat transfer is negligible for the cases considered herein. The outer circular surface of the domain was modeled as a constant-static-pressure boundary to account for outflow and backflow. The pressure for this boundary was set to ambient static pressure [13] with a backflow temperature of 298K, and backflow turbulence intensity of 10%. Symmetry conditions were imposed on the two axial planes.

A grid-independence study was performed to determine the grid density and turbulence intensity required to produce overall heat transfer rates to within 5%. This study also considered turbulence intensity values of 5% and 10% on each grid studied. The geometry
considered is a vertical jet centered under the cylinder axis with $y/d = 0.52$, $z/d = 1.2$, and $Re_d = 1,236,000$. Figure 2.7 shows the variation of local Nusselt number along the $z$-axis of the cylinder for different grid sizes and turbulent intensities of 5% and 10%. Differences in overall Nusselt number between the cases with 380,000 and 1,750,000 elements was less than 5% when considering a particular turbulence intensity, and when considering both turbulence intensities studied. Since such differences were considered acceptable, the grid-density based on 1,750,000 elements and a turbulence intensity of 10% was used for all subsequent calculations due to the more consistent profile. Since the domain size varied with the $z/d$ parameter, the chosen grid-density resulted in overall grid sizes between 945,000 elements and 4,660,000 elements. The position of the outer boundary of the domain was also studied separately to ensure that its position did not influence the heat transfer results at the cylinder. At the highest Reynolds number considered, outer domain

![Figure 2.7: Plot of local Nusselt number as a function of axial distance. Plot shows variation of turbulent intensity and different grid sizes in grid independence model.](image)

diameters beyond $2.2D$ produced insignificant changes in the local and overall heat transfer results.
2.4.1 Validation of Numerical Model

As detailed experimental results are not available for the exact cases considered, the numerical model is verified by comparing values of stagnation Nusselt number against the work of Singh et al. [18] for a single centered jet with a \(y/d\) ratio of 4 and \(d/D\) value between 0.11 and 0.2. The jet Reynolds number was matched at values of 10,000 – 25,000, and the turbulence intensity was fixed at 10%, as noted above. Figure 2.8 shows present numerical results for \(d/D = 0.153\), and experimental and numerical results from Singh et al. [18] for \(d/D = 0.11\) and 0.2. The figure indicates that the general trend of increasing \(N_{\text{ustag}}\) with increasing \(Re_d\) is correctly predicted. The figure also shows that while the experimental results of Singh et al. [18] are considerably lower than their own numerical results for both \(d/D\) cases considered, the current numerical results for \(d/D = 0.153\) across the full range of \(Re_d\) fall between the numerical results for \(d/D = 0.11\) and \(d/D = 0.2\), as they should. The over-prediction of heat transfer is mainly due to the over-prediction of turbulence in the stagnation region [13].

![Figure 2.8: Comparison of stagnation Nu predicted by present numerical model to experimental and numerical results of Singh et al. [18] for a single centered vertical jet at y/d = 4.](image)
A further validation case was run to consider two jets with a large axial spacing so that the results could be compared to the single impinging jet results of Singh et al. [18]. A spacing of \( z/d = 7 \) was used to ensure that the regions of impingement were not impacted by the neighboring jets. The results in Fig. 2.9 are in terms of \( z/D \) and are only given to \( z/D = 0.45 \). Beyond this value, the air stream from neighboring jet influences the jet in question and is, thus not relevant in comparison with the single jet case of Singh et al. [18]. The results in Fig. 2.9 show that the values of stagnation Nusselt number for the numerical

![Figure 2.9: Comparison of axial Nusselt number for validation case of \( y/d = 4 \) and (a) \( Re_d = 10,000 \) and (b) \( Re = 25,000 \).](image-url)
model used are within the same range as the numerical results of Singh et al. [18]. Figure 2.9 also shows that beyond $z/D = 0.2$ the axial variations in Nusselt number match the results of Singh et al. [18] extremely well; this is also the region where the experimental results begin to best match the numerical results. It can be concluded from the validation cases that the present numerical model, the domain and boundary conditions, and the computational mesh produce results that are accurate in comparison to previous numerical and experimental work and are thus sufficient for the proposed study.

Though the computational model has been validated against existing work, it is important to note here that since direct validation is not possible for the specific cases studied herein, the CFD results be considered most accurate in terms of predicting differences between cases, as opposed to absolute heat transfer results. To this end, the most important aspect of the computed results are the trends observed when varying the geometric parameters.

2.5 Results and Discussion

A parametric study on the effect of forced convective cooling due to multiple jets impinging on a horizontal cylinder has been carried out. The parametric ranges considered are as follows:

- Jet-to-cylinder spacing ranged from $0.2 \leq y/d \leq 2.1$
- Jet-to-jet spacing ranged from $1.21 \leq z/d \leq 3.41$
- Ratio of jet diameter to cylinder diameter ranged from $0.15 \leq d/D \leq 0.31$
- Jet offset from the cylinder axis ranged from $0 \leq x/d \leq (D - d)/2d$, given by Eq. 2.1.
- Reynolds number range $2.06\times10^5 \leq Re_d \leq 1.236\times10^6$, where $Re_d$ is based on the jet diameter $d$, the uniform jet exit velocity $V_j$, and the kinematic viscosity of air (see Table 2.1):

$$Re_d = \frac{V_j d}{\nu} \quad (2.13)$$

For each case computed, the overall (average) heat transfer coefficient, and the overall Nusselt number were calculated according to:
As the velocity of the jets in operation was measured to be approximately 10 m/s, the range of jet velocity was chosen to be $5 \leq V_j \leq 15$ m/s. Table 2.2 shows the $d/D$ ratios considered and the corresponding Reynolds numbers (recall that the cylinder diameter is fixed at $D = 4.8$ m). The results are presented in a systematic manner by describing the influence of the different geometric parameters.

### 2.5.1 Effect of jet-to-cylinder spacing, $y/d$

Figure 2.10 shows the effect of varying $y/d$ over the ranges of $x/d$, $z/d$ and $Re_d$ considered. Each pair of plots shows the heat transfer trends for $x/d = 0$ (left) and $(x/d)_{\text{max}}$ (right). As mentioned previously, $(x/d)_{\text{max}}$ corresponds to the case when the edge of the vertical jet is adjacent to the outer edge of the cylinder. In Fig. 2.10(a)-(d), it can be seen that for a row of jets of dimension $d/D \geq 0.23$, the overall Nusselt number ($Nu_{ave}$) decreases with increasing $y/d$ for all $z/d$ considered, and that the reduction in $Nu_{ave}$ decreases with decreasing jet Reynolds number. This is the case for both the centered ($x/d = 0$) and fully offset conditions. It is also observed that as $d/D$ decreases from 0.31 to 0.23, the reduction in $Nu_{ave}$ due to increasing $y/d$ decreases; in fact, at an axial separation of $z/d = 3.4$, the difference in $Nu_{ave}$ between $y/d = 0.3$ and 1.4 is almost negligible at $(x/d)_{\text{max}}$. Fig. 2.10(e)-(f) shows that when $d/D = 0.15$, there is a region between $1.6 < z/d < 1.8$ where $Nu_{ave}$ actually increases with increasing $y/d$. Here, an enhancement in $Nu_{ave}$ (between $y/d = 0.4$
and 2.1) occurs for all Reynolds numbers at approximately $z/d = 1.6$. This trend is observed for both the centered and fully-offset cases in Fig. 2.10(e)-(f), except that the enhancement at $z/d = 1.6$ is most significant for $x/d = 0$. The trends shown in Fig. 2.10 suggest that as $y/d$ increases, there are cases where a local maximum in $Nu_{ave}$ is achieved, however, it is also apparent that this local maximum is dependent upon the $z/d$ and $d/D$ ratios, and location of the jet with respect to the centerline of the cylinder.

To reconcile the heat transfer behavior and the local maximum in $Nu_{ave}$, it is necessary to consider the proximity of the jet outlet with the cylinder and the related flow structure in the impingement region and around the cylinder. For a single circular jet, potential core lengths have been measured to be $y/d \approx 4$ [2,16]. Thus, for the close proximity of the jet with the cylinder considered herein ($0.2 \leq y/d \leq 2.1$), the impingement region occurs within the potential core for all parameters studied. This is a unique aspect of the present study compared to all previous work where the jet is typically positioned such that the impingement region transitions from the tip of the potential core to well outside of it [14-18]. Increasing $y/d$ within the potential core has a significant effect on the flow structure and the heat transfer from the cylinder. Nada [12] observed that as the tip of the potential core is approached, the effect of the turbulent shear layer on the cylinder is greater resulting in higher convective heat transfer.

Fig. 2.11 shows surface heat transfer contours for a jet size of $d/D = 0.31$ (a-b) and $d/D = 0.15$ (c)-(f). For the case shown in (a)-(b), the large jet is positioned under the center axis of the cylinder ($x/d = 0$), where $Re_d = 1,236,000$, $z/d = 3.4$, and $y/d = 0.2$ and 1.0. These parameters lie within the region described in Fig. 2.10(a)-(d) where increases in any parameter led to a decrease in overall heat transfer. In these cases, the cylinder lies well inside the shear layer for both $y/d$ positions shown, and the potential core nearly covers the entire impingement region on the upstream side of the cylinder. Fig. 2.12(a)-(b) shows sectional streamline plots for the same cases shown in Fig. 2.11(a)-(b). Here it is seen that for both $y/d$ shown, a strong and energetic turbulent flow remains attached to the cylinder, producing only a small wake on the leeward side. Within the $z/d$ range considered, the proximity of nearby jets prevents the airflow from deflecting axially across the cylinder, which fosters the upward flow and the formation of the energetic layer adjacent to the
cylinder. For $d/D \geq 0.23$, this was observed to be the case over the full range of $y/d$ considered.
Figure 2.10: Comparison of overall Nusselt number variation as jet-to-jet, z/d, spacing increases at d/D = 0.31, 0.23, and 0.15 for: (a)-(b) \( \text{Re}_d = 411,500 – 1,236,000 \) and y/d = 0.2, 1.0, centered and fully-offset, respectively; (c)-(d) \( \text{Re}_d = 309,000 – 927,000 \) and y/d = 0.3, 1.4, centered and fully-offset, respectively; (e)-(f) \( \text{Re}_d = 206,000 – 618,000 \) and y/d = 0.4, 2.1, centered and fully-offset, respectively.
The case of $d/D = 0.15$ shown in Fig. 2.11(c)-(f) yields a different result for heat transfer and flow. Images (c)-(d) show heat transfer contours for $Re_d = 618,000$, $z/d = 1.6$, $x/d = 0$, and $y/d = 0.4$ and 2.1, while images (e)-(f) show the same jet condition, except with $z/d = 3.4$. Comparison of (c) and (d) shows that while the impingement region has higher heat transfer for $y/d = 0.4$, the heat transfer is better distributed for $y/d = 2.1$, thereby leading to a higher average heat transfer, as indicated in Fig. 2.10(e). Fig. 2.12(c)-(d) shows sectional
streamlines for these cases and clearly indicates a small wake on the leeward side for the large vertical spacing, (d), and a much wider wake for the near spacing (c). The streamline plot indicates that for the near case shown in Figs. 2.11 to 2.12(c), the flow is deflected away from the cylinder producing a large wake that is filled with air moving axially, as suggested by the streamlines seemingly originating at the cylinder wall. This results in low

![Streamline plots](image)

**Figure 2.12:** Images (a)-(b) show sectional streamlines for $Re_d = 1,236,000$, $d/D = 0.31$, $z/d = 3.4$, $x/d = 0$, and $y/d = 0.2$ and 1.0, respectively. Images (c)-(d) show sectional streamlines for $Re_d = 618,000$, $d/D = 0.15$, $z/d = 1.6$, $x/d = 0$, and $y/d = 0.4$ and 2.1, respectively. Images (e)-(f) show sectional streamlines for $Re_d = 618,000$, $d/D = 0.15$, $z/d = 3.4$, $x/d = 0$, and $y/d = 0.4$ and 2.1, respectively.
heat transfer over a good portion of the cylinder and lower average heat transfer than for
\( y/d = 2.1 \).

The images in Fig. 2.11(e)-(f) show that for a higher axial spacing, the heat transfer around
the cylinder is fairly well distributed for both cases. Not surprisingly, Fig. 2.12(e)-(f) shows
that the jet and entrainment flow for these cases produce similarly narrow wakes on the
leeward side, although the larger spacing case has a slightly larger wake. Recall that for
this axial spacing, the heat transfer decreased with increasing vertical distance, \( y/d \), similar
to that observed for the larger jets. In this respect, the axial jet spacing appears to have an
important influence on the flow structure and the resulting heat transfer.

### 2.5.2 Effect of jet offset, \( x/d \)

For each \( d/D \) ratio, the effect that offsetting the jets had on heat transfer was studied for
various jet-to-cylinder, \( y/d \), and axial, \( z/d \), spacings. Figure 2.13 shows the data from Fig.
2.10, except plotted to show the influence of increasing \( x/d \) at a constant \( y/d \) and \( z/d \). Figure
2.13(a)-(d) shows that for the larger jets (\( d/D = 0.31, 0.23 \)), the heat transfer decreases with
increasing \( x/d \) for all conditions shown. For \( d/D = 0.15 \), however, the heat transfer
increases with jet offset for certain other parameters. Figure 2.13(e) shows that at \( y/d = 0.4 \)
the heat transfer increases with jet offset in the range \( 1.4 < z/d < 2.4 \), beyond which the
trend reverses. Figure 2.13(f) shows that for \( y/d = 2.1 \), the fully-offset case has a higher
heat transfer when \( z/d > 1.2 \). Figure 2.14 shows a comparison of a large jet case with \( d/D =
0.31 \) at \( Re_{j} = 1,236,000 \) with the small jet case of \( d/D = 0.15 \) at \( Re_{j} = 618,000 \), both for an
axial spacing of \( z/d = 3.4 \). Though the \( Re_{j} \) is different for the two cases, the velocity of the
airflow at the jet exit is the same for both. In addition, both cases are fully-offset and \( y/d =
1.0 \) for the large jet (a) and \( y/d = 2.1 \) for the small jet (b), to maintain the same vertical spacing for both cases. The figure shows the difference in impingement and wake
structures for the two cases. In plot (a), it is clearly seen that because of the large diameter
ratio of the jet, the impingement still results in part of the jet flowing towards the cylinder
axis, thereby producing a region of attached flow on the left side of the jet combined with
a strong energetic region on the right side. It can be imagined from this image that for the
given \( x/d \), a decrease in \( y/d \) would reduce the flow towards the axis of the cylinder, while
an increase would increase this flow, due to the width of the jet at the impingement region.
The result is a significant wake on the leeward side of the cylinder – in comparison to that shown in Fig. 2.12(a) and a reduction in heat transfer compared to the case of the axially centered jet (Figs. 2.11a, 2.12a). This trend is similar for all the cases of $d/D \geq 0.23$ for the entire ranges of $x/d$, $y/d$ and $z/d$ considered; i.e. an increase in any of the geometric parameters for $d/D \geq 0.23$ led to a reduction in heat transfer.

The flow structure seen in Fig. 2.14 (b) shows that, in contrast to the large jet case, there is almost no flow from the impingement region directed towards the cylinder axis, and the flow on the left side of the cylinder is mainly axial, as indicated by the sectional streamlines. The flow on the right side is strong and energetic and results in a higher heat transfer than the case shown in Fig. 2.12 (f). Interestingly, this flow field leads to higher heat transfer than the case of $x/d= 0$, with all other parameters remaining the same. It is thought that the significant region of high-energy attached flow for the offset cases gives the net effect of a higher average heat transfer than the jets centered axially under the cylinder at the same $y/d$, as indicated in Fig. 2.13 (f).
Figure 2.13: Comparison of overall Nusselt number variation as jet-to-jet, $z/d$, spacing increases at $d/D = 0.31, 0.23, \text{ and } 0.15$ for: (a)-(b) $Re_d = 411,500 - 1,236,000 \text{ and } x/d = 0$, max, $y/d= 0.2, 1.0, \text{ respectively;}$ (c)-(d) $Re_d = 309,000 - 927,000 \text{ and } x/d= 0, \text{ max, } y/d = 0.3, 1.4, \text{ respectively;}$ (e)-(f) $Re_d = 206,000 - 618,000 \text{ and } x/d= 0, \text{ max, } y/d = 0.4, 2.1, \text{ respectively.}
2.5.3 Effect of axial jet spacing, z/d

As seen previously, each case was studied at multiple different z/d ratios. It can be seen in Fig. 2.10 and 2.13 that the trend for d/D $\geq$ 0.23 is a decrease in average Nusselt number with respect to increasing z/d; and for d/D $= 0.15$ the trend varies. The work of Dong et al. [20] displays a similar trend for multiple circular jets impinging on a flat plate. In this work three different axial separations, z/d, were studied. What he observed is that from 2.6 $\leq$ z/d $\leq$ 5 there is an increase in the area-averaged heat flux, while from 5 $<$ z/d $\leq$ 7 there is a decrease. Furthermore, according to the work of Wang et al. [16], circular jets impinging on a cylinder where d/D $\leq 0.5$ follow heat transfer characteristics that are apparent when a circular jet impinges on a flat plate. Based on this finding, it is not surprising that for the d/D ratios studied herein, there are combinations of parameters that lead to both increasing and decreasing trends in heat transfer.

Fig. 2.15 shows sectional streamline plots for three different axial separations for the small jet (d/D = 0.15), at Re_d = 618,000 with y/d = 0.4 and x/d = 0. The plots give sectional streamlines on the axial center plane to show the interaction between neighboring jets with respect to axial separation. When the jets are closest together, there is no downward flow.
between them along the center axis, implying that flow is entrained from below and laterally and moves in a weak pattern around the cylinder having little attachment and a large leeward wake, as seen in Fig. 2.12(c). At the middle axial spacing ($z/d = 1.8$), the jets interact causing an organized downward flow between them; this condition fosters a better attachment to the cylinder, a smaller wake, and higher average heat transfer with increasing $y/d$. At the largest axial spacing considered ($z/d = 3.4$), the jets interact forming a downward flow, but because of the large spacing between them, a large secondary vortex appears which is driven by the downward flow and the weak upward entrained flow along the jet wall. For the centered condition, this condition always leads to a decrease in the average heat transfer.
2.5.4 Correlation for average Nusselt number

The results of average heat transfer for the entire parametric range considered can be concisely described by a correlation that puts the average Nusselt number as a function of Reynolds number, $Re_d$, jet-to-cylinder ratio $d/D$, vertical spacing $y/d$, lateral offset $x/d$, and axial spacing $z/d$. The correlation was produced using the regression analysis package available in Microsoft Excel™ and is expressed in power-law form as:

$$Nu_{ave} = 0.041 Re^{0.862} \left( \frac{d}{D} \right)^{-0.317} \left( \frac{y}{d} \right)^{-0.0729} \left( \frac{z}{d} \right)^{-0.186} \exp \left( -0.00134 \left( \frac{x}{d} \right) \right)$$

(2.16)

where, the range of applicability is:

$$0.15 \leq d/D \leq 0.31; \quad 0.2 \leq y/d \leq 2.1; \quad 1.21 \leq z/d \leq 3.41; \quad 0 \leq x/d \leq (D - d)/2d,$$

and for the Reynolds number range: $2.06 \times 10^5 \leq Re_d \leq 1.236 \times 10^6$.

Note that the lateral offset is included in an exponential function because of the fact that it starts at 0. Fig. 2.16 shows the results predicted by the correlation mapped against the complete set of computational results. The plot shows that the heat transfer correlation given in Eq. 16 can accurately predict the results within an interval of ±26%; however, it was able to predict 90% of the results within ±10%. The correlation can be used in “delta-mode” to quickly establish the enhancement or degradation in heat transfer that will occur for a given bank of jets relative to being centered directly under the cylinder axis at a particular axial and vertical spacing. Without experimental verification, it is not recommended that the correlation be used to predict the absolute convective heat transfer from the cylinder.
Conclusions

A CFD study has been carried out to study the convective heat transfer due to multiple circular jets impinging on an isothermal horizontal cylinder. The unique aspect of the study is the large jet-to-cylinder diameters considered (0.15 ≤ d/D ≤ 0.31), and the close proximity of the jet exit to the cylinder. The results were computed using the commercial software FLUENT™ over a parametric space that is relevant to the cement production industry. The following summary points are made:

1. As $Re_d$ gets smaller, variations in non-dimensional parameters have less of an impact on changes in the average Nusselt number of the horizontal cylinder.

Figure 2.16: Correlation for overall Nusselt number based on numerical simulations.

2.6 Conclusions

A CFD study has been carried out to study the convective heat transfer due to multiple circular jets impinging on an isothermal horizontal cylinder. The unique aspect of the study is the large jet-to-cylinder diameters considered (0.15 ≤ d/D ≤ 0.31), and the close proximity of the jet exit to the cylinder. The results were computed using the commercial software FLUENT™ over a parametric space that is relevant to the cement production industry. The following summary points are made:

1. As $Re_d$ gets smaller, variations in non-dimensional parameters have less of an impact on changes in the average Nusselt number of the horizontal cylinder.
2. For a centered jet (x/d = 0), when d/D ≥ 0.23 and y/d increases, the average Nusselt number decreases for all z/d parameters studied. This same trend is seen for the offset cases in this range of dimensionless jet diameter.

3. When d/D = 0.15, increasing y/d results in a larger average Nusselt number for a centered jet at z/d = 1.6 and 1.8. For a fully-offset jet with the same parameters, the same behavior is observed, although with smaller increases.

4. For d/D = 0.15 offsetting the jets results in a larger average Nusselt number at certain axial spacings; i.e., when y/d = 0.4, for z/d = 1.4 - 2.4, and when y/d = 2.1 for z/d ≥ 1.4, the average Nusselt number is larger for an offset jet.

5. The average Nusselt number does not follow a specific trend as z/d increases, but rather it is subject to regions of increase and decrease, depending on other parameters. Beyond z/d = 2.9, a constant value of average Nusselt number is reached due to low jet-interference from neighboring jets.

2.7 References


Chapter 3

3 Numerical Modelling of a Rotary Cement Kiln with Improvements to Shell Cooling*

Numerical models are developed by researchers to analyze and understand the trends occurring within rotary kilns, and allow for improvements in terms of energy quantification and usage. The present study develops a one-dimensional kiln model using elements of existing models and then links the model to the surroundings via a composite resistance model and a forced convection model that enables proper inclusion of the effects of shell-cooling fans. Shell-cooling fans are common in industry and allow for a reduction in shell temperature and promotion of internal coating formation. Thermal conductivity through the kiln shell is treated as a calibration parameter to allow for a more accurate shell temperature profile to be generated, while a forced convection model developed for a bank of jets impinging on a large cylinder is implemented to quantify the external convective resistance. The governing heat transfer and chemistry equations are implemented into the Matlab R2014a™ software to produce one-dimensional solutions of the temperature distributions and species mass fractions observed in a rotary cement kiln. A validation study is performed against an existing one-dimensional model showing reasonable quantitative and qualitative results of temperature profiles and species outputs. Using operational parameters from a partner organization, a profile of internal and external temperature profiles and the corresponding axial development of species products is also presented. Scanned shell temperature data is then compared against the results of the model considering only free convection, and forced convection from the kiln shell cooling fans in operation. An error of $\geq 20$ percent was observed when the effects of forced convection on the kiln shell are neglected.

*The following is from a version of a manuscript submitted for review with the International Journal of Heat and Mass Transfer.
3.1 Introduction

The goal in cement production is inherently to produce as much cement as possible while consuming the least amount of energy possible. Measurements of energy consumption at a cement plant, and within the cement industry as a whole, are typically expressed as energy/weight of clinker, which is the fundamental building block of the process. Rotary cement kilns are used for the production of cement clinker and are by far the highest consumer of thermal energy in the operation, requiring a continuous input of fuel to facilitate the chemical reactions necessary for clinker production. Not surprisingly, 30 - 40% of the heat released from a cement plant is from the kiln as a by-product of the clinker production process [1,2]. With such large amounts of heat being input, consumed, and generated within the rotary kiln, there is also a large amount of heat released from the kiln.

Engin and Vedat [3] performed a case study on heat recovery for dry-type cement rotary kiln systems and observed that approximately 40% of the total input energy to the kiln was released in the form of hot flue gas (19.15%), cooler stack emissions (5.61%), and via convection and radiation from the kiln shell (15.11%). From these releases, the hot flue gas is typically reused throughout the plant in preheating and drying operations; however, the cooler stack emissions and all of the heat released from the kiln shell due to radiation and convection are lost to the surroundings. Thus, the rotary kiln is the largest source of waste heat in the plant, and this has prompted researchers to conduct analyses on the rotary cement kiln through the use of one-dimensional mathematical models and three-dimensional CFD simulations.

At its core, the rotary cement kiln is a large chemical reactor; a simple schematic of the layout of a rotary cement kiln is shown in Fig. 3.1. Tilted at an angle of 2 - 5° with respect to horizontal, and operating at a slow rotating speed of approximately 1 - 5 rpm, the raw feed (typically limestone, silica, aluminum and iron oxide, [4]) enters at the elevated end, and travels through the cylindrical kiln due to gravity/tumbling. The kiln is comprised of a steel shell for strength and rigidity, lined on the inner surface with refractory brick to enhance the thermal resistance, and to isolate the steel shell from the high temperature process taking place inside. Raw feed enters the kiln at one end, and the fuel (petroleum
coke which is combusted in a burner located approximately 1m into the kiln) enters at the opposite end. There are four main regions within the rotary kiln [5] (refer to Fig. 3.1a):

- **Preheating/Drying**: The initial region of the kiln is where raw material is dried and all remaining moisture is evaporated out of the mixture. The temperature of the raw material increases to approximately 1173K (900°C) where calcination can begin.

- **Calcining/Decomposition**: Calcination occurs in this region, indicating that the limestone, CaCO$_3$, will decompose into calcium oxide (free lime), CaO and carbon dioxide:

  \[
  CaCO_3 \rightarrow CaO + CO_2
  \]

**Figure 3.1: Schematic images of a typical rotary cement kiln.**

- Preheating/Drying: The initial region of the kiln is where raw material is dried and all remaining moisture is evaporated out of the mixture. The temperature of the raw material increases to approximately 1173K (900°C) where calcination can begin.
- Calcining/Decomposition: Calcination occurs in this region, indicating that the limestone, CaCO$_3$, will decompose into calcium oxide (free lime), CaO and carbon dioxide:

  \[
  CaCO_3 \rightarrow CaO + CO_2
  \]
This is one of the most important stages in the cement production process, as limestone that is not properly calcined will be difficult to burn, and can result in a poor quality product.

- **Burning:** In the burning or “clinkerizing” region of the kiln, solid-solid and solid-liquid reactions occur. Material in this region consists of predominantly free lime alongside silica, alumina and iron oxides, and trace amounts of additional components that were originally in the raw feed. This is the hottest region of the kiln where temperatures can reach above 1533K (1260°C) when the solid components begin to liquefy. C₃S (Alite) production occurs in this stage consuming all the free lime remaining within the kiln. Coating formation occurs within the burning region as a result of the presence of liquid.

- **Cooling:** As the material passes the burning region there is a flux between solid and liquid phase changes. The cooling region depends on the location of the flame, causing the cooling to be either slow or rapid. Material begins to form into small balls known as clinker. The clinker is then dispensed into the grate cooler where it undergoes rapid cooling.

These regions are subject to change depending on the type of rotary kiln (dry/wet) and the presence of calciners before the kiln entrance, such as cyclone pre-heaters. The formation of the coating layer in the burning region is essential for the longevity of the rotary kiln as it adds to the thermal resistance of the kiln wall. Coating formation is heavily dependent on the surface temperature of the refractory material. If the temperature of the coating remains less than the solidifying temperature of the particles, more coating will continue to form until this temperature is met [5]. Temperatures above this solidifying temperature will result in removal of coating from the surface of the refractory. It is for this reason that the flame has such a large impact on the area and size of the coating layer, as the flame will directly affect the surface temperature in the burning region. At the partner plant studied, large kiln shell cooling fans are utilized in the burning region of the kiln in order to reduce the outer shell temperature, as well as to reduce the surface temperature of the coating.
inside the kiln. This allows for the operators to manipulate the flame more freely without risking the erosion of coating in certain areas.

Researchers have developed rotary kiln models with the intention of understanding the chemistry of the clinker production process such that reductions in energy consumption can be sought. An early model produced by Spang [6] incorporated the dynamic nature of a rotary kiln and a simplified flame model for heat input. He also developed material balance equations for determining the rate of species formation within the material bed, and qualitatively was able to represent the behavior of actual rotary kilns. Barr et al. [7] performed a study using a pilot-scale rotary kiln and compared it to the results of a mathematical model. A large increase in net heat input at the start of an endothermic bed reaction to the bulk bed and temperature cycling of the inner refractory was observed, however, there was no jump in kiln wall heat loss through the refractory. Furthermore, a close coupling of the bulk bed and internal wall was observed as it emerged from underneath the bed material. Li et al. [8] developed a one-dimensional mathematical model to describe the coupling of the covered wall and bulk bed temperatures. An empirical formula was developed focusing on the heat transfer between the covered wall and the bulk bed. Martins et al. [9] developed their one-dimensional mathematical model for comparison to the work of Watkinson and Brimacombe [10] using a variation in the formulation of heat transfer coefficients. The results of their work were in accordance with the compared study. Two versions of a one-dimensional model were developed by Mujumdar et al. [4,11]. Variations in the models come from an area-weighted average approach for approximating the freeboard gas temperature profile from a previously developed CFD model, and an integrated one-dimensional formulation of heat transfer due to coal devolatization and combustion for the development of the freeboard gas profile. Both models proved to be successful in determining appropriate temperature profiles and output values for the species of C₂S, C₃S, C₄AF, C₃A, and CaO. Following more closely to the work of Spang, Sadighi et al. [12] attempted to estimate the coating thickness formed in the burning zone from previously measured process variables and shell temperature data. It was determined that shell temperatures between 190°C and 220°C were sufficient in producing an appropriate coating layer for refractory protection.
Research specifically into the heat transfer processes within a rotary cement kiln has also been active. Peray and Waddell [5] produced a substantial overview of rotary cement kilns covering all aspects of their operation such as refractory material, combustion, flame heat transfer, heat balances, and clinker chemistry. Work performed by Hottel and Sarofim [13] resulted in expressions for the radiative heat transfer between the gas and bed, as well as the gas and internal wall within a kiln. These expressions have been used in various models of rotary kilns over the years. Tscheng and Watkinson [14] followed up with research on the convective heat transfer processes within a rotary kiln and developed a correlation for Nusselt number due to convection between the gas and bed, and the gas and internal wall. Gorog et al. [15] developed a mathematical model to determine the effects of radiative heat transfer between a non-grey freeboard gas and the internal wall of a rotary kiln. It was determined that unless emissivities of the solid constituents and the wall are less than 0.8, then utilizing a grey-gas assumption will result in errors no higher than 20%. A second study was performed by Gorog et al. [16] incorporating the convective and radiative heat transfer coefficients within a kiln to produce a simplified model that is capable of determining heat transfer to the bed material and heat lost from the kiln shell. Neglecting the effects of chemistry within the kiln, this model produced results that were accurate to within 5%. Limestone calcination within a pilot-scale rotary kiln was studied by Watkinson and Brimacombe [10] to determine the effect of limestone type, feed rate, inclination angle, rotational speed, and particle size on the calcination and heat flow in the kiln. Limestone feed rate was found to have the largest effect on the temperature and calcination fields while the effects of rotation and inclination angle were not as significant. A close coupling of the internal wall and bed temperatures was also observed.

While there are a number of different models available for one-dimensional simulations of rotary cement kilns, major differences among models appear in clinker chemistry formulations and more specifically, in the chemistry kinetics utilized. The heat transfer processes within the kiln have also seen significant study and expressions have been developed for use in the kiln models, as detailed in the preceding paragraphs. However, aside from a brief mention in the work of Mastorakos et al. [17], the effects of the composite kiln-shell wall and kiln-shell cooling fans are generally not included when considering the effect of heat losses from the kiln shell. Almost all of the models described
previously utilize a simplistic formulation for kiln shell resistance and convection from the exposed kiln shell, which is generally based upon a free convection correlation for a heated cylinder. Highly turbulent, forced convection heat transfer over at least part of the kiln shell is common in industry, where banks of fans are used to promote heat transfer in the coating formation region, and to keep the outer shell cool enough to avoid structural damage. The present article first formulates a one-dimensional kiln model by considering the best elements of the existing models reviewed above. This model is then linked to a composite kiln shell resistance model, which enables adjustments to the refractory thermal conductivity, and a convective resistance model that includes the effect of various arrangements of shell-cooling fans. In this manner, the present study develops a kiln model that provides a complete energy quality/quantity image of the kiln that can be used for waste heat recovery considerations. Results of the complete calibrated model are compared to existing studies, and against scanned temperature data of the kiln shell at a partner plant, which demonstrates the importance of including the shell cooling fans.

3.2 Formulation of Mathematical Model

A complete one-dimensional kiln model is presented in this section. The chemistry and internal heat transfer elements of the model are adopted mainly from previous studies reviewed above, but with subtle modifications described below. The heat balance model is then described, which includes shell and external convective resistance models, followed by the solution methodology. The one-dimensional kiln model incorporates the following assumptions:

I. The system is assumed to be a steady state, steady flow process [1];

II. Outside and inside kiln shell diameters remain constant;

III. Bed height of the material within the kiln was considered to be constant throughout the length of the kiln;

IV. The free-board gas phase is modeled as a linear process based on estimates of peak temperature value and location data, as well as input and exit temperature conditions;
V. The effects of mixing and gravity on the particle are neglected, except with respect to the heat transfer processes [19];

VI. A rolling characteristic for transverse bed motion was considered [21] allowing for additional plug flow reactor assumptions. Spatial variation of species concentrations and temperature changes are not present for any cross section within the kiln [22];

VII. Chemical reactions are simplified to five reactions limited only by kinetics, following the work of other researchers [4,6,11,17,19]. Reaction rates were determined by Arrhenius’ law, with specific values such as heats of reactions, latent heat of solid material, activation energies, and pre-exponential factors were to remain constant;

VIII. Calcination is assumed to occur in the pre-heater riser before the material enters into the kiln. Sample material data before entering the kiln was adjusted based on CaCO$_3$ loss on ignition to calculate the expected amount of CaCO$_3$ and CaO entering into the kiln from the riser;

IX. The rotary kiln is a dry-type kiln allowing for heat transfer from the release of H$_2$O to be neglected due to low moisture content in the raw material. Loss of mass due to CO$_2$ releasing into the gas and heat released as a result was incorporated as a source term in energy balance of bulk bed;

X. Thermal contact resistance between the refractory material and kiln shell is unknown; however, modification of the thermal conductivity of the refractory is estimated to account for this quantity;

XI. Emissivities of the freeboard gas, internal kiln wall, and solids remain constant throughout the length of the kiln. Freeboard gas was treated as radiatively gray with no more than 20% error due to the emissivities of the internal kiln wall and solids being high (> 0.8) [15,16];

XII. Following Kirchhoff’s Law for an enclosure for a gray surface, absorptivity of the gray freeboard gas is equal to the emissivity of the gas [23];

XIII. Density of the bulk bed changes as a result of mass being transferred from the release of CO$_2$ from the decomposition of CaCO$_3$ [17].
3.2.1 Internal Heat Transfer - Conduction, Convection, and Radiation

The process of cement production is continuous, and heat transfer via radiation, convection, and conduction occurs both inside and outside of the kiln at all times. Since the model considered herein is based on steady-state, steady-flow conditions, the following relationship is enforced for the mass balance:

$$\sum \dot{m}_{in} = \sum \dot{m}_{out} \quad (3.1)$$

while the general energy balance is described as:

$$\dot{Q}_{net, in} - \dot{W}_{net, out} = \sum \dot{m}_{out} h_{out} - \sum \dot{m}_{in} h_{in} \quad (3.2)$$

Figure 3.2: Cross-sectional view of Rotary Kiln. Layers within the kiln in the burning region when coating is present (left), corresponding heat transfer components from radiation, convection, and conduction in this slice (right).

As described previously, the formulation of a PDE to describe the temperature distribution of the bulk bed material along the length of the kiln is required. Classical forms of heat transfer comprised of radiation, convection, and conduction were the first component required for this PDE. Figure 3.2 shows a cross-sectional view of the kiln and the corresponding internal heat transfer components.
Formulation of the equations corresponding to the variables in Fig. 3.2 is based on previous one-dimensional models [4,8,9,11] based on convection relationships developed by Tscheng & Watkinson [14] and radiation relationships developed by Hottel and Sarofim [13]. $Q_{cw}$ is the conduction heat transfer between the internal wall and the bed material, and is given as:

$$Q_{cw} = h_{cw} A_{cw}(T_W - T_B)$$  \hspace{1cm} (3.3)

$$h_{cw} = 11.6 \left( \frac{k_b}{A_{cw}} \right) \left( \frac{\omega R^2 \Gamma}{\alpha_B} \right)^{0.3}$$  \hspace{1cm} (3.4)

where, $A_{cw}$ is the conduction area from the wall to the bed, $k_b$ is the thermal conductivity of the bed material, $\omega$ is the rotational speed of the kiln (rad/s), $R$ is the radius of the kiln (m), $\Gamma$ is the angle of fill of the kiln (rad), and $\alpha_B$ is the bed thermal diffusivity.

$Q_{rb}$ is the radiative heat transfer between the internal wall and bed material,

$$Q_{rb} = \sigma A_{rb} \varepsilon_B \varepsilon_W \Omega (T_W^4 - T_B^4)$$  \hspace{1cm} (3.5)

$$\Omega = \frac{L_{gcl}}{(2\pi - \beta)R}$$  \hspace{1cm} (3.6)

where, $\Omega$ is the view factor for radiation, $\sigma$ is the Stefan-Boltzmann constant, $A_{rb}$ is the radiative area of the wall, $\varepsilon_B$ and $\varepsilon_W$ is the emissivity of the bed and the wall respectively, $\beta$ is the angle of repose, and $L_{gcl}$ is the chord length of the bed.

$Q_{rb}$ is the radiative heat transfer between the freeboard gas phase and bed material, and $Q_{rgw}$ is the radiative heat transfer between the freeboard gas phase and internal wall,

$$Q_{rg} = \sigma A_{rg} (\varepsilon_n + 1) \left( \frac{\varepsilon_G T_G^4 - \alpha_G T_n^4}{2} \right) \hspace{0.5cm} n = B, W$$  \hspace{1cm} (3.7)

where, $A_{rg}$ is the radiative area from the freeboard gas to the bed or the freeboard gas to the wall, and $\alpha_G$ is the absorptivity of the freeboard gas.
\( Q_{cgb} \) is the convective heat transfer between the freeboard gas phase and bed material, and \( Q_{cgw} \) is the convective heat transfer between the freeboard gas phase and internal wall,

\[
Q_{cgn} = h_{cgn} A_{cgn} (T_G - T_n) \quad n = B, W \tag{3.8}
\]

\[
h_{cgb} = 0.46 \left( \frac{k_g}{D_e} \right) Re_D^{0.535} Re_\omega^{0.104} \eta^{-0.341} \tag{3.9}
\]

\[
h_{cgw} = 1.54 \left( \frac{k_g}{D_e} \right) Re_D^{0.575} Re_\omega^{-0.292} \tag{3.10}
\]

\[
Re_D = \frac{\rho_g u_g D_e}{\mu_g} \tag{3.11}
\]

\[
Re_\omega = \frac{\rho_g \omega D_e^2}{\mu_g} \tag{3.12}
\]

\[
D_e = \frac{(0.5D(2\pi - \Gamma + \sin\Gamma))}{\pi - \frac{\Gamma}{2} + \sin\left(\frac{\Gamma}{2}\right)} \tag{3.13}
\]

where, \( h_{cgn} \) is the convective heat transfer coefficient (W/m²K) for convection from the freeboard gas to the wall or to the bed material, \( Re_D \) is the axial Reynolds number, \( Re_\omega \) is the angular Reynolds number, \( k_g \) is the thermal conductivity of the gas, \( D_e \) is the hydraulic diameter of the kiln, \( \rho_g \) is the density of the freeboard gas, \( u_g \) is the airspeed of the freeboard gas, \( \mu_g \) is the dynamic viscosity of the freeboard gas, and \( D \) is the diameter of the kiln. A final summation for the internal heat transfer components is then [4,11]:

\[
Q' = \frac{Q_{cwb}}{A_{cwb}} + \frac{Q_{rwb}}{A_{cwb}} + \frac{Q_{rgb}}{A_{cwb}} + \frac{Q_{cgb}}{A_{cwb}} \tag{3.14}
\]
3.2.2 Clinker Chemistry

The modeling of clinker formation is highly complex. Numerous simultaneous chemical reactions that each have different thermodynamic requirements [20] restrict the chemistry components in all previous models. One of the largest sources of variation between existing models comes from how each author decided to model the clinker formation process. Through the utilization of assumption VII, the chemistry component becomes highly simplified, and is able to be applied to the one-dimensional model. The main components involved in the clinker formation process can be seen in Table 3.1.

Table 3.1: Main compounds in clinker formation.

<table>
<thead>
<tr>
<th>Name</th>
<th>Formula</th>
<th>Typical Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Input</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Calcium Carbonate (limestone)</td>
<td>CaCO₃</td>
<td>30 – 50*</td>
</tr>
<tr>
<td>Calcium Oxide</td>
<td>CaO</td>
<td>20 – 35*</td>
</tr>
<tr>
<td>Silicon Dioxide</td>
<td>SiO₂</td>
<td>10 – 15*</td>
</tr>
<tr>
<td>Aluminum Oxide</td>
<td>Al₂O₃</td>
<td>2 – 4*</td>
</tr>
<tr>
<td>Iron(III) Oxide</td>
<td>Fe₂O₃</td>
<td>1 – 3*</td>
</tr>
<tr>
<td><strong>Output</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tricalcium silicate (Alite)</td>
<td>C₃S (3CaO·SiO₂)</td>
<td>45 – 65**</td>
</tr>
<tr>
<td>Dicalcium silicate (Belite)</td>
<td>C₂S (2CaO·SiO₂)</td>
<td>10 – 25**</td>
</tr>
<tr>
<td>Tricalcium aluminate</td>
<td>C₃A (3CaO·Al₂O₃)</td>
<td>7 – 12**</td>
</tr>
<tr>
<td>Tricalcium aluminoferrite</td>
<td>C₄AF (4CaO·Al₂O₃·Fe₂O₃)</td>
<td>5 – 11**</td>
</tr>
</tbody>
</table>

* Pre-heater samples from partner plant
** Darabi [19]
The five chemical reactions used in the one-dimensional model are listed in Table 3.2. Temperature ranges and heat change due to the reaction was taken from Spang [6] and Darabi [19]. To determine the amount of heat added and removed from the bed material, the equation used for heat release due to chemistry is based on the work of Spang [6]. Equation 3.15 is a modified version of this equation which includes heat released due to the formation of $C_3A$ and $C_4AF$, and ignores heat released due to water evaporation, since a negligible amount of moisture is present:

$$q_c = \frac{\rho_s}{1 + A_i + F_i + S_i} \left[ -\Delta H_{CaCO_3} k_1 Y_{CaCO_3} - \Delta H_{C_2S} k_2 Y_{SiO_2} Y_{CaO}^2 - \Delta H_{C_3S} k_3 Y_{CaO} Y_{C_3S} - \Delta H_{C_4AF} k_5 Y_{CaO}^4 Y_{Al_2O_3}^2 Y_{Fe_2O_3}^2 \right]$$  \hspace{1cm} (3.15)

Here, $q_c$ is the heat transfer due to chemistry, $\rho_s$ is the density of the bed material, $A_i$, $F_i$, and $S_i$ are the input mass fractions of $Al_2O_3$, $Fe_2O_3$, and $SiO_2$, respectively, $\Delta H_n$ is the heat of reaction for the $j^{th}$ reaction, $Y_n$ is the mass fraction of the $n^{th}$ compound, and $k_j$ is the reaction rate of the $j^{th}$ reaction. Assumption VII implies that constant heat of reactions would be used for each reaction, therefore, the only terms that change in Eq. 3.15 are the reaction rates, and mass fractions. Following plug flow characteristics, reaction rates were based on Arrhenius’ law. This results in the dependence of reaction rate on temperature of the material at that axial position to determine how much of the product is produced. The form of Arrhenius’ equation used is written as follows [24]:

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Temperature Range (K)</th>
<th>Heat of Reaction (J/kg)*</th>
<th>Heat Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$CaCO_3 \rightarrow CaO + CO_2$</td>
<td>823 – 1233</td>
<td>1.782e6</td>
</tr>
<tr>
<td>2</td>
<td>$2CaO + SiO_2 \rightarrow C_2S$</td>
<td>873 – 1573</td>
<td>-1.124e6</td>
</tr>
<tr>
<td>3</td>
<td>$C_2S + CaO \rightarrow C_3S$</td>
<td>1473 – 1553</td>
<td>8.01e4</td>
</tr>
<tr>
<td>4</td>
<td>$3CaO + Al_2O_3 \rightarrow C_3A$</td>
<td>1473 – 1553</td>
<td>-4.34e4</td>
</tr>
<tr>
<td>5</td>
<td>$4CaO + Al_2O_3 + Fe_2O_3 \rightarrow C_4AF$</td>
<td>1473 – 1533</td>
<td>-2.278e5</td>
</tr>
<tr>
<td>6</td>
<td>Completion of $C_2S$ and $C_3S$ components</td>
<td>&gt; 1553</td>
<td>6.00e5</td>
</tr>
</tbody>
</table>

*Spang [6], Darabi [19]
where, $A_j$ is the pre-exponential factor of the $j^{th}$ reaction (1/s), $E_j$ is the activation energy of the $j^{th}$ compound (J/mol), $R_g$ is the universal gas constant, and $T_b$ is the temperature of the bed material. As stated previously, a major source of difference between existing models is in how clinker formation is modelled. This is predominantly present in the selection of pre-exponential factors and activation energies with the exception of the decomposition of CaCO$_3$ (in most cases). The reason for this that there are many factors occurring in the formation of the products in reactions 2 – 5 that are not present in the heavily simplified reaction equations. In the work of Mastorakos [17], they indicate that their pre-exponential factors and activation energies were selected by a process of trial and error. Pre-exponential factors and activation energies for the present model were taken from the work of Spang [6], Darabi [19] as to maintain consistency in units with Eq. 3.15, and are summarized in Table 3.3. With these reaction rate constants, the mass fractions of each component was the last variable that needed to be accounted for. The production rate of each species is a function of the reaction rates of all the chemical reactions where that specific species is present. This indicates that production rate of the species is being influenced differently by the corresponding reaction rate in which the species exists. Therefore, the production rate of a species is a sum of the reaction rates of the chemical reactions where the species is present. The sign of the production rate is positive if the species is a product of the reaction, or negative if it is a reactant. Production rates are written in the form [6,19]:

$$k_j = A_j \exp\left(-\frac{E_j}{R_g T_b}\right)$$  \hspace{1cm} (3.16)

<table>
<thead>
<tr>
<th>Reaction Rate</th>
<th>Rate Constant</th>
<th>Pre-exponential Factor (1/s)*</th>
<th>Activation Energy (J/mol)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$r_1$</td>
<td>$k_1$</td>
<td>4.55e31</td>
</tr>
<tr>
<td>2</td>
<td>$r_2$</td>
<td>$k_2$</td>
<td>4.11e5</td>
</tr>
<tr>
<td>3</td>
<td>$r_3$</td>
<td>$k_3$</td>
<td>1.33e5</td>
</tr>
<tr>
<td>4</td>
<td>$r_4$</td>
<td>$k_4$</td>
<td>8.33e6</td>
</tr>
<tr>
<td>5</td>
<td>$r_5$</td>
<td>$k_5$</td>
<td>8.33e8</td>
</tr>
</tbody>
</table>

*Spang [6], Darabi [19]
\[ r_j = k_j Y_{i_1}^{\beta_1} Y_{i_2}^{\beta_2} \]  

(3.17)

where \( Y_i \) is the mass fraction of the \( j \)th reaction. Utilizing this relationship, the production rates of each species can be cast as:

\[
\frac{dY_{CaCO_3}}{dx} = -\left( \frac{1}{v_p} \right) \left( \frac{M_{CaCO_3}}{M_{CaO}} \right) k_1 Y_{CaCO_3} \tag{3.18}
\]

\[
\frac{dY_{CaO}}{dx} = \left( \frac{1}{v_p} \right) \left[ k_1 Y_{CaCO_3} - k_2 Y_{SiO_2} Y_{CaO}^2 - k_3 Y_{CaO} Y_{C_2S} \right] - k_4 Y_{CaO} Y_{Al_2O_3} - k_5 Y_{CaO} Y_{Al_2O_3} Y_{Fe_2O_3} \tag{3.19}
\]

\[
\frac{dY_{SiO_2}}{dx} = -\left( \frac{1}{v_p} \right) \left( \frac{M_{SiO_2}}{2M_{CaO}} \right) k_2 Y_{SiO_2} Y_{CaO} \tag{3.20}
\]

\[
\frac{dY_{Al_2O_3}}{dx} = -\left( \frac{1}{v_p} \right) \left( \frac{M_{Al_2O_3}}{3M_{CaO}} \right) k_4 Y_{CaO} Y_{Al_2O_3} - \left( \frac{M_{Al_2O_3}}{4M_{CaO}} \right) k_5 Y_{CaO} Y_{Al_2O_3} Y_{Fe_2O_3} \tag{3.21}
\]

\[
\frac{dY_{Fe_2O_3}}{dx} = -\left( \frac{1}{v_p} \right) \left( \frac{M_{Fe_2O_3}}{4M_{CaO}} \right) k_5 Y_{CaO} Y_{Al_2O_3} Y_{Fe_2O_3} \tag{3.22}
\]

\[
\frac{dY_{C_2S}}{dx} = \left( \frac{1}{v_p} \right) \left( \frac{M_{C_2S}}{2M_{CaO}} \right) k_2 Y_{SiO_2} Y_{CaO}^2 - \left( \frac{M_{C_2S}}{M_{CaO}} \right) k_3 Y_{CaO} Y_{C_2S} \tag{3.23}
\]

\[
\frac{dY_{C_3S}}{dx} = \left( \frac{1}{v_p} \right) \left( \frac{M_{C_3S}}{M_{CaO}} \right) k_3 Y_{CaO} Y_{C_2S} \tag{3.24}
\]

\[
\frac{dY_{C_3A}}{dx} = \left( \frac{1}{v_p} \right) \left( \frac{M_{C_3A}}{3M_{CaO}} \right) k_4 Y_{CaO} Y_{Al_2O_3} \tag{3.25}
\]

\[
\frac{dY_{C_3AF}}{dx} = \left( \frac{1}{v_p} \right) \left( \frac{M_{C_3AF}}{4M_{CaO}} \right) k_5 Y_{CaO} Y_{Al_2O_3} Y_{Fe_2O_3} \tag{3.26}
\]

With formulations for reaction rates and mass fractions established, the PDE for determining the temperature of the bed material is given as:
\[ v_b C_p A_{segment} \frac{d(\rho_b T_b)}{dx} = Q' L_{gcl} + A_{segment} q_c - S_{CO_2} \]  \hspace{1cm} (3.27)

### 3.2.3 Coating Formation

As stated previously, the chemical reactions listed in Table 3.2 are dependent upon temperature. The formation of C\textsubscript{3}S will only occur when there is liquid, or melt, present in the burning region of the kiln. To ensure that this reaction occurs at the correct time, the presence of the melt needs to be considered. Furthermore, the presence of melt in the kiln brings about the presence of a coating layer forming over the refractory material. Determination of the melt in the kiln was based on the work of Mastorakos [17], who solved for the liquid fraction, \( Y_{fus} \), based on the excess amount of heat and the latent heat of fusion. The value for latent heat of fusion was taken as \( L_{fus} = 600 \text{ kJ/kg} \) [19]. When fusion was present, C\textsubscript{3}S forming as liquid is considered to be present. The value of \( Y_{fus} \) was determined using the method of Mastorakos [17]; however, it was modified to work with the heat transfer terms that were determined for Eq. 3.27.

\[ L_{fus} A_{segment} v_b \frac{d(\rho_b Y_{fus})}{dx} = [R. H. S. o f E q(27)] \] \hspace{1cm} (3.28)

When liquid formation begins, the start of coating formation also occurs. The entire amount of melt does not solidify into a coating; otherwise C\textsubscript{3}S production would not occur. To this end, the maximum coating thickness (\( C_{T,max} \)) present in the kiln was set to be 0.04\( D_i \), where \( D_i \) is the internal diameter of the kiln [11]. This value also acted as an upper limit for the fusion fraction, above which fusion was neglected.

Lastly, as limestone decomposes into calcium oxide and carbon dioxide, some of the mass is transferred from the solid to the gas. The amount of mass flow of CO\textsubscript{2} released into the gas as a result was determined by a relationship correlating the mass flow rate of the limestone entering into the kiln and the ratio of molar mass of CO\textsubscript{2} over CaCO\textsubscript{3} developed by Darabi [19].

\[ \dot{m}_{CO_2} = \frac{M_{CO_2}}{M_{CaCO_3}} \dot{m}_{CaCO_3} \] \hspace{1cm} (3.29)
3.2.4 Heat Balance

The final critical component of the kiln energy model is the heat balance through the refractory material, kiln shell, and coating layer, where applicable. At steady-state, temperatures of the inner wall, coating layer, and shell temperature can be determined from the heat balance. Equations 3.30 – 3.33 describe the heat balance through each layer:

\[ Q_{rgw} + Q_{cgw} - Q_{rwb} - Q_{cwbb} = Q_{coat} \]  
\[ Q_{coat} = Q_{ref} \]  
\[ Q_{ref} = Q_{stl} \]  
\[ Q_{stl} = Q_{conv-shell} + Q_{rad-shell} \]  

When the coating layer is not present, the left hand side of Eq. 3.30 is equal to the right hand side of Eq. 3.31. The formulation for \( Q_{conv-shell} \) and \( Q_{rad-shell} \) are given as:

\[ Q_{rad-shell} = \sigma A_{sh} \varepsilon_{sh} (T_{sh}^4 - T_0^4) \]  
\[ Q_{conv-shell} = h_{csh} A_{sh} (T_{sh} - T_0) \]  

Refractory conductivity was used as a calibration parameter for the kiln model. Reference values of refractory type and brick height were taken from measured data from the partner plant studied. To account for refractory degradation, material buildup and thermal contact resistance between the bricks and the kiln shell, additional sources were included in the total thermal conductivity value that was modified to give a more accurate shell temperature profile.

Shell cooling fans were utilized the last 20 – 25m of the kiln resulting in forced convection dominating the heat transfer, while the region from the material entrance to this point was subjected to free convection. The coefficient of free convection is obtained from:
\[
\begin{align*}
\frac{h_{csh}}{\rho c_s} & = \left\{ 0.60 + \frac{0.387 Ra^\frac{1}{6}}{D} \right\} \left[ 1 + \left( \frac{0.559}{Pr} \right) \right]^{-\frac{9}{16}} \left( \frac{k_a}{D} \right)^2 \\
\end{align*}
\]

which is derived from the induced flow of air across a heated cylinder of infinite length \[23\]. In the forced convection region, heat transfer coefficients were based on the work of Csernyei and Straatman \[18\], wherein a correlation was developed for a bank of circular jets of high jet-to-cylinder diameter ratio impinging on a large cylinder. The correlation relates jet Reynolds number \((Re_d)\), jet-to-jet axial spacing \((z/d)\), jet-to-cylinder spacing \((y/d)\), jet offset from the centerline of the cylinder \((x/d)\), and the curvature of jet outlet over cylinder diameter \((d/D)\):

\[
Nu_{ave} = 0.041 Re_d^{0.862} \left( \frac{d}{D} \right)^{-0.317} \left( \frac{y}{d} \right)^{-0.0729} \left( \frac{z}{d} \right)^{-0.186} \exp^{-0.00134(\frac{x}{d})} 
\]

The range of applicable parameters for the correlation are given as:

\[
0.15 \leq d/D \leq 0.31; \quad 0.2 \leq y/d \leq 2.1; \quad 1.21 \leq z/d \leq 3.41; \quad 0 \leq x/d \leq (D - d)/2d,
\]

over the Reynolds number range: \(2.06 \times 10^5 \leq Re_d \leq 1.236 \times 10^6\).

Based on the geometric parameters for the kiln shell cooling fans located at a partner production site, Table 3.4 shows a breakdown of the heat transfer coefficients obtained

**Table 3.4: Convective heat transfer coefficients on kiln shell.**

<table>
<thead>
<tr>
<th>Kiln Position (m)</th>
<th>Type of Convection</th>
<th>Convective Heat Transfer Coefficient (W/m²K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 53</td>
<td>Free</td>
<td>~6</td>
</tr>
<tr>
<td>53 – 63</td>
<td>Forced</td>
<td>34</td>
</tr>
<tr>
<td>63 – 69</td>
<td>Forced</td>
<td>37</td>
</tr>
<tr>
<td>69 – 75</td>
<td>Forced</td>
<td>41</td>
</tr>
</tbody>
</table>
from Eqs. 3.36 and 3.37 used for simulations of the cement kiln. The varying heat transfer coefficients are a result of varying geometric positioning of the fans within each region described in Table 3.4. Though the magnitude of the forced convection heat transfer coefficients are in the same range as that used by Mastorakos [17] (approximately 30 W/m²K), the use of a correlation that accounts specifically for the proper geometric and flow conditions has an obvious advantage for model implementation and prediction.

3.2.5 Solution Methodology

Equations 3.3 – 3.43 were implemented into an integral model and solved using Matlab R2014a™ software. The resulting kiln model could be run for various operating parameters and heat transfer conditions. The freeboard gas profile was based on recorded temperatures at the kiln inlet and outlet, as well as a peak temperature for the freeboard gas estimated from six different temperature scanners monitoring the internal kiln temperature in the burning region (data received from partner site). As the exact location of the peak temperature was not known, an estimate was made similar to that done in Mujumdar [4]. Using their approach, the location of peak freeboard gas temperature was adjusted to give the correct composition of C₃S at the kiln outlet. Once the freeboard gas temperature profile was generated, an initial guess for the bed profile and wall temperature were generated based on an approximate shape from the literature. The thermal conductivity and kinematic viscosity of the gas was evaluated at a temperature of 1750K based on the following relationships from Mujumdar [4]:

\[
k_G = \left( \frac{-7.949 \times 10^{-3} + 1.709 \times 10^{-4} T_G - 2.377 \times 10^{-7} T_G^2}{+2.202 \times 10^{-10} T_G^3 - 9.463 \times 10^{-14} T_G^4 + 1.581 \times 10^{-17} T_G^5} \right) \tag{3.38}
\]

\[
v_g = 0.1672 \times 10^{-5} \sqrt{T_G} - 1.058 \times 10^{-5} \tag{3.39}
\]

The bulk bed temperature profile and species mass fractions were solved simultaneously using a fourth-order Runge-Kutta solver [25] and modified to work for multiple PDE’s. This solver incorporated different checks for bed temperature, species mass fraction, and melt presence which dictated when each chemical reaction could take place. The heat balance system of equations (Eq. 3.30 – 3.33) were then solved using a Newton-Raphson
method [25] coupled with a relaxation equation and final approximation in order to improve convergence. Based on the work of Martins [9], the relaxation equations and approximation for wall and shell temperatures were as follows:

\[
T_{w,n} = 0.35T_{w,n} + (1 - 0.35)T_{w,n-1}
\]  

\[
T_{shell,n} = 0.8T_{shell,n} + (1 - 0.8)T_{shell,n-1}
\]

\[
T_{w,n}^4 = T_{w,n}(T_{w,n-1}^3)
\]

\[
T_{shell,n}^4 = T_{shell,n}(T_{shell,n-1}^3)
\]

The equations were solved by iteration until convergence between successive iterations was within the margin of ±1%, based on bed temperature, internal wall temperature, and shell temperature. Approximately 10 – 30 iterations are required to reach convergence, depending on the input parameters.

### 3.3 Results and Discussion

#### 3.3.1 Comparison to Previous Work

A comparison is made against the work of Mujumdar [4] to verify the model and solution procedure used in this study. The comparison to Mujumdar was performed due to the availability of operating parameters listed in that work, and the easily replicated linearized freeboard gas profile. Operating parameters can be seen in Table 3.5. To get the best approximation of the results presented in Mujumdar’s work, two changes were made. The activation energy for the decomposition of limestone was adjusted from \(7.81 \times 10^5\) J/mol to \(7.7 \times 10^5\) J/mol to allow for the full decomposition of limestone into CaO. Without this modification the mass fraction of CaCO\(_3\) reached a value of approximately 0.04 rather than the intended full decomposition. The second modification was in regards to the emissivity of the freeboard gas. Mujumdar reports this value to be 0.4 based on charts from the work of Gorog et al. [15] evaluated at a gas temperature of 1750K. Incorporating a value of 0.4 into this model resulted in an over-prediction of C\(_3\)S at the kiln outlet in comparison to
Mujumdar’s work. Based on the trends observed in the charts, using a gas temperature of 1750K results in a gas emissivity closer to 0.2. This value is in close comparison with the emissivity used in Gorog’s work on regenerative heat transfer [16]. In addition to these changes, free convection was assumed to take place along the entire length of the kiln shell, in accordance with Mujumdar. Results of the compared temperature profile distributions are given in Fig. 3.3, while the predicted inlet and outlet species mass fractions are given in Table 3.6.

### Table 3.5: Input operating parameters for comparison study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length (m)</td>
<td>50</td>
</tr>
<tr>
<td>Inner refractory diameter (m)</td>
<td>3.4</td>
</tr>
<tr>
<td>Outer refractory diameter (m)</td>
<td>3.8</td>
</tr>
<tr>
<td>Outer shell diameter (m)</td>
<td>3.85</td>
</tr>
<tr>
<td>Coating thickness (m)</td>
<td>0.13</td>
</tr>
<tr>
<td>Rotational speed (rpm)</td>
<td>5.5</td>
</tr>
<tr>
<td>Height of fill at inlet (m)</td>
<td>0.46</td>
</tr>
<tr>
<td>Solids flow in, (kg/s)</td>
<td>38.88</td>
</tr>
<tr>
<td>Gas temperature at burner end (K)</td>
<td>1373</td>
</tr>
<tr>
<td>Gas temperature at solid entry (K)</td>
<td>1373</td>
</tr>
<tr>
<td>Maximum flame temperature (K)</td>
<td>2283</td>
</tr>
<tr>
<td>Bed temperature at solid entry (K)</td>
<td>1123</td>
</tr>
<tr>
<td>Bed density, (kg/m³)</td>
<td>1200</td>
</tr>
<tr>
<td>Bed heat capacity, (kJ/kg·K)</td>
<td>0.8</td>
</tr>
<tr>
<td>Bed emissivity</td>
<td>0.9</td>
</tr>
<tr>
<td>Wall emissivity</td>
<td>0.9</td>
</tr>
<tr>
<td>Shell</td>
<td>0.78</td>
</tr>
<tr>
<td>Bed thermal conductivity (W/m·K)</td>
<td>0.5</td>
</tr>
<tr>
<td>Refractory thermal conductivity (W/m·K)</td>
<td>4.0</td>
</tr>
</tbody>
</table>

*Mujumdar [4]*

Figure 3.3 shows that the present model does a reasonable job representing the case reported by Mujumdar [4]. Qualitatively, the temperature profiles follow similar trends and peaks with a close coupling of the bed and internal wall temperature profiles. The dip in the internal wall and shell temperatures are caused by the onset of coating formation. Quantitatively, the temperature profiles of the bulk bed, internal wall, and shell predicted by this model are about 10 – 20% higher than that predicted by Mujumdar, depending on the region. In the area where coating is present, it can be seen that the thermal conductivity
of the coating dominates as the compared values of the internal wall and shell are within ±10% of each other when coating is present. Differences can be attributed to the variation in clinker chemistry resulting in different quantities of heat being released and absorbed by the bed. Furthermore, Mujumdar’s model reaches a maximum bed temperature of approximately 1630 K, while in the range where C_2S and C_3S components finish forming, most models predict temperatures in range of 1800 – 1900 K [17]. Since the Arrhenius parameters used by Mujumdar were based on the work of Mastorakos [17], which were chosen by trial and error for a kiln length of over 80m, these parameters could potentially result in larger amounts of species produced at lower temperatures.

As industrial data typically only exists in the form of mass fraction at the outlet, it is not appropriate to recommend one model over the other. However, on the basis that the present model predicts similar trends to that of Mujumdar [4] and reasonable species composition at the outlet, that the present model is suitable to conduct further comparisons of other unique features.

Figure 3.3: Temperature profile distributions comparing the present predictions to those of Mujumdar [4].
3.3.2 Axial Temperature and Species Profiles

A set of parameters from the rotary cement kiln at the partner plant were chosen to compare the model to empirical data of scanned shell temperatures and Bogue calculations of species output. These input operational parameters (Table 3.7) were chosen based on estimates of reported data and expected values from a cement plant. Since the kiln being modeled utilizes a cyclone preheater to heat up the raw material before it enters the kiln,

### Table 3.7: Input parameters for kiln model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length (m)</td>
<td>75</td>
</tr>
<tr>
<td>Inner refractory diameter (m)</td>
<td>4.52</td>
</tr>
<tr>
<td>Outer refractory diameter (m)</td>
<td>4.7</td>
</tr>
<tr>
<td>Outer shell diameter (m)</td>
<td>4.8</td>
</tr>
<tr>
<td>Rotational speed (rph)</td>
<td>104</td>
</tr>
<tr>
<td>Solids flow in (kg/s)</td>
<td>32.38</td>
</tr>
<tr>
<td>Gas temperature at burner end (K)</td>
<td>973</td>
</tr>
<tr>
<td>Gas temperature at solid entry (K)</td>
<td>1194</td>
</tr>
<tr>
<td>Maximum gas temperature (K)</td>
<td>2075</td>
</tr>
<tr>
<td>Bed temperature at solid entry (K)</td>
<td>962</td>
</tr>
<tr>
<td>Bed density, (kg/m³)</td>
<td>1046</td>
</tr>
<tr>
<td>Bed heat capacity, (kJ/kg·K)</td>
<td>1.088</td>
</tr>
<tr>
<td>Bed emissivity</td>
<td>0.9</td>
</tr>
<tr>
<td>Wall emissivity</td>
<td>0.9</td>
</tr>
<tr>
<td>Shell emissivity</td>
<td>0.78</td>
</tr>
<tr>
<td>Bed thermal conductivity (W/m·K)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

### Table 3.6: Species mass fraction at inlet and outlet.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>CaCO₃</td>
<td>0.340</td>
<td>0.340</td>
<td>C₃S</td>
<td>0.503</td>
<td>0.470</td>
</tr>
<tr>
<td>CaO</td>
<td>0.396</td>
<td>0.396</td>
<td>C₃S</td>
<td>0.222</td>
<td>0.157</td>
</tr>
<tr>
<td>SiO₂</td>
<td>0.179</td>
<td>0.179</td>
<td>C₃A</td>
<td>0.051</td>
<td>0.046</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>0.0425</td>
<td>0.0425</td>
<td>C₄AF</td>
<td>0.149</td>
<td>0.108</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>0.0425</td>
<td>0.0425</td>
<td>CaO</td>
<td>0.075</td>
<td>0.058</td>
</tr>
</tbody>
</table>
some pre-calcination occurs resulting in CaO present in the material feed entering into the kiln. Based on the loss on ignition (LOI) and final quantity of CaO that was expected to be generated, the appropriate degree of calcination at the kiln entrance was determined. The work of Mujumdar [4,16] and Mastorakos [17] also determine an amount of pre-calcination in order to accurately estimate the species mass fractions entering into the kiln.

The thermal conductivity of the gas was evaluated at 1750 K [4], and the emissivity of the gas was taken to be the same as it was in the validation case, since parameters to estimate an actual value from the Gorog charts [15] were not known. Bed height was considered an adjustable parameter and was modified to allow for a more accurate amount of C$_3$S at the kiln outlet.

![Temperature profiles and species mass fractions](image)

Figure 3.4: (Left) Temperature profiles in cement kiln, (Right) Species mass fractions along axial length cement kiln.

The location of peak gas temperature was estimated to be 0.85 times the kiln length to allow for coating formation in the correct region. The peak temperature of the gas was estimated from scanned temperature data in the burning region and fell within the expected range of 2000 – 2200 K. Figure 3.4 shows the temperature profiles both inside and outside of the cement kiln and the species mass fractions as raw material progresses through the kiln. Table 3.8 shows a comparison of the inlet and outlet mass fractions of the material compared to the results of the partner plant.
When \( \text{C}_2\text{S} \) production increases, a large quantity of heat is released to the bulk bed due to its highly exothermic nature. Melt formation begins around 0.6 times the kiln length when \( \text{C}_3\text{S} \) production begins. When melt formation begins, and coating begins to form on the refractory material, a sharp drop in wall temperature is observed [4,16]. A second drop is observed at around 0.7 times the kiln length where the thermal conductivity of the material was modified from the initial region of the kiln coinciding with reported brick data from the plant studied. This region is near where the peak gas temperature is located, and the peak bed temperature reaches approximately 1922 K. This peak bed temperature is similar to previously reported bed temperatures from existing models [6,17,19]. There exists a close coupling between the bed and internal wall temperatures which coincides with the findings of Watkinson and Brimacombe [10]. During the production of \( \text{C}_3\text{S} \), \( \text{C}_2\text{S} \) is still being produced; however, since \( \text{C}_3\text{S} \) is an endothermic reaction, the increase in the temperature of the bed isn’t as sharp as it was before the melt was formed. As \( \text{C}_2\text{S} \) production begins to slow down, the temperature of the bulk bed drops significantly where it exits the kiln at a value of 1690 K where it enters into the grate cooler for further cooling. Similar to Mastorakos [17] it was observed that the bed temperature was the hottest temperature compared to the internal wall and freeboard gas at the kiln outlet.

A comparison of the predicted species mass fractions at the kiln outlet to the estimated empirical data based on Bogue calculations can be seen in Table 3.8. Since Bogue calculations assume that the entire amount of input constituents are converted into their respective species there is some inherent error in the comparison [26]. Similar to the

![Table 3.8: Species mass fractions model predictions for the case in Figure 6.](image)

<table>
<thead>
<tr>
<th>Inlet Mass Fraction</th>
<th>Data</th>
<th>Present Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{CaCO}_3 )</td>
<td>0.3798</td>
<td>0.3798</td>
</tr>
<tr>
<td>( \text{CaO} )</td>
<td>0.3019</td>
<td>0.3019</td>
</tr>
<tr>
<td>( \text{SiO}_2 )</td>
<td>0.1594</td>
<td>0.1594</td>
</tr>
<tr>
<td>( \text{Al}_2\text{O}_3 )</td>
<td>0.0246</td>
<td>0.0246</td>
</tr>
<tr>
<td>( \text{Fe}_2\text{O}_3 )</td>
<td>0.0396</td>
<td>0.0396</td>
</tr>
<tr>
<td>Inert + Other</td>
<td>0.0947</td>
<td>0.0947</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Outlet Mass Fraction</th>
<th>Data</th>
<th>Present Work</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{C}_3\text{S} )</td>
<td>0.582</td>
<td>0.546</td>
</tr>
<tr>
<td>( \text{C}_2\text{S} )</td>
<td>0.130</td>
<td>0.049</td>
</tr>
<tr>
<td>( \text{C}_3\text{A} )</td>
<td>0.063</td>
<td>0.027</td>
</tr>
<tr>
<td>( \text{C}_4\text{AF} )</td>
<td>0.075</td>
<td>0.068</td>
</tr>
<tr>
<td>( \text{CaO} )</td>
<td>0.0</td>
<td>0.034</td>
</tr>
</tbody>
</table>
validation case, output constituents are under predicted in each category. The most predominant differences are within C₃A and C₂S production while C₃S, and C₄AF are more accurate. Differences in the output constituents can mainly be attributed to the Arrhenius parameters used in reactions 2 – 5. Unlike the work of Mastorakos [17] where they were modified by trial and error to allow for a more accurate clinker composition at the kiln outlet, these parameters were based off of those used in previous models. Additionally, a large percentage of the input raw material is due to inert and other compounds. The presence of some of these compounds could allow for a slight increase in species compositions at the outlet. In the formation of Portland cement, silicon trioxide (SO₃) is present in the Bogue calculation. One of the additional components in the raw material feed is 5.2% SO₃. Modifying the SiO₂ input to account for SO₃ in the feed results in a greater amount of C₂S produced. This allows for a greater amount of C₂S at the kiln outlet, and in turn also allows for more C₃S production. Removal of the SO₃ component from the Bogue calculation results in a C₂S of approximately 1.78% at the kiln outlet. It is apparent that the presence of SO₃ in the stream is important to achieving a more accurate clinker composition at the kiln outlet; however, it was discovered that modification of the Arrhenius parameters was required in order to produce more accurate results. Since a change in internal wall and shell temperature of less than 1% was observed, the presence of SO₃ in the mixture was neglected. Additionally, there exists some CaO that has not been included in the production of other species in the developed model. This trend was witnessed in many of the previous models that were developed that focus on the full development of cement clinker [4,11,17,19]. Lastly, it was expected that the results would not match up perfectly, as a majority of the inlet conditions were based on reasonable estimates of typical values. Although there is slight variation, the predictions are consistent with compared literature indicating that the chemical compositions, kinetics, and model assumptions used for this case allow for the reasonable representation of realistic results.
3.3.3 Forced Convection from Shell Cooling Fans

To determine the result of including the effect of the shell cooling fans, a comparison against actual scanned shell temperature data was performed. From Fig. 3.5 it can be seen that the predicted shell profile corresponds very well with the scanned shell temperature data in the early region of the kiln before melt begins to form. The peak shell temperature occurs at around 0.81 times the kiln length indicating the expected region of the flame. An assumption for peak gas temperature was taken to be 0.85 times the kiln length coinciding with results seen in the work of Mastorakos [17] where peak shell temperature occurred at approximately 0.8 times the kiln length.

The first dip in shell temperature from the predicted data corresponds to the start of coating formation. A second large dip in the predicted shell temperature is witnessed from 0.7 – 0.75 times the kiln length. This region (>0.7 times the kiln length) is where the shell cooling fans are located, and coincides with the initial dip seen in the predicted shell temperature profile. As the presence of coating lessens behind the flame, the shell temperature rises before decreasing once again towards the kiln outlet. It can be seen that the presence of
coating significantly dominates the heat transfer through the kiln in the model resulting in a difference between the predicted data at the location where the scanned temperature data peaks. In comparison to the free convection heat transfer coefficients, it can be seen that neglecting the presence of these cooling fans results in an increase of approximately 100 K in the area where the fans are present. This difference is greater in the region behind the region of peak temperature from the scanned data where the fans are packed more closely together. It is apparent that the inclusion of a forced convection term provides a significant effect on the accurate portrayal of the predicted shell temperature profile. An error of >20% is observed when forced convection is not considered.

Fig. 3.6(a) and (b) shows a comparison against scanned shell data when the airspeed velocity of the jets is modified, and the jet-to-jet spacing is increased. In Fig. 3.6(a) it can be seen that as the airspeed velocity of the jets increases a decrease in shell temperature is observed. As the air impinges on the cylinder at an increased rate, the amount of heat energy removed from the shell surface also increases. The drop in shell temperature is not linear as $Re_j$ increases with the largest decrease witnessed in the first change from 411,500 to 823,000, while the increase from 823,000 to 1,236,000 resulted in a temperature decrease of about half of the initial drop. Fig. 3.6(b) shows that as the jet-to-jet spacing, $z/d$, is increased from the minimum to the maximum allowable by the correlation, the shell temperature slightly increases. As the airstreams from each jet travel axially along the bottom of the shell, they collide with each other. This creates a second region of impingement allowing for more heat to be removed from the surface of the shell. As the jets move further apart from one another, the impact of this secondary stagnation region is reduced, resulting in a slight increase in shell temperature.
A secondary function of the shell cooling fans is to help promote the formation of coating within the kiln. Currently there exists no method of coupling this effect with coating formation within the kiln. Present methods of determining coating within the kiln rely on the temperature of the bulk bed, although the bed temperature profile can change depending on the operational parameters used within the model. Efforts to improve upon coating formation within the kiln require the effect of external shell cooling fans on the melt phase,
and how it can influence the rate of cooling, and amount of coating is actually formed in the burning region.

3.4 Summary
An overview of existing numerical models of rotary cement kilns was presented and used to develop a one-dimensional model based on the best existing techniques. Using a series of assumptions based on previous literature, and a modified version of an existing clinker chemistry model to account for thermal bounds and melt formation, the current model was shown to reasonably predict the results of a previously developed one-dimensional model. The one-dimensional kiln model was linked to the surroundings via a resistance model for the composite kiln shell and a correlation for forced convection heat transfer. In this manner, the effect of kiln shell cooling fans and varying refractory material was integrated into the model. A difference of \( \geq 20\% \) was observed when the effects of forced convection were compared to a pure free convection scenario. Further consideration is required to link the effect of external shell cooling fans to their contribution to the effect that they have on the amount and rate at which coating is formed on the refractory brick.

References


Chapter 4

4 Summary

Cement manufacturing is a world-wide industry that utilizes large quantities of both thermal and electrical energy to function effectively. Within Canada, this industry is one of the top six consumers of energy requiring 3.2% in 2010 of the total energy demand across the country. Multiple processes are required for cement production. The most energy intensive operation is performed in the rotary cement kiln. These large, rotating cylinders, have raw material enter in one end, and a burner that generates a flame at the other end. Through the rotation of the kiln, and the effects of gravity, this raw material travels from the entrance of the kiln to the discharge end of the kiln where multiple simultaneous chemical reactions occur causing the formation of cement clinker. Typically 90% of the thermal energy utilized in the cement production process is consumed in the rotary cement kiln, and of the 40% input energy lost from the process, typically 15% of it is lost through the kiln shell due to convection and radiation. Large vertical and angled fans external from the kiln impinge on the kiln shell in the region where the flame is located resulting in the temperature inside of the kiln to be the greatest. These fans are used to reduce the temperature of the kiln shell and help promote the formation of coating inside the kiln over the refractory material. Numerical models of rotary cement kilns have been developed by researchers to better quantify the thermal energy consumed both within the kiln, and lost from the kiln shell. An extensive literature survey of previously existing models was performed, and to the author’s best knowledge, the effect of external kiln shell cooling fans was neglected from almost every model. Previous models assumed free convection over the entire length of the kiln shell, with only one model utilizing an estimated coefficient for forced convection.

The objective of this thesis was to study the forced convection effect of these external kiln shell cooling fans by means of computational simulations, and integrate the results into a one-dimensional numerical model of a rotary cement kiln so that an improved energy quality/quantity image can be used for waste heat recovery consideration.
4.1 Conclusions and Contributions

As a collection of papers, both Chapter 2 and Chapter 3 relate to numerical simulations regarding their respective areas of study. Chapter 2 focuses on the use of Computational Fluid Dynamics (CFD) to analyze the effect of different geometric conditions for external shell cooling fans that are applicable to the cement industry. This problem was approached by considering multiple large diameter circular jets impinging on a large cylinder. Different geometric models were developed in SolidWorks™ 2013 and exported into ANSYS ICEM™ as a PARASOLID™ file for mesh generation. The use of symmetry to model only a slice of the jet impinging on the cylinder was utilized in order to improve simulation run time. The resulting mesh was imported into ANSYS Fluent™ where simulations were conducted. Grid independence tests and validation of the numerical model was performed against previous work of a single jet impinging on a cylinder. A correlation describing the average heat transfer over the entire parametric range considered was developed. The correlation was able to predict results of average surface heat transfer within an interval of ±26% while 90% of the results fell within an interval of ±10%.

Chapter 3 documents the formulation of the one-dimensional numerical model used to describe the temperature profiles within and outside of a rotary kiln, and species mass fractions axially along the kiln. Through the utilization of educated assumptions and formulations developed by previous researchers, the effects of convection, conduction, radiation, and clinker chemistry were coupled together. Modifications to the chemistry model were made to allow for the consideration of heat released/consumed from all five chemical reactions, and to account for thermal bounds and melt formation. The internal heat transfer model was linked to the external surroundings via a resistance model for the composite kiln shell, and the forced convection effects of the kiln shell cooling fans. Conductivity through the kiln refractory was treated as a calibration parameter to allow for a more accurate solution to scanned temperature data of the kiln shell. The model was solved using Matlab R2014a™ software through the use of an iterative procedure. A fourth-order Runge-Kutta solution method for the bulk bed temperature, and clinker chemistry while the Newton-Raphson method was used for the heat balance across the
kiln shell. Validation of the model was performed by comparing temperature profile
trends and species mass fraction quantities at the kiln outlet to a previously existing
model. A difference of ≥20% was observed when the effects of forced convection were
compared to a pure free convection scenario. The effect of modifying the geometric
parameters of the kiln shell cooling fans on kiln shell temperature was also studied.

4.2 Future Work

Research into rotary cement kilns is an ongoing process that is subject to major
limitations when trying to perform experimental studies and procure on-site measured
data. The use of numerical models to further this research is invaluable as it allows for a
better understanding of the processes occurring within the volatile environment inside of
rotary kilns. Advancements to rotary kiln modelling is a slow process due to the large
range of parameters that influence how the process operates. This section contains some
recommendations by the author for areas of advancement in regards to the research kiln
shell cooling fans and numerical modelling of rotary cement kilns:

I. Angled external kiln shell cooling fans: The work performed in Chapter 2
encompasses only the effect of vertical shell cooling fans. It was observed that in
the industry there exists kiln shell cooling fans that impinge on the kiln at various
angles to the horizontal plane. Efforts to analyze the effects of these angled fans
and how they can influence forced convective heat transfer from the kiln shell
should be performed in order to further improve the work described in Chapter 2.

II. Effect of kiln shell cooling fans on coating formation: The influence from kiln
shell cooling fans on the shell temperature profile was described in Chapter 3;
however, the secondary effect of these fans, in regards to the promotion of coating
formation within the kiln, should also be reviewed. Current kiln models base the
formation of melt, and in turn, coating on the refractory brick, on the temperature
of the bulk bed and heat transfer processes occurring inside the kiln. As input
operational parameters are modified for these models, the length of the coating
and area where it exists inside the kiln can change. Research into how these fans
can influence coating in the regions where they impinge on kiln would help to
improve the development of coating formation in numerical models, allowing for an improved characterization of the burning region of the kiln.

III. **Standard formulation for heat transfer and clinker chemistry:** Unfortunately a large source of time when a numerical model is used for rotary kiln research is devoted to the development of the numerical model itself. From a review of previously existing models, it was apparent that each researcher borrowed previously developed formulations for the internal heat transfer or clinker chemistry. As a result, each model had minor differences in their overall formulation, although they were each capable of producing reasonably accurate temperature profiles and species outputs. Although geometric and operating parameters of the kilns will inevitably vary depending on the kiln being studied, the internal heat transfer and chemistry processes will remain the same. If a standard formulation describing the internal heat transfer characteristics and formation of clinker was available for future researchers to access, it would be invaluable to the rate at which research could be performed on rotary kilns. More focus could then be placed on the unique features of the kiln being studied such as the development of the freeboard gas profile which hinges on the burner type and fuel used. Presently, it is of the opinion of the author that the need to develop a one’s own numerical model from the ground up acts as a bottleneck to new researchers who wish to further the study of rotary cement kilns.
Appendix A: Parametric Study of Kiln Model

Rotary cement kilns possess a large number of operating parameters that allow for the modification of output constituents from the kiln. It comes as no surprise that researchers resort to various approximations and assumptions to calibrate their models more accurately. A significant parameter is present in the form of mass flow rate of the raw material entering into the kiln. The amount of material entering influences parameters such as bed height, internal angle with the bed, area of the bed segment, and bed velocity. Changes in all of these parameters affect the production of C$_3$S within the kiln. Using the input parameters in Appendix A.1, inlet velocity was modified by ±10% and ±20%. Sensitivity to the temperature profiles and C$_3$S at the kiln outlet were observed and can be seen in Appendix A.2.

### Appendix A.1: Input parameters for kiln model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length (m)</td>
<td>75</td>
</tr>
<tr>
<td>Inner refractory diameter (m)</td>
<td>4.52</td>
</tr>
<tr>
<td>Outer refractory diameter (m)</td>
<td>4.7</td>
</tr>
<tr>
<td>Outer shell diameter (m)</td>
<td>4.8</td>
</tr>
<tr>
<td>Rotational speed (rph)</td>
<td>104</td>
</tr>
<tr>
<td>Solids flow in (kg/s)</td>
<td>32.38</td>
</tr>
<tr>
<td>Gas temperature at burner end (K)</td>
<td>973</td>
</tr>
<tr>
<td>Gas temperature at solid entry (K)</td>
<td>1194</td>
</tr>
<tr>
<td>Maximum gas temperature (K)</td>
<td>2075</td>
</tr>
<tr>
<td>Bed temperature at solid entry (K)</td>
<td>962</td>
</tr>
<tr>
<td>Bed density, (kg/m$^3$)</td>
<td>1046</td>
</tr>
<tr>
<td>Bed heat capacity, (kJ/kg·K)</td>
<td>1.088</td>
</tr>
<tr>
<td>Bed emissivity</td>
<td>0.9</td>
</tr>
<tr>
<td>Wall emissivity</td>
<td>0.9</td>
</tr>
<tr>
<td>Shell emissivity</td>
<td>0.78</td>
</tr>
<tr>
<td>Bed thermal conductivity (W/m·K)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Appendix A.2 shows the comparison for temperature profiles and mass fraction of C$_3$S at the kiln discharge. Appendix A.2 (a) – (d) shows the change in temperature profiles as the inlet mass flow rate is reduced. The major difference between each plot is the length of the melt region which results in a larger production of C$_3$S. A constant bed height has been assumed for each case resulting in the same area of the bed segment. As mass flow rate of
the material decreases, the axial velocity of the bed will also decrease, and as mass flow rate increases, axial velocity increases. Since the Arrhenius law is influenced by the velocity of the species, a slower species will result in a greater amount of product; restricted by the maximum amount of species that could be produced. This trend is witnessed in Appendix A.2 as the mass flow rate is modified.

A reduction in the mass flow rate of the material entering into the kiln by 20% of the base value results in the melt phase occurring 3 m earlier and ends at the same position of the base case. Peak bed temperature increases by approximately 20 K while and approximately 3% more C₃S is produced. Appendix A.2 (e) shows that the trend for this case is linear. An increase of mass flow rate by 20% results in the melt phase occurring approximately 4 m later, approximately 3% less C₃S at the kiln discharge, and a decrease of peak bed temperature by 20 K. Again, the melt phase ends at around the same position as the base case. Although additional factors such as the angle of kiln tilt, and changing axial bed height, it is apparent that the inlet velocity of the material can influence the process within the kiln model. When a precalciner is present, typically the mass flow rate of the material is only measured at the inlet of the precalciner and at the kiln discharge. Recorded data indicates a drop of 40 – 50% in mass flow rate between these two sources, and 15 – 25% [1] from the kiln inlet to the kiln outlet. Achieving a proper estimate of the mass flow rate entering into the kiln, and utilizing accurate relationships to describe bed height and material velocity help improve the accuracy of the model and reduce the error that can be present with estimated values.
Appendix A.2: Influence of mass flow rate on temperature profiles (a) – (d) and mass fraction of C3S at kiln discharge (e).
When possible, use of an approximated gas temperature profile should be avoided. As the primary source of heat within the kiln, proper estimation of this profile is essentially to improving the accuracy of the model. Unfortunately, not every cement plant utilizes the same burner and fuel source. This results in issues when trying to adapt previous one-dimensional models for the freeboard gas to the kiln being studied, and if implemented incorrectly, can result in a great source of error. Resources such as using CFD tools to accurately model the burner that is present have been seen to be quite useful in kiln research when approximating the freeboard gas profile \([2,3,4]\); however, the formulation and implementation of these more complex models are very time consuming and not practical from a consumer standpoint. Using the linear profile approximation for the base case, the peak freeboard gas temperature and position were adjusted to show the sensitivity of the model in response to the freeboard gas profile. Appendix A.3 (a) – (d) represents the modification of the temperature value while Appendix A.4 (a) – (d) represents the modification of the position of peak freeboard gas temperature.

Focusing on the influence of temperature value first, Appendix A.3 (a) – (c) shows that as \(T_{g_{\text{max}}}\) increases, the peak bed temperature also increases, and melt formation occurs sooner. These trends correspond with the increase in \(\text{C}_3\text{S} \) at the kiln discharge seen in (d). An increase of peak freeboard gas temperature of 200 K results in an increase of \(\text{C}_3\text{S} \) production by approximately 11%. A large increase in \(\text{C}_3\text{S} \) production was also reported by Mujumdar [2] where increasing the peak freeboard gas temperature by approximately 150 K resulted in an increase of about 25% in \(\text{C}_3\text{S} \) production. Difference can be attributed to the amount of \(\text{C}_3\text{S} \) available to be produced and the effect of temperature on the reaction rates determined by the Arrhenius parameters. This influence of temperature corresponds to an increase in thermal energy transmitted to the bulk bed, allowing for a greater production of \(\text{C}_3\text{S} \), which is the direct result of a larger peak freeboard gas temperature. It should be noted that as the peak freeboard gas temperature rises, the temperature of the freeboard gas at the kiln inlet would also be higher. This would influence the thermal energy transferred to the bed along the entire length of the kiln up to the peak, which would result in an even earlier production of melt formation, and in turn allow for more \(\text{C}_3\text{S} \) to be produced.
In regards to the location of peak freeboard gas temperature, there is less of an influence on C3S production and more influence on location of melt formation. Peak bed temperature coincides near the region where the peak freeboard gas temperature exists corresponding to the burning region and when C₃S is produced. Appendix A.4 (a) – (c) shows as the location of $T_{g_{\text{max}}}$ moves, the position of peak bed temperature also moves and so does the burning region indicated by the presence of melt. Appendix A.4 (a) and (b) show an essentially unrealistic scenario for the kiln studied as the melt region ends 10 – 15m before the kiln exit. Typically the melt should be present the last 40 – 50% of the length of the kiln [1,2,3] with a decrease in the amount of melt present past the peak temperature. Appendix A.4 (c) represents the burning region more accurately with melt formation occurring the final 40% of the kiln length.

Appendix A.3: Influence of peak freeboard gas temperature on temperature profiles (a) – (c) and mass fraction of C3S at kiln discharge (e).
Appendix A.4: Influence of peak freeboard gas location on temperature profiles (a) – (c) and mass fraction of C3S at kiln discharge (e).


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