

**A Modeling and Design Study on the  
Determination of the Most Influential Parameters  
on the Industrial Furnaces Performance**

by

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17347

Dissertation submitted in partial fulfillment of  
the requirements for the  
Bachelor of Engineering (Hons)  
(Chemical Engineering)

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Universiti Teknologi PETRONAS,  
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Perak

CERTIFICATION OF APPROVAL

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Approved by:

---

Dr. Abbas Azarpour

UNIVERSITI TEKNOLOGI PETRONAS  
BANDAR SERI ISKANDAR, PERAK

September 2015

## CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or person.

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SATHIYA A/L GUNASEGRAN

## **ABSTRACT**

Modeling of heat and mass transfer of fired heaters for refinery use was carried out to determine the equipment efficiency as well as the process and flue gas temperature variations. Previous research involving non-computational fluid dynamics (CFD) analysis of fired heaters modeled individual sections of the heater with little attention to the other. In this study, transfer models were developed and compiled in the MATLAB environment for validation. Upon which, simulations were run to determine the most influential parameters affecting the performance of fired heaters. Research papers referenced in this study developed models by incorporating correlations established in the early 1950s'. This study differs in a sense that the formulas used to develop the model are generally modified using common engineering sense to accommodate the dimensions of a refinery fired heater. Initially, the research involved the modeling of separate sections of the heater encompassing heat and mass balances of the flue gas. The models were solved by an iterative procedure with initial boundary conditions taken from the nominal parameters of the paper used to validate this study. Upon completion of the modeling phase, the model was compiled in MATLAB. The code was designed to be as flexible as possible. Users will enter nominal parameters of the heater on the dimensions as well as fuel and air characteristics. The parameters entered in the beginning of the code form the basis of variables manipulated in the search of the most influential parameters on the performance of fired heaters. The results obtained via the simulations examined at least five parameters selected based on the previous research utilizing fluid dynamics and differential boundary equations. The developed model validation was done against peer-reviewed papers to confirm the accuracy of the model. Once proven, the code can then be employed for the commercial use since the computing time and technical costs afforded by the utilization of CFD analysis are significantly reduced.

## **ACKNOWLEDGEMENT**

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# CHAPTER 1

## INTRODUCTION

Increasing environmental concerns to conserve energy and their subsequent key source, fossil fuels, have initiated the need to design and optimize energy intensive processes. The focus of this study is set on developing a model of a process heater based selected parameters which affect the performance and efficiency of this equipment. The results of the design study will be compiled as a MATLAB code to generate data to compare against suitable sources.

### 1.1 Background of Study

Energy is an extremely precious commodity that the modern world cannot run without. In 2012, the International Energy Agency estimated the global energy consumption stood at 155,505 terawatt-hours (TWh), or  $5.6 \times 10^{20}$  joules; overwhelming values which just serve to show how important energy is to us (IEA, 2014). In 2012, nearly 59% of the total final consumption of energy in the world was derived from oil and natural gas (IEA, 2014). Likewise, industrial users consume 51% of the global total energy production. The primary driver associated with costs in industrial output is energy utilities consumption. Presently, research is geared towards developing approaches to increase the efficiencies of industrial processes to reduce the consumption of energy in this sector. Of primary importance to this study would be the reduction in energy usage in the petroleum refinery industry

particularly in the design of fired heaters which are some of the most energy intensive equipment.

As existing reserves of petroleum are being depleted, and the utilization of light and sweet crude oils increase, refiners will increasingly use heavy crudes, tar sands and shale oil to meet the growing energy demand. However, these materials require more energy-intensive processing to meet industrial specifications. Energy is the most important cost factor in the petrochemical industry. The primary use of this energy lies within the heating and cooling utilities, which play a dominant role in driving petrochemical processes; in fact, roughly 75% of energy consumption in these complexes is used for powering furnaces and heaters (Masoumi & Izakmehri, 2011).

Certain chemical processes require process heat to be supplied with a high heat duty, high temperature or a high heat flux. In these situations, radiant heat transfer is derived from the combustion of fuel in a process heater. The most common type of process heater used in petroleum refining and petrochemical sectors is the direct fired heater. These units function to provide simple heating or sensible heat for reactions to occur and to heat and partially vaporize a stream before entering distillation columns. Heaters are sometimes used to supply heat for cracking or reforming processes. Hence, it should not be strange to see 25 – 75 direct fired heaters in a petroleum refinery (Bahadori, 2010). Masoumi & Izakmehri (2011) ran a study to determine the effects of furnace performance optimization numerically. They concluded that preheating combustion air to 250°C, while reducing excess air to 15% reduces stack temperature and increased efficiency by 23%. Conclusively, due to the substantial energy utilization of this unit, considerable energy savings can be derived from the proper design and optimization of the fired heater operating conditions. The performance of the fired heater can be enhanced via a thorough analysis of the system, by way of intensive modeling and parameters evaluation.

## 1.2 Problem Statement

The design of fired heaters has been intrinsically complex due to the wide variety of intermingling heat transfer phenomena driven by radiation and convection transports. These systems are generally non-linear with varying incidences, which can directly influence operating conditions and performance. Optimizing the performance of fired heaters is paramount when tasked with increasing the efficiency of a process plant. Due to the high energy demand of this equipment, enhancing the design to increase efficiency even by a small margin can lead to significant cost savings.

The design of fired heaters has numerous constraints due to the fact that its efficiency, maximum permissible rate of absorption in the radiant section and maximum permissible pressure drop of the process fluid effectively impact the optimization of the radiant tube system geometry and similarly the optimum combustion conditions. Based on the API 560 standard for the design of fired heaters for general refinery service, the visible flame height should not be more than two-thirds of the height of the radiant section (API, 2012). However, fired heaters are liable to variations in firing rate - due to a wide range of fuel heating values - consequential of combining refinery gas, waste gas and fuel oils. These deviations caused by fluctuations in fuel constituents result in significant variances in flame height, which in turn bring about movement of the heating regions in the heater.

The API 560 and the ISO 13705 remain the most applicable standards when designing a fired heater for general refinery service. However, the principles attached to these standards employ 2-dimensional simplified radiation modeling to evaluate the inconstancy of heat loading to the radiant tubes (Jegla, 2015). The reason behind this is that evaluating furnace systems with 3D modeling is computationally expensive. Much of the material prior to Jegla (2015), did not attempt to corroborate the standard design calculations of the above two standards with detailed modeling.

Little effort has been spent on developing a simplified engineering approach to model 3D fired heater system using numerical methods. The key focus of this project is the determination of a few operating parameters of a refinery fired heater and to model how influential these parameters are by way of MATLAB simulations.

### **1.3 Objectives**

As energy demands and costs continue to increase globally, it has become palpable that efforts must be taken to maximize the efficiency of energy intensive processes. Of key significance to this study is the optimum design of refinery heaters which consume nearly 75% of the energy input to a refinery complex. Accordingly, this project serves to address the following objectives:

- a) To model and design the operating conditions in a cylindrical refinery fired heater using a simplistic engineering approach which is a very close approximation to real-life working conditions.
- b) To develop a MATLAB code to numerically solve the developed model considering the operating conditions.
- c) To validate the developed code against a peer-reviewed case study and achieve a deviation from selected parameters by less than 5%.
- d) To determine a few of the most important parameters that affect the performance of the heater based on the data generated from the simulation.

After development of the appropriate model of the fired heater system, all simulations will be carried out in MATLAB environment. A simulation and sensitivity analysis will be conducted to select the most influential operating parameters of the developed model.

## **1.4 Scope of Study**

This study will develop a process model on the modes of heat and mass transfer in fired heaters which will be compiled in a MATLAB environment. The completed code will be run with parameters taken from an established case study from a peer-reviewed paper for validation. Following validation, the effect of certain parameters on the performance of the fired heater model will be simulated and analyzed to determine their ranking of influence. For the initial phase, a few parameters will be selected based on reviewed research papers. If time permits, more parameters will be examined. The end result of this project will be a completed code that simulates heat and mass transfer of a fired heater that can be run in a MATLAB environment. In addition to that, the other outcome will be the ranking of the most influential parameters on the performance of fired heaters.

## **CHAPTER 2**

### **LITERATURE REVIEW**

Literature is replete with papers on optimal design of process heaters. However, most of these efforts have been directed towards the use of computational fluid dynamics (CFD) on a non-industrial scale. Only recently, some effort has been focused on the use of simplified models of combustion and radiant effects of heat to properly model a direct fired heater; CFD simulations are computationally demanding on a large scale.

#### **2.1 Types of Fired Heaters**

Refinery and petrochemical plants incorporate extensive heating of process fluids. Based on the temperature requirement, this heating is attained either by direct heating or steam tracing. In the former case, the pressurized fluid is confined in tubes which are heated directly via radiation from flames. By and large, refinery fired heaters consists of four sections which are the radiant section, the shield or shock section, the convection section and the stack (AMETEK, 2014).

The radiant section which is also called the combustion chamber or firebox, combusts fuel gas to generate heat and hot flue gases. The main mode of heat transfer is radiation via exposure of the process tubes to the burner flames. Tubes that are placed within the firebox are called radiant tubes. The radiant zone is lined with refractory which are both the most expensive sections of the equipment. The shock

section consists of two or three rows of bare process tubes containing the lowest temperature process fluids which are directly exposed to the flue gases and flames. The temperature of the flue gas after the radiant heat is absorbed by the radiant tubes at this section, which is either called the bridgewall or breakwall temperature.

The convection section contains the most number of tube rows where the mode of heat transfer is convection via hot flue gases. Finally, the flue gases exit the heater via the stack. Designers often optimize the furnace configuration to recycle the hot flue gases to preheat the combustion air which leads to higher conversion of fuel gas. Figure 2.1 and 2.2 show examples of furnace configurations.

Generally, there are two types of the fired heater which are (Jegla, 2011):

- a. Cylindrical heaters with either one central burner or a ring of burners at the base which are preferred for small to medium duty heating applications. The process tubes are arranged vertically in the radiant section and horizontally in the convection section.
- b. Cabin heaters which are long and rectangular with many burners in a row on the floor of the heater are preferred for large heat duty applications. The tubes containing the process fluid are arranged horizontally in both the radiant and convection sections of the heater.



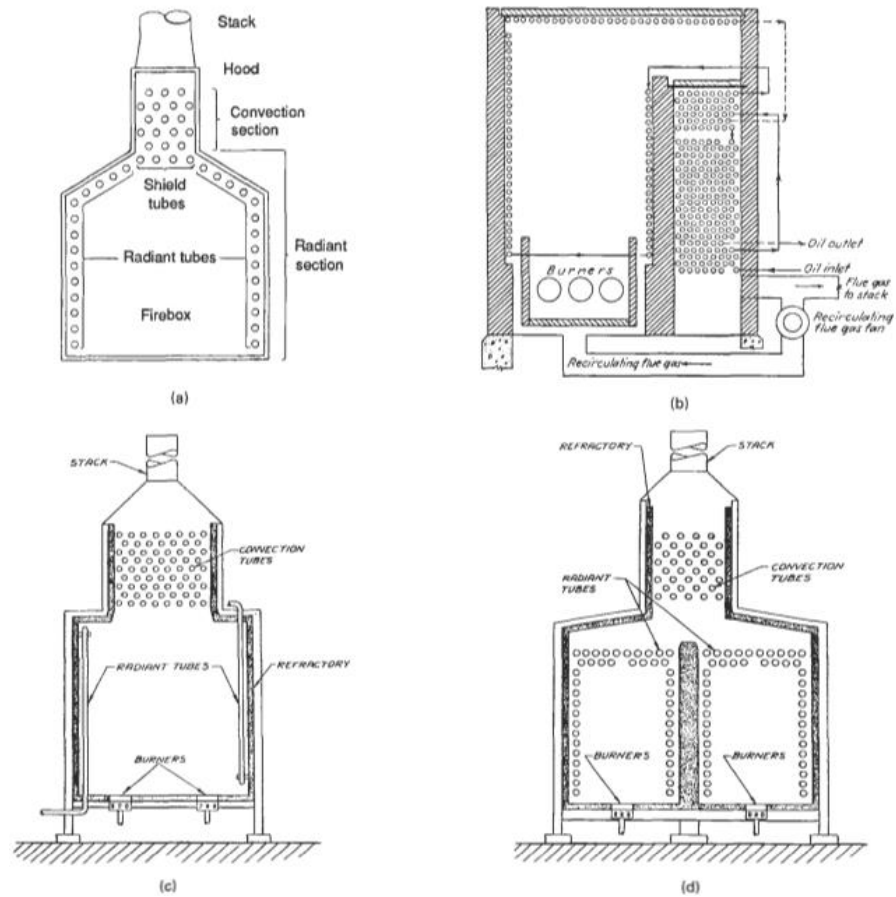


Figure 2.1 Types of Process Fired Heaters. (a) Box Type Heater. (b) Heater with a Split Convection Section for Preheating Before and Soaking After the Radiant Section. (c) Vertical Radiant Tubes in a Cylindrical Shell. (d) Two Radiant Chambers with a Common Convection Section (Fair, 2004)

Cylindrical heaters are preferred to box type heaters due to a more uniform heating rate and generally enhanced thermal efficiencies. Additionally, it usually costs less to construct cylindrical heaters, and they require smaller construction areas (Hassan, 2010). 70-90% of the heat transfer mechanism is via radiation which means that greater significance is attached to radiative transfer mechanism in equipment design. Finned or studded tubes are often used in the convection to maximize heat transfer area. This in turn, approximately equalizes the heat flux in the radiant and convective sections.

## 2.2 Fired Heater Design and Modeling

Most refinery heaters are generally designed according to the API 560. In spite of continuous revisions, the heat transfer phenomenon to the radiant tubes in the firebox is modeled based on an abridged 2-dimensional radiation model (Jegla, 2015). As per Jegla (2015), the heater is assumed to have three zones; which are the hot gas zone, the heat sink and the refractory walls. The hot zone is assumed to be homogeneous with respect to temperature and is perfectly mixed. Furthermore, the heat sink is homogeneous with respect to temperature while the refractory is assumed to be radiatively adiabatic (Hottel & Sarofim, 1967). Tucker & Ward (2012) studied the effect of utilizing low cost modeling techniques via the zone model. They stated that modeling the combustion gases as non-grey with an adiabatic wall allows the model to describe changes when emissivity is raised.

Heynderickx et.al. (1992) improved the zone model by including a 1-dimensional plug flow reactor model to predict the radiant tube skin temperatures and tube coking rates radially. Yet, this model was comparatively simple as the flow and combustion models were left out in the furnace design. Hassan (2010) challenged the stirred furnace or zone model as it assumes discontinuous changes from one zone to the next. Hassan discussed that the flux model gives a more accurate representation of the furnace as it allows for gas property variation as a smooth function as opposed to modeling the furnace as separate subsections.

Mussati et.al. (2009) employed Mixed Integer Nonlinear Programming in order to optimize the design of fired heaters. The geometric design of the heater was discretized while the process conditions were modeled with continuous variables. They stated that based on the Wimpress procedure, certain sections of the heater configuration, size and performance need to be assumed before an iterative procedure is utilized to compute the performance of the radiative and convection zones of the heater (Wimpress, 1963).

Chaibaksh et.al. (2015) investigated the simulation of the furnaces employing CFD. The derived partial differential equations were solved using pre-specified boundary and initial conditions. However, the developed model solution resulted in particular solutions only. Thus, many variables may need to be posed in order to study diverse scenarios. Moreover they stated that thermo-hydraulic models were generated in order to scrutinize the performance of heat exchangers, eventually owing to the selection of suitable arrangement of networks to moderate fouling in heat exchanger trains. However, they declared that the use of thermo-hydraulic models was slightly misleading due to its over-simplification and omission of many operating parameters. They asserted that the use of semi-empirical models is superior in the modeling of furnaces as these models can be generalized over a wide range of operating conditions.

Hajek (2014) criticizes the methods used by the API 530 standard which is employed to estimate maximum tube temperature evaluated from the product of average radiant heat flux and numerous experimental correlation factors. He stated that the lacking projection of heat flux distribution in the radiant section heavily contributes to the rapid degradation of process tubes. However, the determination of the radiant heat flux in this paper was computed using CFD analysis.

Cliff et.al. (2011) studied the effect of completely switching from using a fuel gas composed of 50% methane to one which contained 95% hydrogen on the performance of a few types of fired heaters. The study concluded that the use of a hydrogen fuel increased the radiant section duty while the duty of the convection section decreased. Torleif (2013) expanded upon the work of Cliff et.al. (2011), by introducing detailed combustion chemistry and developing a detailed model of the radiative transport mechanism. They concluded that the efficiency of the heater is dependent on burner geometry, air-to-fuel ratio and the burner firing rate.

Process heater operation efficiency is by part influenced by draft, burner operation and air-to fuel ratio (Wildy, n.a.). Varying the air-to-fuel ratio (AFR) can significantly affect the performance of a fired heater as it controls the extent of combustion. Conversely, there is no single set point for AFR as it is subsequently dependent on the furnace duty, burner design, types of fuel and burner performance. Ibrahim & Al-Qassimi (2008) asserted that the evaluation of furnace efficiency could be done by either the direct (input-output) method or by the indirect method. The direct method is more robust than the indirect route. Its main advantages are that it is rapid and requires a few parameters to compute. However, its drawback is that it is very difficult to evaluate the losses by streams, and can only give an overall view of the furnace efficiency. The indirect method, on the other hand, allows the user discernment of individual losses by streams, and further allows improvement of the system by the individual streams.

## CHAPTER 3: METHODOLOGY

### 3.1 Project Process Flow

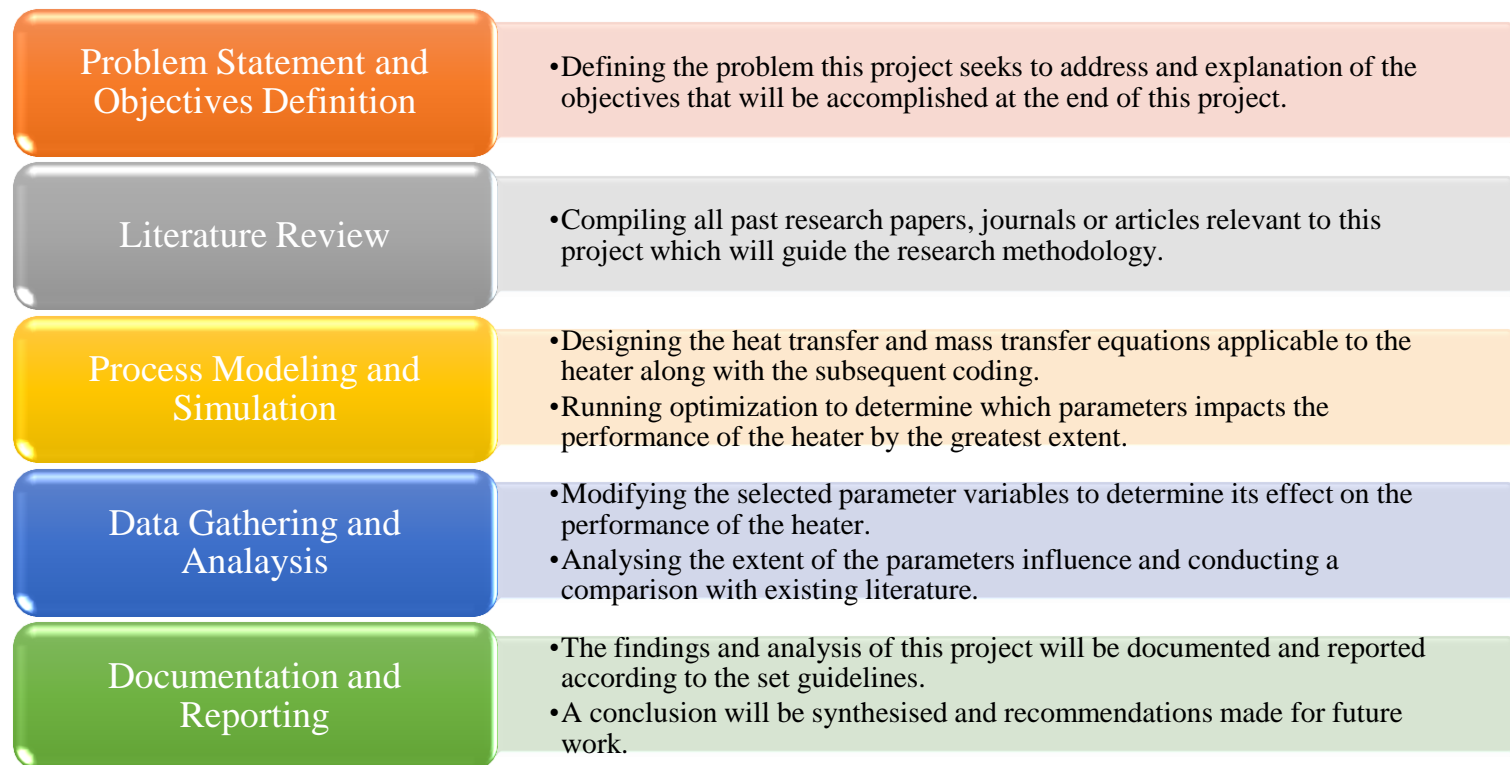


Figure 3.1 Process Flow of the Project

## **3.2 Research Methodology**

### **3.2.1 Selection of Suitable Literature**

Although several papers have been written on the design criteria for fired heaters, not many have discoursed on this topic via numerical simulations. Most papers have studied the heat transfer phenomena using computational fluid dynamics (CFD). Literature on the development of numerical models as well as the numerical simulations of such models will be compiled.

This project is in progress and it should be open to certain modifications along the way. Should a sufficiently strong paper arise along the way which is very relevant and beneficial to this research, pointers can be taken to adjust the methodology accordingly. This is to ensure that a more valid design study can be conducted provided that justifications for the change be proposed and agreed upon.

### **3.2.2 Design Study, Modeling and Elimination of Variables**

It is not possible to evaluate all parameters and variables in the development of the mathematical model for the fired heater. Using previous literature as a guide, certain parameters were omitted to facilitate the completion of a very approximate mathematical model.

Below are examples of parameters which will be considered but are not limited to:

- Heating values of the fuel which are affected by the type of fuel
- Flow rate of the fuel
- Geometry of the process tubes
- Air-to-fuel ratio which affects the nature of combustion gases

- Excess air percentage
- Inlet air temperature

### 3.2.3 MATLAB Coding

After evaluating the comprehensiveness of the developed model, the model will be compiled in MATLAB environment. Next, numerical simulations to solve the fired heater were conducted. The calculation for furnace efficiency should similarly be integrated in a MATLAB program. Subsequently, a comparison of the solution was performed using an established paper on this topic. This move addresses the need to validate the accuracy of the model as compared to the real working conditions.

### 3.2.4 Sensitivity Analysis

After validating the model, the program will be run with varying operating conditions to evaluate the effect of all the selected parameters on the performance of the furnace. The scenario selection can be done using an orthogonal factorial design method. The advantage of using this method is that variance of operating conditions in factorial designs is lower than in non-orthogonal design of experiments. The values should be tabulated with the corresponding efficiencies to determine and select a few of the most influential parameters on furnace operation. Examples of parameters, which may be included in the model, are listed out in Section 3.2.2.

$$\eta = \frac{T_{FT} - T_{stack}}{T_{FT} - T_o} \quad (1)$$

The efficiency of the fired heater can be determined using Equation 1. TFT is the theoretical flame temperature which is evaluated using combustion chemistry and the heating value of the fuel, whereas  $T_{stack}$  is the temperature of the stack gases and  $T_0$  is the standard temperature of 25°C.

### 3.2.5 Documentation and Report Writing

All findings and analyses for this research will be documented. A detailed comparison against existing literature will be conducted to evaluate the effectiveness of this model and its suitability in simulating the real-life application of a fired heater.

## 3.3 Modeling and Simulation Methodology

### 3.3.1 Modeling Study

The two dominant modes of heat transfer in furnaces are radiation and convection, with the former contributing to 70-90% of the total heat transfer. The well-stirred zonal (WSZ) method of modeling the fired heater was utilized. In this method, a 2-dimensional analysis of energy and mass balances are derived. Instead of integrating the distance of the flames from the tubes both vertically and horizontally, the combustion gases were treated as the heat sources. Doing so reduces the calculation of the radiation view factor,  $F_{ij}$  to a constant of 0.97. Thus, the heat transfer coefficients used in the model are as follows:

$$Q_{rad} = \alpha \sigma A_{cp} F_{ij} (T_g^4 - T_w^4) \quad (2)$$

$$Q_{conv} = h_{conv} A_{cp} (T_g - T_w) \quad (3)$$



$$h_{conv} = \frac{k}{D} \left( 0.3 + \frac{0.62Re^{0.5}Pr^{\frac{1}{3}}}{\left[1 + \left(\frac{0.4}{Pr}\right)^{\frac{2}{3}}\right]^{\frac{1}{4}}} \times \left[1 + \left(\frac{Re}{282000}\right)^{\frac{5}{8}}\right]^{\frac{4}{5}} \right) \quad (4)$$

$$h_{process} = \frac{k}{D} [0.023Re^{0.8}Pr^{0.4}] \quad (5)$$

$$T_w = \frac{T_{process-in} + T_{process-out}}{2} \quad (6)$$

$$Q_{process} = UA(T_G - T_{process}) \quad (7)$$

$$\frac{1}{UA} = \left[ \frac{1}{A_{ext}[\alpha\sigma F_{ij}(T_g^2 - T_{wh}^2)(T_G + T_{wh}) + h_{conv}]} + \frac{r_o - r_i}{kA_{lm}} + \frac{1}{h_{process}A_{int}} \right] \quad (8)$$

The heat transfer equations shown above are not the only one used, but are among the most prominent ones that dictate the performance of the radiant section. The equations for  $h_{conv}$  and  $h_{process}$  were developed from Nusselt correlations for flow across vertical tubes are heated flow inside tubes respectively. Depending on the heat and mass transfer equations used in the developed model, only the parameters required for these equations were considered in the user-input section of the code so as to prevent over-specification.

The heater was assumed to be operating with a natural draft operation and the flow rate of flue gas and its subsequent velocity was assumed to be driven by the negative pressure that is influenced by the opening of dampers at the top and bottom of the furnace. Yet, variations in velocity were assumed to occur at different sections of the furnace due to the system geometry. At the radiant section, the geometry of the tubes does not influence the flow much as compared to the tubes in the convection section which are arranged as a bank of in-line or staggered tubes.

Combustion equations were developed to automatically calculate the flow rate of air necessary to accommodate the burning of the fuel depending on the excess air percentage which is meant to be user-specified. This in turn is used to calculate

the adiabatic flame temperature depending on the composition of the fuel and the subsequent composition of the fuel gas. At each point in the furnace, the temperature of the flue gas is calculated as heat transfer continually occurs from the combustion gases to the furnace walls and the process tubes. The method used to evaluate the variation in temperatures is the same method used to evaluate the adiabatic flame temperature.

### **3.3.2 Code Compilation**

The model was then compiled as a script file in MATLAB. The first section of the code is for the user to enter the nominal parameters of the furnace, such as the height and width of the furnace, the inner and outer diameters of the process tubes, fuel composition, excess air percentages and as many as 60 other parameters which can be varied.

The code will split the furnace into two major sections which are the radiant and convection sections depending on the geometry of the furnace. Subsequently, the code will integrate meshing which will be explained in the next section to iteratively solve the temperature and heat flux variations across the furnace as well as the mass transfer of process fluids and flue gas. The same loop used to calculate the adiabatic flame temperature will be repeated at different sections of the furnace to calculate the flue gas temperature.

### **3.3.3 Meshing**

The transfer of heat to the process and to the walls was computed iteratively by developing a mesh that would divide the radiant section into 'blocks' of equal height. These 'blocks' were then evaluated sequentially following the relation in Figure 3.2 below. The flue gases travel upwards and enter a 'block' where some heat

is transferred via radiation and convection to the process fluids through the tube walls (process heat) and some to the firebox walls which is termed losses. The portion of the coding which computes the radiant section model is included in the Appendix.

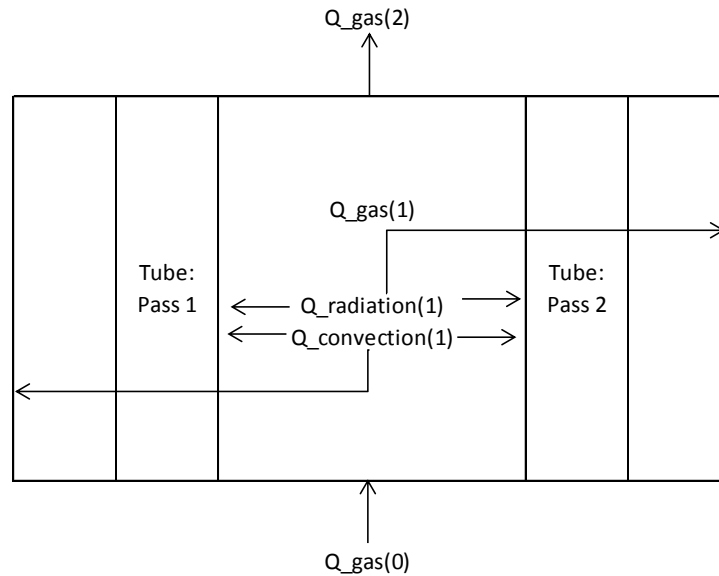


Figure 3.2 Heat and Mass Balance across a Single ‘Block’

As mentioned above, depending on the geometry of the furnace, the furnace was split into 2 major subsections. The radiant section was then split into 3 subsections which are the region below the process tubes, the region containing the vertically arranged process tubes, and the region immediately above the process tubes until right before entering the convection section. The convection section on the other hand was split into 7 subsections which are listed below:

- a) The region immediately below the shield tubes
- b) The region containing the horizontally arranged shield tubes
- c) The region between the shield tubes and the 2<sup>nd</sup> pass of the convection tubes
- d) The region containing the 2<sup>nd</sup> pass of the convection tubes
- e) The region between the 2<sup>nd</sup> pass and the 1<sup>st</sup> pass of the convection tubes
- f) The region containing the 1<sup>st</sup> pass of the convection tubes
- g) The region above the 1<sup>st</sup> pass of tubes until the end of the stack

Each subsection was then divided into ‘blocks’ which were then solved iteratively to determine variation in process fluid temperature, variations in flue gas

temperatures and to calculate radiation and convection heat fluxes which is especially important when trying to determine the maximum heat flux that the process tubes can be exposed to.

### 3.3.4 Validation Study

The research paper of choice to validate the accuracy of the developed model is by Hassan & Mourhaf (2013). The paper was published taking nominal refinery parameters from the article by Hassan (2010), which is more comprehensive. Table 3.1 below lists the nominal and calculated parameters of the fired heater based on the paper as well as the simulated data from the model developed in this study.

Table 3.1 Furnace Parameters for Validation

Process Parameters	Reference Case	Simulated	Percentage deviation
Radiant section inlet charge temperature ( $K$ )	483		
Radiant section outlet charge temperature ( $K$ )	628		
Flue gas temperature at outlet of convection section ( $K$ )	654		
Flow rate of flue gases ( $kmol/h$ )	1720.9		
Adiabatic flame temperature ( $K$ )	2128		
Average percentage deviation			

Provided that the average percentage deviation is less than  $\pm 5\%$ , we can assume that the code is reasonably accurate and can be utilized for the sensitivity analysis. Although, in foresight it would definitely be for the best if lower than  $\pm 1\%$  deviation be achieved for accuracy purposes.

### 3.3.5 Sensitivity Analysis

The sensitivity analysis will be conducted using the factorial design method for experiments. A base case for the evaluated parameters will be established and based on the study done by Hassan (2013) used in the validation study. Table 3.2 shows the variation in parameters which will be used in this analysis. The row labeled base are the base case parameters taken from the study while the row labeled ' $\pm$ ' represent the degree to which each parameter is varied with respect to the base.

Table 3.2 Parameter Variations for Sensitivity Analysis

Exp. No	Fuel flow rate (kmol/h)	Tube pitch (m)	Excess air (%)	Air temperature (K)	Ratio of methane to hydrogen	Methane (%)	Hydrogen (%)
Base	100	0.55	100%	303	20.1075		
$\pm$	10	0.1	5%	10	20		
1	100	0.55	100%	303	20.1075	80.430	4.000
2	100	0.55	100%	303	20.1075	80.430	4.000
3	110	0.65	105%	313	40.1075	81.315	3.115
4	90	0.65	105%	313	40.1075	81.315	3.115
5	110	0.45	105%	313	40.1075	81.315	3.115
6	110	0.65	95%	313	40.1075	81.315	3.115
7	110	0.65	105%	293	40.1075	81.315	3.115
8	110	0.65	105%	313	0.1075	78.841	5.589

The parameters listed above are the parameters chosen for the determination of the most influential parameters on the industrial furnaces performance. As 5 parameters were selected, the minimum number of runs for a full factorial design is  $2^5$  or 32 simulations to fully evaluate the influence. Once all simulations have been

completed, the data will have to be analyzed. The non-linear complexity of the system gives rise to difficulty in analyzing the results. Hence, a curve fitting method will be adopted to give a reasonably accurate characterization of all 5 parameters on a single response. If regression analysis applied to determine the correlation between the simulated response and the curve fitted equation finds a Pearson product moment of correlation or  $R$  value greater than 0.85, the results can be analyzed as having linear properties and their subsequent influence on the performance of the furnace can be evaluated easily. However, analyses using varying types of models such as quadratic, cubic, exponential and logarithmic models are further employed for the curve fitting. The model that leads to the lowest square of errors or the greatest Pearson product moment of correlation will be used to rank the parameters by their individual degree of influence.

The milestones for this project are presented visually in Figure 3.3 below. Each cycle comprises 4 weeks as the Gantt chart below illustrates the details of the project timelines elapsed for about 28 weeks all the way until the end of FYP 2. Figure 3.4 illustrates the general Gantt chart for submissions and grading.

### 3.4 Project Timelines

#### 3.4.1 Project Milestones

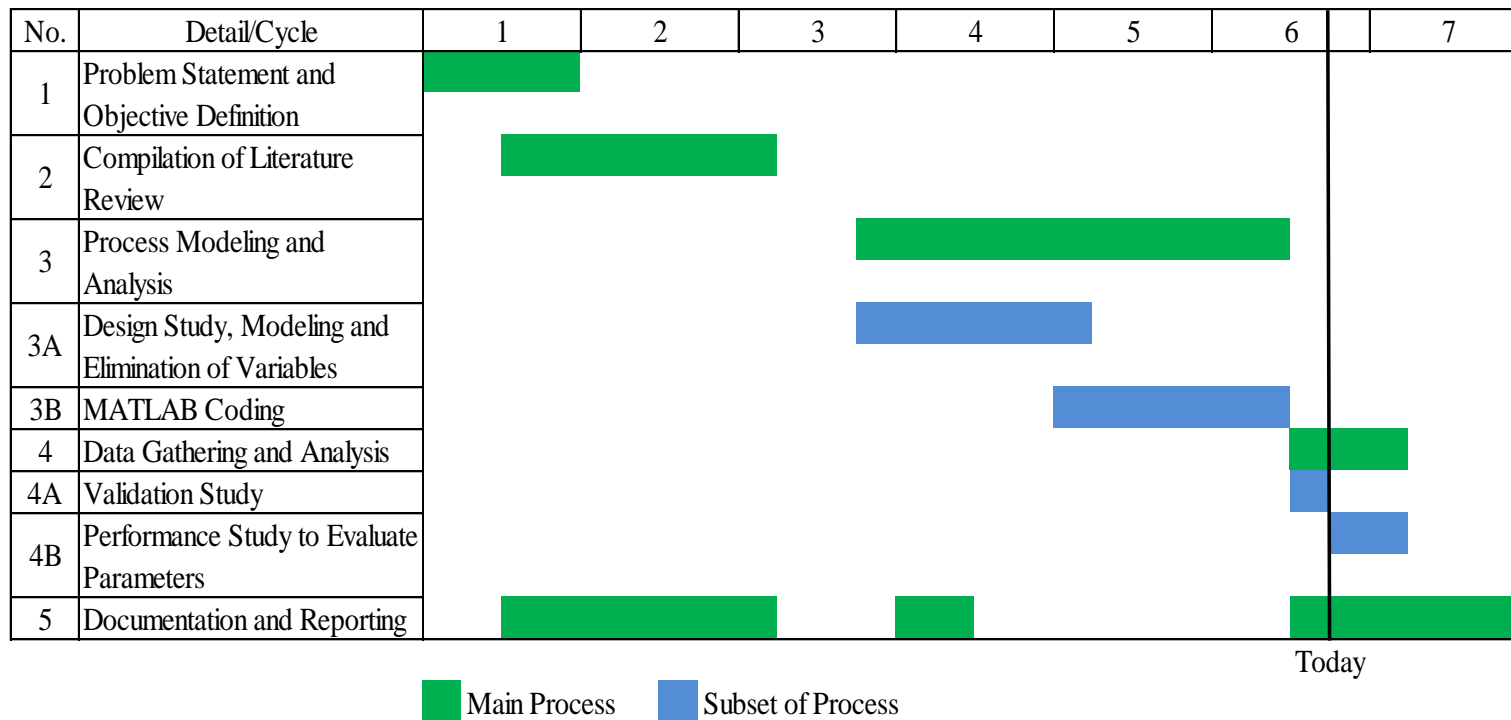


Figure 3.3 Gantt chart Detailing Key Milestones

### 3.4.2 FYP 2 Gantt Chart

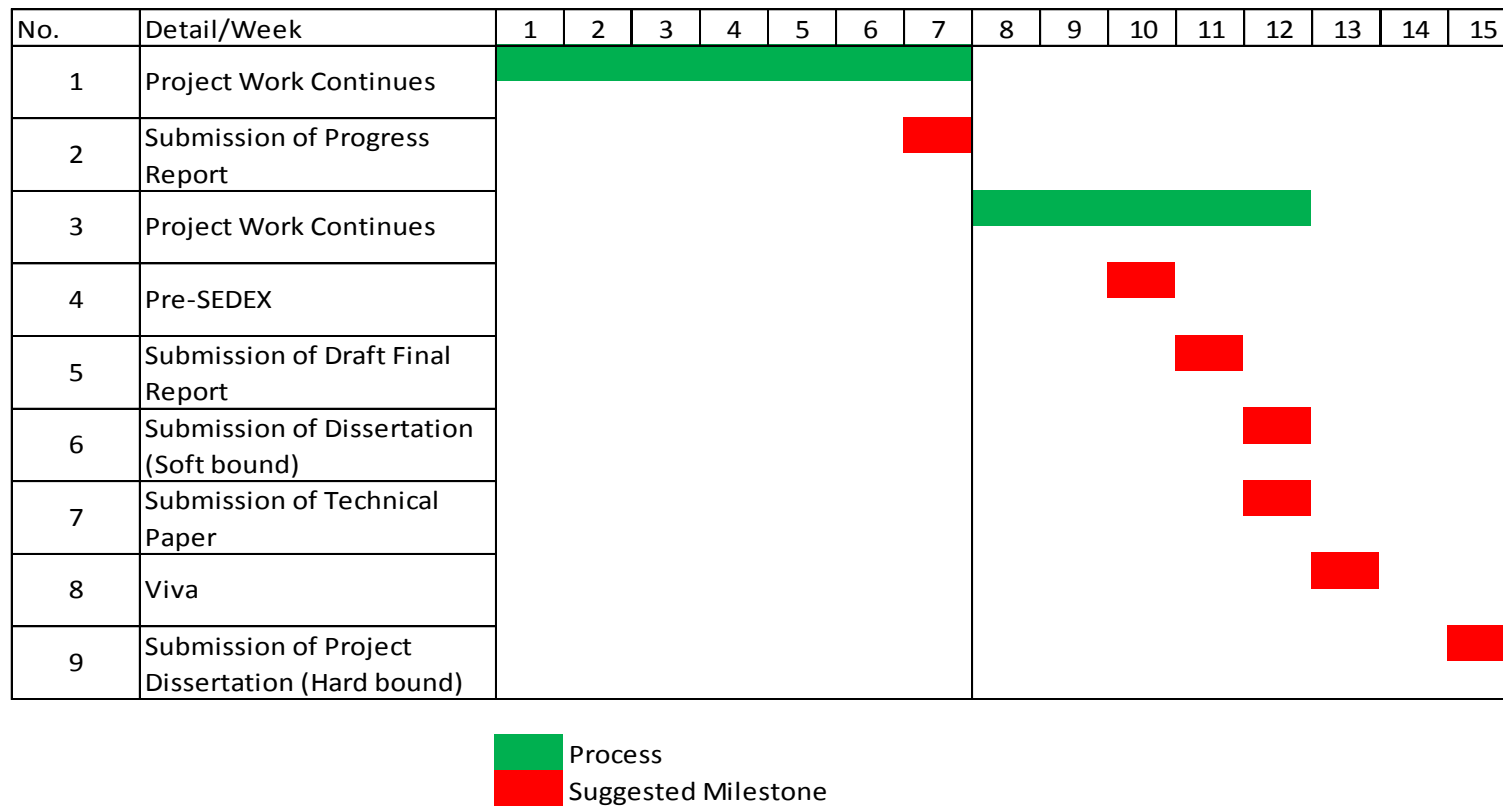


Figure 3.4 Gantt chart for FYP 2



## **CHAPTER 4**

### **RESULTS AND DISCUSSION**

#### **4.1 Completed Coding**

The completed coding has been attached in the Appendix. The code was compiled in a single script file to facilitate debugging efforts. This is especially important for long codes. The total length of the code is approximately 1545 lines. Although, a contributing factor to its length is a loop of length 59 lines repeated 11 times to determine the variation in flue gas temperature and to calculate the adiabatic flame temperature. Having an entire code in a single file may seem messy but it is easier to troubleshoot for syntax or runtime errors.

#### **4.2 Validation Study**

Table 4.1 below lists the nominal and calculated parameters of the fired heater based on the paper as well as the simulated data from the model developed in this study.

Table 4.1 Simulated Data Against Benchmark Data

Process Parameters	Reference Case	Simulated	Percentage deviation (%)
Radiant inlet charge temperature (K)	483	467.04	3.30
Radiant outlet charge temperature (K)	628	629.74	0.28
Gas temperature at convection exit (K)	654	666.00	1.83
Flue gas flow rate (kmol/h)	1720.9	1738.0	0.99
Adiabatic flame temperature	2128	2180	2.44
Average percentage deviation			1.77

As can be seen from Table 4.1, the simulated values of the model were all less than 5% off from the reference values with an average percentage deviation of 1.77%. Consequently, it can be said that the model is valid as the industry requires a pre-specified tolerance of  $\pm 5\%$ . The difference between the use of correlations and that of using generalized heat transfer formulas are clearly demonstrated in the deviation of inlet and outlet process temperatures. Using the ‘tic-toc’ command in the code, the elapsed time for the entire simulation was 0.596 seconds.

### 4.3 Analysis of Results

The two figures below were plotted at the mesh blocks containing the process tubes. To analyze the effect on process fluid temperature, the heat transfer and temperature calculations for the blocks immediately below and above the process tubes were omitted. The only heat transfer phenomenon occurring in these blocks are heat loss to the walls, which according to the API 560 standards, is only 1.5% of the total heat contained by the flue gas.

Figure 4.1 demonstrates the variation in temperature of the flue gas and of the process fluid for both the tube passes 1 and 2 in the relevant mesh blocks. Heat transfer occurs from a region of high temperature to one of lower temperature. As observed at all points along the radiant section, the temperature of the flue gas is significantly higher than that of the process fluid in both passes.

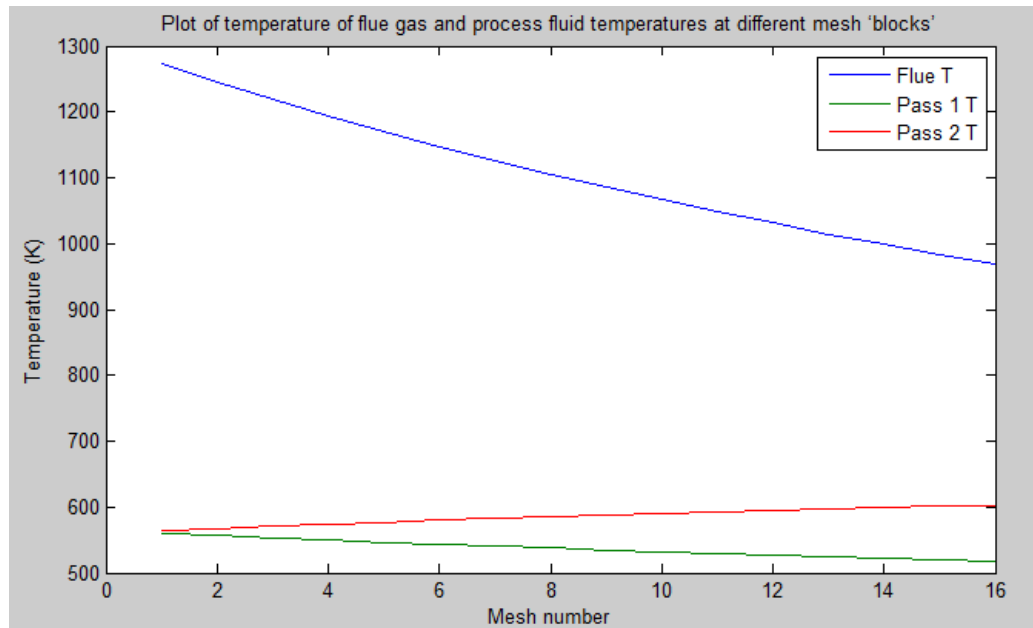


Figure 4.1 Plot of Temperature of Flue Gas and Process Fluid Temperatures at Different Mesh 'Blocks'

A closer look is presented in Figure 4.2, where the variation of process fluid temperature in the tube pass 1 and 2 seem to mirror each other. This may be caused by the simplification of the process fluid flow where the effects of pressure drop are neglected. Ignoring the effects of pressure drop gives in to a constant velocity of the process fluid as shown in the mass continuity equation below. Not having a variation in pressure and ignoring the effects of gravity will lead to little variation between the heat transfer characteristics at each flow pass. And as the fluid temperatures are calculated at each mesh block where the flue gas temperature is shared and constant, the temperature gradient will definitely be constant.

$$\frac{P}{\rho} + gz + \frac{v^2}{2} = \text{constant} \quad (9)$$

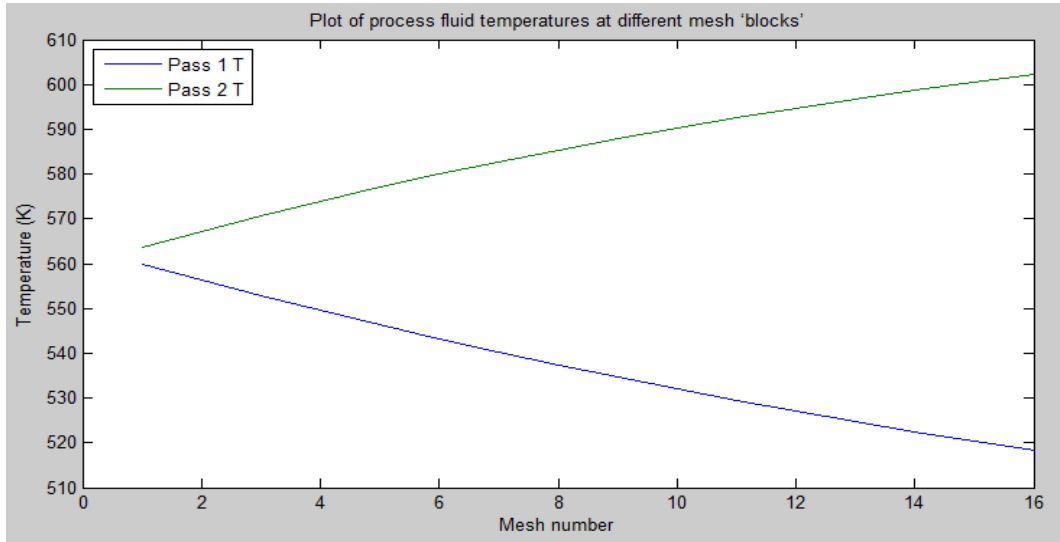


Figure 4.2 Plot of Process Fluid Temperatures at Different Mesh ‘Blocks’

Figure 4.3 on the other hand exhibits the variation in radiation and convection heat transfer coefficients on the process tubes in the radiant section. Two observations can be made based on this figure. Firstly, it is very obvious that the radiation heat transfer plays a more significant role in heat transfer than convection heat transfer due to the elevated temperatures in the fired heater. Equation 1 and 2 above clearly shows that the effect of temperature on radiation heat transfer is 3 orders higher than that of convection heat transfer. The second observation that can be made is that both radiation and convection heat transfer coefficients are higher on the first pass of tubes than the second pass. This can also be explained by both equation 1 and 2, where the temperature of the process fluid in the second pass is definitely higher than that in the first pass as shown in Figure 4.2. This leads to a lowered temperature difference between the heat source which is the flue gas and the heat sink which in this case is the process fluid; and heat transfer coefficients are most strongly dictated by temperature difference.

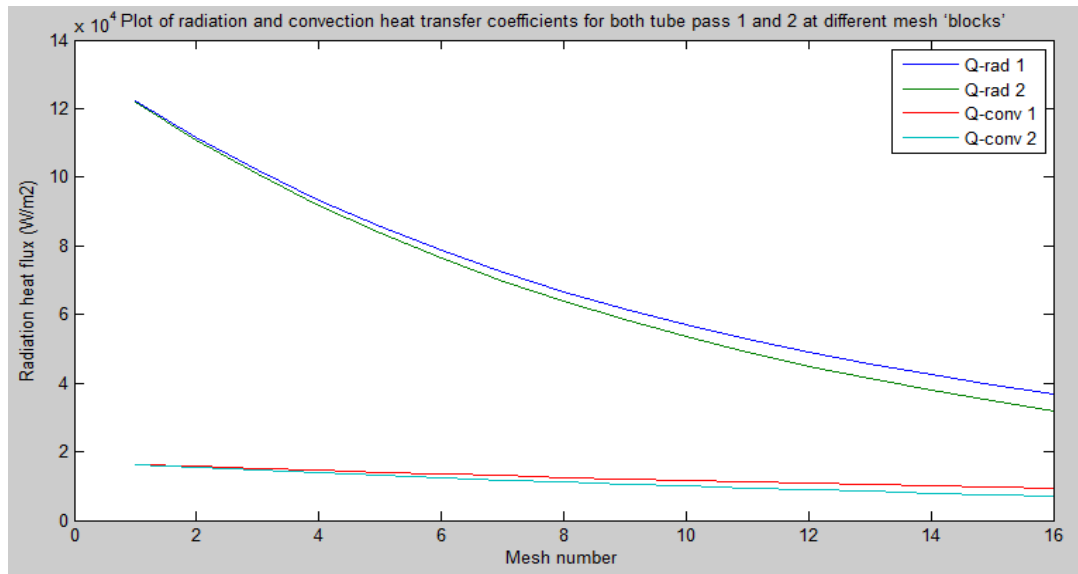


Figure 4.3 Plot of Radiation and Convection Heat Transfer Coefficients For Both Tube Pass 1 and 2 at Different Mesh ‘Blocks’

For the next part, we will analyze the heat transfer phenomena of the convection section. It is especially difficult to trace the flow of process fluid here as it passes through 2 horizontal tube passes before going through a single horizontal pass in the shield tubes. Figure 4.4 shows the plot of temperature variation of the process fluid in the convection section.

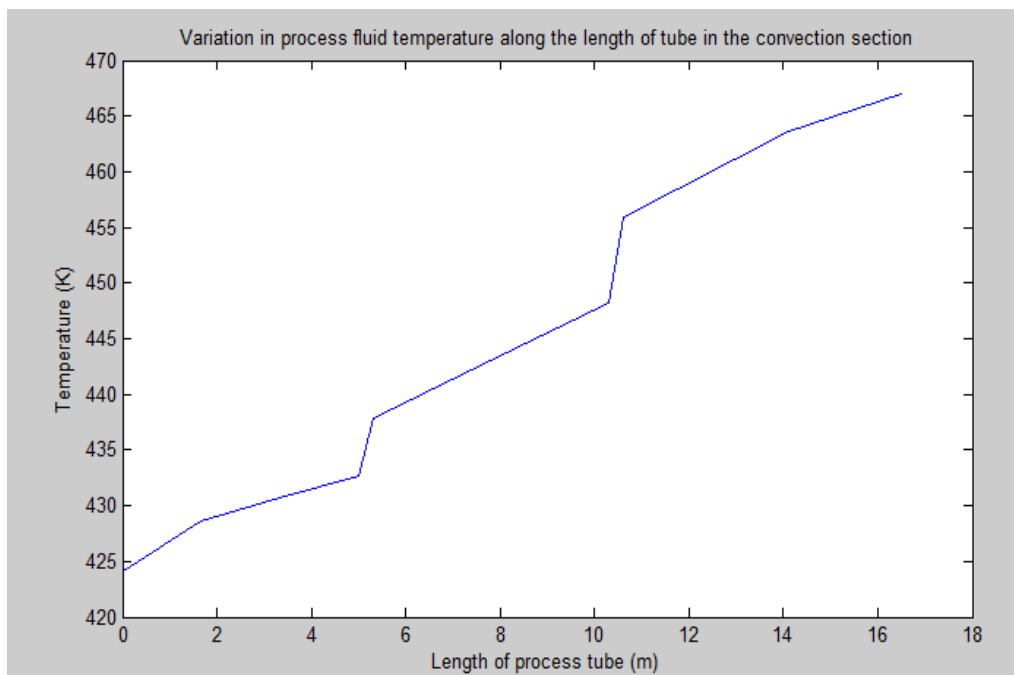


Figure 4.4 Variation in Process Fluid Temperature Along the Length of the Tube in the Convection Section

Figure 4.5 on the other hand shows the variation in convection and radiation heat transfer on the process tubes along the convection section. The sharp increase in heat flux for both the radiation and convection heat transfer on the shield tubes is caused by the fact that the heat transfer in that area is supplemented not just by the flue gas temperature but also by the radiant heat transfer coming directly from the burners. This is the reason as to why the radiation heat transfer in this section is significantly greater than the convection heat transfer. Also, as the temperature of the flue gas starts to drop as it passes through the convection section, the convection heat transfer starts to compete with the radiant heat transfer. Due to the arrangement of the tubes in a bank, the velocity of the flue gas will increase. As there is no accumulation of flue gas anywhere in the furnace, reducing the free-area not encumbered by process tubes for the flue gas to pass will lead to an increase in gas velocity in-line with the mass continuity equation shown in Equation 10.

$$\rho A_1 v_1 = \rho A_2 v_2 \quad (10)$$

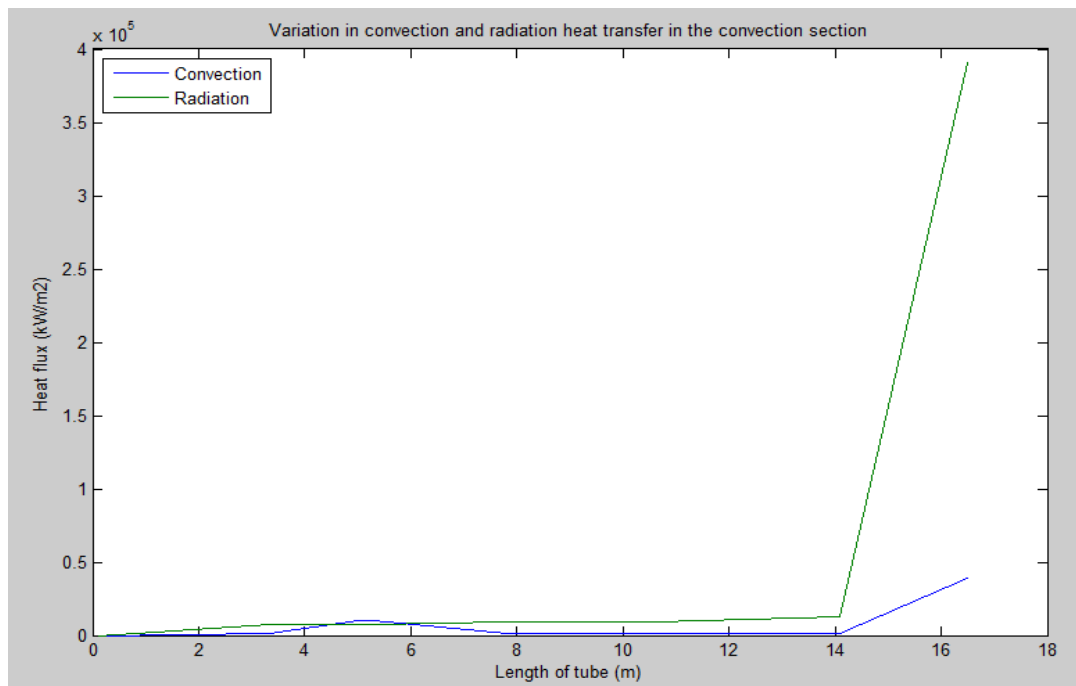


Figure 4.5 Variation in Convection and Radiation Heat Transfer Along Points in the Convection Section

## 4.4 Sensitivity Analysis

### 4.4.1 Linear Analysis

The determination of the most influential parameters on the performance of the furnace is a difficult process due to the complexity of how each parameter affects the efficiency. Some parameters influence the efficiency in a linear manner, whereas others can have either a quadratic or exponential effect on the efficiency. A simplification of analysis can be done by approximating the parameters as having a linear effect on the performance of the furnace. In order to do that, we have to first develop the multivariate linear regression model using the least squares technique. An optimization file was developed in MATLAB and run with an initial value of 0 for all the coefficients. After optimizing iteratively, the linear coefficients were found as shown below. Table 4.2 shows the calculated linear coefficients attached to the parameters listed in Equation 11. Figure 4.6 is the resulting plot of predicted data based on the multivariate linear regression against the simulated response.

$$Y = ax_1 + bx_2 + cx_3 + dx_4 + ex_5 \quad (11)$$

Table 4.2 Coefficients for Multivariate Linear Regression

Coefficients	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>
Parameter	Fuel flow rate	Tube pitch	Excess air percentage	Inlet air temperature	Methane to hydrogen fuel ratio
Values	0.0539	-20.4794	-10.2261	0.3084	-0.7098

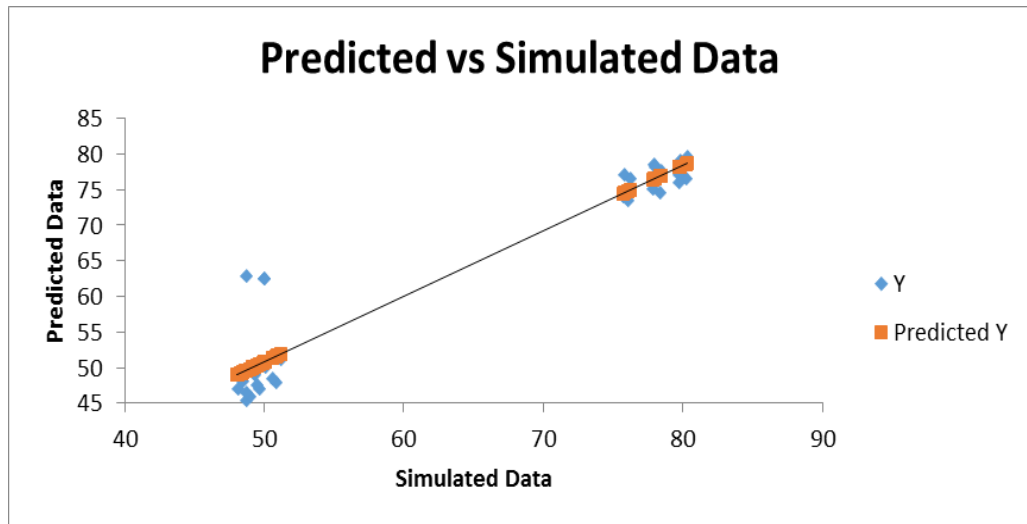


Figure 4.6 Plot of Multivariate Linear Regression against Simulated Data

Subsequently, the data was plotted and the Pearson’s product moment of correlation or R value was found to be equal to 0.955. Based on this R value, we assume that the parameters have a linear effect on the simulated response and treat the analysis as such. Of course in reality, the true regression model will be far more complex due to the wide variety of parameters influencing the performance of the furnace. The next step is to carry out a multivariate linear model analysis on the effect of the multiplicative variation on the simulated data. This is better illustrated in Appendix C. The values of the calculated coefficients reflect the effect of its related parameters and are shown in Table 4.3.

Table 4.3 Coefficients of Multiplicative Variation

Coefficients	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>
Values	4.698	8.394	3.436	4.782	−4.556

By taking the absolute value of the coefficients, we can then rank the influence of the parameters on the performance. The largest absolute value is the most influential parameter while the lowest absolute value is the least influential



parameter, at least among the selected parameters. Thus, the ranking of the selected parameters is shown below in order of decreasing influence.

- Tube pitch
- Inlet air temperature
- Fuel flow rate
- Fuel composition
- Excess air percentage

Further analysis to determine the direction in which each parameter affects the efficiency of the furnace is done and it is found that only fuel flow rate and air inlet temperature should be increased to give rise to increased efficiency. Tube pitch and excess air percentage should be decreased to increase furnace efficiency. The fuel composition on the other hand should lean towards higher hydrogen content to increase efficiency.

#### **4.4.2 Non-Linear Analysis**

Further measures were taken to evaluate the relationship between the selected parameters and the simulated response from a non-linear point of view. Table 4.4 provides the results of applying non-linear models on the selected parameters and the calculated square of the error between the regression values and the simulated response.

Table 4.4 Type of Non-linear Regression Model and Measure of Fit

Relationship	Model Equation	Square of Error	Coefficients
Linear	$Y = ax_1 + bx_2 + cx_3 + dx_4 + ex_5$	643.290	$a = 0.28$ $b = -11.46$ $c = -13.46$ $d = 0.23$ $e = -0.71$
Quadratic	$Y = ax_1^2 + bx_2^2 + cx_3^2 + dx_4^2 + ex_5^2$	1555.979	$a = 0.0007$ $b = -11.47$ $c = -13.48$ $d = 0.0009$ $e = -0.016$
Cubic	$Y = ax_1^3 + bx_2^3 + cx_3^3 + dx_4^3 + ex_5^3$	2350.282	$a = 0$ $b = -11.48$ $c = -13.53$ $d = 0$ $e = -0.0004$
Exponential	$Y = e^ax_1 + e^bx_2 + e^cx_3 + e^dx_4 + e^ex_5$	7824.986	$a = -0.69$ $b = 1.46$ $c = 1.97$ $d = -10.69$ $e = -6.96$
Logarithmic (natural base)	$Y = a.\ln(x_1) + b.\ln(x_2) + c.\ln(x_3) + d.\ln(x_4) + e.\ln(x_5)$	16.173	$a = 0.28$ $b = -11.44$ $c = -13.40$ $d = 9.50$ $e = -3.37$
Logarithmic (10)	$Y = a.\lg(x_1) + b.\lg(x_2) + c.\lg(x_3) + d.\lg(x_4) + e.\lg(x_5)$	16.177	$a = 0.12$ $b = -26.32$ $c = -30.80$ $d = 22.29$ $e = -7.76$
Logarithmic natural base with $\varepsilon$	$Y = a.\ln(x_1) + b.\ln(x_2) + c.\ln(x_3) + d.\ln(x_4) + e.\ln(x_5) + \varepsilon$	15.927	$a = -0.41$ $b = -26.12$ $c = -30.19$ $d = 9.53$ $e = -7.76$ $\varepsilon = 32.76$

Referencing Table 4.4, we can conclude that the most accurate model equation to be used to describe the effect of the selected operating parameters on the performance of the furnace is the natural base log with an error constant. In fact, doing a regression analysis of the plot of predicted response values based on the natural base log against the simulated response gives an R value of 0.999 which is more accurate than the linear model. Yet again, the true model would be more complex in order to achieve a squared error value below 1.

Based on the calculated value of the coefficients, for the model based on the log to the natural base with an error constant, ranking of the evaluated parameters are as follows:

- Excess air percentage
- Tube pitch
- Inlet air temperature
- Fuel composition
- Fuel flow rate

Only the inlet air temperature should be increased to improve the efficiency of a furnace. The fuel flow rate coefficient is quite near to zero and can be assumed to have little effect on the performance. The tube pitch, excess air percentage and the methane composition in the fuel on the other hand should each be reduced in order to increase the performance of the furnace. In fact, the run with the highest efficiency value for the simulated response and the predicted data point towards the operating conditions listed.

Further analysis on the effect of each parameter can be explained by looking at the equations that relate each parameter on the performance of the furnace. Assuming there is no accumulation of mass flow in the furnace, the fuel flow rate should have little effect on the performance as it only increases the velocity of the flue gas. This in turn increases the convection heat transfer coefficient only on the

bank of tubes in the convection section where the temperature of the flue gas is already diminished.

Increasing the excess air percentage will lead to more combustion products which do not contribute significantly to the combustion enthalpy. Increasing excess air leads to a higher air flow rate which only increases sensible heat to the system. Most of the enthalpy is delivered by the combustion of the fuel. The effect of increased air percentage on lowering the performance of the heater can be reduced by increasing the inlet air temperature which further increases the contribution of the sensible heat.

Tube pitch on the other hand is related to the absorptivity of the cold plane area for which the radiation heat transfer is absorbed by. Increasing tube pitch leads to a drop in absorptivity which further reduces the enthalpy delivered to the process. This means that the temperature of the flue gas will still be elevated at the stack which will lead to reduced efficiency. Referencing Cliff et. al. (2015), it is obvious to see why reducing the methane composition in the fuel while increasing the hydrogen content increases the furnace performance. Hydrogen has higher energy content by weight and this leads to an increased adiabatic flame temperature with reduced molecular weight of the fuel.

## **CHAPTER 5**

### **CONCLUSION AND RECOMMENDATIONS**

To conclude, during the course of this study an appropriate and considerably accurate model of a fired heater in refinery service has been developed and simulated. The model was then compiled as a MATLAB code for validation and sensitivity analysis to be carried out. The validation study proved that the model deviated by less than 5% from the reference case. For this study, 5 parameters were selected for the sensitivity analysis. It has proved that some parameters have more effect on the performance of the furnace more than others.

Characteristically, the use of computational fluid dynamics (CFD) to model the entire structure of a fired heater is a computationally and cost demanding procedure. This program serves to provide a lower cost and less computationally demanding avenue to simulate fired heaters as a preliminary design analysis. The findings of this study might be applied to the industry application to improve the performance of the heaters and the relevant process efficiency.

As this study involves the elimination of certain operating parameters which slightly influence the performance of fired heaters, the effect of the neglected parameters will not be evaluated. Accordingly, further studies should seek to develop more comprehensive models which more accurately represent the fired heater. A suggestion for improvement would be to incorporate the neglected parameters and conduct the same design method to simulate the heater. The inclusion of more and more parameters increases the rigorousness of the model, but may increase the

processing time. As the advantage of employing MATLAB to numerically simulate heaters over computational fluid dynamics (CFD) lies in its processing speed, the inclusion of further parameters reduces this advantage. Hence, another suggestion would be to optimize a balance between processing speed and rigorousness.

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# APPENDIX

## APPENDIX A – Fired Heater Configuration

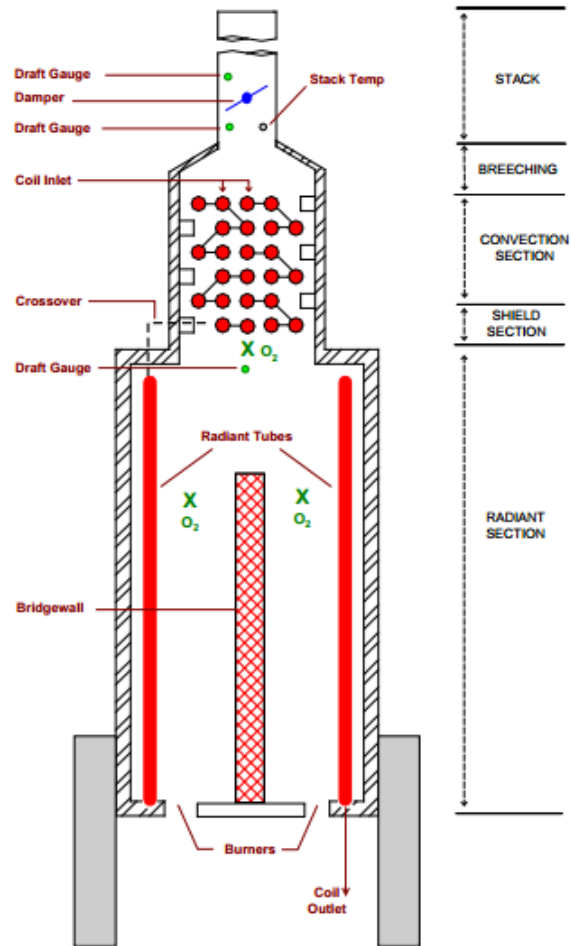


Figure A1 Configuration of a Vertical-Cylindrical Furnace

## APPENDIX B – Coding for Radiant Section Containing Process Tubes

```
%% heat flux calculations for the mesh blocks containing the process tubes

for c=1:1:(m-top_rad_mesh-bot_rad_mesh)

    Q_rad_pro(1)=H4;
    T_gas_rad(1)=T2;
    T_process_rad1(1)=T_guess_rad1;

    % for the calculation of external radiant tube heat flux via convection
    [CORRECT]
    Reynolds_rad=(velocity_flue_rad*L_rad/2)/(1.710293646186000e-04); %
    Reynolds coefficient for pass 1 and 2 in the radiant section
    Prandtl_rad=0.74; % Prandtl coefficient for pass 1 and 2 in the radiant section

    h_conv_rad=(0.3+((0.62*(Reynolds_rad^0.5)*(Prandtl_rad^(1/3)))/(1+(0.4/Prandtl_rad)^(2/3)))^(1/4))*((1+(Reynolds_rad/282000)^(5/8))^(4/5))*(0.080489191/D_out_rad); % Nusselt correlation for pass 1 and 2 in the radiant section

    % for the calculation of inner radiant tube heat fluxes [CORRECT]
    velocity_process;
    Reynolds_process=velocity_process*D_in_rad/v_process; % Reynolds number for
    pass 1 and 2 in the radiant section
    Prandtl_process=mu_process*Cp_process/k_rad; % Prandtl number for pass 1 and
    2 in the radiant section

    h_process_rad1=(0.023*Reynolds_process^0.8*Prandtl_process^0.4)*(k_rad/D_in_rad);

    h_process_rad2=(0.023*Reynolds_process^0.8*Prandtl_process^0.4)*(k_rad/D_in_rad);

    % Process fluid temperature profile: calculation for rate of heat absorption from
    combined heat flux inside the tube [CORRECT]
    A_int_mesh=Nt_rad*(L_rad_pass)/(m-bot_rad_mesh-top_rad_mesh)*D_in_rad*pi; % internal surface area for convection in the radiant
    tubes per mesh
    A_ext_mesh=Nt_rad*(L_rad_pass)/(m-bot_rad_mesh-top_rad_mesh)*D_out_rad*pi; % external surface area for convection in the radiant
    tubes per mesh
    A_log_mesh=(A_ext_mesh-A_int_mesh)/log(A_ext_mesh/A_int_mesh); %
    logarithmic heat transfer area
    V_pro_mesh=(D_in_rad/2)^2*pi*(L_rad_pass)/(m-bot_rad_mesh-top_rad_mesh);
    % internal volume of fluid contained in a single mesh within the process tubes
```

```

Q_process_rad1(c)=(T_gas_rad(c)-
T_process_rad1(c))/(1/((h_conv_rad+sigma*alp*F_ij*(T_gas_rad(c)^2+(100+T_pro
cess_rad1(c))^2)*(T_gas_rad(c)+100+T_process_rad1(c)))*A_ext_mesh)+(D_out_ra
d-D_in_rad)/(2*k_rad*A_log_mesh)+1/(h_process_rad1*A_int_mesh)); % amount
of heat being absorbed by the charge during the first pass

```

```

T_process_rad2(1)=T_process_rad1(1)+Q_process_rad1(1)/(V_pro_mesh*1000*SG
_process*Cp_process*1000);

```

```

Q_process_rad2(c)=(T_gas_rad(c)-
T_process_rad2(c))/(1/((h_conv_rad+sigma*alp*F_ij*(T_gas_rad(c)^2+(100+T_pro
cess_rad2(c))^2)*(T_gas_rad(c)+100+T_process_rad1(c)))*A_ext_mesh)+(D_out_ra
d-D_in_rad)/(2*k_rad*A_log_mesh)+1/(h_process_rad2*A_int_mesh)); % amount
of het being absorbed by the charge during the second pass

```

```

T_process_rad1(c+1)=T_process_rad1(c)-
Q_process_rad1(c)/(V_pro_mesh*1000*SG_process*Cp_process*1000); % process
fluid temperature profile by assuming constant surface heat flux in pass 1

```

```

T_process_rad2(c+1)=T_process_rad2(c)+Q_process_rad2(c)/(V_pro_mesh*1000*S
G_process*Cp_process*1000); % process fluid temperature profile by assuming
constant surface heat flux in pass 2

```

```

% for the calculation of external radiant tube heat flux via radiation
h_rad_rad1(c)=sigma*F_ij*alp*(T_gas_rad(c)^4-
(100+0.5*(T_process_rad1(c)+T_process_rad1(c+1))))^4);
h_rad_rad2(c)=sigma*F_ij*alp*(T_gas_rad(c)^4-
(100+0.5*(T_process_rad2(c)+T_process_rad2(c+1))))^4);
Q_rad_rad(c)=h_rad_rad1(c)*A_ext_mesh+h_rad_rad2(c)*A_ext_mesh; %
combined radiation heat transfer to the process tubes

```

```

Q_conv_rad1(c)=h_conv_rad*A_ext_mesh*(T_gas_rad(c)-
(100+0.5*(T_process_rad1(c)+T_process_rad1(c+1))));
Q_conv_rad2(c)=h_conv_rad*A_ext_mesh*(T_gas_rad(c)-
(100+0.5*(T_process_rad2(c)+T_process_rad2(c+1))));
Q_conv_rad(c)=Q_conv_rad1(c)+Q_conv_rad2(c); % combined convection heat
transfer to the process tubes

```

```

a=1;

```

```

for pii=0.5:0.1:1
    pii_store(a) = pii ;

```

```

T_gas2_rad(1) = T_gas_rad(1) ; %[K] Initial flame temperature guess
del_T2 = 0.5 ;
T_gas2(1) = 1000 ; %[K] Initial Adiabatic flame temperature setting
b = 1 ; %[] counter
T_inf = T_ambient ;

```

```

while T_gas2_rad(b) < T_gas2(b)

```

H4=Q\_rad\_bot(end-1); % enthalpy of combustion air after accounting for the mesh size and the radiant loss through refractory

%Specific heats in terms of kJ/kmol

% 'for calculation of CpCO2';

if (298<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<2000)

CpCO2=24.99375+55.18696\*(10^-3)\*T\_gas2\_rad(b)-33.69137\*(10^-6)\*(T\_gas2\_rad(b)^2)+7.948387\*(10^-9)\*(T\_gas2\_rad(b)^3)-0.136638\*(10^6)/(T\_gas2\_rad(b)^2);

else (2000<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<6000);

CpCO2=58.16639+2.720074\*(10^-3)\*T\_gas2\_rad(b)-0.492289\*(10^-6)\*(T\_gas2\_rad(b)^2)+0.038844\*(10^-9)\*(T\_gas2\_rad(b)^3)-6.447293\*(10^6)/(T\_gas2\_rad(b)^2);

end

% 'For calculation of CpH2O';

if (298<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<500)

CpH2O=-203.6060+1523.290\*(10^-3)\*T\_gas2\_rad(b)-3196.413\*(10^-6)\*(T\_gas2\_rad(b)^2)+2474.455\*(10^-9)\*(T\_gas2\_rad(b)^3)+3.855326\*(10^-6)/(T\_gas2\_rad(b)^2);

elseif (500<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<1700)

CpH2O=30.09200+6.832514\*(10^-3)\*T\_gas2\_rad(b)+6.793435\*(10^-6)\*(T\_gas2\_rad(b)^2)-2.534480\*(10^-9)\*(T\_gas2\_rad(b)^3)+0.082139\*(10^6)/(T\_gas2\_rad(b)^2);

else (1700<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<6000);

CpH2O=41.96426+8.622053\*(10^-3)\*T\_gas2\_rad(b)-1.499780\*(10^-6)\*(T\_gas2\_rad(b)^2)+0.098119\*(10^-9)\*(T\_gas2\_rad(b)^3)-11.15764\*(10^6)/(T\_gas2\_rad(b)^2);

end

% 'For calculation of CpN2';

if (100<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<500)

CpN2=28.98641+1.853978\*(10^-3)\*T\_gas2\_rad(b)-9.647459\*(10^-6)\*(T\_gas2\_rad(b)^2)+16.63537\*(10^-9)\*(T\_gas2\_rad(b)^3)+0.000117\*(10^6)/(T\_gas2\_rad(b)^2);

elseif (500<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<2000)

CpN2=19.50583+19.88705\*(10^-3)\*T\_gas2\_rad(b)-8.598535\*(10^-6)\*(T\_gas2\_rad(b)^2)+1.369784\*(10^-9)\*(T\_gas2\_rad(b)^3)+0.527601\*(10^6)/(T\_gas2\_rad(b)^2);

else (2<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<6);

CpN2=35.51872+1.128728\*(10^-3)\*T\_gas2\_rad(b)-0.196103\*(10^-6)\*(T\_gas2\_rad(b)^2)+0.014662\*(10^-9)\*(T\_gas2\_rad(b)^3)-4.553760\*(10^6)/(T\_gas2\_rad(b)^2);

end

% 'For calculation of CpO2';

if (100<T\_gas2\_rad(b))&&(T\_gas2\_rad(b)<700)

```

        CpO2=31.32234-20.23531*(10^-3)*T_gas2_rad(b)+57.86644*(10^-
6)*(T_gas2_rad(b)^2)-36.50624*(10^-9)*(T_gas2_rad(b)^3)-
0.007374*(10^6)/(T_gas2_rad(b)^2);
        elseif (700<T_gas2_rad(b))&&(T_gas2_rad(b)<2000)
            CpO2=30.03235+8.772972*(10^-3)*T_gas2_rad(b)-3.988133*(10^-
6)*(T_gas2_rad(b)^2)+0.788313*(10^-9)*(T_gas2_rad(b)^3)-
0.741599*(10^6)/(T_gas2_rad(b)^2);
            else (2000<T_gas2_rad(b))&&(T_gas2_rad(b)<6000);
                CpO2=20.91111+10.72071*(10^-3)*T_gas2_rad(b)-2.020498*(10^-
6)*(T_gas2_rad(b)^2)+0.146449*(10^-
9)*(T_gas2_rad(b)^3)+9.245722*(10^6)/(T_gas2_rad(b)^2);
            end

        % For calculation of CpSO2';
        if (298<T_gas2_rad(b))&&(T_gas2_rad(b)<1200)
            CpSO2=21.43049+74.35094*(10^-3)*T_gas2_rad(b)-57.75217*(10^-
6)*(T_gas2_rad(b)^2)+16.35534*(10^-
9)*(T_gas2_rad(b)^3)+0.086731*(10^6)/(T_gas2_rad(b)^2);
            else (1200<T_gas2_rad(b))&&(T_gas2_rad(b)<6000);
                CpSO2=57.48188+1.0093288*(10^-3)*T_gas2_rad(b)-0.076290*(10^-
6)*(T_gas2_rad(b)^2)+0.005174*(10^-9)*(T_gas2_rad(b)^3)-
4.045401*(10^6)/(T_gas2_rad(b)^2);
            end

        %      T_gas2(b+1)      =      T_inf      +(H4)/(P_CO2_mesh_rad*CpCO2
+P_H2O_mesh_rad*CpH2O
+P_N2_mesh_rad*CpN2+P_O2_mesh_rad*CpO2+P_SO2_mesh_rad*CpSO2 ) ;
        T_gas2(b+1)      =      T_inf      +      (H4)/(P_CO2_mesh_rad*CpCO2
+P_H2O_mesh_rad*CpH2O
+P_N2_mesh_rad*CpN2+P_O2_mesh_rad*CpO2+P_SO2_mesh_rad*CpSO2 ) ;

        T_gas2_rad(b+1) = T_gas2_rad(b) + del_T2 ;
        b=b+1 ;

        if b > 1E5
            break
        end
    end
    format long

    T_gas_rad(1)=T_gas2_rad(1);

    a=a+1 ;
end
Q_rad_pro(c+1)=Q_rad_pro(c)-(Q_process_rad1(c)+Q_process_rad2(c));
T_gas_rad(c+1)=T_gas_rad(c)-
(Q_process_rad1(c)+Q_process_rad2(c))/(P_CO2_mesh_rad*CpCO2
+P_H2O_mesh_rad*CpH2O
+P_N2_mesh_rad*CpN2+P_O2_mesh_rad*CpO2+P_SO2_mesh_rad*CpSO2);

```

```

if T_gas_rad(c)<T_process_rad1(c)
    break
end
c=c+1;
if c>m-top_rad_mesh-bot_rad_mesh
    break
end
end
end
T3=T_gas_rad(end-1);

```

## APPENDIX C – Factorial Design of Simulations

Table C1 Factorial Design of Simulations

Exp No.	Response	Fuel flow rate (kmol/h)	Tube pitch (m)	Excess air (%)	Inlet air T (K)	Methane content (%)	Hydrogen content (%)
Variation		100	0.55	1.05	303		
Response		5	0.05	0.05	5		
1	50.01	100	0.55	1.05	303	80.430	4.000
2	50.01	100	0.55	1.05	303	80.430	4.000
3	48.29	105	0.6	1.1	308	82.381	2.049
4	48.42	95	0.6	1.1	308	82.381	2.049
5	49.88	105	0.5	1.1	308	82.381	2.049
6	49.11	105	0.6	1	308	82.381	2.049
7	48.73	105	0.6	1.1	298	82.381	2.049
8	75.84	105	0.6	1.1	308	0.629	83.801
9	50.06	95	0.5	1.1	308	82.381	2.049
10	51.20	95	0.5	1	308	82.381	2.049
11	50.84	95	0.5	1	298	82.381	2.049
12	80.21	95	0.5	1	298	0.629	83.801
13	75.73	105	0.6	1.1	298	0.629	83.801
14	77.89	105	0.6	1	298	0.629	83.801
15	79.74	105	0.5	1	298	0.629	83.801
16	49.32	95	0.6	1	308	82.381	2.049
17	48.01	95	0.6	1.1	298	82.381	2.049
18	76.21	95	0.6	1.1	308	0.629	83.801
19	49.66	95	0.5	1.1	298	82.381	2.049
20	77.93	95	0.5	1.1	308	0.629	83.801
21	80.29	95	0.5	1	308	0.629	83.801
22	77.99	105	0.6	1	308	0.629	83.801

23	79.82	105	0.5	1.1	308	0.629	83.801
24	79.74	105	0.5	1.1	298	0.629	83.801
25	78.34	95	0.6	1	298	0.629	83.801
26	78.42	95	0.6	1	308	0.629	83.801
27	49.48	105	0.5	1.1	298	82.381	2.049
28	48.94	95	0.6	1	298	82.381	2.049
29	76.11	95	0.6	1.1	298	0.629	83.801
30	50.95	105	0.5	1	308	82.381	2.049
31	48.73	105	0.6	1	298	82.381	2.049
32	50.58	105	0.5	1	298	82.381	2.049
33	48.35	100	0.6	1.1	308	82.381	2.049
34	49.18	105	0.55	1.1	308	82.381	2.049
35	48.67	105	0.6	1.05	308	82.381	2.049
36	48.09	105	0.6	1.1	303	82.381	2.049
37	48.76	105	0.6	1.1	308	80.430	4.000

## APPENDIX D – Factorial Design of Simulations with Multiplicative Factor

Table D1 Multiplicative Factor for Factorial Design

Exp No.	Response	Fuel flow rate (kmol/h)	Tube pitch (m)	Excess air (%)	Inlet air temperature (K)	Methane to hydrogen ratio
1	50.01	0	0	0	0	0
2	50.01	0	0	0	0	0
3	48.29	1	1	1	1	1
4	48.42	-1	1	1	1	1
5	49.88	1	-1	1	1	1
6	49.11	1	1	-1	1	1
7	48.73	1	1	1	-1	1
8	75.84	1	1	1	1	-1