FAULT DETECTION AND DATA VALIDATION
IN REFINERY POWER PRODUCTION

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ABSTRACT

FAULT DETECTION AND DATA VALIDATION
IN REFINERY POWER PRODUCTION

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In refinery utility generation, boilers, steam and gas turbines are the primary equipment, producing steam as well as electricity. In boilers, high pressure steam is produced by combustion of a mixture of waste gases from the production line and natural gas – called fuel gas. The steam is at relatively high pressures and is then reduced to lower pressures in steam turbines. The resulting medium and low pressure steam are sent to the refinery for use in processes. In a gas turbine, electricity is produced by compressed air using energy released from combustion of natural gas.

In this study, the aim is to model the efficiencies of the steam production equipment, tracking their performance in an effort to optimize the equipment utilization. For this purpose, historical data from a refinery are verified. Material and energy balances are checked on individual units using ASPEN software to verify the data as a reference. Then, MATLAB software is used to adapt our situation in the plant. In these analyses, clustering methods are used. Results of the model and analysis of historical

data allows us to make recommendations on which sensors need to be calibrated and how data integrity issues can be resolved.

In the examined case, it was postulated that oxygen sensor at the stack gas line was accurate and then combustion air flow calculation was set forth to check mass balance. To check energy balance, some imaginary heat exchangers are defined at critical locations for which there should be no net heat loss/gain. Based on these restrictions, the dataset of the plant over a period of 3 months was corrected. After ensuring data integrity, efficiency values of multiple boilers in production are analyzed. These efficiency values can be used reliably in an overall optimization scheme to optimize equipment usage.

Keywords: steam boilers, modeling, data consolidation

ÖZ

RAFİNERİDEKİ GÜÇ ÜRETİMİNDE
HATA TESPİTİ VE VERİ DOĞRULAMASI

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Şubat 2014, 107 sayfa

Güç üretim tesislerinde, buhar üretmek ve elektrik elde etmek için kazanlar, buhar türbinleri ve gaz türbinleri ana ekipman olarak kullanılır. Kazanlarda, üretim hattından gelen yakıt yakılarak açığa çıkan enerji kullanılarak buhar üretilir. Üretilen bu yüksek basınçlı buhar, buhar türbinlerinde daha düşük basınca indirgenirken elektrik üretilir. Ortaya çıkan orta ve düşük basınçtaki buhar, rafineri proseslerine gönderilir. Gaz türbinlerinde ise yakıtın yakılmasıyla açığa çıkan enerji kullanılarak sıkıştırılmış hava ile yine elektrik üretilir.

Bu çalışmada, buhar üretim ekipmanlarının verimliliklerinin modellenmesi, ve ekipmanların performanslarını izleyerek en uygun şekilde bu ekipmanların kullanımının sağlanması amaçlanmıştır. Bu amaç doğrultusunda, endüstriden alınan geçmiş veriler incelenmiştir. ASPEN bilgisayar programı referans alınarak her birim için kütle ve enerji denkliği yapılmışır. Sonrasında, MATLAB bilgisayar programı kullanılarak tesisteki duruma uyarlanmıştır. Bu analizlerde, kümelenme metodu

kullanılmıştır. Geçmiş verilerin modellenme ve analiz sonuçları, hangi sensörlerin kalibrasyona ihtiyaç duyduğu ve veri bütünlüğü sorunlarının çözümü hakkında önerilerde bulunmamızı sağlamaktadır.

Bu çalışmada ele alınan durumda, kütle denkliğini sağlamak için baca gazındaki oksijen miktarı sensörünün doğru olduğu kabul edilip kazana giren yanma havası miktarının hesaplanması öngörülmüştür. Enerji denkliğini sağlamak için, kritik bölgelerde ısı kaybının ya da ısı kazancının olmadığı sanal eşanjörler tanımlanmıştır. Bu kısıtlamalarla, tesisin 3 aylık veri seti düzeltilmiştir. Veri bütünlüğü sağlandıktan sonra, üretim hattındaki çoklu kazanların verimleri incelenmiştir. Bu verim değerleri, ekipmanların optimizasyonu için genel optimizasyon çerçevesinde güvenle kullanılabilir.

Anahtar Sözcükler: buhar kazanları, modelleme, veri birleştirme

To my family,

ACKNOWLEDGEMENTS

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LIST OF SYMBOLS

Symbol	Definition	Unit
ai	Coefficient of heat capacity	
BD.H	Enthalpy of blowdown	MJ
BD.m	Mass flow rate of blowdown	kg
BD.P	Pressure of blowdown	atm
BD.T	Temperature of blowdown	^{o}C
BDLOSS	Heat loss of heat exchanger on blow down flow	MJ
BDOUT.H	Enthalpy of blowdown released	MJ
BDOUT.m	Mass flow rate of blowdown released	kg
BDOUT.P	Pressure of blowdown released	atm
BDOUT.T	Temperature of blowdown released	^{o}C
bi	Coefficient of heat capacity	
BOILER.T	Temperature of boiler	^{o}C
CA.H	Enthalpy of combustion air	MJ
CA.Hi	Enthalpy values of combustion air components	MJ
CA.m	Mass flow rate of combustion air	kg
CA.mi	Mass flow rate of combustion air components	kg
CA.ni	Molar flow rate of combustion air components	kmol
CA.P	Pressure of combustion air	Atm
CA.rho	Density of combustion air	kg/m^{3}
CA.T	Temperature of combustion air	^{o}C
CA.V	Volumetric flow rate of combustion air	m^{3}
CA.yi	Mole fraction of combustion air components	
ci	Coefficient of heat capacity	
C_p	Heat capacity	J/(mol.K)
di	Coefficient of heat capacity	
DV	Design value	
ECOLOSS	Heat loss of heat exchanger on stack gas flow	MJ
ei	Coefficient of heat capacity	
FG.H	Enthalpy of fuel gas	MJ

J_G	The enthalpy of flue gas at flue gas temperature	MJ
J_{Gb}	The enthalpy of flue gas at reference temperature	MJ
J_L	The enthalpy of combustion air	MJ
KBS.H	Enthalpy of boiler feed water	MJ
KBS.m	Mass flow rate of boiler feed water	kg
KBS.P	Pressure of boiler feed water	atm
KBS.T	Temperature of boiler feed water	^oC
KBS2.H	Enthalpy of boiler feed water after economizer	MJ
KBS2.m	Mass flow rate of boiler feed water after economizer	kg
KBS2.P	Pressure of boiler feed water after economizer	atm
KBS2.T	Temperature of boiler feed water after economizer	^oC
KBS3.H	Enthalpy of KBS3 flow	MJ
KBS3.m	Mass flow rate of KBS3 flow	kg
KBS3.P	Pressure of KBS3 flow	atm
KBS3.T	Temperature of KBS3 flow	^oC
KBS4.H	Enthalpy of KBS4 flow	MJ
KBS4.m	Mass flow rate of KBS4 flow	kg
KBS4.P	Pressure of KBS4 flow	atm
KBS4.T	Temperature of KBS4 flow	^oC
l_U	The ratio of unburned to supplied fuel mass flows	
m	Mass flow rate	kg
m_{ALK}	Mass of tetracontene	kg
m_{ARO}	Mass of chyrenese	kg
m_B	Fuel mass flow	kg
m_{H2S}	Mass of hydrogen sulphide	kg
mi	Mass flow rate of components of flow	kg
MW_avg	Average molecular weight	kg/kmol
MW_j	Molecular weight of component j	kg/kmol
n	Total molar flow rat	kmol
n_{ALK}	Moles of tetracontene	kmol
n_{ARO}	Moles of chyrenese	kmol
n_C	Moles of carbon	kmol
n_H	Moles of hydrogen	kmol
n_H^*	Moles of remaining hydrogen in stream	kmol
n_{H2S}	Moles of hydrogen sulphide	kmol
ni	Molar flow rate of components of flow	kmol

n_S	Moles of sulphur	kmol
P	Pressure	atm
PS	Pseudo Sigma	
Q_{Ab}	Blowdown heat	MJ
QBOILER	Released heat of boiler	MJ
QCAHEAT	Heat loss of preheater on air flow	MJ
Q_{CO}	Loss due to unburned combustibles	MJ
Q_D	Live steam heat	MJ
Q_G	Flue gas losses	MJ
Q_N	The useful heat output	MJ
QRAD	Radiation loss	MJ
QSP	Heat loss of heat exchanger DESUP	MJ
Q_{St}	Losses due to radiation and convection	MJ
Q_Z	Total heat credit	MJ
Q_{ZB}	Heat input	MJ
Q_{Ztot}	The total heat input	MJ
R	Ideal gas constant	J/(mol.K)
rho	Density	kg/m^3
s	Relative density of fuel oil	kg/m^3
SG.H	Enthalpy of stack gas exit second economizer	MJ
SG.ni	Molar flow rate of stack gas exit second economizer	kmol
SG.T	Temperature of stack gas exit second economizer	^{o}C
SG1.H	Enthalpy of stack gas exit first economizer	MJ
SG1.ni	Molar flow rate of stack gas exit first economizer	kmol
SG1.T	Temperature of stack gas exit first economizer	^{o}C
SG2.H	Enthalpy of stack gas exit boiler	MJ
SG2.Hi	Enthalpy values of components of stack gas exit boiler	MJ
SG2.m	Mass flow rate of stack gas exit boiler	kg
SG2.mi	Mass flow rate of components of stack gas exit boiler	kg
SG2.ni	Molar flow rate of components of stack gas exit boiler	kmol
SG2.T	Temperature of stack gas exit boiler	^{o}C
SG2.xi	Weight fraction of components of stack gas exit boiler	
SG2.yi	Mole fraction of components of stack gas exit boiler	
SGLOSS	Heat loss of heat exchanger on stack gas flow	MJ
SGOUT.H	Enthalpy of stack gas released to surrounding	MJ
SGOUT.ni	Molar flow rate of stack gas released to surrounding	kmol

SGOUT.T	Temperature of stack gas released to surrounding	^{o}C
SP.H	The enthalpy of spray water	MJ
SP.m	The mass flow rate of spray water	kg
SP.P	The pressure of spray water	atm
SP.T	The temperature of spray water	^{o}C
SP1.H	The enthalpy of spray water after vaporization	MJ
SP1.m	The mass flow rate of spray water after vaporization	kg
SP1.P	The pressure of spray water after vaporization	atm
SP1.T	The temperature of spray water after vaporization	^{o}C
SPLOSS	Heat loss of heat exchanger on spray water flow	MJ
ST.H	Enthalpy Of Steam inlet	MJ
ST.m	Mass Flow Rate Of Steam inlet	kg
ST.P	Pressure Of Steam inlet	atm
ST.T	Temperature Of Steam inlet	^{o}C
ST3.H	The enthalpy of steam feed the superheater	MJ
ST3.m	The mass flow rate of steam feed the superheater	kg
ST3.P	The pressure of steam feed the superheater	atm
ST3.T	The temperature of steam feed the superheater	^{o}C
ST4.H	The enthalpy of steam exit the superheater	MJ
ST4.m	The mass flow rate of steam exit the superheater	kg
ST4.P	The pressure of steam exit the superheater	atm
ST4.T	The temperature of steam exit the superheater	^{o}C
STGAIN	Heat gain from steam line	MJ
STOUT.H	Enthalpy of steam released	MJ
STOUT.m	Mass flow rate of steam released	kg
STOUT.P	Pressure of steam released	atm
STOUT.T	Temperature of steam released	^{o}C
T	Temperature	^{o}C
V	Volumetric flow rate	m^3
V_{GT}	The dry flue gas volume	m^3
X_{ALK}	Mass fraction of tetracontene	
X_{ARO}	Mass fraction of chyrenese	
X_C	Mass fraction of carbon in fuel oil	
X_H	Mass fraction of hydrogen in fuel oil	
X_{H2S}	Mass fraction of sulphur	
xi	Weight fraction of components of flow	
X_O	Mass fraction of oxygen in fuel oil	

X_S	Mass fraction of sulphur in fuel oil	
y.H2O	Steam composition in combustion air	
y.N2	Nitrogen composition in the combustion air	
y.O2	Oxygen composition in the combustion air	
y_{COT}	Carbon monoxide content by volume of dry flue gas	
y_i	Mole fraction of components of flow	
η_K	Efficiency of steam generator	
μ_{ZD}	The mass of atomizing steam or air per kg of fuel	kg

CHAPTER 1

INTRODUCTION

Basic human needs can be met only through industrial growth, for which energy supply is crucial. The population increase in the last few decades has caused an industrial growth spur, bringing about the need for additional capacity in the areas of power and steam generation throughout the world. As a result of increased demand, the earth's oil and gas reserves face an end after roughly one hundred years. The coal reserves will last for five hundred years in the future [1]. Low cost, high efficiency, reliable and available technology and one of the least hazardous processes to environment are the main reasons for the usage of steam boilers [1], [2].

As is the case with many plants petrochemical plants use steam boilers to produce energy in addition to electrical power which is purchased from electrical power company. In this study, İzmit TÜPRAŞ refinery is taken as basis. In power production plants, boilers, steam turbines and gas turbines are the main equipment to produce steam and obtain electricity. In boilers, steam is produced using the energy released by combustion of fuel coming from the production line. These produced steams at relatively high pressures are also reduced to lower pressures, to obtain electricity in steam turbine. In gas turbine, electricity is produced by compressed air using energy released from fuel combustion. Moreover, the high temperature of air is used to produce steam from water.

In this study, the aim is to comprehensively model a steam boiler with a MATLAB based code, confirmed by ASPEN as a reference. By modeling the process in

MATLAB, the overall efficiency of the system can be tracked easily. When the process starts to run regularly and systematically, not only the bad data (outliers of the system) can be eliminated but also missing data can be estimated in the real system.

1.1 Refinery Production

1.1.1 Boilers

Invention of boilers that are used to produce huge energy today is based on very ancient times. The first combined reaction turbine and boiler was invented by Hero of Alexandria about 100 BC, and domestic boilers were known in Pompeii in the first century AD [3], [4].

A boiler is an enclosed vessel that provides a means for combustion heat to be transferred into water until it becomes heated water or steam. The hot water or steam under pressure is then usable for transferring the heat to a process [5]. In chapter 2, boilers are explained in detail. A typical boiler room schematic is shown in Figure 1.1.
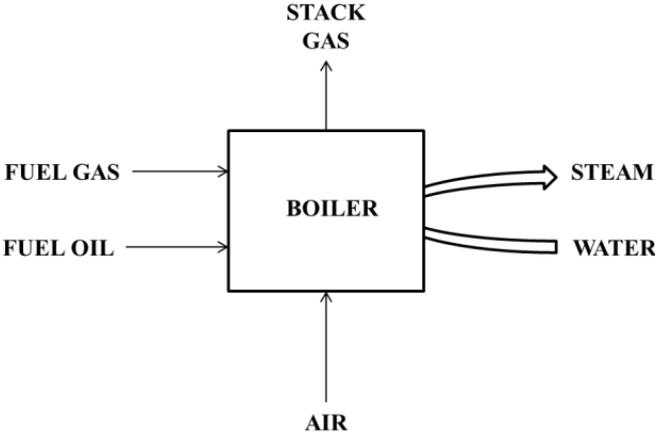
Figure 1.1 – Schematic of boiler

1.1.2 Gas Turbines

A gas turbine is a machine that converts fuel energy to mechanical energy such as an automobile engine [6]. Compressor, combustor, turbine and generator are the main components of gas turbines.

Ambient air is compressed to higher pressure values in the compressor. Compressed air and fuel enter the combustor. Under constant pressure, combustion reactions occur and temperature increases. Energy from hot gases from the combustor is converted to work in the turbine. Some amount of this work is used to rotating the turbine and the remaining is converted to electricity with a generator. Most industrial-type gas turbines work on this principle [7], and a typical gas turbine schematic is shown in Figure 1.2 [6].
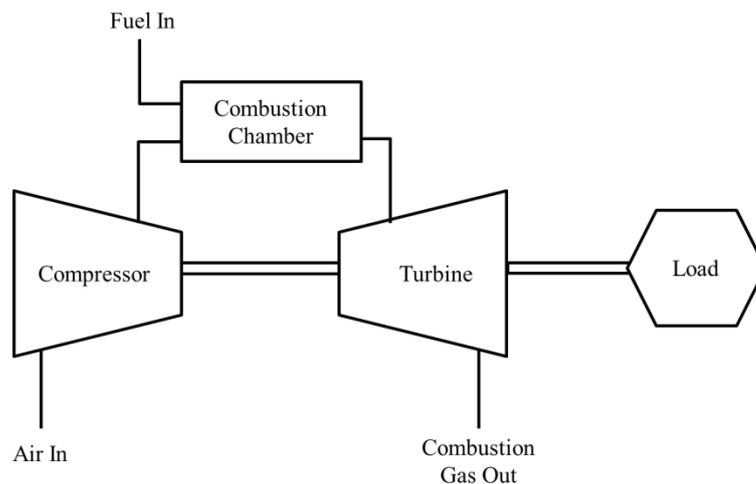
Figure 1.2 – Schematic of gas turbine [6]

1.1.3 Steam Turbines

Steam turbines are similar to gas turbines except combustor and compressor parts. They provide steam for power generation. Steam at high temperature and pressure is reduced to lower temperature and pressure levels. In this process, heat energy is first converted into kinetic energy which is then converted into mechanical work [8]. It is

suitable for use in heaters, pumps and blowers [9]. A typical steam turbine schematic is below in Figure 1.3.
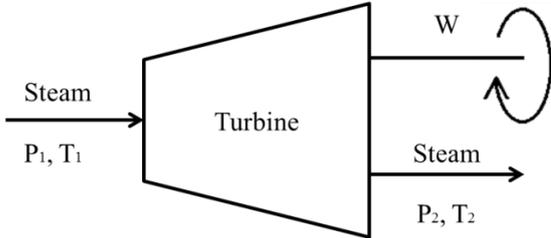
Figure 1.3 – Schematic of steam turbine

1.2 Typical Refinery Set-up

A typical refinery utility flowchart is shown below, in Figure 1.4. There may be multiple boilers, turbines and steam turbines. When multiple equipment is used to achieve the same process objective, there exists the possibility of different operational combinations, thereby generating optimization problems.
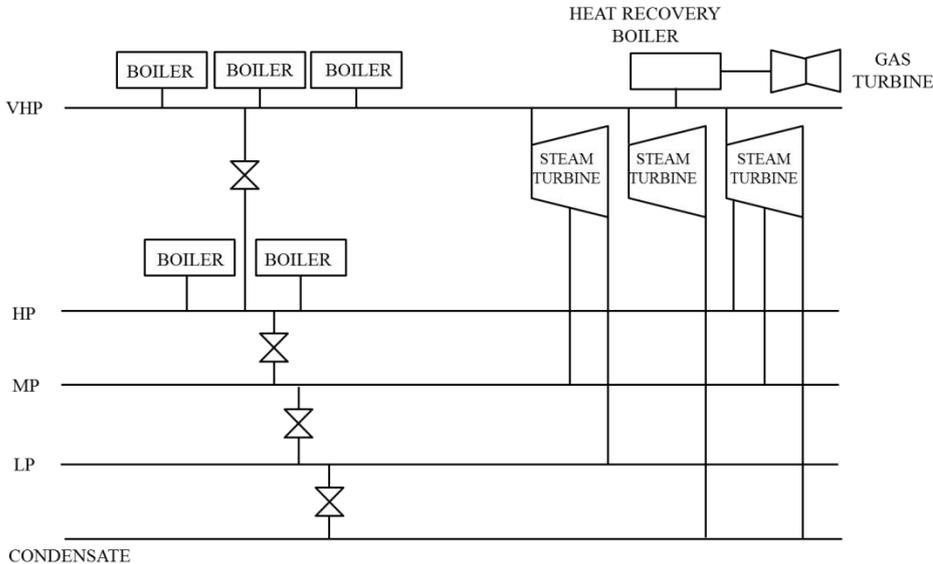
Figure 1.4 – Typical refinery flowchart

4

VHP   : Very High Pressure Line

HP   : High Pressure Line

MP   : Medium Pressure Line

LP   : Lower Pressure Line

1.3 Purpose of the Study

The ultimate aim of the project is to optimize refinery power production; however this thesis concentrates on boilers as they make up a large portion of the energy conversion.

In accordance with this purpose, in this Chapter, general information about power plants is given. In the second Chapter, a literature survey for steam boiler modeling is discussed in detail. Approaches of modeling in ASPEN and MATLAB are discussed in Chapter 3. Then, results are presented in Chapter 4, followed by conclusions in Chapter 5. Additional information about modeling methods, MATLAB codes and snapshots of ASPEN are presented in the Appendices.

CHAPTER 2

BACKGROUND OF MODELING

2.1 Boilers in General

Steam is used in nearly every industry, and it is well known that steam generators and heat recovery boilers are important in power and process plants [10]. As the name suggests, a boiler is a device that boils water to produce steam. More precisely, a boiler converts the chemical energy of the fuel into the thermal energy in steam, or the thermal energy of hot gases into the thermal energy of steam when no firing is involved [2].

In order to describe the principles of a steam boiler, a very simple case, where the boiler simply is a container, partially filled with water can be considered (Figure 2.1).
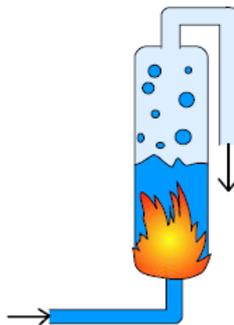
Figure 2.1 – Simplified boiler drawing [2]

Combustion of fuel produces heat, which is transferred to the container and makes the water evaporate. The vapor or steam can escape through a pipe that is connected to the container and it can be transported elsewhere. Another pipe brings water (called "feed-water") to the container to replace the water that has evaporated and escaped [1].

When considering a simple power plant cycle, the steam boiler provides steam to power an engine. The steam turbine extracts heat from the steam and turns it into work [1]. A generator is usually connected to the turbine to produce electricity from the work. After leaving turbine, the steam is recycled by cooling it until condenses into water and then returns it as feed-water to the boiler. However, there should be a pump in this line because the pressure of steam drops expeditiously while exiting from the turbine. Since the work needed to compress a fluid is about a hundred times less than the work needed to pressurize a gas, the pump is set after the condenser. This cycle is called a Rankine cycle and is the basis of most modern steam power plant processes. Figure 2.2 represents the schematic of typical modern steam power plants.
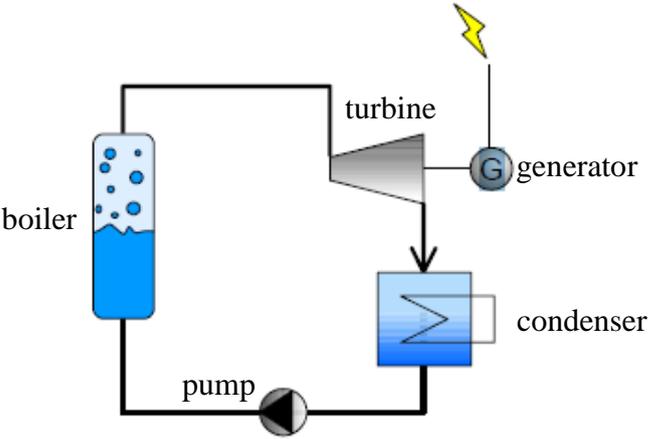
Figure 2.2 – Modern steam power plant processes [2]

The types of boiler available in industrial use are: [2], [11], [12]

- *Fire-tube boilers* in which flue gases are inside and water is outside
- *Water-tube boilers* in which water is inside and flue gases are outside
- *Combination boilers* in which flue gases and water flow both outside and inside the tubes; and which contain an external furnace and shell-type boiler in a sequence

Fire-tube boilers are the most common type of boilers. However, they correspond to much larger outputs than fire-tube boilers since 29% of the total boilers are water-tube boilers. Indeed, it is known that water-tube boilers are usually used in large industrial plants operating continuously. So, demands for power and heat should be in good balance in such as chemical works, oil refineries and steel industry. The fire-tube boilers cannot satisfy the need of high pressure and temperature [13].

In large industrial plants, some arrangements are made on water-tube boilers for the purpose of increasing overall efficiency. In an air heater, the incoming air is preheated and feed water is heated in an economizer using released heat of stack gas. If it is preferred to heat the steam above saturation temperature by just a turbine installation, a superheater is linked on the boiler [12]. In addition to these, there are also deaerators, feed pump, attemperator, steam system, condenser, condensate pump, sets of controls to monitor water and steam flow, fuel flow and airflow [14].

2.2 Boilers Modelled

This work is based on a water-tube boiler. In Figure 2.3, a simple schematic of modelled boiler with its components, which are air preheater, fuel oil atomizer, economizer, blowdown unit and superheater is shown.
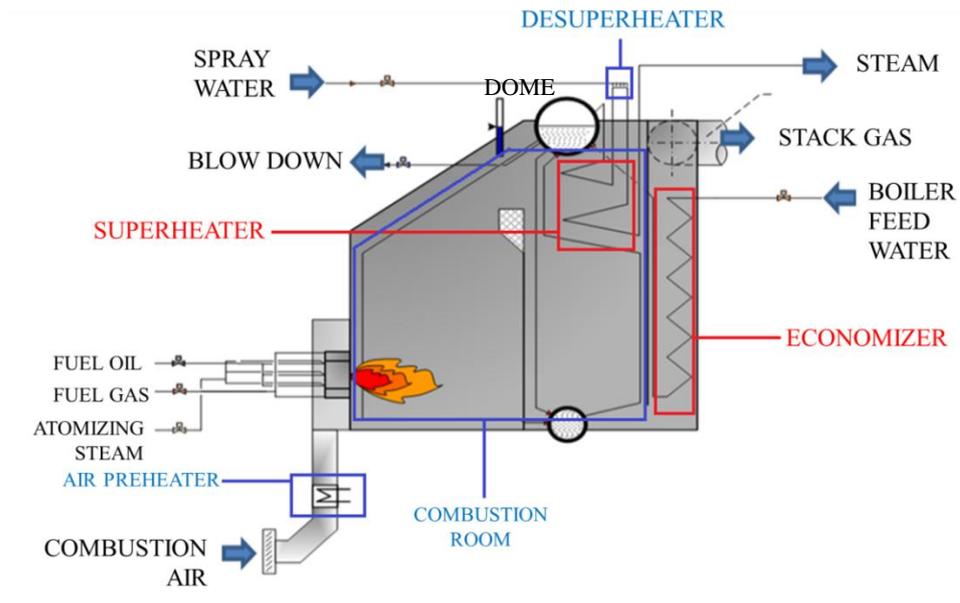
Figure 2.3 – Modelled boiler schematic

2.2.1 Air Preheater

To increase the overall efficiency, recovering the released heat of stack gas, combustion air is preheated in a preheater [2]. Raising the temperature of combustion air also increases the burning velocity. This helps to obtain flame stability and reduce flame volume [11]. Indeed, providing excess air in different levels is important to ensure sufficient oxygen supply for combustion. However, excess air reduces the overall efficiency by decreasing the temperature of boiler furnace and absorbing heat that would otherwise be available for steam production. Therefore, it is necessary to supply the optimum amount of combustion air [12].

2.2.2 Economizer

Economizers are also installed in the same manner with air pre-heaters on the stack gas line instead of air flow line. They take heat from the flue gases which they transfer via extended surface elements to the feed-water immediately prior to the

water entering the boiler [15]. In addition to decreasing the gas temperature, the economizer performs another important task of narrowing the difference between feed and drum temperatures, thereby reducing the thermal shock to drum and water walls [2]. Because these operate at relatively low pressures and exit temperatures economizers are used in connection with water-tube boilers, largely [11].

2.2.3 Blowdown

Boiling water generated steam and dissolved solids contained in the water remain in the boiler. If feed-water contains more solids, they become water-insoluble and precipitation occurs. This precipitation causes impaired water circulation and lowers the boiler safety. To prevent such a situation from arising, the solids inside the boiler water are limited, the level being controlled by the removal from the water with a high solids concentration. This process of water removal from the boiler is called blowing down. It is achieved by the manual or automatic operation of a valve positioned so as to remove the water from the point of highest dissolved solids concentration [11]. The simplest way of blowing down is to open the main bottom blowdown valve for a set period of time at regular intervals. This method may also be extended to larger boilers where conditions are such that there is little build-up of solids. Such conditions could be high-condense returns and good-quality make-up feed-water [15]. Using continuous blowdown has many of practical advantages [11].

1. The blowdown, and hence the quantity of feed-water necessary to replace it, is a steady flow instead of having short-term peaks.
2. The boiler water total dissolved solids (TDS) is constant at a given load and hence so is steam purity.
3. Once the blowdown valve is set for given conditions there is no need for regular operator intervention.

2.2.4 Superheater

Heat is added after all the water is converted to saturated steam in an evaporator. While latent heat is added in the evaporator circuits, superheat is added in the superheater. The efficiency of the steam cycle is improved by higher steam pressure and temperature. Superheating of steam should be as high as possible. When the pressure of steam is 120 bar and higher, the cycle efficiency increase about 1% [2].

2.2.5 Fuel Oil Atomizer

Atomizers are used to break down a film of liquid into a fine spray. Atomization of fuel oil gives an opportunity for a complete combustion in a very short time [2]. Moreover, they ensure minimum amount of deposits on the heating surfaces [16].

CHAPTER 3

MODELING AND APPROACH

3.1 Approach

The focus of this modeling effort is the steam boiler. Boilers are first modelled using ASPEN software, and then this model is used to confirm the MATLAB model. The purpose of using ASPEN software is that it gives highly reliable results which can be used as reference. MATLAB Software on the other hand can be easily integrated in real time optimization programs, which is the reason of using MATLAB software. Therefore, MATLAB-based models to be used for applications are to be confirmed by the ASPEN model.

The two main goals of the modeling are confirmation of quality of data and usage of calculated equipment efficiencies in an optimization program. The MATLAB code, confirmed with ASPEN, is used in optimization decisions. Defective measuring equipment can be determined through inconsistencies in mass and energy balances. Therefore, these equipment units can be calibrated, repaired or replaced. Subsequently, critical measurement equipment units provide consistent data using optimization decisions.

To complement the modeling, some studies are detailed in Chapter 4, Appendix A and Appendix B. Sensivity analysis of the model is made in Chapter 4. With this analysis, equipment units which should have more accurate measurement are

determined. In Appendix A, the results of modeling the combustion of fuel oil which are adopted after literature search are explained. The studies in Appendix B are related with consideration and verification of some correlations of specific heat capacity which is very important for calculating enthalpy values.

3.2 Modeling

Boiler working principle is the production of vapor from boiler feed water using combustion heat of fuel oil and fuel gas. Its flowchart is illustrated in Figure 3.1. The denominations of the streams are used in both ASPEN and MATLAB codes.
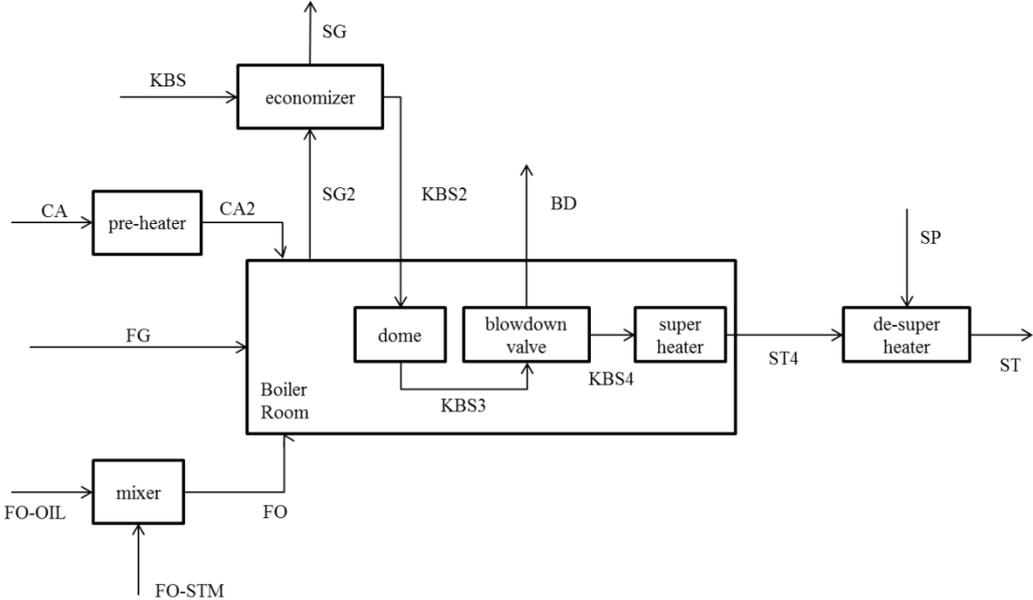
Figure 3.1 – Flowchart of boiler

In the combustion room, energy is obtained from combustion of fuel gas (FG) and fuel oil (FO) with combustion air (CA). Before the combustion room, fuel oil is atomized with some steam (FO-STM) for the purpose of best possible heat release and minimum amount of deposits on the heating surfaces. To increase the combustion efficiency, the temperature of combustion air is increased in preheater.

The stream leaving the preheater is called as CA2. Boiler feed water (KBS) is first heated with hot stack gas (SG2) and then released energy is decreased in stack gas (SG). This equipment is called the economizer.

After preheating, boiler feed water (KBS2) is heated more in dome, and the stream leaving the dome is called KBS3. If necessary, a part of stream is separated in blowdown stream (BD). The purpose of blowdown is to refresh the circulated water in the plant. The rest of the KBS3 is dented by KBS4 and it feeds the superheater. The steam exit the superheater is called ST4. Sometimes temperature of ST4 can be higher than the temperature of steam used in plant, and then it is decreased to needed temperature with necessary amount of water, SP.

The system is modelled with the following assumptions:

- There is a steady-state operation.
- Complete combustion occurs in the boiler. This is supported by the fact that oxygen amount in the stack gas is maintiained at 3-4% by adjusting the incoming combustion air and that CO levels in the same stack gas are monitored and seen to be at the ppm level during refinery operation.
- There are uniform physical and material properties. Temperature and composition distribution are not considered.
- The system is modelled based on adiabatic equipment. This approach is justified by the fact that at the end of the operation, an imaginary heat flow is defined to capture all combined losses. So in reality, the overall system is not adiabatic but only the individual unit operations are.
- Air, fuel gas and stack gas streams are modelled using ideal gas properties in MATLAB, because there is not much difference between Peng Robinson equation of state, mostly used in modelling refinery opearions and the ideal gas approach as confirmed with ASPEN simulations. The temperatrure and pressures of these streams also justify this assumption. Only the high pressure steam streams are at high enough pressures to make this assumption unrealistic and those streams are modelled based on the steam tables.

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3.3 Combustion Reaction Stoichiometry

In the plant, there are two types of fuel, fuel gas and fuel oil. Fuel gas has nineteen components whereas fuel oil analysis is based on a mixture of carbon, hydrogen and sulphur. Combustion reactions of each component are shown below. Complete combustion is assumed throughout this study which is confirmed by tracking the carbon monoxide content of the flue gas, always observed to be at about 100 ppm levels.

Fuel Gas:

1.	Hydrogen	:	$H_2 + 0.5\ O_2 \rightarrow H_2O$
2.	Carbon monoxide	:	$CO + 0.5\ O_2 \rightarrow CO_2$
3.	Hydrogen Sulfide	:	$H_2S + 1.5\ O_2 \rightarrow H_2O + SO_2$
4.	Methane	:	$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$
5.	Ethane	:	$C_2H_6 + 3.5\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$
6.	Ethylene	:	$C_2H_4 + 3\ O_2 \rightarrow 2\ CO_2 + 2\ H_2O$
7.	Propane	:	$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$
8.	Propadiene	:	$C_3H_4 + 4\ O_2 \rightarrow 3\ CO_2 + 2\ H_2O$
9.	Propylene	:	$C_3H_6 + 4.5\ O_2 \rightarrow 3\ CO_2 + 3\ H_2O$
10.	n-Butane	:	$C_4H_{10} + 6.5\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$
11.	iso-Butane	:	$C_4H_{10} + 6.5\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$
12.	iso-Butylene	:	$C_4H_8 + 6\ O_2 \rightarrow 4\ CO_2 + 4\ H_2O$
13.	1-Butene	:	$C_4H_8 + 6\ O_2 \rightarrow 4\ CO_2 + 4\ H_2O$
14.	T-2 Butene	:	$C_4H_8 + 6\ O_2 \rightarrow 4\ CO_2 + 4\ H_2O$
15.	C-2 Butene	:	$C_4H_8 + 6\ O_2 \rightarrow 4\ CO_2 + 4\ H_2O$
16.	1,3-Butadiene	:	$C_4H_6 + 5.5\ O_2 \rightarrow 4\ CO_2 + 3\ H_2O$
17.	n-Pentane	:	$C_5H_{12} + 8\ O_2 \rightarrow 5\ CO_2 + 6\ H_2O$
18.	iso-Pentane	:	$C_5H_{12} + 8\ O_2 \rightarrow 5\ CO_2 + 6\ H_2O$
19.	C6	:	$C_6 + 6\ O_2 \rightarrow 6\ CO_2$

Fuel Oil:

1.   C   : $C + O_2 \rightarrow CO_2$

2.   H   : $2\,H + 0.5\,O_2 \rightarrow H_2O$

3.   S   : $S + O_2 \rightarrow SO_2$

Fossil fuels, oil and natural gas are available in combined of carbon, hydrogen and in some cases sulphur. Therefore, combustion reactions of fuel oil are represented on an atomic scale. A pseudo component approach is outlined in Appendix A. In Table 3.1, mass compositions of some typical fuel oils are tabulated [17].

Table 3.1 – Analyses of some typical liquid fuels (by mass)

	Unit	Gasoline	Diesel	Light Fuel Oil	Heavy Fuel Oil	Residual Fuel Oil
Carbon		0.862	0.838	0.834	0.829	0.883
Hydrogen		0.128	0.121	0.117	0.114	0.095
Sulfur		-	-	-	-	-
Nitrogen		-	-	-	-	-
Oxygen		-	-	-	-	-
Ash		-	0.006	0.009	0.012	0.010
Density	kg/L	0.760	0.870	0.900	0.950	0.950
Gross Calorific Value	kJ/kg$_F$	46490	44942	44290	43746	42511
Net Calorific Value	kJ/kg$_F$	43623	42232	41669	41193	40383

3.4 Heating Values of the Fuel Gases

According to Perry's Handbook [18], the heating values of fuel gases are tabulated in Table 3.2.

Table 3.2 – Heating values of fuel gas components

	Chemical Formula	H_{rxn-i} (MJ/kmol)
Hydrogen	H_2	241.8
Carbon monoxide	CO	283
Hydrogen Sulfide	H_2S	518
Methane	CH4	802.6
Ethane	C_2H_6	1428.6
Ethylene	C_2H_4	1323
Propane	C_3H_8	2043.1
Propadiene	C_3H_4	-
Propylene	C_3H_6	1925.7
n-Butane	C_4H_{10}	2657.3
iso-Butane	C_4H_{10}	2649
iso-Butylene	C_4H_8	-
1-Butene	C_4H_8	2540.8
T-2 Butene	C_4H_8	2530.3
C-2 Butene	C_4H_8	2533.9
1,3-Butadiene	C_4H_6	2409
n-Pentane	C_5H_{12}	3244.9
iso-Pentane	C_5H_{12}	3239.5
C6	C_6	-

3.5 Efficiency Modeling Methods

Efficiency tests help us to find out the efficiency deviation from the best efficiency and target problem area for corrective action. Therefore, efficiency is the main performance parameter of any equipment [19].

Design characteristics of the boiler, the fuel burned, the type of burner and the conditions of the operation are the main factors which are used in determination of the steam boilers' efficiency. The controllable items that affect the maximum efficiency of a steam generator are excess air, flue gas temperature, unburned combustibles, poor maintenance, and low capacity operation [12]. This section details some of the approaches published in the literature for tracking boiler efficiencies.

3.5.1 Determination of Boiler Efficiency

The German DIN 1942 and the American ASME standards are the main standards used for definition of boiler efficiency. Although the ASME standard is in regard to higher heating value, the DIN 1942 is based on lower heating value that is widely used in Europe [20].

If the water vapor formed during combustion is condensed, the amount of heat produced by the complete combustion of a unit quantity of fuel oil is called as higher heating value (HHV); if water vapor is not condensed, it is called as lower heating value (LHV) [21].

In this section, determination and calculation of boiler efficiency is explained by using the DIN 1942 standard. According to the standard [20], there are three factors that determine the boiler system used in efficiency: heat input, useful heat output and losses.

Heat Input

The heat input, Q_{ZB}, consists of heat in fuel (chemical heat), heat in combustion air and heat in atomizing steam. This is expressed by the Equation (3.1).

$$Q_{ZB} = m_B[(H_u + h_B + \mu_{ZD}h_{ZD})/(1 - l_u) + J_L]$$

(3.1)

Where m_B is the fuel mass flow, H_u is the net calorific value of fuel at reference temperature (t_B), h_B is the enthalpy of fuel, μ_{ZD} is the mass of atomizing steam or air per kg of fuel, and h_{ZD} is the enthalpy of atomizing steam, l_u is the ratio of unburned to supplied fuel mass flows, J_L is the enthalpy of combustion air.

Useful Heat Output

The useful heat output, Q_N, is the total heat which is transferred in the system generator to the water or steam, the enthalpy of blowdown water being added to the useful output. This is expressed by equation (3.2).

$$Q_N = Q_D + Q_Z + Q_{Ab} \qquad (3.2)$$

Where Q_D is live steam heat, Q_Z is total heat credit and Q_{Ab} is blowdown heat.

Losses

Losses can be categorized in three terms: flue gas losses (Q_G), loss due to unburned combustibles (Q_{CO}) and losses due to radiation and convection (Q_{St}). Flue gas losses and loss due to unburned combustibles are calculated using Equations (3.3) and (3.4).

$$Q_G = m_B(J_G - J_{Gb}) \qquad (3.3)$$

$$Q_{CO} = m_B V_{GT} y_{COT} H_{uCOn} \qquad (3.4)$$

In this equation m_B represents the fuel mass flow, J_G represents the enthalpy of flue gas at flue gas temperature (t_G), J_{Gb} represents the enthalpy of flue gas at reference temperature (t_b). V_{GT} represents the dry flue gas volume, y_{COT} represents the carbon monoxide content by volume of dry flue gas and H_{uCOn} is the net calorific value per cubic meter of carbon monoxide, related to standard conditions.

Normally, to measure heat losses due to radiation and convection are not possible because of unknown parameters of the system, so empirical values are to be used. For the most common steam generator designs as a function of the maximum useful heat output, the radiation loss is expressed by the Equation (3.5).

$$Q_{St} = C Q_N^{0.7} \qquad (3.5)$$

Where C is 0.0113 for fuel oil and natural gas boilers, 0.0220 for hard coal boilers and 0.0315 for brown coal and fluidized-bed combustion boilers and Q_N is the maximum useful heat output.

There is research [11] that tabulates the typical values of thermal efficiency in Table 3.3. As it is seen from table, by far the greatest heat loss is that carried away by the flue gases, a reduction of the flue gas temperature of 20°C is equivalent to an increase in thermal efficiency of approximately 1%.

Table 3.3 – Typical values of thermal efficiency

		Natural Gas	Oil	Coal
Flue gas temperature	C	125	180	160
Excess air supplied	%	10	10	35
Dry gas loss	%	3.39	5.68	6.21
Moisture loss	%	10.67	6.56	4.90
Unburnt combustible loss	%	0.00	0.10	2.00
Moisture in air loss	%	0.07	0.11	0.12
Radiation loss	%	0.60	0.60	1.20
Total losses	**%**	**14.73**	**13.05**	**14.43**

3.5.2 Calculation of Boiler Efficiency

The steam boiler efficiency is the ratio of useful energy output to the energy input. The difference between energy input and output is the sum of the various energy losses from the boiler as explained previous section. The efficiency of a boiler can therefore be expressed alternatively as 100% minus the sum of the losses expressed as a percentage of the input energy. The two definitions of efficiency given above lead to two methods of measuring it [12] :

- by direct method
- by indirect method

The Direct Method

This method is also known as "input-output method" because it needs only the useful output and the heat input to calculate the efficiency. In this method, various losses cannot be calculated or when efficiency of system is lower, this method does not give the reason. However with this method, operators can evaluate quickly the efficiency

of boiler because of few instruments for monitoring and few parameters for computation. The efficiency is calculated by the Equation (3.6).

$$\eta_K = \frac{Q_N}{Q_{Ztot}}$$
(3.6)

Where η_K represents efficiency of steam generator, Q_N represents useful heat output and Q_{Ztot} represents the total heat input.

The Indirect Method

This method is also known as "heat loss method" because it calculates the efficiency subtracting the heat losses. It is now generally accepted [22], [23], [24] that the indirect method yields more accurate results. Moreover, this method is used to understand what affects the efficiency, loss areas which need more attention [12]. The efficiency is calculated by the Equation (3.7).

$$\eta_K = 1 - \frac{Q_G + Q_{CO} + Q_{St}}{\dot{Q}_{Ztot}}$$
(3.7)

In this equation, η_K represents efficiency of steam generator, Q_{Ztot} represents the total heat input, Q_G represents the flue gas losses, Q_{CO} represents loss due to unburned combustibles and Q_{St} represents the losses due to radiation and convection.

3.6 ASPEN Model

In the modeling approach of this study, the indirect method is adapted, carrying out detail material and energy balances on every equipment. The ASPEN model is represented in Figure C.1. Applied and expanded version of Figure 3.2 is modeled in ASPEN software. In the bottom-left of flow-sheet, fuel gas and atomized-fuel oil are

feed with combustion air to combustion room, called as BOILER in the flow-sheet. Hot stack gas (SG2) at certain temperature is sent to the economizer, ECO1. In ECO1, using energy of SG2, certain temperature and pressure boiler feed water (KBS) is heated to hot boiler feed water (KBS2). Cooled stack gas (SG1) is fed to an imaginary economizer, ECO2. In the refinery, this kind of economizers does not exist; however it is put into simulation. The reason of using imaginary heat exchangers is that they are used in energy balance checking.

Part of the energy of BOILER is released with stack gas and the rest is called HCOMB, which is used in heating process of KBS. Exit stream of ECO1, called KBS2, is first heated in DOME at liquid phase. Released computable heat, QBOILER, is calculated with enthalpies of KBS2 and KBS3 and then it is fed to vaporization unit, L2V. Although heating and vaporization process occurs at the same time, it is put into model separately to provide the measured plant conditions of blowdown stream. The rest of energy in superheated steam in QBOILER is released with QRAD. The amount of QRAD is defined as the energy cannot be transferred to boiler feed water from HCOMB and it comes out as radiation loss of the system.

On the right of the flow-sheet, there is a section at which produced superheated steam is cooled to steam distribution line of refinery. This process occurs with spraying the boiler feed water to superheated steam in the plant. However, it starts with calculation of energy between SP4 and SP3in equipment called as DESUP in the ASPEN. The only difference between them is temperature value. Released energy from DESUP, called as QSP, is used for vaporization of boiler feed water, and then thrown out as SPLOSS. At the end of the process, at the same temperature and pressure SP1 and SP3 are mixed in SPMIXER, then the steam, SP, is feed to main steam line of refinery.

In the simulation, as well as all real plant equipment units there are some imaginary heat exchangers in front of each outlet that convert temperature and pressure values to inlet conditions. Using these energy values of economizers (SGLOSS, BDLOSS and STGAIN), efficiencies for each steam can be calculated in detail.
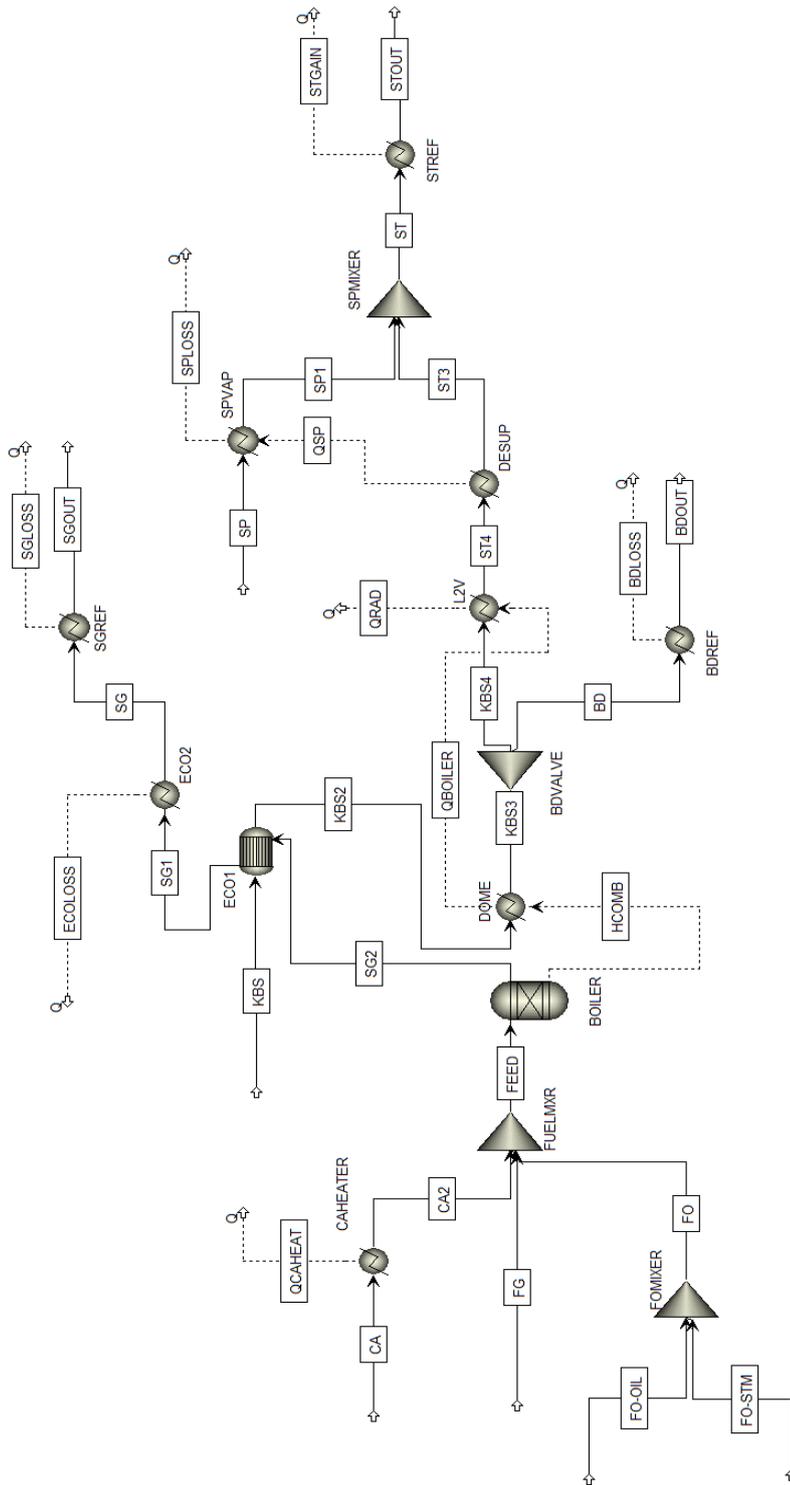
Figure 3.2 – Snapshot of all streams in the ASPEN model

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3.7 MATLAB Model

The MATLAB code implements the same model in the MATLAB environment. The flowchart of the MATLAB Model is represented in Figure 3.3 that shows each step in the code.
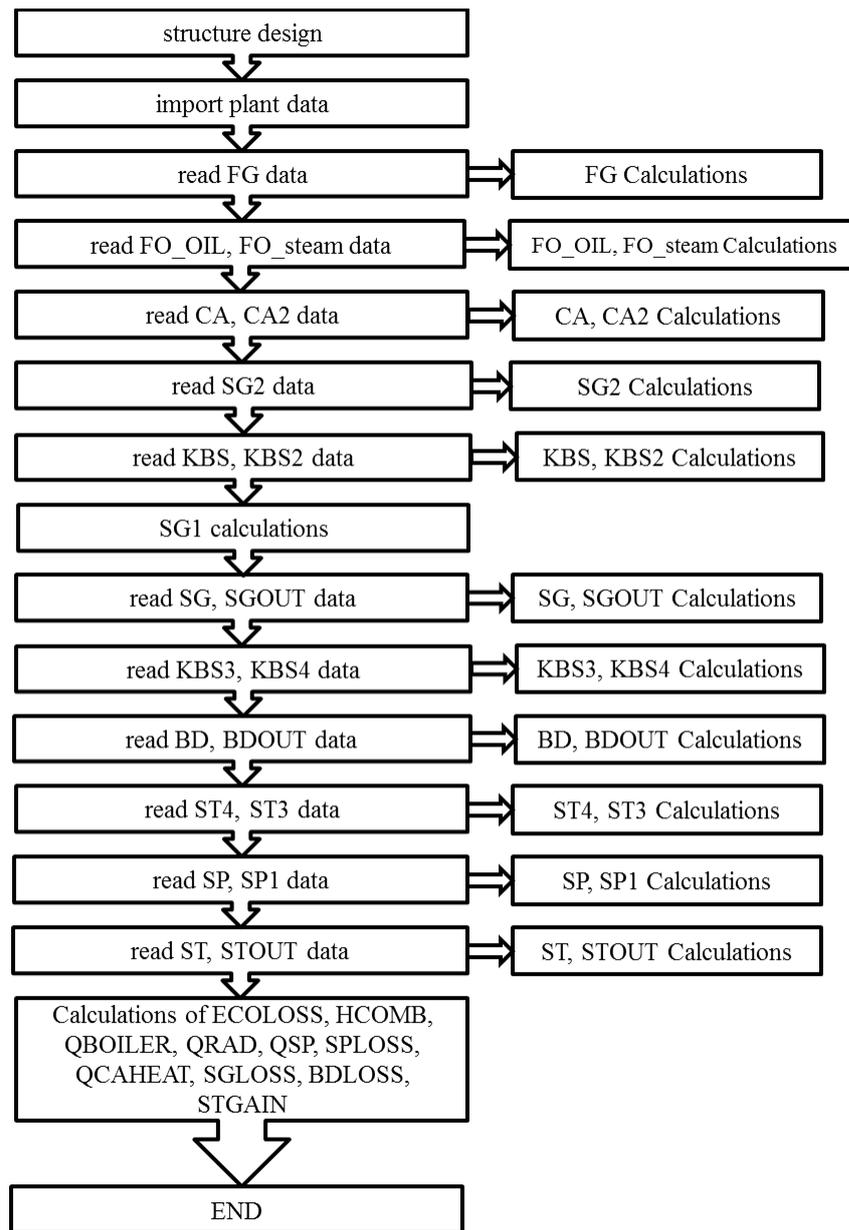
Figure 3.3 – Flowchart of MATLAB model

In the beginning, all streams are defined as structure variables. The structure variable in MATLAB allows one to combine different data types under a single name. First eight fields define the overall properties of streams. They are mass flow rate, pressure, temperature, volumetric flow rate, density, enthalpy, heat of combustion and number of components of streams, respectively m, P, T, V, rho, H, Hrxn and i. Next six fields define composition properties. They are mass flow rate, number of moles, mass fraction, mole fraction, enthalpy and heat of combustion of each component of steams, respectively mi, ni, xi, yi, Hi and Hirxn. Finally, identifiers which are plant, case and stream are defined in fifteenth, sixteenth and seventeenth fields. These definitions form the structure is designed for each component of all streams and tabulated in Table 3.4.

Table 3.4 – Field definitions of MATLAB code

	definitions		definitions		definitions
Field 1	m	Field 7	Hrxn	Field 13	Hi
Field 2	P	Field 8	i	Field 14	Hirxn
Field 3	T	Field 9	mi	Field 15	Plant name
Field 4	V	Field 10	ni	Field 16	Case
Field 5	rho	Field 11	xi	Field 17	Stream
Field 6	H	Field 12	yi		

After designing structure, plant data are imported from an excel sheet called "FeedData.xls". This sheet includes all information used in simulation for all scenarios, called as plant data. Then, data are called from the plant data and all properties of each stream are calculated in a loop that covers all scenarios.

In the first part, properties of fuel gas (FG) are calculated. For this purpose, a code is written in FG_Calculations2.m file. For each component of fuel gas, this m-file firstly imports molecular weight, coefficients of heat capacity (ideal gas) and heat of

combustion values from a excel sheet called "FG_Constants.csv". Then, average molecular weight (MW_avg) is calculated by using Equation (3.8).

$$MW\_avg = \sum_i MW_i * FG.yi \tag{3.8}$$

MW_i denotes the molecular weight of each component and FG.yi denotes mole fraction of each component in the fuel gas. Using ideal gas law, density and volumetric flow rate of fuel gas are calculated by Equation (3.9) and (3.10), respectively.

$$FG.rho = \frac{FG.P * MW\_avg}{R * FG.T} \tag{3.9}$$

$$FG.V = \frac{FG.m}{FG.rho} \tag{3.10}$$

In these equations, density, pressure, temperature and volumetric flow rate of fuel gas are represented as FG.rho, FG.P, FG.T and FG.V, respectively. Then, total mole flow is calculated by Equation (3.11).

$$n = \frac{FG.m}{MW_{avg}} \tag{3.11}$$

FG.m denotes the mass flow rate of fuel gas. After determining total mole flow, mole flows, mass flows and heat of combustion values of each component are calculated in Equations (3.12), (3.13) and (3.15), respectively. Modifying the Aly-Lee Cp correlation, Equation (B.5), enthalpy value is calculated in Equation (3.14).

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$$FG.ni = n * FG.yi \tag{3.12}$$

$$FG.mi = FG.ni * MW_i \tag{3.13}$$

$$FG.Hi = FG.ni * \left(a_i * (FG.T) + \frac{2 * b_i * c_i}{\exp\left(\frac{2 * c_i}{FG.T}\right) + 1} + \frac{2 * d_i * e_i}{\exp\left(\frac{2 * e_i}{FG.T}\right) - 1} \right) \tag{3.14}$$

$$FG.Hirxn = -Hrxn * FG.ni \tag{3.15}$$

In these equations, FG.ni denotes component mole flow rate, FG.mi denotes component mass flow rate, FG.yi denotes component mole fractions, FG.Hi denotes enthalpy of components, and FG.T denotes temperature of fuel gas. Hrxn denotes heat of combustion of each component in the fuel gas and a_i, b_i, c_i, d_i and e_i are the coefficients of heat capacity of components in the fuel gas. Then, total enthalpy and heat of combustion values are calculated by Equation (3.16) and (3.17), respectively.

$$FG.H = \sum_i FG.H_i \tag{3.16}$$

$$FG.Hrxn = \sum_i FG.Hrxn_i \tag{3.17}$$

In the second part of main driver code, properties of fuel oil are calculated. For this purpose, a code is written in FO_OIL_calculations2.m file as fuel oil calculations. For each component of fuel oil, this m-file firstly imports the some constants that are molecular weight and heat of combustion values from a excel sheet called "FG_Constants.csv". Then, like fuel gas calculations, mass flow rates (FO_OIL.mi), mole flow rates (FO_OIL.ni), heat of combustion of components (FO_OIL.Hirxn) in

fuel oil and total heat of combustion (FO_OIL.Hrxn) are calculated by Equations (3.18), (3.19), (3.20) and (3.21), respectively.

$$FO\_OIL.mi = FO\_OIL.m * FO\_OIL.xi \qquad (3.18)$$

$$FO\_OIL.ni = FO\_OIL.mi/MW_i \qquad (3.19)$$

$$FO\_OIL.Hirxn = -Hrxn * FO\_OIL.ni \qquad (3.20)$$

$$FO\_OIL.Hrxn = \sum_i FO\_OIL.Hirxn \qquad (3.21)$$

In these equations FO_OIL.m denotes total mass flow rate, FO_OIL.xi mass fraction of each component in the fuel oil (FO_OIL). To calculate total mole flow rate (nT) Equation (3.22) and to calculate mole fractions (FO_OIL.yi) of each component Equation (3.23) are used as below.

$$nT = \sum_i FO\_OIL.ni \qquad (3.22)$$

$$FO\_OIL.yi = \frac{FO\_OIL.ni}{nT} \qquad (3.23)$$

In fuel oil calculations, API value is assumed as 11.5, which is the average value used in plant. Accordingly, relative density of fuel oil (s) is calculated in Equation (3.24) [18].

$$s = \frac{141.5}{131.5 + \text{API}} \qquad (3.24)$$

To determine the heat capacity of fuel oil (C_p), Equation (3.25) [18] is used and the enthalpy of fuel oil is calculated by Equation (3.26).

$$Cp = \frac{1.685 + FO\_OIL.T * 0.039}{\sqrt{s}} \qquad (3.25)$$

$$FO_{OIL}.H = FO_{OIL}.m * Cp * FO_{OIL}.T \qquad (3.26)$$

Temperature of fuel oil (FO_OIL.T) is in $^{\circ}$C and therefore C_p is calculated in kJ/(kg.$^{\circ}$C).

The fuel oil properties are calculated as above. To atomize the fuel oil, steam is sprayed on the fuel oil, as much as one-third fuel oil amount. In the next part of main driver code, this steams properties are called from plant data and enthalpy of fuel-oil steam (FO_steam.H) is calculated using XSteam function. Xsteam function is a database that gives enthalpy values of water and steam at defined temperature and pressure values [25]. Then, in FO_calculations.m file fuel oil properties (FO_OIL) and steam used in fuel oil (FO_steam) are put together to use as a one fuel oil stream (FO) before the boiler.

In the next part of main driver code, combustion air (CA) properties are calculated. Before this calculation, composition of air is determined. According to relative humidity, temperature and pressure water fraction (y.H2O) is determined from XSteam function. Then, nitrogen (y.N2) and oxygen (y.O2) composition in the combustion air are calculated in Equations (3.27) and (3.28), respectively and results are written into plant data.

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$$y.N2 = \frac{0.79}{1 + y.H2O} \tag{3.27}$$

$$y.O2 = \frac{0.21}{1 + y.H2O} \tag{3.28}$$

Then, total mass flow rate, pressure, temperature and mole fraction of combustion air is read from plant data. Same as fuel gas and fuel oil procedure, first a code is written in CA_calculations2.m file as combustion air calculations. For each component of combustion air, this m-file first imports the some constants that are molecular weight and heat of combustion values from a excel sheet called "FG_Constants.csv". Then, average molecular weight (MW_avg) is calculated by using Equation (3.29).

$$MW\_avg = \sum_i MW_i * CA.yi \tag{3.29}$$

MW$_i$ denotes the molecular weight of each component and CA.yi denotes mole fraction of each component in the combustion air. Using ideal gas law, density and volumetric flow rate of combustion air are calculated by Equation (3.30) and (3.31), respectively.

$$CA.rho = \frac{CA.P * MW\_avg}{R * CA.T} \tag{3.30}$$

$$CA.V = \frac{CA.m}{CA.rho} \tag{3.31}$$

In these equations density, pressure, temperature and volumetric flow rate of combustion air are represented as CA.rho, CA.P, CA.T and CA.V, respectively. Then, total mole flow is calculated by Equation (3.32).

$$nT = \frac{CA.m}{MW_{avg}}$$

(3.32)

CA.m denotes the mass flow rate of combustion. After determining total mole flow, mole flows (CA.ni), mass flows (CA.mi) and enthalpy (CA.Hi) of each component are calculated in Equations (3.33), (3.34) and (3.35), respectively.

$$CA.ni = nT * CA.yi$$

(3.33)

$$CA.mi = CA.ni * MW_i$$

(3.34)

$$CA.Hi = CA.ni * \left(a_i * (CA.T) + \frac{2 * b_i * c_i}{\exp\left(\frac{2 * c_i}{CA.T}\right) + 1} + \frac{2 * d_i * e_i}{\exp\left(\frac{2 * e_i}{CA.T}\right) - 1} \right)$$

(3.35)

The Aly-Lee correlation [26] for C_p estimation is used here. Reasons for this are detailed in Appendix B.

In these equations CA.T is the temperature of the combustion air and a_i, b_i, c_i, d_i and e_i are the coefficients of heat capacity of components in the combustion air. Then, total enthalpy is calculated by Equation (3.36).

$$CA.H = \sum_i CA.H_i$$

(3.36)

In the process, combustion air is heated before the reactor. CA2 stream denotes preheated combustion air and with new temperature and pressure, properties are calculated in CA2_calculations2.m file in spite of combustion air stream (CA).

In the next part of main driver code, properties of hot stack gas (SG2) exit the boiler are calculated. For this purpose, a code is written in SG2_calculations2.m file. For each component of stack gas, this m-file again imports the some constants that are molecular weight, coefficients of heat capacity (ideal gas), and coefficients of oxygen consumption, water generation, carbon dioxide generation and sulfur oxide of both fuel gas and fuel oil from reaction stoichiometry from a excel sheet called "FG_Constants.csv". Before calculations, this m-file also called properties and calculations of preheated combustion air (CA2), fuel gas (FG) and fuel oil (FO). Then, each component mole flow rate is determined using component mole flows of other streams. After that, remaining properties are calculated using Equations (3.37), (3.38), (3.39) and (3.40), respectively.

$$SG2.mi = SG2.ni * MW_i \tag{3.37}$$

$$SG2.m = \sum_i SG2.m_i \tag{3.38}$$

$$SG2.xi = \frac{SG2.mi}{SG2.m} \tag{3.39}$$

$$SG2.yi = \frac{SG2.ni}{\sum_i SG2.n_i} \tag{3.40}$$

In these equations, component mass flow rate, components mole flow rate, total mass flow rate, component mass fraction and component mole fraction in hot stack gas after boiler are represented as SG2.mi, SG2.ni, SG2.m, SG2.xi and SG2.yi, respectively. Then enthalpy values of each component (SG2.Hi) and total enthalpy (SG2.H) are calculated by Equation (3.41) and (3.42), respectively.

$$SG2.Hi = SG2.n_i * \left(a_i * (SG2.T) + \frac{2 * b_i * c_i}{\exp\left(\frac{2 * c_i}{SG2.T}\right) + 1} + \frac{2 * d_i * e_i}{\exp\left(\frac{2 * e_i}{SG2.T}\right) - 1} \right) \quad (3.41)$$

$$SG2.H = \sum_i SG2.H_i \quad (3.42)$$

In these equations SG2.T is the temperature of the hot stack gas and a_i, b_i, c_i, d_i and e_i are the coefficients of heat capacity of components in the hot stack gas.

Using energy of hot stack gas, boiler feed water (KBS) is heated in the next step. In the main driver, mass flow rate, temperature and pressure values of both before and after economizer are imported from plant data. Then, using XSteam function, total enthalpy of both boiler feed water (KBS) and the stream out of economizer (KBS2) are calculated.

Some amount of energy is used for heating boiler feed water and the rest is conserved in stack gas, the stream outlet of first economizer, SG1. This stream has the same properties with hot stack gas (SG2), except temperature. After economizer, temperature decreases. To calculate temperature of SG1, a code is written in SG1_calculations2.m file. In this m-file, again coefficients of heat capacity (i.e. a_i, b_i, c_i, d_i, e_i) are imported from "FG_Constants.csv" and also properties and calculations of hot stack gas (SG2), boiler feed water (KBS) and hot boiler feed water (KBS2). From the energy conversion law, equation (3.43), first the enthalpy of SG1 is calculated.

$$SG1.H = SG2.H + KBS.H - KBS2.H \tag{3.43}$$

Then, using total enthalpy equation (3.44), temperature is estimated.

$$SG1.H = \sum_i \left(SG1.n_i * \left(a_i * (SG1.T) + \frac{2 * b_i * c_i}{\exp\left(\frac{2 * c_i}{SG1.T}\right) + 1} + \frac{2 * d_i * e_i}{\exp\left(\frac{2 * e_i}{SG1.T}\right) - 1} \right) \right) \tag{3.44}$$

In the next two parts of main driver, properties of stack gas after second economizer (SG) and stack gas released to atmosphere (SGOUT) are calculated at different temperature and pressure. For this purpose, a code is written in SG_calculations2.m file and SGOUT_calculations2.m file. In these m-files, coefficients of heat capacity (i.e. a_i, b_i, c_i, d_i, e_i) are imported from "FG_Constants.csv". Then, using Equation (3.45) and (3.46), enthalpy values of each component (SG.Hi) and total enthalpy (SG.H) are calculated at defined temperature (SG.T). These equations are also used for calculation of stack gas released to atmosphere (SGOUT) with its temperature and component mole flow rates.

$$SG.Hi = S2.n_i * \left(a_i * (SG2.T) + \frac{2 * b_i * c_i}{\exp\left(\frac{2 * c_i}{SG.T}\right) + 1} + \frac{2 * d_i * e_i}{\exp\left(\frac{2 * e_i}{SG.T}\right) - 1} \right) \tag{3.45}$$

$$SG.H = \sum_i SG.H_i \tag{3.46}$$

After calculations of stack gas properties, properties of water stream line are calculated in the main driver program. The stream KBS2 is heated again in the equipment called DOME and the exit stream is called KBS3. Importing temperature and pressure value of KBS3 from plant data, enthalpy value is calculated with XSteam function.

Next, the KBS3 stream is divided into two streams, KBS4 and blow-down (BD). In time, circulated water in the plant gets dirty and some amount of water is discarded with the stream blow-down after cooling. Importing temperature and pressure values of blow-down (BD) and cooled blow-down (BDOUT), the enthalpy values of BD and BDOUT are calculated with XSteam function. The rest flow of KBS3 continues in line with decreased mass (KBS4) and using its temperature and pressure values, enthalpy of this line is calculated by again XSteam function.

Up to this water line, all streams are in liquid form. Using rest energy from combustion heat, water is converted to steam in the equipment called L2V. The exit steam is called as ST4. In the equipment DESUP, temperature of ST4 is decreased and the stream continues in line with the name ST3. Calling properties of temperature and pressure values from plant data, both enthalpy of ST4 and enthalpy of ST3 are calculated with XSteam function.

At the end of the process, using released energy from DESUP, spray water (SP) is converted to steam (SP1). Then, SP1 line and ST3 line are mixed in SPMIXER. This unit combination is designed to decrease temperature with adding water. After mixing, total steam (ST) is decreased to room temperature for efficiency calculations in detail. Calling temperature and pressure values from plant data, main driver program calculates enthalpy values for each stream (i.e. SP, SP1, ST, STOUT) using XSteam function.

Finally, main driver program calculates released and gained heat values between CA and CA2 as QCAHEAT, SG1 and SG as ECOLOSS, SG and SGOUT as SGLOSS, heat of combustion as HCOMB, KBS2 and KBS3 as QBOILER, BD and BDOUT as BDLOSS, KBS4 and ST4 as QRAD, ST4 and ST3 as QSP, SP and SP1 as SPLOSS and ST and STOUT as STGAIN by using between equations (3.47) - (3.56).

$$QCAHEAT = CA.H - CA2.H \qquad (3.47)$$

$$ECOLOSS = SG1.H - SG.H \qquad (3.48)$$

$$SGLOSS = SG.H - SGOUT.H \qquad (3.49)$$

$$HCOMB = SG2.H + FO.Hrxn + FG.H.rxn - CA2.H - FG.H - FO.H \qquad (3.50)$$

$$QBOILER = HCOMB + KBS2.H - KBS3.H \qquad (3.51)$$

$$BDLOSS = BD.H - BDOUT.H \qquad (3.52)$$

$$QRAD = QBOILER + KBS4.H - ST4.H \qquad (3.53)$$

$$QSP = ST4.H - ST3.H \qquad (3.54)$$

$$SPLOSS = QSP + SP.H - SP1.H \qquad (3.55)$$

$$STGAIN = ST.H - STOUT.H \qquad (3.56)$$

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Confirmation and Simulation Conditions

In previous parts of this thesis, Aspen Model and Matlab Model are described in detail. Before putting into use on the Matlab Model in the plant, consistency is checked between Aspen and Matlab Models. For this purpose, ten variables used as input values in models are set at different levels. Numbers of levels for each variable are tabulated in Table 4.1. Related with these levels; all combinations of these variables are examined in 4608 cases.

When setting the values of variables, for the air properties meteorology data are analyzed. Operation conditions are based on TÜPRAŞ plant data and for the variables with different levels, one standard deviation above and below of the mean value are used.

In the Appendix E, there is a simple process flow diagram.

Table 4.1 – Input variables and number of levels of these variables of models

Variables	# of Levels	Variables	# of Levels
CA.m	Calculated	KBS.m	3
CA.P	1	KBS.T	2
CA.T	2	KBS.P	1
CA.yi	2	DOME.T	1
CAHEATER.T	2	DOME.P	1
CAHEATER.P	1	ECO1.T	1
FO-OIL.m	2	ECO2.T	1
FO-OIL.P	1	ECO2.P	1
FO-OIL.T	1	SP.m	2
FO-OIL.xi	1	SP.T	1
FO-STM.m	FO.m/3	SP.P	1
FO-STM.P	1	L2V.T	1
FO-STM.T	1	L2V.P	1
FG.m	2	DESUP.T	1
FG.P	1	DESUP.P	1
FG.T	1	SPVAP.T	1
FG.yi	6	SPVAP.P	1
BOILER.T	2	BDVALVE.m	KBS.m/10
BOILER.P	1		

There is not much change in the compositions of fuel oil according to measurements in the plant; therefore fuel oil composition is assumed constant. Except fuel gas compositions, all levels are tabulated in Table 4.2. Because of having more components and variety in fuel gas, impact of fuel gas composition is analyzed at different levels. Changing the values of components having higher composition, six different levels are specified. Table 4.3 shows tabulated levels of fuel gas composition below.

Table 4.2 – Levels of variables

Variables	Unit	1st level	2nd level	3rd level
CA.m	kg/h	Calculated		
CA.P	atm	MEAN		
CA.T	^{o}C	LOW	HIGH	
CA.yi. N_2		LOW	HIGH	
CA.yi. O_2		LOW	HIGH	
CA.yi. H_2O		LOW	HIGH	
CAHEATER.T	^{o}C	LOW	HIGH	
CAHEATER.P	atm	MEAN		
FO-OIL.m	kg/h	LOW	HIGH	
FO-OIL.P	atm	MEAN		
FO-OIL.T	^{o}C	MEAN		
FO-OIL.xi. $C_{40}H_{80}$		MEAN		
FO-OIL.xi. $C_{18}H_{12}$		MEAN		
FO-OIL.xi. H_2S		MEAN		
FO-STM.m	kg/h	LOW	HIGH	
FO-STM.P	atm	MEAN		
FO-STM.T	^{o}C	MEAN		
FG.m	kg/h	LOW	HIGH	
FG.P	atm	MEAN		
FG.T	^{o}C	MEAN		
BOILER.T	^{o}C	LOW	HIGH	
BOILER.P	atm	MEAN		
KBS.m	kg/h	LOW	MEDIUM	HIGH
KBS.T	^{o}C	LOW	HIGH	
KBS.P	atm	MEAN		
DOME.T	^{o}C	MEAN		
DOME.P	atm	MEAN		
ECO1.T	^{o}C	MEAN		
ECO2.T	^{o}C	MEAN		
ECO2.P	atm	MEAN		
SP.m	kg/h	LOW	HIGH	
SP.T	^{o}C	MEAN		
SP.P	atm	MEAN		
L2V.T	^{o}C	MEAN		
L2V.P	atm	MEAN		
DESUP.T	^{o}C	MEAN		
DESUP.P	atm	MEAN		
SPVAP.T	^{o}C	MEAN		
SPVAP.P	atm	MEAN		
BDVALVE.m	kg/h	LOW	MEDIUM	HIGH

Table 4.3 – Levels of fuel gas compositions

	1st level	2nd level	3rd level	4th level	5th level	6th level
H_2	0.4291	0.4822	0.4222	0.3827	0.2832	0.3775
N_2	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008
CO_2	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003
O_2	0.0010	0.0023	0.0003	0.0003	0.0023	0.0010
CO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H_2S	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CH_4	0.4586	0.3903	0.4619	0.5235	0.5335	0.5335
C_2H_6	0.0435	0.0436	0.0534	0.0336	0.0632	0.0336
C_2H_4	0.0102	0.0063	0.0144	0.0101	0.0610	0.0101
C_3H_8	0.0347	0.0477	0.0281	0.0281	0.0281	0.0247
C_3H_4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C_3H_6	0.0020	0.0030	0.0015	0.0015	0.0030	0.0015
C_4H_{10}	0.0091	0.0117	0.0067	0.0087	0.0117	0.0067
C_4H_{10}	0.0079	0.0079	0.0079	0.0079	0.0089	0.0079
C_4H_8	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
C_4H_8	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
C_4H_8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C_4H_8	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C_4H_6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C_5H_{12}	0.0007	0.0011	0.0006	0.0006	0.0011	0.0006
C_5H_{12}	0.0019	0.0026	0.0016	0.0016	0.0026	0.0016
C_6H_{12}	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

After comparing the results from Matlab and Aspen simulation, using Equation (4.1), error values of each equipment are calculated and the results are tabulated in Table 4.4. In Figure 4.1, these results are illustrated as a box plot. Box plots display data in which the box contains the middle 50% of the data with the mean dividing it, and the whiskers extend to the some defined lower and upper limits [27].

$$Error\ (\%) = \left| \frac{ASPEN\ result - MATLAB\ result}{ASPEN\ result} \right| \qquad (4.1)$$

Table 4.4 – Error distributions of equipment

	Min (%)	Median (%)	Max (%)	mean	upper 95%	lower 95%
BD-BDOUT	0.001	0.001	0.001	0.001	0.001	0.001
CA-CA2	0.003	0.065	0.090	0.054	0.054	0.053
KBS-KBS2	0.049	0.052	0.055	0.052	0.052	0.052
KBS2-KBS3	0.030	0.030	0.030	0.030	0.030	0.030
SG1-SG	0.323	0.513	2.119	0.589	0.597	0.582
SG-SGOUT	0.232	0.269	0.299	0.270	0.270	0.269
SG2-SG1	0.049	0.052	0.055	0.052	0.052	0.052
ST-STOUT	0.059	0.059	0.059	0.059	0.059	0.059
ST3-ST4	0.957	0.957	0.957	0.957	0.957	0.957
HCOMB	0.091	0.278	0.458	0.279	0.282	0.276
BOILER	0.100	0.310	0.528	0.314	0.317	0.310
RAD	0.213	0.779	5.993	1.107	1.135	1.080
SPLOSS	0.146	0.273	0.590	0.319	0.323	0.314
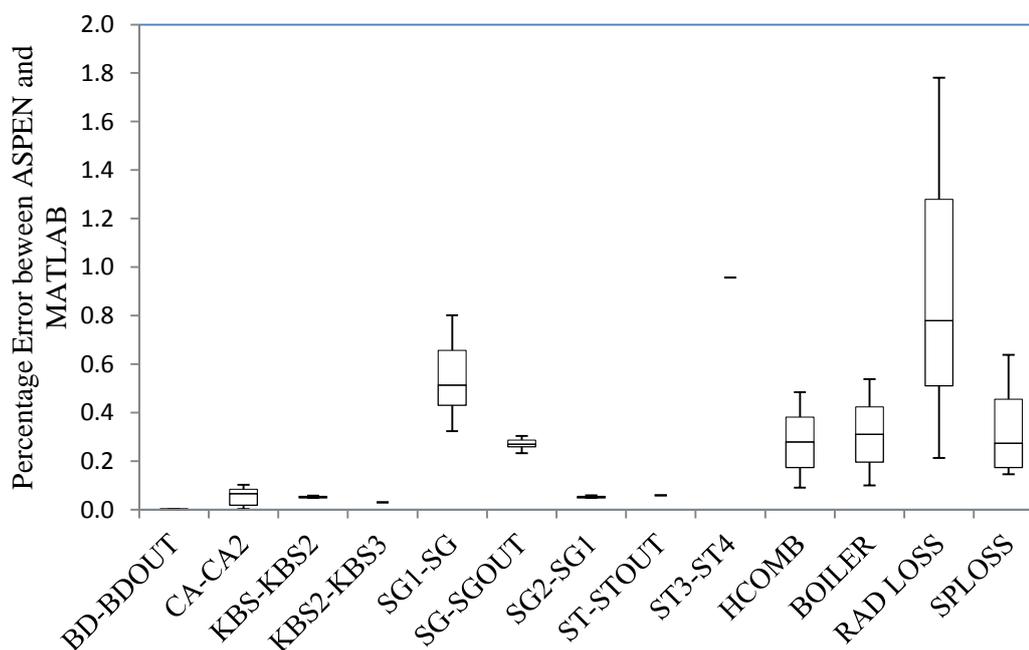
Figure 4.1 – Error distributions

In the Figure 4.1 the error of radiative loss and error (SG1-SG) have the maximum values in all error values. To understand the reason of errors, using all parameters models are created for both error of radiative loss and error of (SG1-SG). Their predicted plots are illustrated in Figure 4.2 and t-ratio values of parameters are tabulated in Table 4.5. t-distribution is useful in determining the potential value of each of the regressor variables in the regression model. A large t-ratio value indicates that this estimate has lower chance or higher sampling error [27]. In this manner, t ratio lists the statistics for the hypotheses that each parameter is zero. It is the ratio of the parameter estimate to its standard error. Prob>|t| lists the observed significance probability calculated from each t ratio. It is the probability of getting a t ratio greater than computed value, given a true hypothesis [28].
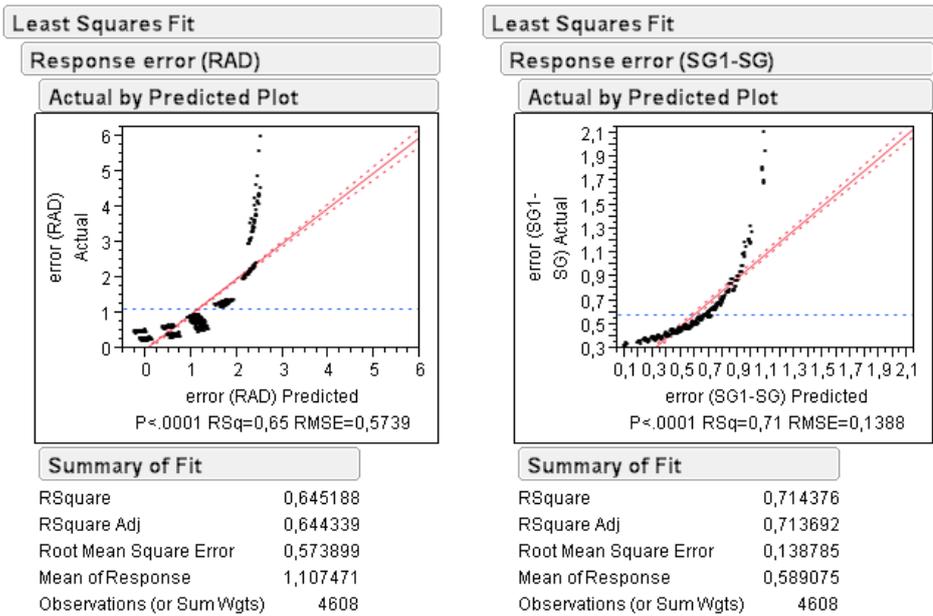
Figure 4.2 – Predicted plots of error of radiative loss and error of (SG1-SG)

Table 4.5 – t-ratio values of error of radiative loss and error of (SG1-SG)

Term	error (QRAD)		error (SG1-SG)	
	t-ratio	Prob>|t|	t-ratio	Prob>|t|
Intercept	1.63	0.10	15.86	0.00
BOILER.T	4.33	0.00	-33.35	0.00
CA.m	-0.16	0.87	-0.54	0.59
CA.T	0.00	1.00	0.00	1.00
CA.y.N2	-1.25	0.21	-1.62	0.10
CA2.T	-7.64	0.00	0.00	1.00
FG.m	-3.27	0.00	-2.01	0.04
FG.y.H2	-0.75	0.45	-0.84	0.40
FO-OIL.m	-0.43	0.67	-2.58	0.01
KBS.m	59.07	0.00	75.76	0.00
KBS.T	0.00	1.00	-23.12	0.00
SP.m	0.00	1.00	0.00	1.00

Sum of undefined errors in the system is called radiation errors, so having high errors is expected to result in some cases. Even though some of radiative errors are expected, to understand the impacts of KBS flow rate, FG flow rate and boiler temperature Figure 4.3 is plotted. As it is seen in the figure, when KBS flow rate increases error of radiative loss also increases in a large amount. Contrary to of KBS impact, when FG flow rate increases the error decreases. Also it is seen that boiler temperature has less impact on error of radiative loss relative to KBS flow rate and FG flow rate.
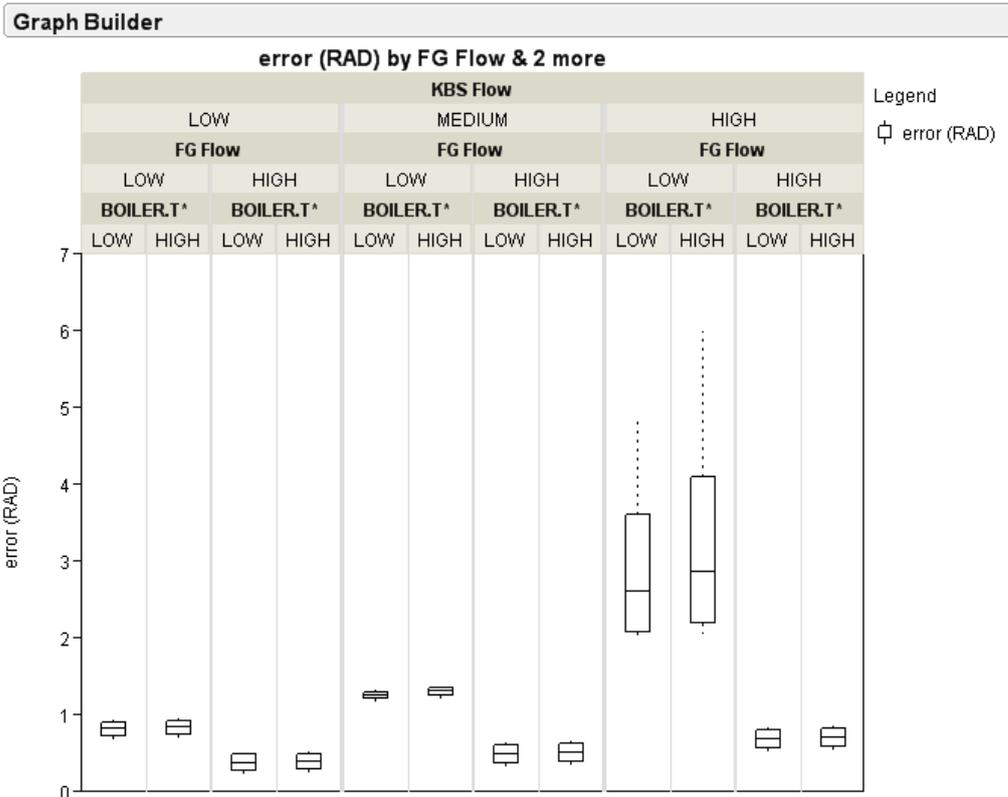
Figure 4.3 – Impacts of KBS flow rate, FG flow rate and boiler temperature on error of radiative loss

To analyze the error of (SG1-SG), Figure 4.4 is plotted using the highest three t-ratio values. As it is seen in the figure, when KBS flow rate increases error of radiative loss also increases as in error of radiative loss. On the other hand, the error decreases when boiler temperature and temperature of KBS increase.

Indeed, the equipment ECO2 is an imaginary heat exchanger. This allows one to observe the efficiency of the equipment ECO1 which is placed in a real system. Decreases in the heat difference between SG1 and SG lines mean that efficiency of the equipment ECO1 increases. To quantify this efficiency confirmation of the equipment ECO1 is important.
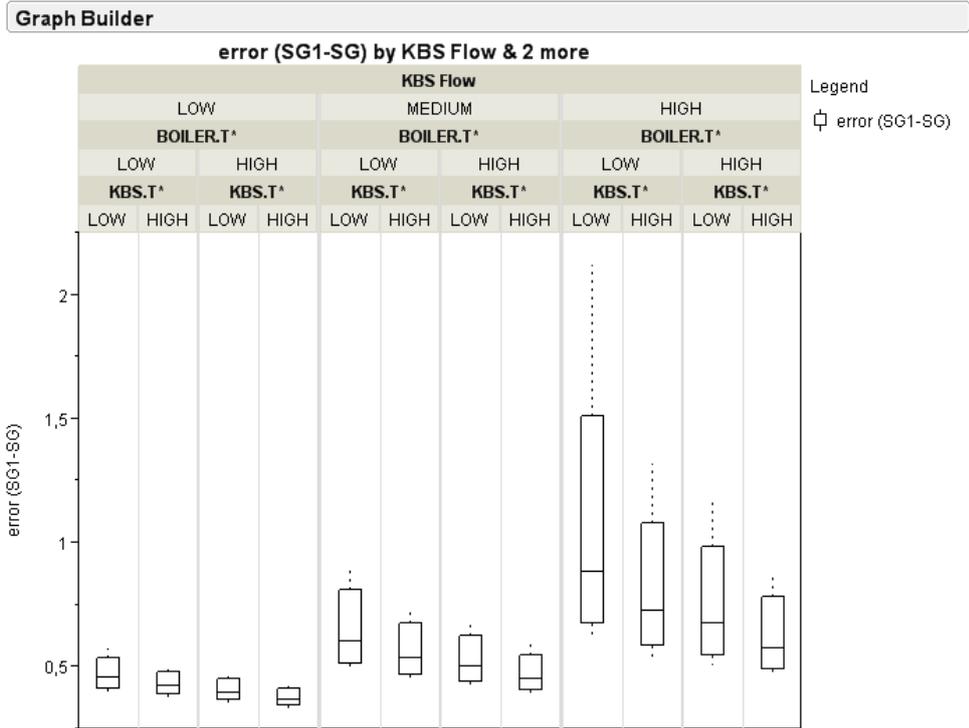
Figure 4.4 – Impacts of KBS flow rate, boiler temperature and temperature of KBS on error of (SG1-SG)

4.2 Overlapping of SGLOSS, HCOMB, STGAIN and QRAD

The main equipment of the system are SGREF, BOILER, STREF and L2V that are described in Aspen Modeling section. Validation of released energy from these equipment SGLOSS, HCOMB, STGAIN and RAD, respectively, is also important. To understand whether the ASPEN and MATLAB results are overlapping or not, relations between ASPEN and MATLAB results are illustrated in Figure 4.5 and Figure 4.6.

As it is understood from graphs, the most effective parameters (SGLOSS, HCOMB, STGAIN and QRAD) in steam boiler calculations are overlapped very well because coefficient of determination (R^2) are around 1 in all cases.
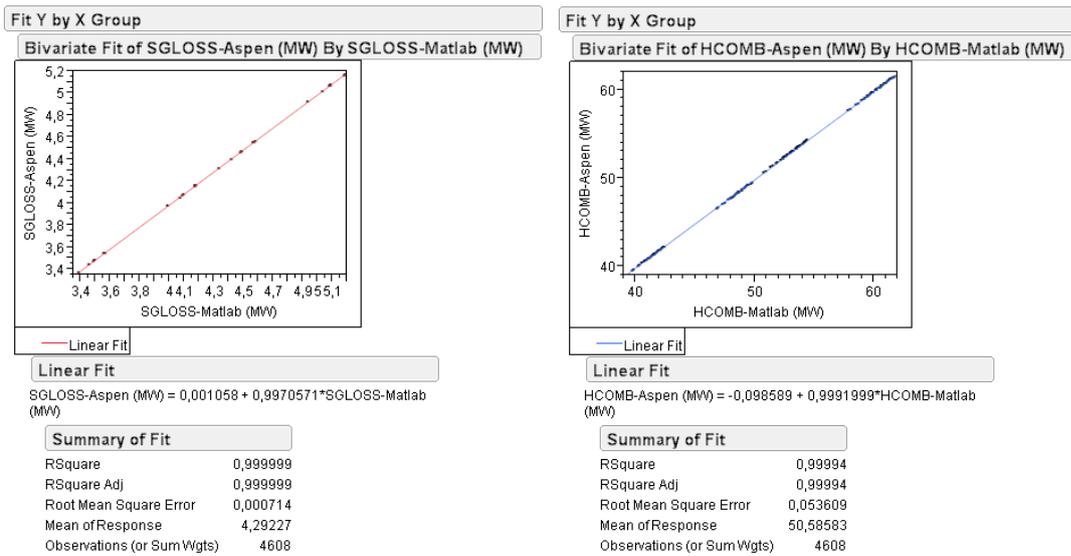
Figure 4.5 – Relations between ASPEN and MATLAB results of SGLOSS and HCOMB
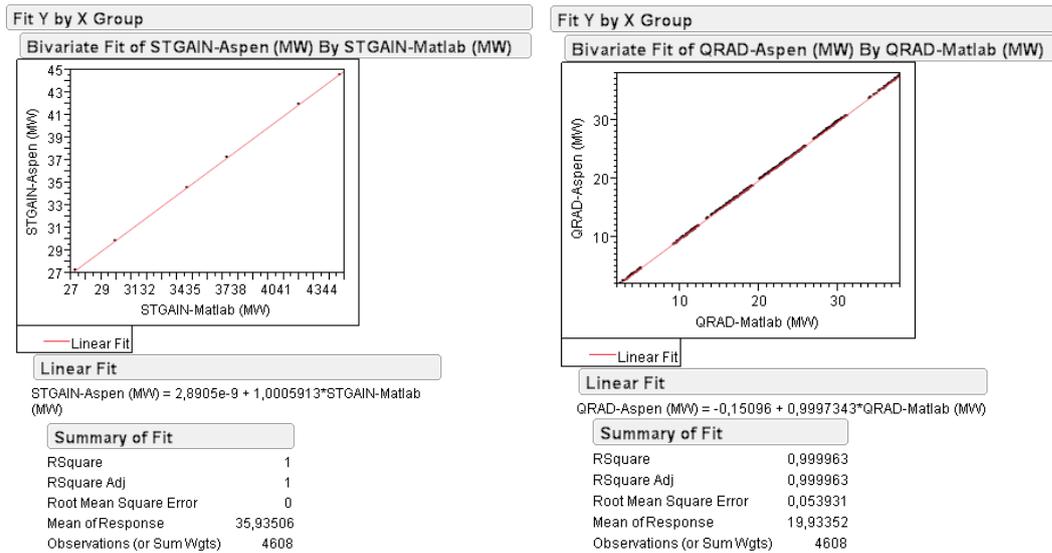
Figure 4.6 – Relations between ASPEN and MATLAB results of STGAIN and QRAD

4.3 Sensivity Analysis

The purpose of sensivity analysis is to understand which of the operational variables is most critical in satisfying the material and energy balances. In addition to confirmation cases, temperature levels of fuel oil and fuel gas and levels of excess oxygen in the stack gas are increased to three levels. Totally, there are 124416 cases. For this purpose firstly overall efficiency is calculated with indirect method, which is explained in Chapter 3.5.2. Then, distributions of overall efficiency, economizer loss and radiative loss are analyzed. Their predicted plots are shown in Figure 4.7. In the Table 4.6, their T-ratios are tabulated.
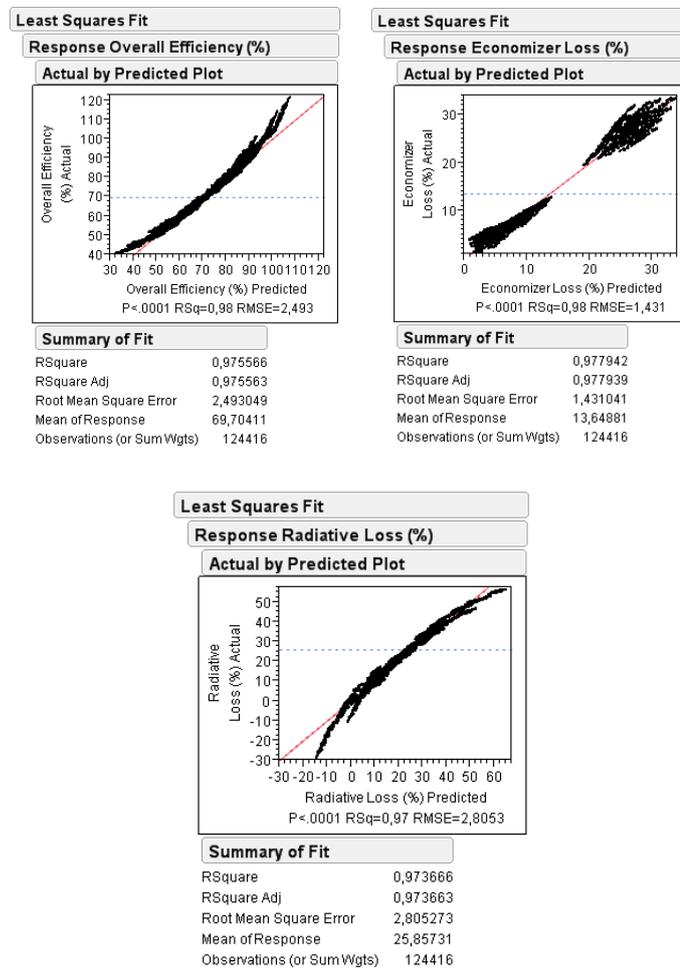
Figure 4.7 – Predicted plots of overall efficiency, economizer loss and radiative loss

Table 4.6 – t-ratio values of overall efficiency, economizer loss and radiative loss in the sensivity analysis

Term	Overall Efficiency (%)		Economizer Loss (%)		Radiative Loss (%)	
	t-ratio	Prob>|t|	t-ratio	Prob>|t|	t-ratio	Prob>|t|
BD.m	.	.	.	.	.	.
BOILER.T	98.54	0.00	**284.31**	0.00	-97.27	0.00
CA.m	88.87	0.00	**579.77**	0.00	**-297.96**	0.00
CA.T	0.00	1.00	0.00	1.00	0.00	1.00
CA.y.N2	-12.97	0.00	-39.63	0.00	25.69	0.00
CA2.T	-186.72	0.00	-85.20	0.00	184.85	0.00
FG.m	**-945.31**	0.00	-236.51	0.00	**860.75**	0.00
FG.T	-1.19	0.23	-0.42	0.67	1.13	0.26
FG.y.H2	-103.85	0.00	-24.49	0.00	93.85	0.00
FO-OIL.m	0.00	1.00	0.00	1.00	0.00	1.00
FO-OIL.T	-33.16	0.00	-11.60	0.00	31.45	0.00
FO-STM.m	0.00	1.00	0.00	1.00	0.00	1.00
Intercept	60.93	0.00	-38.50	0.00	13.66	0.00
KBS.m	**1649.18**	0.00	**-253.77**	0.00	**-1356.51**	0.00
KBS.T	0.00	1.00	57.88	0.00	0.00	1.00
SG2.yi.(2)	51.54	0.00	92.53	0.00	-78.05	0.00
SP.m	**362.17**	0.00	0.00	1.00	0.00	1.00

Comparing t-ratio values of parameters for overall efficiency; flow rates of boiler feed water (KBS.m), fuel gas (FG.m) and spray water (SP.m) have top three values. In Figure 4.8, impacts of these parameters on overall efficiency are shown. As it is seen in the figure, when SP.m and KBS.m increase, overall efficiency also increases in contrast to FG.m. These increment or decrement amounts are related with t-ratio values. With the larger t-ratio, the larger gradient occurs.
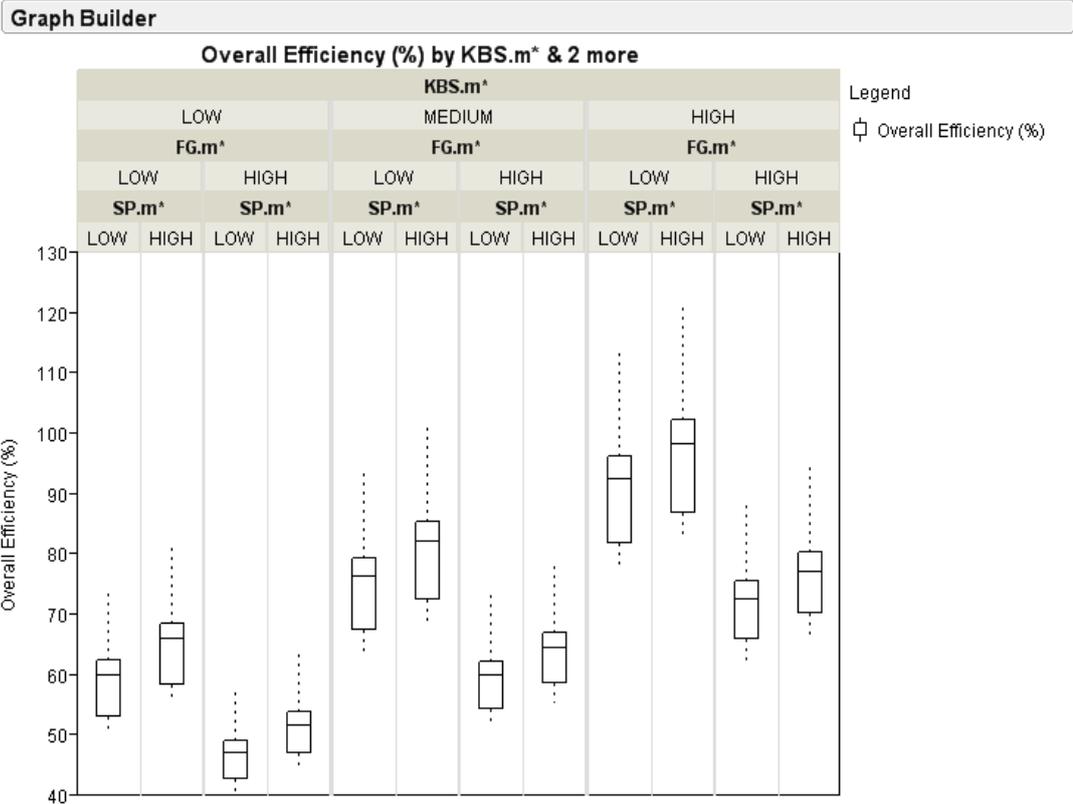
Figure 4.8 – Overall efficiency distribution with respect to KBS.m, FG.m, SP.m

For economizer loss, combustion air flow rate (CA.m), boiler temperature (Boiler.T), flow rate of boiler feed water (KBS.m), fuel gas flow rate (FG.m) and excess air ratio have the highest t-ratio values. In Figure 4.9, effects of boiler temperature (Boiler.T), flow rate of boiler feed water (KBS.m), fuel gas flow rate (FG.m) and excess air ratio are illustrated. As it is seen in the figure, when Boiler.T and FG.m increase, economizer loss also increases whereas when KBS.m increases, it decreases. Beside these, another parameter, excess air ratio affects the loss notably. When excess air ratio increases from 4% to 15%, the economizer loss increases approximately 5 times.
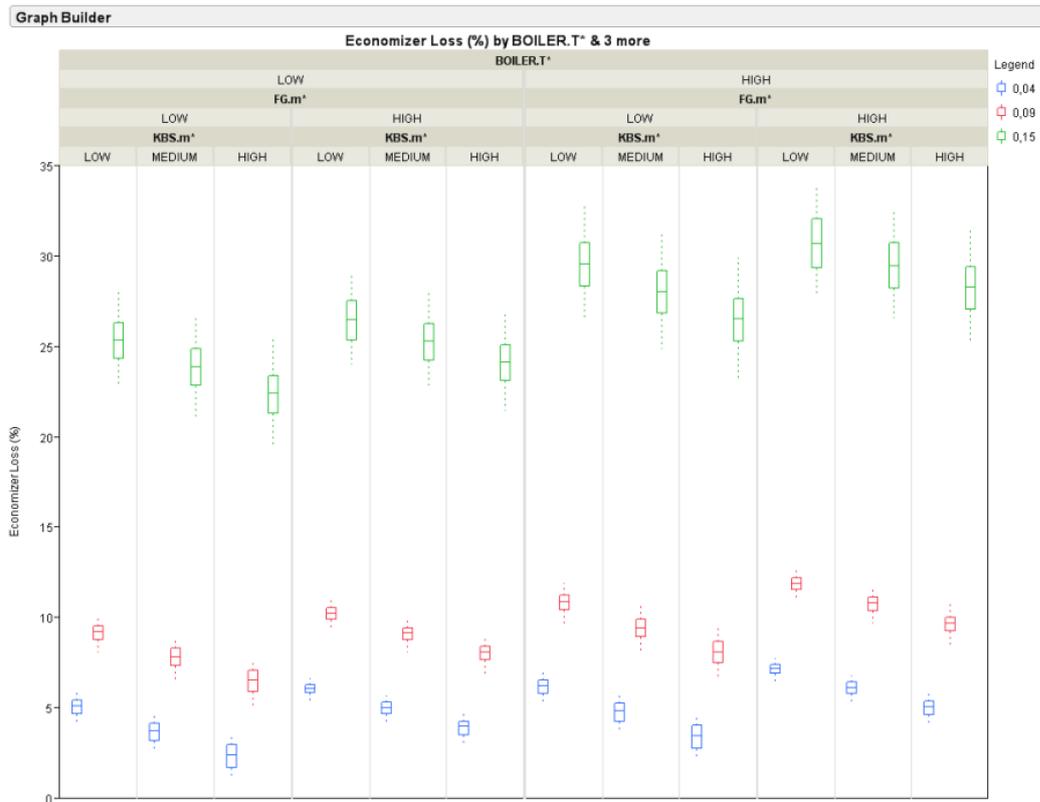
Figure 4.9 – Economizer loss distribution with respect to BOILER.T, FG.m, KBS.m and oxygen fraction in stack gas

For radiative loss, KBS.m, FG.m, CA.m and temperature of pre-heated combustion air (CA2.T) have the top four highest t-ratio values. In Figure 4.10, radiative loss distribution with respect to KBS.m, FG.m and CA2.T is illustrated. Greatness of t-ratio value of KBS.m asserts itself. When KBS.m increases, radiative loss decreases relatively high amount whereas when FG.m and CA2.T increase, radiative loss also increases relatively fewer.
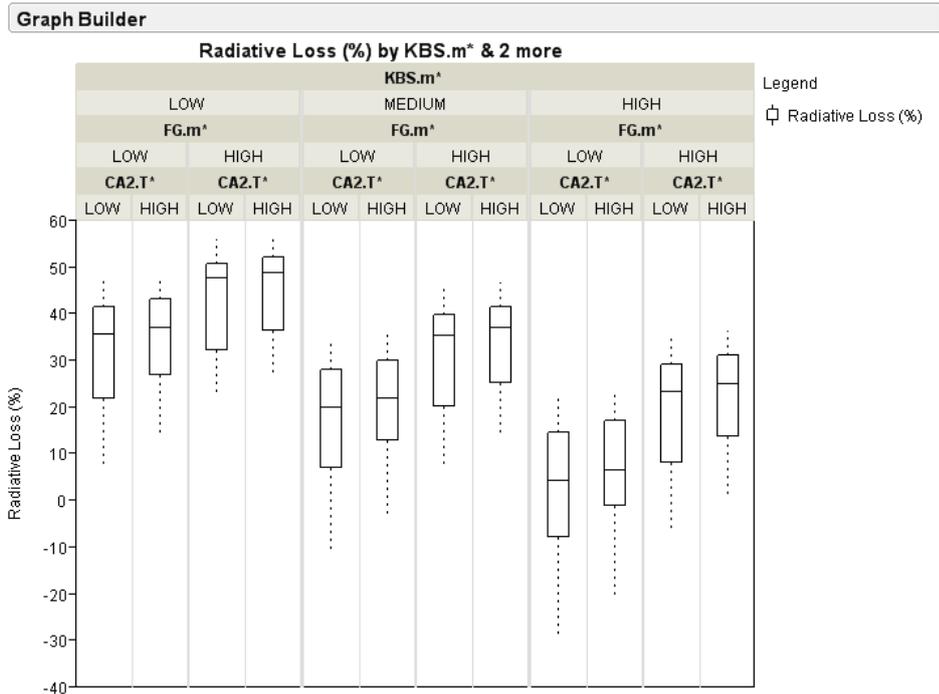
Figure 4.10 – Radiative loss distribution with respect to FG.m, KBS.m and CA2.T

In these three sensivity analysis, overall efficiency, economizer loss and radiative loss, KBS.m and FG.m seem to be the main dominant parameters. KBS.m plays an important role in the process because boiler feed water turns into vapor phase at the end of the process and has higher heat capacity and heat of vaporization values. Fuel gas is important because it is used as the main energy source of the system. The other important parameters vary in each analysis, because of having different conditions. This finding does not indicate that that the other parameters are necessarily not important but simply that they are not as important as KBS.m or FG.m. So, it can be easily stated that flowmeters of KBS and FG are the most important equipment in the process and accuracy of these equipment is critical.

4.4 Analysis of Plant Data

The aforementioned modeling approach was applied to actual production data from a TÜPRAŞ refinery – covering a period of 3 months. All analysis results are reported in terms of normalized variables and the actual boiler names were replaced with generic counterparts in order to satisfy the data security requirements of the refinery.

4.4.1 Data Filtering and Correction

Initial Screening

The initial data screening involves filtering out the data which filters out boilers that are not in steady-state operation or those for which one of the critical flow-meters are showing very unrealistic values – those beyond a certain range around the regular operational values, which is likely either a physical problem with the sensor or a problem with the interface that updates the data in the manufacturing database. Finally all other variables are filtered out with a 4 pseudo-sigma filter. The 4 pseudo-sigma filter is a filtering technique that filters out extreme outlier data points based on the data distribution and is a method that is frequently utilized in statistical process control applications [27]. These filters are defined in Table 4.7 below. In the table, DV represents the Design Value, PS represents the Pseudo Sigma.

Table 4.7 – Initial data screening filter definitions

Variable	Lower Limit	Upper Limit
KBS.m		
FG.m	DV – 0.2*DV	DV + 0.2*DV
FO.m		
Others	Mean – 4*PS	Mean + 4*PS

Further Data Screening and Improvement

After a simple filter based on the values of the process variables being within certain limits, a more complex approach involving the results of the material and energy balances are done. The first such check involves the confirmation of the flue gas oxygen composition against the one calculated based on complete combustion fuel-gas and fuel-oil that is fed into the system. This is followed by further checks based on energy balances.

- *Flue Gas Oxygen Composition*

If all flow and composition measurements are correct and complete combustion assumption is satisfied, then the calculated and measured oxygen compositions must overlap. A value of 1 indicates good agreement. When one looks at the trend of the calculated vs measured oxygen composition ratio trends, Figure 4.11 it is evident that there is an inconsistency.
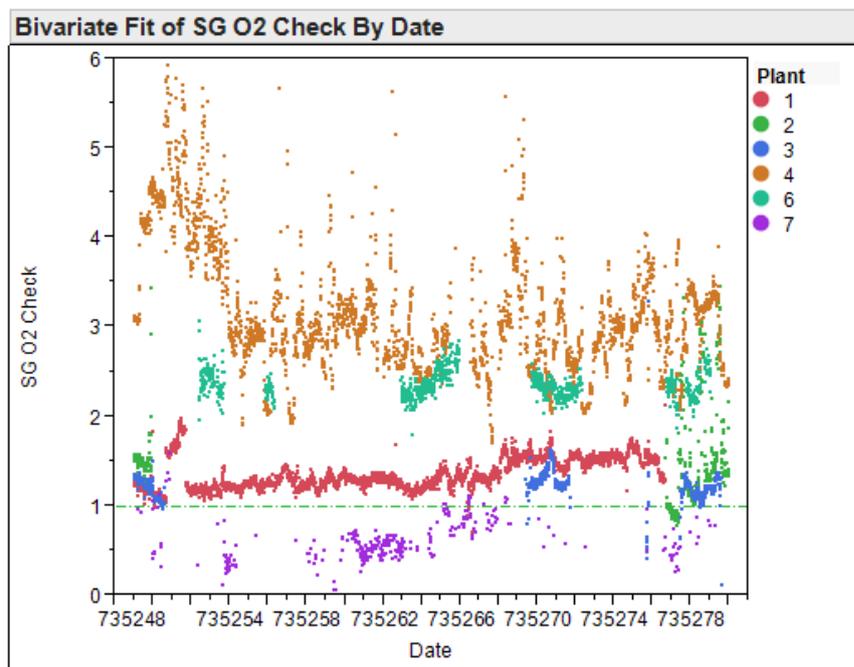
Figure 4.11 – Calculated to measured oxygen composition of the flue gas – time trend

One can further break-down these distributions by looking at box plots and note that some boilers show a greater deviation than the others, Figure 4.12. This indicates a problem with one or more of the measurements involved in these calculations. The oxygen sensor and fuel flow-meters were picked as the more trustworthy measurements in this loop upon discussions with the process engineers responsible for boiler operation. The reasoning is simple – the fuels cost money and the excess oxygen sensor is used in the control loop that regulates the inlet air flow-rate for ensuring complete combustion in the boiler. This leaves the air flow-rate as the variable we can tune in order to satisfy the flue gas oxygen composition.

In summary, the inlet combustion air flow-rate can be calculated based on the inlet flow-rates of the fuels and the flue gas composition. This eliminates the problem illustrated in Figure 4.11.
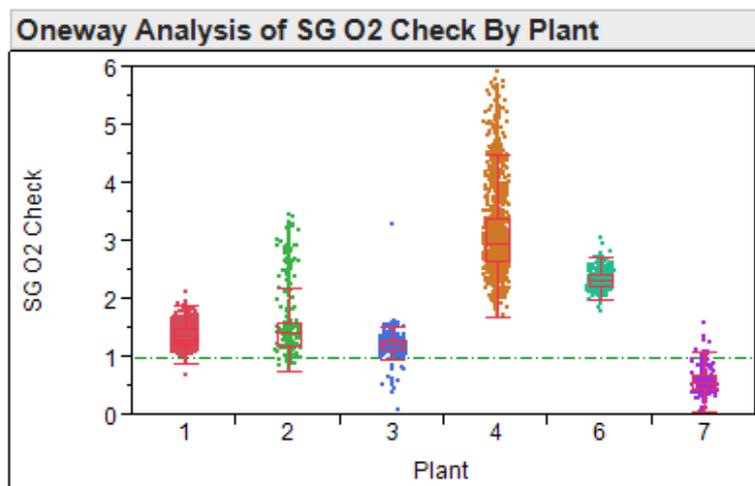
Figure 4.12 – Calculated to measured oxygen composition of the flue gas – box plot

- *Energy Balance Consistency Checks*

The models developed in the previous section include a number of imaginary heat exchange equipment whose purpose is to ensure that calculations can be made in presence of measurement errors. The duty of these exchangers should ideally be equal to zero if all variables involved are error free. These are the ECO2 and SPVAP

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exchangers appearing in the ASPEN flow sheet (Figure C.1). These two exchangers compensate for the lack or excess energy of their respective input streams. If every measurement is consistent then the variables ECOLOSS and SPLOSS must be equal to zero.

Another variable that can be monitored for the overall consistency of the energy balance is QRAD. QRAD refers to the energy left over after all of the KBS flow has been converted to steam. This is somewhat of a more indirect data integrity check as its value depends on the level of insulation of the boiler equipment. Literature sources suggest that this loss should be 2-5% of the overall duty of the boiler. Therefore unlike the ECOLOSS and SPLOSS terms, this cannot be used for direct adjustment of the suspect variables; just as a confirmation for data integrity after all other corrections have been applied.

The following plots show the distribution of the ECOLOSS, SPLOSS and QRAD terms for the respective boilers. Apart from the temperatures of the respective streams, the KBS and flue gas flow-rates can impact the ECOLOSS parameter. Out of these two, the sensitivity analysis of the previous section shows that KBS.m will have a much larger impact on the consistency of the ECOLOSS parameter, due to the higher heat capacity of the liquid in comparison to the flue gas. If the same impact were to be compensated by the flue gas flow-rate, then the combustion air and fuel flow-rates must all be modified in order to maintain the flue gas oxygen composition. So rather than manipulating three flowrates, decision was made to modify just the KBS measurement in order to satisfy the requirement that ECOLOSS is zero. This corresponds to around 10-20% modifications in the KBS flow-rate.

If one were to modify this inconsistency with the flue-gas flow-rate, the change would have to be an order of magnitude higher. Also since this means the flue flow-rates are going to change, the radiative loss trend goes in the opposite direction. Changing the KBS flow-rate fixes ECOLOSS with one manipulation and fixes the radiative loss trend at the same time and the level of modification is within reasonable limits.
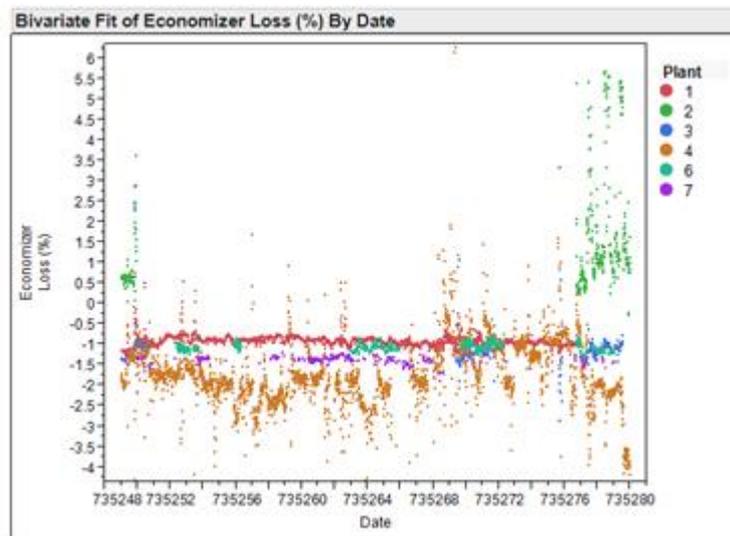
Figure 4.13 – ECOLOSS trends – ECOLOSS has been normalized

The disadvantage of this approach is that we are modifying a liquid flow-rate measurement, based on the premise that a gas flow-rate measurement is correct. The general impression of the process engineers is that liquid flow-rate measurements are more reliable however modification of the fuel-gas flow-rate brings about more doubts and inconsistencies and thus this choice had to be made.
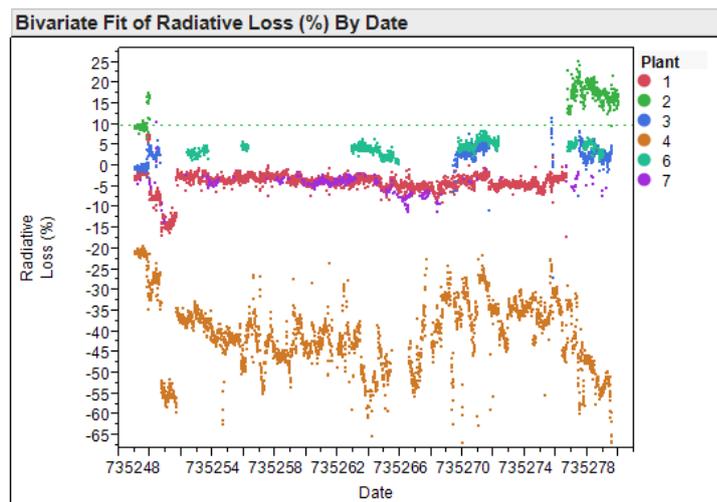
Figure 4.14 – Radiative loss trends – values have been normalized

The SPLOSS inconsistency is a much less significant problem than the above two issues. This inconsistency can simply be fixed by manipulating SP.m – which is not a measured variable during operation. This flow-rate is manipulated in real-time through a control valve which tries to maintain a target outlet steam temperature. The actual flow-rate is not measured; only the percentage of valve opening is tracked.
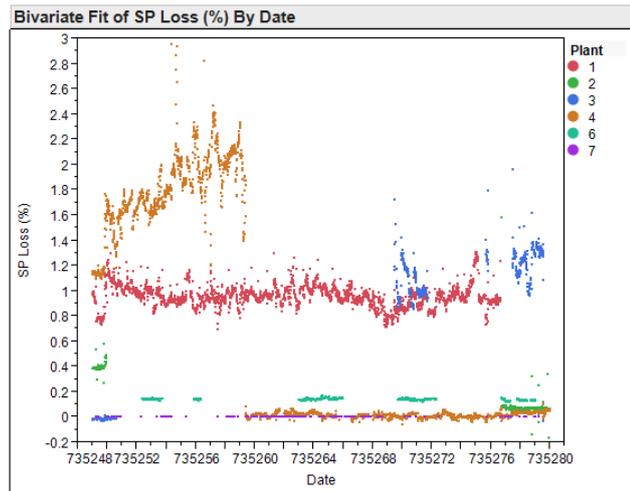
Figure 4.15 – SPLOSS trends – SPLOSS values have been normalized

4.4.2 Time Trend Analysis

Once all corrections have been made to the data-set, we can look at some of the time trends and see if we can track equipment performance and relate them to various parameters of operation.

One can see in Figure 4.16, that certain equipment demonstrates a better efficiency level than the others. The absolute efficiency numbers are omitted in this figure. This can provide some guidance as to which equipment to utilize more heavily and which ones to schedule for repairs and maintenance. For example Plant 3, shown in blue, definitely needs some attention at the next possible instance when it can be taken out of production. However due to operational constraints, it may sometimes be necessary to keep operating such equipment with low efficiency numbers because of capacity requirements.

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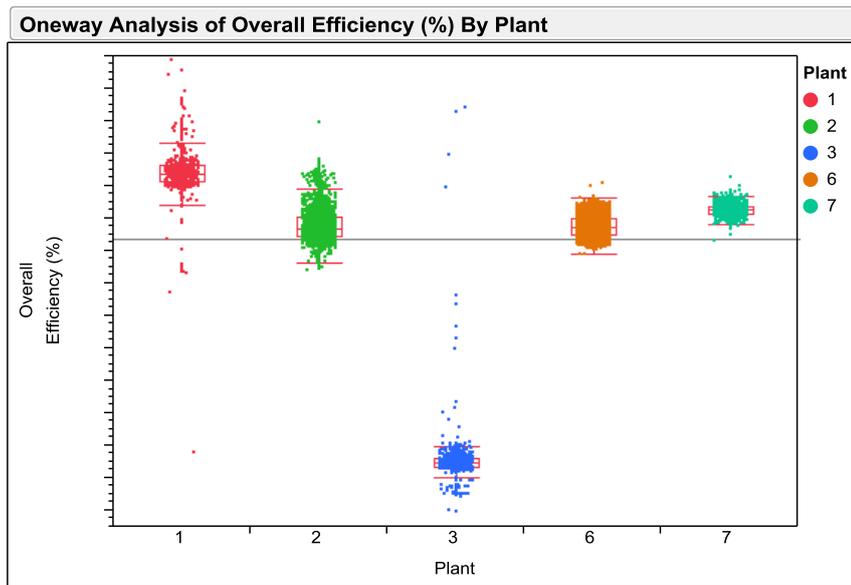
Figure 4.16 – Overall efficiency trends by equipment – Overall efficiency has been normalized

In Figure 4.17, one can look at the time trends of the equipment performance in order to better understand the distributions of Figure 4.16 – on an individual equipment basis. For instance Plant 6 shows periodic trends as well as step changes to new efficiency levels. This performance metric can then be correlated to other operational variables such as capacity, ratio of the fuels used (fuel gas to fuel oil), the composition of the fuel gas (which changes since fuel gas is a mixture of natural gas and refinery off gases), time of operation etc. These breakdowns would give further insight into whether the trends are due to equipment malfunction or simply operational condition fluctuations. Details of such analysis contain propriety operational details and could not be included here in the open literature.
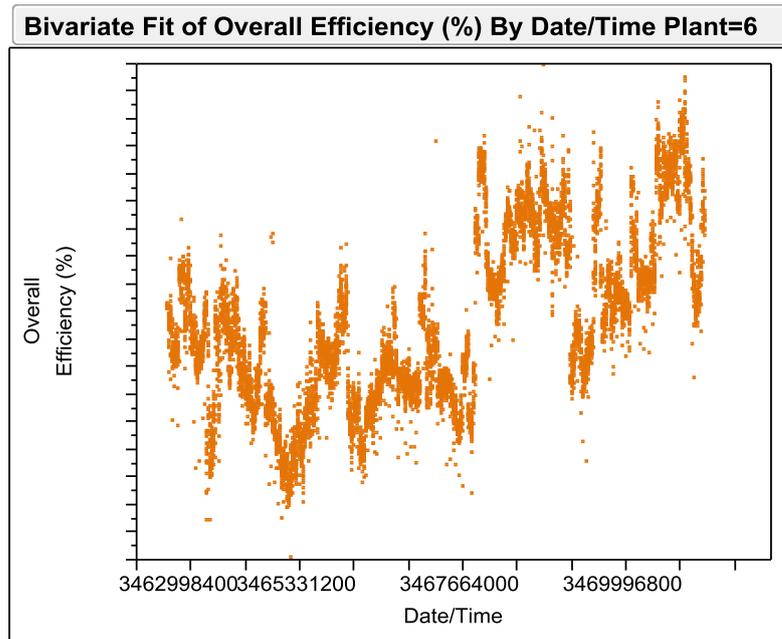
Figure 4.17 – Overall Efficiency Trends by time for Plant 6

One further item that was looked at is the capacity with respect to efficiency trends. This is shown in Figure 4.18 and Figure 4.19 for Plants 3 and 6 respectively. The first impression one gets from these two plots is that capacity shows a significant impact for Plant 3 but not for Plant 6. However upon further inspection of the details, one can see that Plant 6 actually operates in a small range around the design value however Plant 3 has been operated for a much larger range. Therefore the conclusion is that a boiler needs to be operated as close to its nominal design capacity as possible. However again there are operational constraints here. During operation, there needs to be excess capacity in case one of the boilers operating at capacity goes down unexpectedly or there are unforeseen spikes in the refinery steam demands. Therefore one may conclude that Plant 3, during this time, was being operated at times as this back-up boiler whereas Plant 6 has been operated one of the primary boilers.
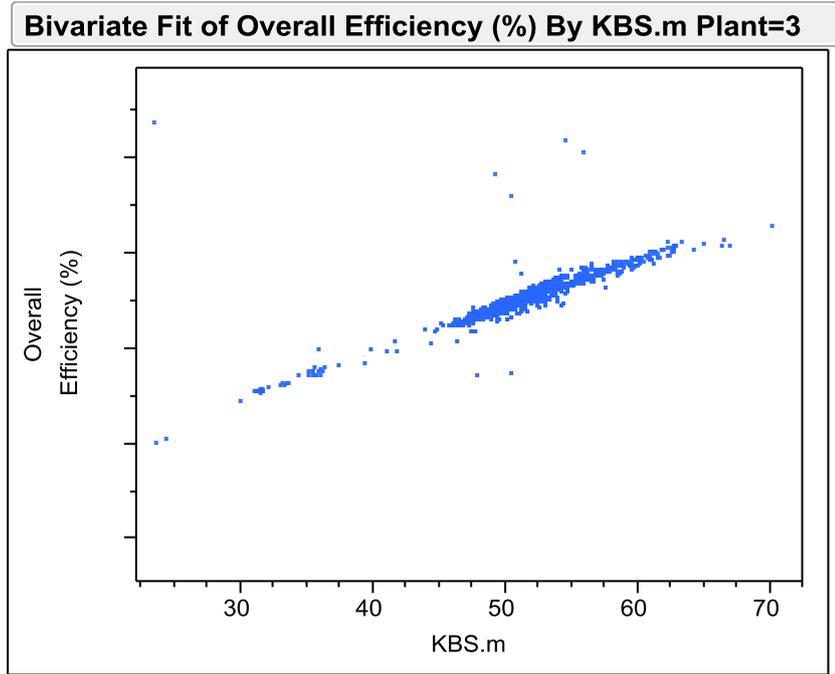
Figure 4.18 – Overall Efficiency vs Capacity – Plant 3
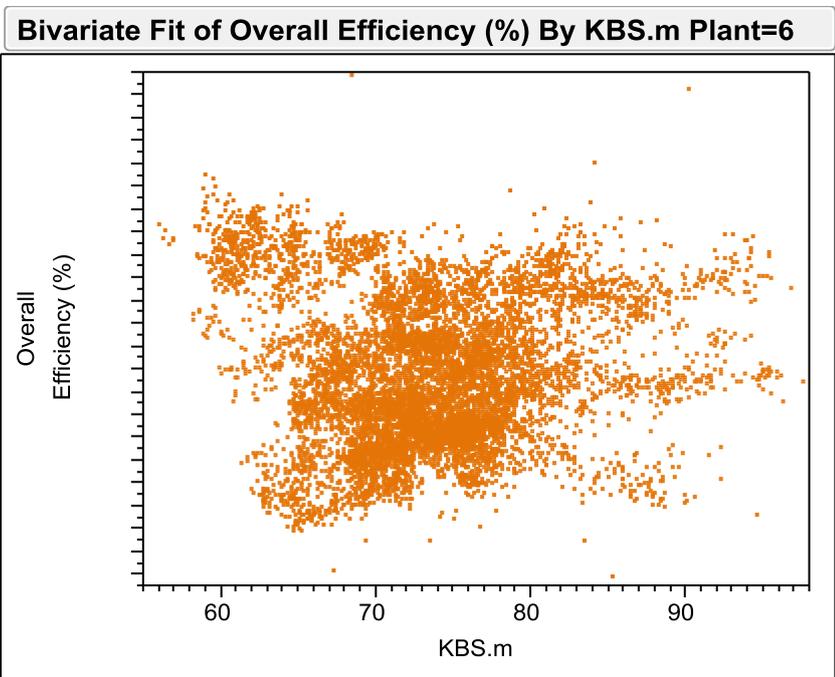
Figure 4.19 – Overall Efficiency vs capacity – Plant 6

CHAPTER 5

CONCLUSIONS

In this study, it was aimed to model the efficiencies of electricity and steam production equipment to track their performance in an effort to optimize the equipment utilization. To model the steam boiler, Aspen Plus software which is a chemical process modeling system and MATLAB software which is a high-level programming language were used.

In accordance with this aim, all components of the steam boiler were defined and created in the Aspen model that is used as reference. Then, using MATLAB, the system was ready to integrate in real time optimization program. To confirm these two programs, consistency was checked in Chapter 4. Changing levels of ten variables, 4608 different cases were set. Using results of these cases, errors (inconsistency between Aspen and Matlab models) of equipment were calculated. Inconsistency on radiative loss has maximum value, around 6%. Errors of (SG1-SG) and (ST3-ST4) have the next two highest inconsistency values which are around 2% and 1%, respectively. Error values of the rest of the ten equipment are all below 0.6%. When errors of radiative loss and SG1-SG were analyzed, it was observed that flow rate of boiler feed water is the most effective parameter. Increasing the flow rate of boiler feed water, the consistency decreases. The possible reason of this downfall is that the energy of fuel fails to satisfy the increment in temperature of boiler feed water. In addition to the confirmation, Aspen and Matlab results of main equipment, which are heat exchangers on stack gas flow (SGREF) and steam flow (STREF),

vaporization unit on water flow (L2V) and boiler were compared. When Aspen results versus Matlab results were plotted for each equipment, coefficient of determination (R^2) of all comparison are about 1, which means Aspen model matches the Matlab model for each equipment. At the end of these analyses, Matlab model becomes ready for using in real time optimization program.

To determine the most critical measurement equipment, sensivity analysis is made with using 124416 cases. These cases are set by adding three more parameters to confirmation parameters. For sensivity analysis, overall efficiency, economizer loss and radiative loss are evaluated. In actual versus predicted plots, R^2 values are around 0.97. Comparing t-ratio values of sixteen parameters, the most important parameters are specified. In these three analyses, it was observed that flow rate of boiler feed water and fuel gas flow rate are the main factors. The flow rate of boiler feed water is important because of having higher heat capacity and fuel gas flow rate is important because it is the main energy source of the system.

In last part of Chapter 4, actual production data from a TÜPRAŞ refinery were analyzed. Firstly, unrealistic values were filtered out using a certain range around the regular operational values and 4-pseudo-sigma filter. To improve the data screening, flue gas oxygen composition and energy balance consistency were checked. According to corrections after consistency check, the overall efficiency values of the boilers are calculated and impact of flow rate of boiler feed water are analyzed for plant 3 and plant 6. In Section 4.4, all analysis results were represented in terms of normalized data.

To sum up, in this study it was aimed to model steam turbines in MATLAB verified with ASPEN and it was succeeded. When similar approaches are applied to steam and gas turbines, whole plant equipment will be ready to optimize refinery power production.

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APPENDIX A

FUEL OIL MODELING

In TÜPRAŞ, one of the most important energy sources is combustion of fuel oil. Fuel oil is a mixture composed of different hydrocarbon compounds in different ratios. In general, fuel oils are classed according to density, fluidity and boiling points. This classification starts with Grade1, lower density, ends with Grade 6, high density [29].

In refinery, fuel oil with higher density, Grade 6, is used. This kind of fuel oil is also called "residual oil", because it includes waste hydrocarbon compounds which cause uneconomical decomposing during refining [30]. It consists of hydrocarbon compounds of which boiling points change between 350-650°C and molecular weights change between 300-1000. 20% of fuel oil is saturated hydrocarbon, 65% of fuel oil is aromatics and the rest is asphaltene [31]. Moreover, H_2S is also important because of the released SO_2 as a result of combustion [32]. Also, fuel oil has oxygen, nitrogen and metal-containing molecules [33]. Additionally, there are different analyses in the literature. However, these kinds of analysis methods are not practically in production area because they are costly and time consuming. The main purpose is to get quick and convenient results from analysis in the plant.

A1. Approach 1 – Using Correlations

Fuel Oil Heating Value and Correlations to API and S%

In the literature, there are various correlations. One of them is Dulong formula, equation (A.1), which assumes that carbon, hydrogen, oxygen and sulphur are combusted in atomic basis [34], [35].

$$HHV = 14600 \cdot X_C + 62000 \left(X_H - \frac{X_O}{8} \right) + 4000 \cdot X_S \qquad \text{(A.1)}$$

In this equation, X_C, X_H, X_O and X_S are in the weight fraction of carbon, hydrogen, oxygen and sulphur, respectively. The calculated energy (HHV) is in Btu/lb.

To use this correlation, weight fractions of carbon, hydrogen, oxygen and sulphur should be determined. Using API density, firstly relative density is calculated with equation (A.2).

$$API = \frac{141.5}{s} - 131.5 \qquad \text{(A.2)}$$

Then, hydrogen amount (X_H) in fuel oil, which includes just carbon and hydrogen, is calculated using equation (A.3) [18]. Schmidt [36] claims the precision of the formula can be improved by replacing initial constants with different constants. For Grade 6, initial constant is 25.

$$X_H = 25 - 15 \cdot s \qquad \text{(A.3)}$$

Modeled data includes weight of sulphur and they show that there is no oxygen in the fuel oil composition. Therefore, equation (A.3) becomes equation (A.4).

$$\frac{X_H}{1 - X_S} = 25 - 15 \cdot s \tag{A.4}$$

Using sulphur fraction from data and calculated hydrogen fraction, carbon fraction (X_C) is also calculated by equation (A.5).

$$X_C = 1 - X_H - X_S \tag{A.5}$$

After determining all fractions in the fuel oil, high heating value of fuel oil is calculated by using Equation (A.1). The margin of error of this approach is between 5% and 10%. In the literature, there is another correlation that reduced the margin of error to 1% and it is based on experimental heating value of fuel oil [37]. In the Figure A.1, this correlation is represented [18].
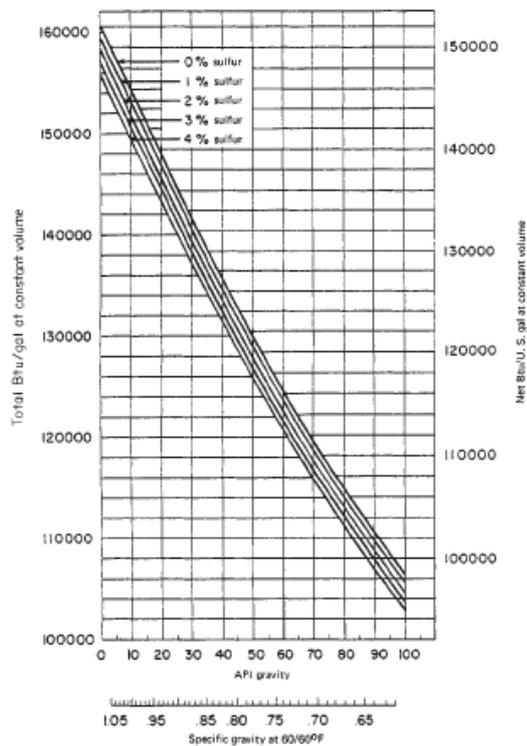
Figure A.1 – Correlation of heating value of fuel oil [18]

Because the correlation in the graphical form, firstly the graph is scanned and converted into number digitally. In this way, this correlation is ready for using in computer software practically. According to digitized graph, the correlation depends on API and S% is modeled as below, equation (A.6).

$$HHV = 41.6 + 0.123 \cdot API - 0.00112 \cdot (API - 10.158)^2 - 0.335 \cdot S\% \qquad (A.6)$$

In addition to the heating value, also the heat capacity of fuel oil should be calculated. In the literature [18], there is a relation between specific gravity and heat capacity which is represented below. In this relation, specific gravity can be calculated with equation (A.7) and in this equation, temperature is in ^{o}C, heat capacity is in kJ/(kg.C). This relation is based on the experimental data of which specific gravity is between 0.75 and 0.96 and temperature is between 0 and 205°C.

$$C_p = \frac{1.685 + (0.039 \cdot T)}{\sqrt{s}} \qquad (A.7)$$

A2. Approach 2 – Hydrocarbon Mixture

The first approach is more suitable for MATLAB model. All equations of mass and energy balances and physical properties will be defined into MATLAB program. On the other hand, ASPEN software is not as flexible as MATLAB software, and all components should be defined as input data. Therefore, a mixture of components in the ASPEN library should be used for fuel oil.

For this purpose, saturated hydrocarbon and aromatic compounds whose specific gravity is between 0.75 and 0.96 and temperature is between 0 and 205°C are investigated. To obtain hydrogen amount related with API values, hydrocarbon compounds should have different C:H ratios. In general, fuel oil has 40-45% H and 55-60% C in mole-fraction. For sulphur source, H_2S is used in the simulation.

Analyzing compounds in the ASPEN library, tetracontene and chyresene are selected as saturated hydrocarbon and aromatic hydrocarbon, respectively. Their properties are tabulated in Table A.1. There is only one contradiction that molecular weight of aromatic hydrocarbon is out of the residual fuel oil range in Table 3.1. Additionally, selected hydrocarbon compounds are at the lower limit in range of molecular weight and range of boiling points. However, these selections are the most suitable selections in the ASPEN library.

Using crude oil properties in ASPEN library is another approach; however, the confirmation of C:H:S ratios is more difficult in this situation. Surely, this is a more undesirable situation when it is compared with the previous approach. After the definition of these compounds, the composition of fuel oil is determined using API values. Then, the energy released by the combustion of fuel oil in this composition is verified.

Table A.1 – Hydrocarbon compounds used in fuel-oil ASPEN model

Name	Abbreviation	Formula	Molecular Weight	Boiling Point	Classification
Tetracontene	ALK	$C_{40}H_{80}$	561	523	Saturated Hydrocarbon
Chyresene	ARO	$C_{18}H_{12}$	228	441	Aromatic Hydrocarbon
Hydrogen Sulphide	H_2S	H_2S	34	N/A	Sulphur Source

Based on 1 g fuel oil, sulphur amount in fuel oil is calculated in weight fraction using molecular weight of sulphur as Equation (A.8).

$$n_S = \frac{X_S}{32.06} \tag{A.8}$$

When the fuel oil consists of only sulphur, carbon and hydrogen, using equation (A.2), (A.4) and (A.5) weight fractions of hydrogen and carbon are calculated. After determining the weight fractions, similar to the calculation of the amount of sulphur, the amounts of hydrogen and carbon are calculated as equation (A.9) and (A.10), respectively.

$$n_H = \frac{X_H}{1.008} \tag{A.9}$$

$$n_C = \frac{X_C}{12.01} \tag{A.10}$$

The next step is the calculation of mixture that provides the analyzed molar composition of carbon, hydrogen and sulphur. Using simple mass balance, chemical formulas of selected compounds are used for determining the compositions. Because only hydrogen sulphide includes sulphur and each molecule has one sulphur atom, number of moles of hydrogen sulphide is equal to the number of sulphur atom as equation (A.11). The mass of hydrogen sulphide is calculated with molecular weight in equation (A.12).

$$n_{H2S} = n_S \tag{A.11}$$

$$m_{H2S} = 34.081 \cdot n_{H2S} \tag{A.12}$$

Then, remaining hydrogen amount ($n_H{}^*$) is calculated as Equation (A.13)

$$n_H{}^* = n_H - 2 * n_{H2S} \tag{A.13}$$

For tetracontene (n_{ALK}) and chyrenese (n_{ARO}), two equations with two unknowns should be solved as equation (A.14), because both tetracontene and chyrenese have carbon and hydrogen atoms.

$$\begin{bmatrix} n_C \\ n_H{}^* \end{bmatrix} = \begin{bmatrix} 40 & 18 \\ 80 & 12 \end{bmatrix} \cdot \begin{bmatrix} n_{ALK} \\ n_{ARO} \end{bmatrix} \tag{A.14}$$

The constants of 2x2 matrices are the atom numbers of compounds tabulated in Table A.1. The solution of equation (A.13) gives below relations, (A.15) and (A.16).

$$n_{ALK} = -0.0125 \cdot n_C + 0.0187 \cdot n_H{}^*$$ (A.15)

$$n_{ARO} = 0.0833 \cdot n_C - 0.0417 \cdot n_H{}^*$$ (A.16)

And using molecular weight, mass of compounds can be calculated as equation (A.17) and (A.18).

$$m_{ALK} = 561 \cdot n_{SAT}$$ (A.17)

$$m_{ARO} = 228 \cdot n_{ARO}$$ (A.18)

Using calculated mass values, weight fractions of compounds are calculated as below, Equations (A.19), (A.20) and (A.21).

$$X_{ALK} = \frac{m_{ALK}}{m_{ALK} + m_{ARO} + m_{H2S}}$$ (A.19)

$$X_{ARO} = \frac{m_{ARO}}{m_{ALK} + m_{ARO} + m_{H2S}}$$ (A.20)

$$X_{H2S} = \frac{m_{H2S}}{m_{ALK} + m_{ARO} + m_{H2S}}$$ (A.21)

Thus, fuel oil composition modeled in ASPEN is in consistency with the composition results. For this purpose, a simple ASPEN program modelled is represented in Figure A.2. Three components in the fuel oil are mixed with the needed stoichiometric air in equipment B1. In the B2 unit, fuel oil is combusted adiabatically and released with stack gas in line 6. When all streams are specified at 25°C and 1 atm, the line 7 represents the combusted heating value of the mixture.
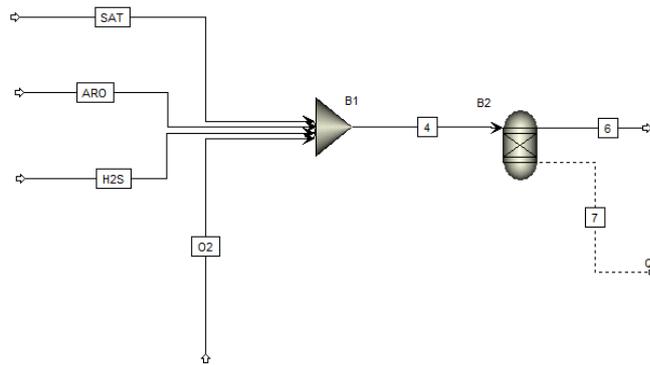
Figure A.2 – ASPEN simulation flowchart of calculation of fuel oil heating values

To confirm the second approach for determining fuel oil composition, 42 cases are set at different API and S% levels. Using Equation (A.6); theoretical value of combustion heat of fuel oil is calculated and then ASPEN model results are compared as in Table A.2. As it is seen in the table, error distribution is between 0.002% and 0.744%. That means this approach is applicable in programming MATLAB model.

Table A.2 – Comparison of heat of combustion values with ASPEN and theoretical prediction

	API	S%	Theoretical Prediction (MJ/kg)	ASPEN (MJ/kg)	Error (%)
Case 1	9.8	2.79	41.860	42.067	0.495
Case 2	10.1	2.55	41.977	42.123	0.350
Case 3	10.5	2.13	42.166	42.228	0.147
Case 4	10.5	2.15	42.159	42.222	0.149
Case 5	10.6	2.14	42.175	42.221	0.108
Case 6	10.6	2.16	42.168	42.215	0.110
Case 7	10.7	2.1	42.201	42.228	0.064
Case 8	10.7	2.15	42.184	42.213	0.069
Case 9	10.8	2.15	42.196	42.208	0.028
Case 10	10.9	2.14	42.212	42.206	0.013

Table A.2 – Comparison of heat of combustion values with ASPEN and theoretical prediction (cont'd)

	API	S%	Theoretical Prediction (MJ/kg)	ASPEN (MJ/kg)	Error (%)
Case 11	10.9	2.22	42.185	42.182	0.006
Case 12	11	2.24	42.190	42.172	0.044
Case 13	11	2.93	41.959	41.960	0.002
Case 14	11.1	2.25	42.199	42.164	0.084
Case 15	11.2	2.13	42.251	42.195	0.134
Case 16	11.2	2.19	42.231	42.177	0.129
Case 17	11.2	2.25	42.211	42.159	0.125
Case 18	11.2	2.93	41.984	41.949	0.082
Case 19	11.3	2.08	42.280	42.205	0.179
Case 20	11.3	2.15	42.257	42.184	0.173
Case 21	11.4	2.09	42.289	42.197	0.218
Case 22	11.4	2.2	42.252	42.164	0.210
Case 23	11.5	1.87	42.375	42.258	0.277
Case 24	11.5	1.98	42.338	42.225	0.267
Case 25	11.5	2.07	42.308	42.198	0.260
Case 26	11.5	2.15	42.281	42.174	0.254
Case 27	11.6	1.85	42.394	42.259	0.318
Case 28	11.6	2.01	42.340	42.211	0.305
Case 29	11.6	2.06	42.324	42.196	0.301
Case 30	11.7	2.09	42.326	42.182	0.339
Case 31	11.8	0.84	42.756	42.542	0.502
Case 32	11.8	2.13	42.325	42.166	0.376
Case 33	11.8	2.15	42.318	42.159	0.375
Case 34	11.9	2.18	42.320	42.145	0.413
Case 35	12	2.01	42.389	42.192	0.465
Case 36	12	2.14	42.346	42.153	0.456
Case 37	12.1	2.11	42.368	42.157	0.498
Case 38	12.2	2.08	42.390	42.161	0.540
Case 39	12.4	2.11	42.405	42.142	0.619
Case 40	12.6	2.04	42.452	42.154	0.704
Case 41	12.6	2.06	42.446	42.148	0.702
Case 42	12.7	2.04	42.465	42.149	0.744

APPENDIX B

C$_p$ CORRELATION CONFIRMATION

The specific heat values that are depended on temperature of fuel gas are one of the most important material properties because of affecting efficiency calculations, especially enthalpy of stack gas at high temperature is calculated with these relations. These enthalpy values are calculated by ASPEN using its own material properties library. Because these calculated values are regarded as true values, they should be compatible with correlations in the MATLAB program.

There are three important criteria to provide correlations. First one is better prediction of real data and their analytical integration into the programs. If correlations cannot be integrated analytically, it should be integrated numerically for each enthalpy calculation. Addition to these two properties, correlations should be suitable with different thermodynamic properties such as enthalpy, entropy that decrease the number of constants in the MATLAB program.

In literature, there are three kinds of correlations for specific heat with respect to temperature. First one is a third-degree polynomial that shown in Equation (B.1) [38].

$$C_p = a + bT + cT^2 + dT^3 \tag{B.1}$$

This correlation is suitable for second criteria; however there is a deviation from real data especially in high temperature values. Second correlation is similar to the first one, with the difference of degree of polynomial, represented in Equation (B.2) [39].

$$C_p = a + 2bT + 3cT^2 + 4dT^3 + 5eT^4 \qquad \text{(B.2)}$$

Even though second correlation is improved with conformity of experimental data, there are again deviations at extreme temperature values. The main reason of these deviations is that first and second correlations cannot characterize the processes affecting the specific heat inside the materials. A solution to this problem, Equation (B.3) is recommended in 1981 [26].

$$C_p = a + b\left[\frac{c}{T\sinh\left(\frac{c}{T}\right)}\right]^2 + d\left[\frac{e}{T\cosh\left(\frac{e}{T}\right)}\right]^2 \qquad \text{(B.3)}$$

This function is obtained by modeling the all processes that depends on temperature, including molecular movements that provide storing energy. Therefore, this correlation is ensued as overlapping experimental data in a wide temperature range. Integration of this correlation is shown in Equation (B.4) and (B.5).

$$\int_{H_{ref}}^{H} dH = \int_{T_{ref}}^{T} C_p(T) * dT \qquad \text{(B.4)}$$

$$H - H_{ref} = \left(aT + \frac{2bc}{e^{2c/T} - 1} + \frac{2de}{e^{2e/T} + 1}\right)\Big|_{T_{ref}}^{T} \qquad \text{(B.5)}$$

Through the Equation (B.5) is integrated analytically into the programs, the need of real time performance is provided.

The constants of Aly-Lee correlation are tabulated in Table B.1 [18]. This table includes all components of fuel gas and stack gas of the system. Calculated specific heat values are in J/(mol.K)

Table B.1 - Constants of Aly-Lee C_p correlation

Component	Formula	a	b	c	d	e
Hydrogen	H_2	27620	9560	2466.0	3760.0	567.6
Nitrogen	N_2	29110	8610	1701.6	100.0	909.8
Carbon Dioxide	CO_2	29370	34540	1428.0	26400.0	588.0
Oxygen	O_2	29100	10040	2526.5	9360.0	1153.8
Carbon Monoxide	CO	29110	8770	3085.1	8460.0	1538.2
Hydrogen Sulfide	H_2S	33290	26090	913.4	-17980.0	949.4
Methane	CH_4	33300	79930	2086.9	41600.0	992.0
Ethane	C_2H_6	40330	134220	1655.5	73220.0	752.9
Ethylene	C_2H_4	33380	94790	1596.0	55100.0	740.8
Propane	C_3H_8	51920	192450	1626.5	116800.0	723.6
Methyl Acetylene	C_3H_4	44780	109170	1550.8	67500.0	658.2
Propylene	C_3H_6	43390	152000	1425.0	78600.0	623.9
n-Butane	C_4H_{10}	71340	243000	1630.0	150330.0	730.4
2-Methylpropane	C_4H_{10}	65490	247760	1587.0	157500.0	-707.0
2-Methylpropene	C_4H_8	61250	206600	1545.0	120570.0	676.0
1-Butene	C_4H_8	59980	208460	1588.4	129400.0	707.3
trans-2-Butene	C_4H_8	65920	207000	1673.3	125100.0	742.2
cis-2-Butene	C_4H_8	57650	211500	1629.9	128720.0	739.1
1,3-Butadiene	C_4H_6	50950	170500	1532.4	133700.0	685.6
n-Pentane	C_5H_{12}	88050	301100	1650.2	189200.0	747.6
2-Methylbutane	C_5H_{12}	74600	326500	1545.0	192300.0	666.7
Cyclohexane	C_6H_{12}	43200	373500	1192.0	163500.0	-530.1
Water	H_2O	33360	26790	2610.5	8900.0	1169.0
Sulfur Dioxide	SO_2	33380	25860	932.8	10880.0	423.7

Correlations of specific heat are verified with ASPEN simulation results. In the Figure B.1, ASPEN simulation used in verification is represented. Pure components are heated at ten different temperature stages and their heat values are calculated with the simulation. Because released heat is equal to difference between inlet and outlet enthalpy, enthalpy differences are calculated in each stage and they are compared

with ASPEN simulation results. In the last unit, needed oxygen for combustion is mixed in simulation and its released energy is compared with combustion heat values in literature used in MATLAB program.

Another assumption, ideal gas, is verified with ASPEN simulations. It is assumed that fuel gas presents ideal gas behavior and there is no interaction between components in MATLAB model. This idea is supported with boiler operating conditions, high temperatures (200-1000°C) and low pressures. On the other hand, ASPEN software has different approaches that model non-ideal gas behavior easily. Among the all approaches, Peng-Robinson Equation of State is the most commonly used in refinery plants. This law, with its extra parameters, has the ability to model interactions between molecules and thus it models non-ideal gas behavior more accurately at low temperatures and high pressures. Related with this law, ASPEN simulations are operated between 1 and 3 atm.

With this approach, Aly-Lee specific heat correlations, combustion heat and deviations because of ideal gas are evaluated in the same ASPEN simulation.
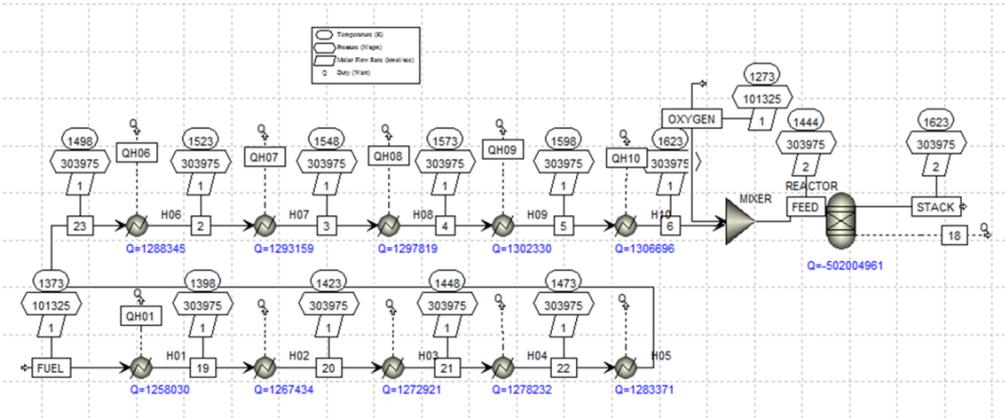
Figure B.1 - ASPEN simulation used in verification of specific heat correlations

Ideal gas behavior is evaluated between 1-3atm and 0-1500°C. This evaluation for methane, sample results, is represented in Figure B.2. As it is seen in the bigger graph, pressure does not affect the enthalpy values. Average error is about 0.01% in

the temperature range. The difference is just realized when graph is enlarged, in zoomed graph. The rest of the components also show similar behavior. The conclusion drawn from figure is the assumption of ideal gas is valid for fuel at 1atm, 2atm and 3atm and between 0-1500°C in MATLAB model. This range covers boiler operating conditions. In the figure, temperature is in ^{o}C, enthalpy is in kJ/kg.
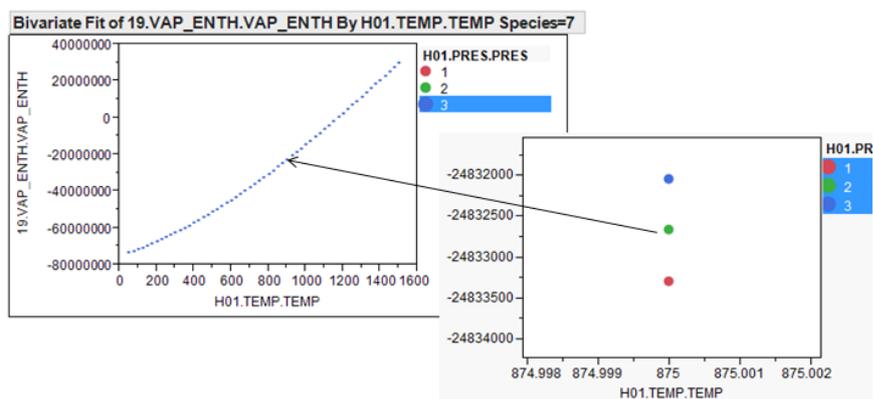
Figure B.2 - Effects of different pressure values to enthalpy

After verification of ideal gas, accuracy of Aly-Lee C_p correlations is evaluated. Results are shown in Figure B.3. In this figure, x-axis represents component number in the Table B.1 and different colors and symbols represent different pressure values, i.e. red circle denotes 1 atm. In Figure B.3, each point shows calculated error for different temperature. Average values are summarized and average error values are calculated between 1 and 3 and in the range of 0.17% and 0.27%. Especially at 1atm, except propadiene, all errors are below 1%. In Figure B.4, error distribution with respect to temperature is shown. Symbols and color code again show pressure levels, as previous graph. Between 200-1200°C, errors are always below 1% except propadiene. However propadiene composition is very small in whole fuel gas compositions. As a result, Aly-Lee constants, summarized in Table B.1, are used in models.
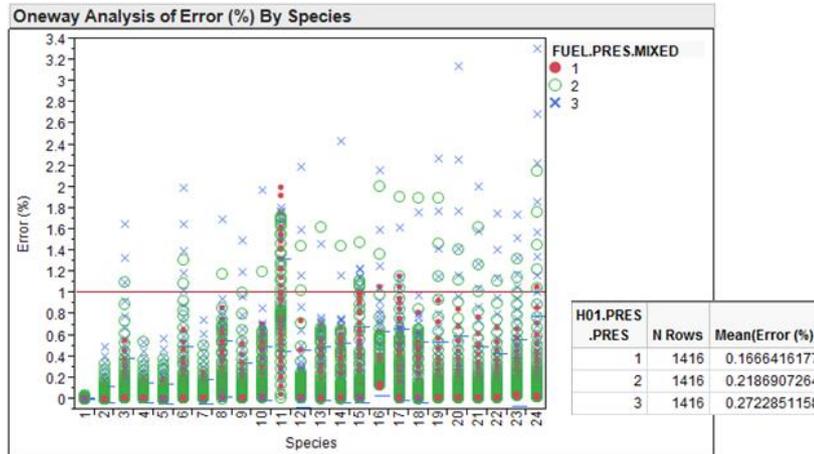
Figure B.3 - Comparison of Aly-Lee C_p correlations with ASPEN enthalpy values
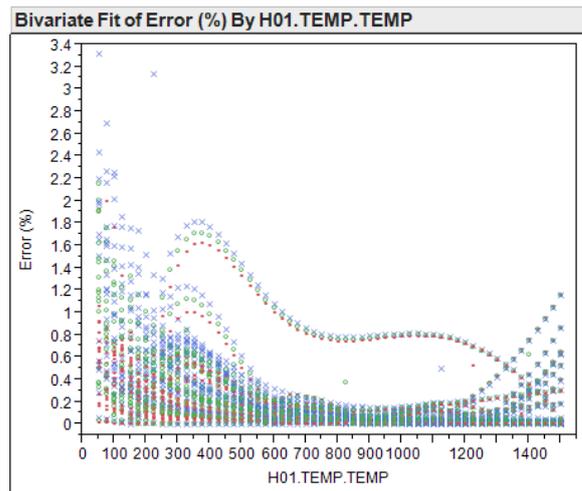
Figure B.4 - Error distribution of Aly-Lee C_p correlations and ASPEN with respect to temperature

Last, comparison of combustion heat values are tabulated in Table B.2. In the next table, Table B.3, all heat capacity correlations of fuel gas and stack gas results and error of Aly-Lee correlations and error of polynomial approach is also calculated. Constants of polynomial heat capacity correlations are taken from the website of Korean Database of Thermophysical Properties [40] As it is seen in the table Aly-

Lee heat capacity correlations gives better results than polynomial heat capacity correlations. Additionally, combustion heat values used in MATLAB models are overlapped with ASPEN simulation values.

Table B.2 – Comparison of combustion heat values of literature and ASPEN

Order	Component	Literature (J/kmol)	ASPEN (J/kmol)	Error (%)
1	Hydrogen	-2.42E+08	-2.49E+08	3.02
2	Nitrogen	N/A	N/A	N/A
3	Carbon Dioxide	N/A	N/A	N/A
4	Oxygen	N/A	N/A	N/A
5	Carbon Monoxide	-2.83E+08	-2.82E+08	0.52
6	Hydrogen Sulfide	-5.18E+08	-5.20E+08	0.45
7	Methane	-8.03E+08	-8.03E+08	0.06
8	Ethane	-1.43E+09	-1.43E+09	0.22
9	Ethylene	-1.32E+09	-1.33E+09	0.22
10	Propane	-2.04E+09	-2.05E+09	0.40
11	Methyl Acetylene	-1.85E+09	-1.86E+09	0.71
12	Propylene	-1.93E+09	-1.93E+09	0.34
13	n-Butane	-2.66E+09	-2.67E+09	0.54
14	2-Methylpropane	-2.65E+09	-2.66E+09	0.54
15	2-Methylpropene	-2.50E+09	-2.54E+09	1.26
16	1-Butene	-2.54E+09	-2.55E+09	0.43
17	trans-2-Butene	-2.53E+09	-2.54E+09	0.39
18	cis-2-Butene	-2.53E+09	-2.54E+09	0.27
19	1,3-Butadiene	-2.41E+09	-2.43E+09	0.68
20	n-Pentane	-3.24E+09	-3.29E+09	1.45
21	2-Methylbutane	-3.24E+09	-3.29E+09	1.49
22	Cyclohexane	-3.86E+09	-3.71E+09	3.81
23	Water	N/A	N/A	N/A
24	Sulfur Dioxide	N/A	N/A	N/A

Table B.3 – Error summary of Aly-Lee and polynomial C_p correlations

Order	Component	Aly-Lee			Polynomial		
		Max (%)	Min (%)	Avg (%)	Max (%)	Min (%)	Avg (%)
1	Hydrogen	0.01	0.01	0.01	4.57	0.78	2.36
2	Nitrogen	0.02	0.00	0.01	5.53	0.66	3.78
3	Carbon Dioxide	0.02	0.00	0.01	27.66	3.10	14.54
4	Oxygen	0.01	0.01	0.01	7.70	1.09	5.16
5	Carbon Monoxide	0.01	0.01	0.01	5.94	0.46	4.11
6	Hydrogen Sulfide	0.01	0.00	0.00	11.83	3.81	8.97
7	Methane	0.02	0.01	0.01	28.73	9.23	20.32
8	Ethane	0.44	0.06	0.21	43.55	11.55	27.40
9	Ethylene	0.03	0.00	0.01	52.35	10.81	27.97
10	Propane	0.72	0.02	0.28	55.27	10.87	29.65
11	Methylacetylene	1.65	0.04	0.91	64.74	9.07	27.19
12	Propylene	0.22	0.00	0.09	61.24	10.55	29.43
13	n-Butane	0.62	0.03	0.24	63.50	10.55	30.23
14	2-Methylpropane	0.74	0.01	0.28	64.31	10.23	30.71
15	2-Methylpropene	0.86	0.02	0.39	72.44	10.71	31.16
16	1-Butene	0.29	0.01	0.13	54.87	10.50	28.97
17	trans-2-Butene	0.99	0.00	0.26	57.23	10.25	28.64
18	cis-2-Butene	0.66	0.03	0.25	63.84	10.83	31.16
19	1,3-Butadiene	0.04	0.00	0.01	265.37	15.72	107.80
20	n-Pentane	0.03	0.00	0.01	52.89	10.47	26.81
21	2-Methylbutane	0.03	0.00	0.01	59.72	11.39	28.34
22	Cyclohexane	0.04	0.00	0.02	44.45	5.49	20.77
23	Water	0.01	0.01	0.01	92.46	5.48	17.16
24	Sulfur Dioxide	0.00	0.00	0.00	20.56	1.32	9.79

APPENDIX C

ASPEN SNAPSHOTS

Figure C.1 – Snapshot of all streams in the ASPEN model
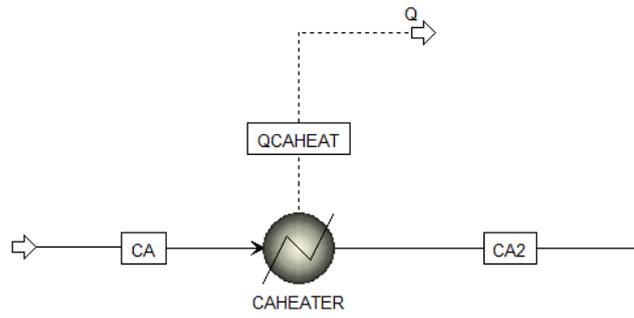
Figure C.2 – Snapshot of pre-heater in combustion air stream
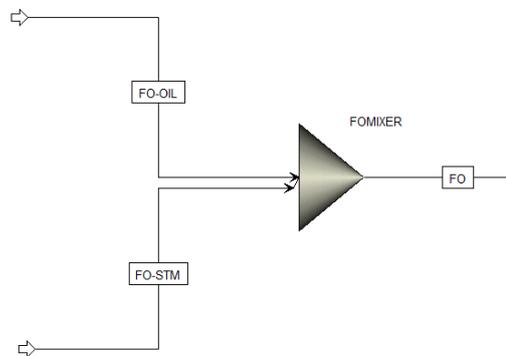
Figure C.3 – Snapshot of fuel oil mixer
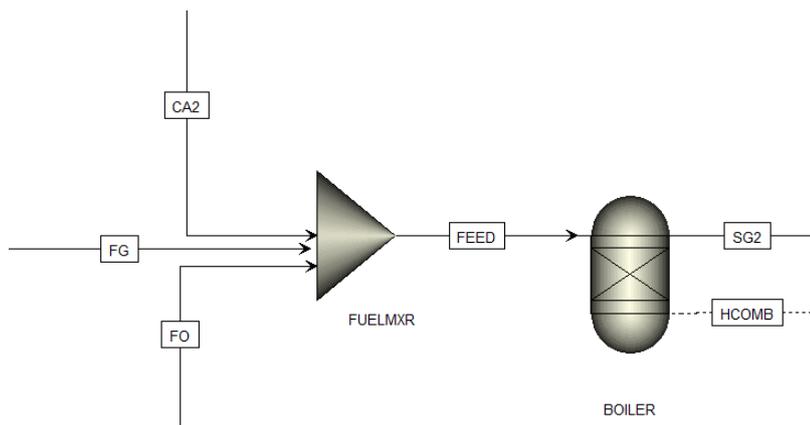
Figure C.4 – Snapshots of fuel mixer and boiler
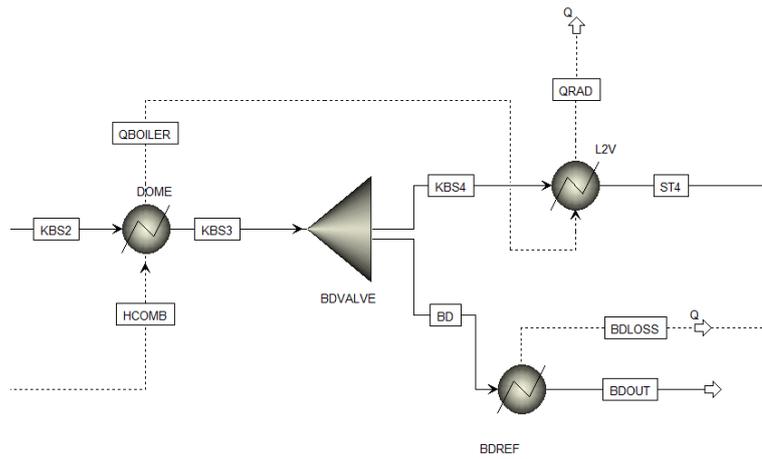
Figure C.5 – Snapshots of dome, blowdown valve and heat exchangers after blowdown valve
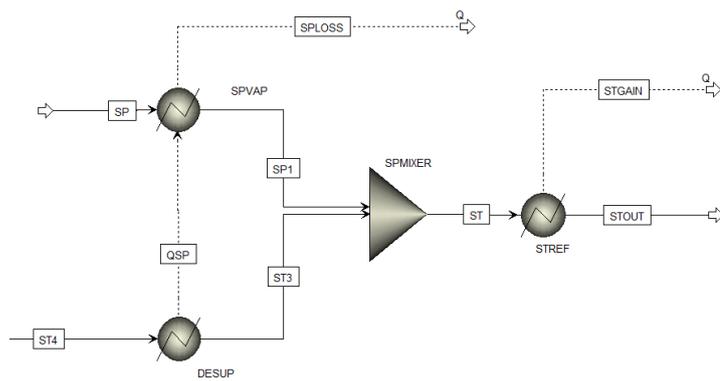
Figure C.6 – Snapshots of DESUP, SPVAP, SPMIXER and STREF
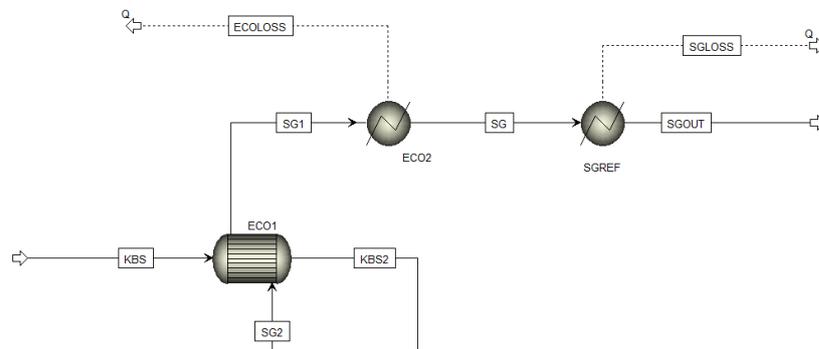
Figure C.7 – Snapshots of economizer after boiler and heaters in the stack gas line

APPENDIX D

MATLAB CODES

D1. Main Driver Code

```matlab
clear all
clc

global R
R = 8.205746e-5;              % Universal Gas Constant in m3.atm/K/kmol
atm_bar = 1.01325010000438;
psia_atm = 1.068045957064;

% Overall Properties
field1 = 'm';
field2 = 'P';
field3 = 'T';
field4 = 'V';
field5 = 'rho';
field6 = 'H';
field7 = 'Hrxn';
field8 = 'i';

% Composition Properties
field9 = 'mi';
field10 = 'ni';
field11 = 'xi';
field12 = 'yi';
field13 = 'Hi';
field14 = 'Hirxn';

% Identifiers
field15 = 'Plant';
field16 = 'Case';
field17 = 'Stream';

% Creating the structures that will hold stream properties
i = 22;
FG =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Fuel_Gas_Inlet_Rxr');
```

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```matlab
i = 4;
FO =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Fuel_Oil_Inlet_Rxr');

i = 3;
CA =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Air_Inlet');


CA2 =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Air_Pst_Heater');

FO_OIL =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Fuel_Oil_Inlet');

i = 5;
SG2 =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Stack_Pre_Eco1');

SG =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Stack_Pst_Eco2');

SG1 =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Stack_Pst_Eco1');

SGOUT =
struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,field7,0,...
    field8,i,field9,zeros(1,i),field10,zeros(1,i),field11,zeros(1,i),...
    field12,zeros(1,i),field13,zeros(1,i),field14,zeros(1,i),...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Stack_Out');

i = 1;
FO_steam = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
  field15,'XXXXXXX',field16,'XXXXXXX',field17,'Atomized_Steam_forFO_Inlet');

KBS = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'KBS_pre_Eco');

KBS2 = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'KBS_pst_Eco');
```

```matlab
KBS3 = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'KBS_pst_Dome');

BD = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Blow_Down');


BDOUT = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'Blow_Down_Out');

KBS4 = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'KBS_except_BD');

ST4 = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'KBS_except_Radiation');

ST3 = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'');

SP = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'SP');

SP1 = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'SP_pst_Heater');

ST = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'KBS_and_SP');

STOUT = struct(field1,0,field2,0,field3,0,field4,0,field5,0,field6,0,...
    field15,'XXXXXXX',field16,'XXXXXXX',field17,'KBS_and_SP_Out');


% Importing the file containing the plant operation variables
newData1 = importdata('FeedData.xls');

vars = fieldnames(newData1);
for i = 1:length(vars)
    assignin('base', vars{i}, newData1.(vars{i}));
end
plant_data = data;

temp = size(plant_data);

for i = 1:temp(1)

if i>1
    FO(i) = FO(i-1);
    CA(i) = CA(i-1);
    CA2(i) = CA2(i-1);
    SG2(i) = SG2(i-1);
    SG1(i) = SG1(i-1);
    SG(i) = SG(i-1);
    FG(i) = FG(i-1);
    FO_OIL(i) = FO_OIL(i-1);
    FO_steam(i) = FO_steam(i-1);
    KBS(i) = KBS(i-1);
    SGOUT(i) = SGOUT(i-1);
    KBS2(i) = KBS2(i-1);
    KBS3(i) = KBS3(i-1);
    BD(i) = BD(i-1);
    BDOUT(i) = BDOUT(i-1);
    KBS4(i) = KBS4(i-1);
```

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```
    ST3(i) = ST3(i-1);
    ST4(i) = ST4(i-1);
    SP(i) = SP(i-1);
    SP1(i) = SP1(i-1);
    ST(i) = ST(i-1);
    STOUT(i) = STOUT(i-1);
end


FG(i).m = plant_data(i,18)/3600;     %kg/s
FG(i).P = plant_data(i,19);     %atm
FG(i).T = plant_data(i,20);     %C
FG(i).yi = plant_data(i,21:42) ;
FG(i) = FG_Calculations2(FG(i));


FO_OIL(i).m = plant_data(i,9)/3600;        %kg/s
FO_OIL(i).P = plant_data(i,10);        %atm
FO_OIL(i).T = plant_data(i,11);        %C
FO_OIL(i).xi = plant_data(i,12:14);  %C40H80, C18H12 ,H2S
FO_OIL(i) = FO_OIL_calculations2(FO_OIL(i));

FO_steam(i).m = plant_data(i,15)/3600;  %kg/s
FO_steam(i).P = plant_data(i,16);  %atm
FO_steam(i).T = plant_data(i,17);  %C
FO_steam(i).H = FO_steam(i).m * XSteam('h_pT', FO_steam(i).P*atm_bar,
FO_steam(i).T);


FO(i) = FO_calculations2(FO_OIL(i), FO_steam(i), FO(i)); % C40H80, C18H12,
H2S, H2O


CA(i).m = plant_data(i,1)/3600;  %kg/s
CA(i).P = plant_data(i,2);     %atm
CA(i).T = plant_data(i,3);     %C
CA(i).yi = plant_data(i,4:6); %N2,O2,H2O
CA(i) = CA_calculations2(CA(i));


CA2(i).m = CA(i).m;       %kg/s
CA2(i).P = plant_data(i,8);  %atm
CA2(i).T = plant_data(i,7);  %C
CA2(i).yi= CA(i).yi;
CA2(i).ni= CA(i).ni;
CA2(i) = CA2_calculations2(CA2(i));

SG2(i).T = plant_data(i,43);
SG2(i).P = plant_data(i,44);
SG2(i) = SG2_calculations2(SG2(i), CA2(i), FG(i), FO(i));

KBS(i).m = plant_data(i,45)/3600;  %kg/s
KBS(i).T = plant_data(i,46);     %C
KBS(i).P = plant_data(i,47);     %atm
KBS(i).H = XSteam('h_pT',KBS(i).P*atm_bar,KBS(i).T) * KBS(i).m;

KBS2(i).m = KBS(i).m;               %kg/h
KBS2(i).T = plant_data(i,50); %C
KBS2(i).P = KBS(i).P;               %atm
KBS2(i).H = XSteam('h_pT',KBS2(i).P*atm_bar,KBS2(i).T) * KBS2(i).m;

SG1(i).m = SG2(i).m;
SG1(i).mi = SG2(i).mi;
SG1(i).yi = SG2(i).yi;
SG1(i).ni = SG2(i).ni;
```

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```matlab
SG1(i).P = SG2(i).P;                    %atm
SG1(i) = SG1_calculations2(SG1(i), KBS2(i), KBS(i), SG2(i));

SG(i).m = SG2(i).m;
SG(i).mi = SG2(i).mi;
SG(i).yi = SG2(i).yi;
SG(i).ni = SG2(i).ni;
SG(i).T = plant_data(i,51);     %C
SG(i).P = plant_data(i,52);     %atm
SG(i)= SG_calculations2(SG(i));

SGOUT(i).m = SG2(i).m;
SGOUT(i).mi = SG2(i).mi;
SGOUT(i).yi = SG2(i).yi;
SGOUT(i).ni = SG2(i).ni;
SGOUT(i).T = 25;    %C
SGOUT(i).P = 1;     %atm
SGOUT(i) = SGOUT_calculations2(SGOUT(i));


KBS3(i).m = KBS2(i).m;          %kg/h
KBS3(i).T = plant_data(i,48);   %C
KBS3(i).P = plant_data(i,49);   %atm
KBS3(i).H = XSteam('h_pT',KBS3(i).P*atm_bar,KBS3(i).T) * KBS3(i).m;

BD(i).m = plant_data(i,62)/3600; %kg/h
BD(i).P = KBS3(i).P;                %atm
BD(i).T = KBS3(i).T;               %C
BD(i).H = XSteam('h_pT',BD(i).P*atm_bar,BD(i).T) * BD(i).m;

BDOUT(i).m = BD(i).m;               %kg/h
BDOUT(i).T = 142.565867029826;      %C
BDOUT(i).P = 93.1776656501586;      %atm
BDOUT(i).H = XSteam('h_pT',BDOUT(i).P*atm_bar,BDOUT(i).T) * BDOUT(i).m;

KBS4(i).m = KBS3(i).m - BD(i).m; %kg/h
KBS4(i).P = KBS3(i).P;               %atm
KBS4(i).T = KBS3(i).T;               %C
KBS4(i).H = XSteam('h_pT',KBS4(i).P*atm_bar,KBS4(i).T) * KBS4(i).m;

ST4(i).m = KBS4(i).m;           %kg/h
ST4(i).T = plant_data(i,56);    %C
ST4(i).P = plant_data(i,57);    %atm
ST4(i).H = XSteam('h_pT',ST4(i).P*atm_bar,ST4(i).T) * ST4(i).m;

ST3(i).m = ST4(i).m;            %kg/h
ST3(i).T = plant_data(i,58);    %C
ST3(i).P = plant_data(i,61);    %atm
ST3(i).H = XSteam('h_pT',ST3(i).P*atm_bar,ST3(i).T) * ST3(i).m;

SP(i).m = plant_data(i,53)/3600;  %kg/s
SP(i).T = plant_data(i,54);        %C
SP(i).P = plant_data(i,55);        %atm
SP(i).H = XSteam('h_pT',SP(i).P*atm_bar,SP(i).T) * SP(i).m;

SP1(i).m = SP(i).m;             %kg/h
SP1(i).T = plant_data(i,60);    %C
SP1(i).P = plant_data(i,61);    %atm
SP1(i).H = XSteam('h_pT',SP1(i).P*atm_bar,SP1(i).T) * SP1(i).m;

ST(i).m = SP(i).m + ST3(i).m;  %kg/h
ST(i).P = ST3(i).P;                %atm
```

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```matlab
ST(i).T = ST3(i).T;                %C
ST(i).H = XSteam('h_pT',ST(i).P*atm_bar,ST(i).T) * ST(i).m;

STOUT(i).m = ST(i).m;              %kg/h
STOUT(i).T = 142.565867029826;     %C
STOUT(i).P = 93.1776656501586;     %atm
STOUT(i).H = XSteam('h_pT',STOUT(i).P*atm_bar,STOUT(i).T) * STOUT(i).m;

results(i,1) = FG(i).Hrxn*1000;
results(i,2) = FO_OIL(i).Hrxn*1000;
results(i,3) = BD(i).H*1000;
results(i,4) = BDOUT(i).H*1000;
results(i,5) = CA(i).H*1000;
results(i,6) = CA2(i).H*1000;
results(i,7) = FG(i).H*1000;
results(i,8) = FO_OIL(i).H*1000;
results(i,9) = FO_steam(i).H*1000;
results(i,10) = KBS(i).H*1000;
results(i,11) = KBS2(i).H*1000;
results(i,12) = KBS3(i).H*1000;
results(i,13) = KBS4(i).H*1000;
results(i,14) = SG(i).H*1000;
results(i,15) = SG1(i).H*1000;
results(i,16) = SG2(i).H*1000;
results(i,17) = SGOUT(i).H*1000;
results(i,18) = SP(i).H*1000;
results(i,19) = SP1(i).H*1000;
results(i,20) = ST(i).H*1000;
results(i,21) = ST3(i).H*1000;
results(i,22) = ST4(i).H*1000;
results(i,23) = STOUT(i).H*1000;
results(i,24) = SG2(i).yi(2);

results(i,26) = (BD(i).H - BDOUT(i).H)/1000;     %BDLOSS in MW
results(i,27) = (CA(i).H - CA2(i).H)/1000;       %QCAHEATER in MW
results(i,28) = (KBS(i).H - KBS2(i).H)/1000;     %KBS-KBS2 in MW
results(i,29) = (KBS2(i).H - KBS3(i).H)/1000;    %KBS2-KBS3 in MW
results(i,30) = (SG1(i).H - SG(i).H)/1000;       %SG1-SG in MW
results(i,31) = (SG(i).H - SGOUT(i).H)/1000;     %SGLOSS in MW
results(i,32) = (SG2(i).H - SG1(i).H)/1000;      %ECO2LOSS in MW
results(i,33) = (ST(i).H - STOUT(i).H)/1000;     %STGAIN in MW
results(i,34) = (ST3(i).H - ST4(i).H)/1000;      %ST3-ST4 in MW
results(i,35) = -(SG2(i).H - CA2(i).H - FG(i).H - FO_OIL(i).H -
FO_steam(i).H - FG(i).Hrxn - FO_OIL(i).Hrxn)/1000; %HCOMB in MW
results(i,36) = (-(SG2(i).H - CA2(i).H - FG(i).H - FO_OIL(i).H -
FO_steam(i).H - FG(i).Hrxn - FO_OIL(i).Hrxn) + KBS2(i).H - KBS3(i).H)/1000;
%QBOILER in MW
results(i,37) = (-(SG2(i).H - CA2(i).H - FG(i).H - FO_OIL(i).H -
FO_steam(i).H - FG(i).Hrxn - FO_OIL(i).Hrxn) + KBS2(i).H - KBS3(i).H -
ST4(i).H + KBS4(i).H)/1000;      %QRAD in MW
results(i,38) = (SP1(i).H - SP(i).H + ST3(i).H - ST4(i).H)/1000;  %SPLOSS in
MW

xlswrite('results.xls', results)
end
```

D2. Calculation Code of Fuel Gas

```matlab
function [FG] = FG_Calculations2(FG)
global R
% This function makes the necessary additions to the FG inlet conditions
% Loading MW, Hrxn, Cp and Combustion Rxn Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;

MW = FG_constants(1:22,7);
a = FG_constants(1:22,2);
b = FG_constants(1:22,3);
c = FG_constants(1:22,4);
d = FG_constants(1:22,5);
e = FG_constants(1:22,6);

Hrxn = FG_constants(1:22,1);

for i = 1:22
    MW_a(i) = MW(i)*FG.yi(i);
end

MW_avg=sum(MW_a);
FG.rho = FG.P * MW_avg / R / (FG.T + 273.15);
FG.V = FG.m/FG.rho;          %m3
n=FG.m/MW_avg;

for i = 1:FG.i
    FG.ni(i) = n*FG.yi(i);
    FG.mi(i) = FG.ni(i)*MW(i);
    FG.Hi(i) = (a(i)  * (FG.T + 273.15) +...
        2 * b(i) * c(i) /(exp(2*c(i)/(FG.T + 273.15))-1) +...
        2 * d(i) * e(i) /(exp(2*e(i)/(FG.T + 273.15))+1)) * FG.ni(i);
    FG.Hirxn(i) = -Hrxn(i) * FG.ni(i);
end
    FG.H = sum(FG.Hi)/1000;      %kJ
    FG.Hrxn = sum(FG.Hirxn);     %kJ
end
```

D3. Calculation Code of Pure Fuel Oil

```matlab
function [FO_OIL] = FO_OIL_calculations2(FO_OIL)
% This function carries out the necessary calculations on the Fuel Oil
% Loading MW, Hrxn, Cp and Combustion Rxn Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;
MW = FG_constants(25:27,7); % C40H80, C18H12, H2S in FO_OIL
Hrxn = FG_constants(25:27,1);

for i = 1:FO_OIL.i
    FO_OIL.mi(i) = FO_OIL.m * FO_OIL.xi(i); %kg
    FO_OIL.ni(i)= FO_OIL.mi(i) / MW(i); %kmol
    FO_OIL.Hirxn(i) = -Hrxn(i) * FO_OIL.ni(i);
end
```

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```matlab
FO_OIL.Hrxn = sum(FO_OIL.Hirxn);     %kJ
nT = sum(FO_OIL.ni);  %kmol

for i = 1:FO_OIL.i
FO_OIL.yi(i)= FO_OIL.ni(i)/nT;
end

API = 11.5;
s = 141.5/(API+131.5);    % Perry's HB Eqn 27.10
FO_OIL.H = FO_OIL.m * (1.685+FO_OIL.T*0.039)/sqrt(s)* FO_OIL.T;     % kg*
kJ/kg.C * C Perry's HB Eqn 27.11
end
```

D4. Calculation Code of Fuel Oil after Atomizing

```matlab
function [FO] = FO_calculations2(FO_OIL, FO_steam, FO)
% This function carries out the necessary calculations on the Fuel Oil
% inlet boiler

MW = [561.080 228.294 34.076 18.02]; % C40H80, C18H12, H2S, H2O in FO_OIL
and FO_steam

FO.P = 1 ; %atm
FO.m = FO_OIL.m + FO_steam.m;
FO.ni(1)= FO_OIL.ni(1);
FO.ni(2)= FO_OIL.ni(2);
FO.ni(3)= FO_OIL.ni(3);
FO.ni(4)= FO_steam.m/MW(4);
FO.mi = [FO_OIL.mi(1) FO_OIL.mi(2) FO_OIL.mi(3) FO_steam.m];
nT = sum(FO.ni);

for i = 1:FO.i
FO.yi(i) = FO.ni(i) / nT;
end

MW_avg = MW(1)*FO.yi(1) + MW(2)*FO.yi(2) + MW(3)*FO.yi(3) + MW(4)*FO.yi(4);

FO.H = FO_OIL.H + FO_steam.H;    % kJ
FO.Hrxn = FO_OIL.Hrxn;           % kJ

end
```

D5. Calculation Code of Air Composition

```matlab
function [air_comp] = air_comp(RH,P,T)
% Calculation of inlet air composition given RH and P
% Dry air basis is 79% N2 and 21% O2

for i = 1:length(RH)
```

```matlab
    yH2O = XSteam('psat_T',T(i)) / P(i) * RH(i) / 100;
    yN2 = 0.79 / (1 + yH2O);
    yO2 = 0.21 / (1 + yH2O);

    air_comp(i,1) = yN2;
    air_comp(i,2) = yO2;
    air_comp(i,3) = yH2O;
end

end
```

D6. Calculation Code of Combustion Air

```matlab
function [CA] = CA_calculations2(CA)
global R
% This Function assigns the remaining properties of the CA stream
% Loading MW and Cp Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;

MW = [FG_constants(2,7) FG_constants(4,7) FG_constants(23,7)];

a = [FG_constants(2,2) FG_constants(4,2) FG_constants(23,2)];
b = [FG_constants(2,3) FG_constants(4,3) FG_constants(23,3)];
c = [FG_constants(2,4) FG_constants(4,4) FG_constants(23,4)];
d = [FG_constants(2,5) FG_constants(4,5) FG_constants(23,5)];
e = [FG_constants(2,6) FG_constants(4,6) FG_constants(23,6)];

% Determining Molar Flowrates

for i = 1:3
    MW_a(i) = MW(i)*CA.yi(i);
end

MW_avg=sum(MW_a);
CA.rho = CA.P * MW_avg / R / (CA.T + 273.15);
CA.V = CA.m / CA.rho;
nT = CA.m / MW_avg;

% Calculating Enthalpy
for i = 1:CA.i
    CA.ni(i) = nT * CA.yi(i);
    CA.mi(i) = CA.ni(i) .* MW(i);
    CA.xi(i) = CA.mi(i) / CA.m;
    CA.Hi(i) = (a(i) * (CA.T + 273.15) +...
        2 * b(i) * c(i)/(exp(2*c(i)/(CA.T + 273.15))-1)+...
        2 * d(i) * e(i)/(exp(2*e(i)/(CA.T + 273.15))+1)) * CA.ni(i);
end

CA.H  = sum(CA.Hi)/1000; %kJ
end
```

D7. Calculation Code of Combustion Air after Pre-heater

```matlab
function [CA2] = CA2_calculations2(CA2)
global R

% This Function assigns the remaining properties of the CA2 stream
% Loading MW and Cp Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;

MW = [FG_constants(2,7), FG_constants(4,7), FG_constants(23,7)];

a = [FG_constants(2,2) FG_constants(4,2) FG_constants(23,2)];
b = [FG_constants(2,3) FG_constants(4,3) FG_constants(23,3)];
c = [FG_constants(2,4) FG_constants(4,4) FG_constants(23,4)];
d = [FG_constants(2,5) FG_constants(4,5) FG_constants(23,5)];
e = [FG_constants(2,6) FG_constants(4,6) FG_constants(23,6)];

% Determining Molar Flowrates
for i = 1:3
    MW_a(i) = MW(i)*CA2.yi(i);
end
MW_avg=sum(MW_a);
nT = CA2.m / MW_avg;

for i = 1:CA2.i
    CA2.ni (i) = nT * CA2.yi(i);
    CA2.mi (i) = CA2.ni (i) * MW (i);
end

CA2.rho = CA2.P * MW_avg / R / (CA2.T + 273.15);
CA2.V = CA2.m / CA2.rho;


% Calculating Enthalpy
for i = 1:CA2.i
    CA2.Hi(i) = (a(i) * (CA2.T + 273.15) +...
        2 * b(i) * c(i) /(exp(2*c(i)/(CA2.T + 273.15))-1) +...
        2 * d(i) * e(i) /(exp(2*e(i)/(CA2.T + 273.15))+1)) * CA2.ni(i);
end

CA2.H  = sum(CA2.Hi)/1000; %kJ

end
```

D8. Calculation Code of Stack Gas after Boiler

```matlab
function [SG2] = SG2_calculations2(SG2, CA2, FG, FO)
global R
% This function makes the necessary additions to the FG inlet conditions
% Loading Cp and Combustion Coefficients Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;
```

```matlab
O2_cons_FG = FG_constants(1:22,8);
H2O_gen_FG = FG_constants(1:22,9);
CO2_gen_FG = FG_constants(1:22,10);
SO2_gen_FG = FG_constants(1:22,11);
O2_cons_FO = [FG_constants(25:27,8); FG_constants(23,8)];
H2O_gen_FO = [FG_constants(25:27,9); FG_constants(23,9)];
CO2_gen_FO = [FG_constants(25:27,10); FG_constants(23,10)];
SO2_gen_FO = [FG_constants(25:27,11); FG_constants(23,11)];


a = [FG_constants(2,2) FG_constants(4,2) FG_constants(23,2)
FG_constants(3,2) FG_constants(24,2)];
b = [FG_constants(2,3) FG_constants(4,3) FG_constants(23,3)
FG_constants(3,3) FG_constants(24,3)];
c = [FG_constants(2,4) FG_constants(4,4) FG_constants(23,4)
FG_constants(3,4) FG_constants(24,4)];
d = [FG_constants(2,5) FG_constants(4,5) FG_constants(23,5)
FG_constants(3,5) FG_constants(24,5)];
e = [FG_constants(2,6) FG_constants(4,6) FG_constants(23,6)
FG_constants(3,6) FG_constants(24,6)];
MW = [FG_constants(2,7) FG_constants(4,7) FG_constants(23,7)
FG_constants(3,7) FG_constants(24,7)];

% Material Balance to Calculate Stack Gas Contents
% Nitrogen Balance - N2 comes from CA2 and FG
SG2.ni(1) = (CA2.ni(1) + FG.ni(2));
% Oxygen Balance - O2 is present in SA2 and FG - gets consumed by FO and FG
SG2.ni(2) = (CA2.ni(2) + FG.ni(4) - sum(FG.ni .* O2_cons_FG') - sum(FO.ni .*
O2_cons_FO'));
% H2O Balance - H2O comes from CA2 and generated from FO&FG combustion and
% FO atomized
SG2.ni(3) = (CA2.ni(3) + sum(FG.ni .* H2O_gen_FG') + sum(FO.ni .*
H2O_gen_FO'));
% CO2 Balance - CO2 comes from FG and is generated from FO and FG combustion
SG2.ni(4) = (FG.ni(3) +  sum(FG.ni .* CO2_gen_FG') + sum(FO.ni .*
CO2_gen_FO'));
% SO2 Balance - SO2 is generated through the combustion FO and FG
SG2.ni(5) = (sum(FG.ni .* SO2_gen_FG') + sum(FO.ni .* SO2_gen_FO'));

% Calculating the remaining properties
SG2.mi = SG2.ni .* MW;
SG2.m = sum(SG2.mi);
SG2.xi = SG2.mi / SG2.m;
SG2.yi = SG2.ni / sum(SG2.ni);

% Enthalpy Calculations
for i = 1:SG2.i
    SG2.Hi(i) = (a(i) * (SG2.T + 273.15) +...
        2 * b(i) * c(i) /(exp(2*c(i)/(SG2.T + 273.15))-1) +...
        2 * d(i) * e(i) /(exp(2*e(i)/(SG2.T + 273.15))+1)) * SG2.ni(i);
end
SG2.H  = sum(SG2.Hi)/1000; %Kj

end
```

D9. Calculation Code of Stack Gas after Second Heat Exchanger

```matlab
function [SG] = SG_calculations2(SG)
global R
% This function makes the necessary additions to the SG (outlet Eco2)
conditions
% Loading Cp Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;

a = [FG_constants(2,2) FG_constants(4,2) FG_constants(23,2)
FG_constants(3,2) FG_constants(24,2)];
b = [FG_constants(2,3) FG_constants(4,3) FG_constants(23,3)
FG_constants(3,3) FG_constants(24,3)];
c = [FG_constants(2,4) FG_constants(4,4) FG_constants(23,4)
FG_constants(3,4) FG_constants(24,4)];
d = [FG_constants(2,5) FG_constants(4,5) FG_constants(23,5)
FG_constants(3,5) FG_constants(24,5)];
e = [FG_constants(2,6) FG_constants(4,6) FG_constants(23,6)
FG_constants(3,6) FG_constants(24,6)];

% Enthalpy Calculations
for i = 1:SG.i
    SG.Hi(i) = (a(i) * (SG.T + 273.15) +...
        2 * b(i) * c(i) /(exp(2*c(i)/(SG.T + 273.15))-1) +...
        2 * d(i) * e(i) /(exp(2*e(i)/(SG.T + 273.15))+1)) * SG.ni(i);
end
SG.H  = sum(SG.Hi)/1000; %kJ
end
```

D10. Calculation Code of Stack Gas Released to Environment

```matlab
function [SGOUT] = SGOUT_calculations2(SGOUT)
global R
% This function makes the necessary additions to the SGOUT
% Loading Cp Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;

a = [FG_constants(2,2) FG_constants(4,2) FG_constants(23,2)
FG_constants(3,2) FG_constants(24,2)];
b = [FG_constants(2,3) FG_constants(4,3) FG_constants(23,3)
FG_constants(3,3) FG_constants(24,3)];
c = [FG_constants(2,4) FG_constants(4,4) FG_constants(23,4)
FG_constants(3,4) FG_constants(24,4)];
d = [FG_constants(2,5) FG_constants(4,5) FG_constants(23,5)
FG_constants(3,5) FG_constants(24,5)];
e = [FG_constants(2,6) FG_constants(4,6) FG_constants(23,6)
FG_constants(3,6) FG_constants(24,6)];
```

```
% Enthalpy Calculations
for i = 1:SGOUT.i
    SGOUT.Hi(i) = (a(i) * (SGOUT.T + 273.15) +...
        2 * b(i) * c(i) /(exp(2*c(i)/(SGOUT.T + 273.15))-1) +...
        2 * d(i) * e(i) /(exp(2*e(i)/(SGOUT.T + 273.15))+1)) * SGOUT.ni(i);
end
SGOUT.H  = sum(SGOUT.Hi)/1000; %kJ
end
```

D11. Calculation Code of Stack Gas after First Heat Exchanger

```
function [SG1] = SG1_calculations2(SG1, KBS2, KBS, SG2)
global R
% This function makes the necessary additions to the SG1 (outlet of Eco1)
% Loading Cp Information

newData1 = importdata('FG_Constants.csv');
FG_constants = newData1.data;

a = [FG_constants(2,2) FG_constants(4,2) FG_constants(23,2)
FG_constants(3,2) FG_constants(24,2)];
b = [FG_constants(2,3) FG_constants(4,3) FG_constants(23,3)
FG_constants(3,3) FG_constants(24,3)];
c = [FG_constants(2,4) FG_constants(4,4) FG_constants(23,4)
FG_constants(3,4) FG_constants(24,4)];
d = [FG_constants(2,5) FG_constants(4,5) FG_constants(23,5)
FG_constants(3,5) FG_constants(24,5)];
e = [FG_constants(2,6) FG_constants(4,6) FG_constants(23,6)
FG_constants(3,6) FG_constants(24,6)];

% SG1.ni =[0.5288    0.0186    0.1290    0.0727    0.0003];

KBS2_H = KBS2.H;
KBS_H = KBS.H;
SG2_H = SG2.H;
SG1.H = - KBS2_H + SG2_H + KBS_H;
SG1_H = SG1.H*1000;

% Temperature Calculations
for i = 1:5
    syms SG1_T
    SG1_Hi(i) = (a(i) * (SG1_T + 273.15) +...
        2 * b(i) * c(i) /(exp(2*c(i)/(SG1_T + 273.15))-1) +...
        2 * d(i) * e(i) /(exp(2*e(i)/(SG1_T + 273.15))+1)) * SG1.ni(i);
end

A  = sum(SG1_Hi);

SG1_T=solve(A-SG1_H);
SG1.T=SG1_T;

end
```

APPENDIX E

PROCESS FLOW DIAGRAM

In this section, there are tables illustrated sample operating conditions of boiler. Boiler feed water stream properties are shown in Table E.1, properties of feed streams of boiler are shown in Table E.2 and stack gas properties are shown in Table E.3.

Table E.1 − Process flow diagram of boiler feed water stream

	BD	BDOUT	KBS	KBS2	KBS3	KBS4
Total Flow (kmol/sec)	0.069386	0.069386	0.693855	0.693855	0.693855	0.62447
Temperature (K)	553.0375	298.15	413.15	473.15	553.15	553.0375
Pressure (N/sqm)	6586130	101325	9119250	9119250	6586130	6586130
Vapor Fraction	3.85E-04	0	0	0	0	3.85E-04
Component Mole Flow (kmol/sec)						
H_2O	0.069386	0.069386	0.693855	0.693855	0.693855	0.62447

Table E.1 − Process flow diagram of boiler feed water stream (cont'd)

	SP	SP1	ST	ST3	ST4	STOUT
Total Flow (kmol/sec)	0.077095	0.077095	0.701565	0.62447	0.62447	0.701565
Temperature (K)	418.15	693.15	693.15	693.15	708.15	298.15
Pressure (N/sqm)	6586130	6586130	6586130	6586130	6586130	101325
Vapor Fraction	0	1	1	1	1	0
Component Mole Flow (kmol/sec)						
H_2O	0.077095	0.077095	0.701565	0.62447	0.62447	0.701565

Table E.2 – Process flow diagram of feed streams

	CA	CA2	FEED	FG	FO	FO-OIL	FO-STM
Total Flow (kmol/sec)	1.229161	1.229161	1.310359	0.063445	0.017753	2.33E-03	0.015419
Temperature (K)	288.15	373.15	371.6061	293.15	429.9255	423.15	473.15
Pressure (N/sqm)	101325	101325	101325	101325	101325	101325	1013250
Vapor Fraction	1	1	0.998587	1	0.891426	0.198513	1
Component Mole Flow (kmol/sec)							
H_2	0	0	0.027281	0.027281	0	0	0
N_2	0.958746	0.958746	0.958809	6.34E-05	0	0	0
CO_2	0	0	6.34E-05	6.34E-05	0	0	0
O_2	0.258124	0.258124	0.258187	6.34E-05	0	0	0
CO	0	0	0	0	0	0	0
H_2S	0	0	4.89E-04	0	4.89E-04	4.89E-04	0
CH_4	0	0	0.02855	0.02855	0	0	0
C_2H_6	0	0	2.79E-03	2.79E-03	0	0	0
C_2H_4	0	0	6.34E-04	6.34E-04	0	0	0
C_3H_8	0	0	1.90E-03	1.90E-03	0	0	0
C_3H_4	0	0	0	0	0	0	0
C_3H_6	0	0	1.27E-04	1.27E-04	0	0	0
C_4H_{10}	0	0	5.71E-04	5.71E-04	0	0	0
C_4H_{10}-01	0	0	5.08E-04	5.08E-04	0	0	0
C_4H_8--01	0	0	6.34E-05	6.34E-05	0	0	0
C_4H_8--02	0	0	6.34E-05	6.34E-05	0	0	0
C_4H_8--03	0	0	6.34E-05	6.34E-05	0	0	0
C_4H_8--04	0	0	6.34E-05	6.34E-05	0	0	0
C_4H_6--01	0	0	0	0	0	0	0
C_5H_{12}-01	0	0	5.08E-04	5.08E-04	0	0	0
C_5H_{12}-02	0	0	1.27E-04	1.27E-04	0	0	0
C_6H_{12}-01	0	0	0	0	0	0	0
H_2O	0.012292	0.012292	0.027711	0	0.015419	0	0.015419
SO_2	0	0	0	0	0	0	0
$C_{40}H_{80}$-01	0	0	1.19E-03	0	1.19E-03	1.19E-03	0
$C_{18}H_{12}$-01	0	0	6.57E-04	0	6.57E-04	6.57E-04	0

Table E.3 – Process flow diagram of stack gas

	SG	**SG1**	**SG2**	**SGOUT**
Total Flow (kmol/sec)	1.326867	1.326867	1.326867	1.326867
Temperature (K)	448.15	556.1822	631.6677	298.15
Pressure (N/sqm)	101325	101347	101347	101325
Vapor Fraction	1	1	1	1
Component Mole Flow (kmol/sec)				
N2	0.958809	0.958809	0.958809	0.958809
CO2	0.109413	0.109413	0.109413	0.109413
O2	0.066253	0.066253	0.066253	0.066253
H2O	0.191904	0.191904	0.191904	0.191904
SO2	4.89E-04	4.89E-04	4.89E-04	4.89E-04