QATAR UNIVERSITY

COLLEGE OF BUSINESS AND ECONOMICS

USING DATA MINING TECHNIQUES TO PREDICT NOX EMISSION LEVELS IN GAS FIRED BOILERS

BY

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ABSTRACT

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Title: Using Data Mining Techniques to Predict NOx Emissions Levels in Gas Fired Boilers

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Natural gas industry becomes one of the largest sectors in the today's world economy. With the growth of production, pollutants from gas processing plants continue to grow, forcing government and legislative authorities to compel stringent restrictions on the release of emissions. These restrictions become among top vital factors influencing plant operations nowadays in the state of Qatar. One of the most important tasks for gas processing plants is not only to ensure a continuous gas supply to customers, but also to monitor, control and address concerns about the environmental impact of the operations. The use of the gas fired steam boilers in the gas operations has led to a significant increase in the emissions of toxic substances such as NOx. Therefore, significant worries have been raised about the environmental effect on climate and air quality of noxious emissions associated with the steam generation process of the boilers.

Data mining is a powerful tool that has been used for decades for advanced process analytics of large quantities of plant data in order to extract useful information and to reach a better understanding of the process. In this research, some of data mining techniques such as artificial neural networks and decision trees are applied on real plant data representing 27 industrial process parameters from a gas fired steam boiler of one

gas processing plant at Ras-Laffan Industrial City in order to predict the most important factors impacting the NOx formation in the combustion process of the boiler. Closer attention to those factors can be given promptly in order to enhance the plant environmental performance.

The results obtained by the artificial neural network and decision tree models showed that the NOx emissions are directly related to the air flow parameters such as O_2 concentration, the excess air level in the boiler and the amount of the flue gas at the boiler outlet. It was also shown that the company is following a traditional technique of lowering the amount of oxygen in the boiler aiming to reduce the NOx emission levels. However, this technique was proven to be limited under certain threshold of boiler load due to other important factors such as the adiabatic flame temperature (AFT) which induces the formation of NOx emissions.

Keywords: Data Mining; Artificial Neural Network; Decision Tree; Modeling; Steam Boiler; NOx Emissions.

DEDICATION

I dedicate this research to my beloved parents whose affection, encouragement and prays, make me able to continue my MBA program

To my dearest brother and sister for always being there and the continuous support they've given me

Last but not least, I dedicate this work to my wonderful wife whose limitless giving, huge sacrifice and endless patience, helped me accomplish my degree

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CHAPTER 1: INTRODUCTION

Oil and gas sector represents the major constituent that runs the Qatari economy today, despite that the State of Qatar stresses the importance of finding substitutions to these prime sources of energy which comes in line with the Qatar National Vision 2030 in order to reduce the country's necessity towards the natural resources of crude oil which totals about (850 thousand barrels per day), and natural gas which totals about (18 billion cube foot per day) extracted from the North Gas Field which has gas reserves of about (380 trillion cube foot) (Sergie, 2018; John, 2018).

Founded in 1971, the North Gas Field (NGF) anchors offshore to the northeast of the Qatar peninsula under water depths extending between 15 to 70 meters. Its total area coverage is about 6,000 square kilometers, an estimated half of the entire mainland Qatar (Sergie, 2018). NGF is the main location and possesses single concentration of non-associated natural gas worldwide with a total accumulated volume reserve of more than 900 trillion cubic feet, constituting 20% of global whole, thereby, placing Qatar the third country position in the world for natural gas reserves after Russia and Iran (Said, 2017). The expansion of this giant natural resource has been a noteworthy element in Qatar's economic growth. The gas produced from this major field is treated to produce *Liquefied Natural Gas*, *Gas to Liquid*, *Natural Gas Liquid*, and other gas products, in addition to natural gas pipeline for export (Said, 2017). Based on the huge extractable reserve quantities in the North Gas Field and benefits of production of clean gas, safe usage and long shelf life (Sergie, 2018). Qatar Petroleum (QP), the state owned petroleum company of Qatar founded in 1974, articulated a step-by-step strategical plan to progress the field extractions, maintain reserves as well as optimal utilization of the energy extractions without compromising the environment (John, 2018).

With the rapid and developing growth of natural gas industry in Qatar, there emerged a number of environmental problems such as pollution from industrial releases, waste management issues and other ecological concerns. So, environmental defense is being paid rising attention nowadays.

One of the most important challenges facing gas processing plants in Qatar is not only to ensure a continuous gas supply to customers, but also to monitor, control and address concerns about the environmental impact of the operations. In fact, natural gas producers are encountering regulatory, and competitive challenges to deliver consistent and clean energy while reducing the cost of operations. Many technologies and advanced control systems have been developed and implemented to improve the efficiency of power plant assets while lowering the level of toxic substance emissions to the environment (Waldner et al., 2013).

Furthermore, the use of fired gas boilers for steam generation has led to a major growth in the emissions of toxic gases in the atmosphere such as NOx, CO_2 and SOx (Waldner et al., 2013). Consequently, noteworthy fears have been raised about the environmental consequences on climate and air quality of noxious emissions associated with the steam generation process of the boilers (Schlechtingen et al., 2013).

However, steam generation process in gas processing plants involves very complicated, dynamic and non-linear operations because of the complex operating conditions with the various stages of field equipments and associated processes, the massive boiler design, and fuel gas characteristics (Chongwatpol & Phurithititanapong, 2014; Schlechtingen et al., 2013). This makes the control of the operational parameters and the understand of the thermal combustion reactions are very difficult in order to minimize the environmental effect on climate and air quality (Waldner et al., 2013).

Similar to other natural gas processing plants in Ras-Laffan Industrial City such as Qatar-Gas, Ras-Gas and Shell GTL, the research will study one gas processing plant that uses giant gas fired boilers to produce superheated high pressure (HHP) steam to drive Steam Turbine driven Generators (STG) for electrical power generation.

Moreover, HHP steam is marginally depressurized to produce saturated high pressure (HP) steam to be used in different process and chemical reactions. In general, boilers are crucial for the plant operations, as they are essentially used to generate steam that is in turn used:

- For electrical power generation
- As a heating medium in heat exchangers for various process reactions
- For equipment purging and gas slug removals
- For producing desalinated water that is intended for several operations

Steam Boiler Operation Overview

The superheated high pressure (HHP) steam at our research plant is produced in four boilers, by the flow of demineralized water through a series of tubes inside the boilers to capture the heat from the furnace and then boil under high pressure to become superheated steam. The furnace provides the necessary heat by burning combustion fuel gas. The generated superheated steam leaves the boiler then enters the steam turbine throttle of the STG, where it powers the turbine connected to generator to produce electricity. By this, the company is capable to generate 80% of its demand to electricity from the HHP steam. The exhaust gas, also called the flue gas, escapes out of the boiler to the atmosphere via chimneys. The maximum continuous capacity of the boilers is 223 ton/h with outage pressure of 43 bar and temperature of 385 °C. Boilers fuel gas combustion is managed by Burner Management System (BMS) controlling each boiler with respect to fuel gas to main and pilots burners, air flow rate to burners, instrument air to pilots and all boiler operating variables.

Environmental considerations and emissions are serious factors to be considered when we talk about boiler operations. An example of the pollutants is the NOx emission that is known for its massive harm to the human well-being and to the atmospheric environment. Thus, all operated companies including our research study company are obligated to maintain the NOx emission levels and to report the figures on regular basis to Qatar Petroleum to confirm the environmental compliance and the adherence to QP HSE Regulations. According to QP HSE Regulations: "*Operators shall conform to the provisions of the (1) 'Environmental Protection Law of 2002' and (2) Annexes of the Executive By-Law for the Environmental Law, Decree Law No. 30 for 2002*". The corporate HSE department at the company is responsible for ensuring the availability and the integrity of environmental emissions information for reporting.

NOx Emissions Issue

One of the crucial problems facing the company is that it suffers from high levels of NOx emissions released into the atmosphere which is generated from the combustion process at the gas fired steam boiler. The NOx emission is greater than the regulation limit of 50 mg/Nm^3 and the design specification limit of 35 mg/Nm^3.

In fact, the company always operates its boilers near the accepted threshold value of the NOx emissions; that is, any disturbance in boiler operation, such as an increase in the steam demand or upsets in the downstream and/or upstream process can lead to high NOx emissions beyond the alarm level. The following figure illustrates the trend of NOx emissions from the company's historian system, known as Process Information (PI) System:

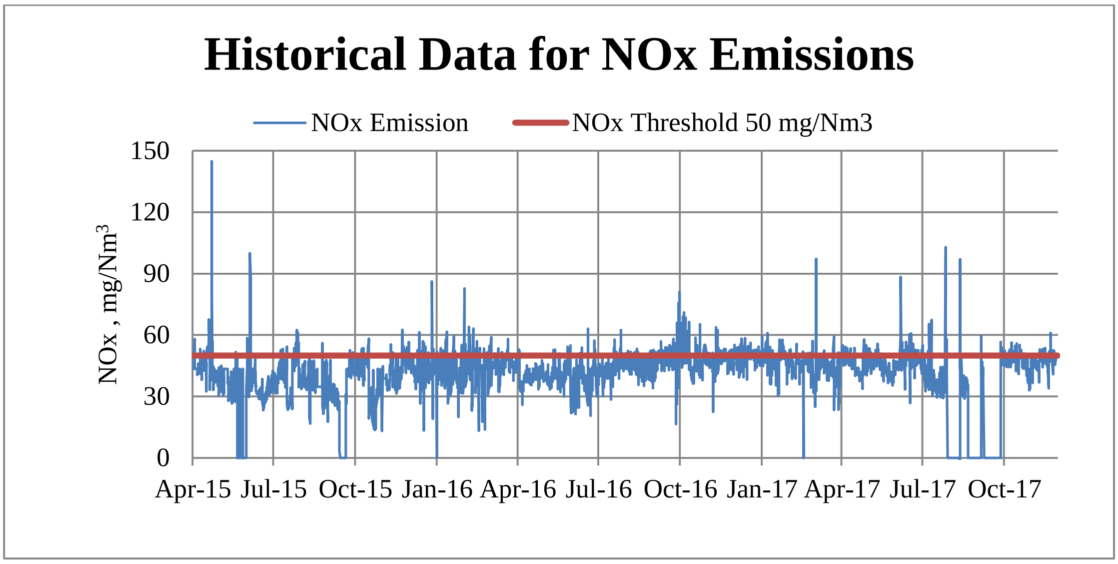

Figure 1. Historical data represents NOx emissions

Research Question

After discussing the NOx emissions issues in the above section, it is obvious that both of failure to control NOx emissions within the accepted limit and failure to report proper NOx emissions data to the authority are two of the serious challenges that facing the company. Thus, the research problem appears in answering the following questions:

1. What are the factors (process parameters) responsible for the high NOx emissions in the gas fired boilers?
2. How the model of NOx emissions can be derived in order to predict or calculate the NOx emission using available process parameters?

Answering the two question will indeed provide practical solutions to help the company resolve its problems.

Project Objectives

This project aims to follow an academic approach in order to:

1. Study and review the literature review of boiler operation, and NOx emissions

formation and reduction. Then, try to relate the issue of NOx emissions in the company of study to other companies in the same industry inside and outside Qatar.

2. Recognize the role that data mining methods can play to derive the NOx emission model and to identify the factors affecting the NOx emission value in the gas fired boiler.
3. Provide practical solutions based on the data mining concepts and techniques to answer the research questions.
4. Evaluate and compare the results obtained by the various data mining methods.
5. Provide short-term and long-term recommendations to the company based on the research outcomes to help the company resolve the issue of high NOx levels.

Since NOx is one of the crucial contributors to the company’s gas releases, the main focus of this study is on determining the key factors that have a great influence on NOx pollutants. Although this research is built within the context of a particular gas fired steam generation, the challenges of limiting the NOx emissions and improving environmental protections at the plant are quite similar to what is observed in most gas processing plants within Qatar.

Research Importance

After reviewing the available previous studies about the determination of the important factors contributing to NOx formation in the gas fired boilers, it was revealed that this research is the first one discussing this topic in Qatar and in the GCC region, and it is among few studies that discuss this topic in the world.

Furthermore, the research has used two different data mining techniques, namely neural networks and decision trees, to build models that predict the NOx emissions from 27 real process parameters. The aim behind using two different techniques is to compare the outputs and to have a better explanation of each model.

This research also fills the gap between two classical explanations of NOx formation in the combustion process which are the NOx vs Oxygen affiliation and NOx vs AFT (adiabatic flame temperature) relationship. The later one represents the most recent elucidation of the NOx emissions in the literature, and the former one provides the traditional explanation about the famous relationship between the NOx formation and the oxygen concentration.

CHAPTER 2: LITERATURE REVIEW

The need to increase in size as well as the capacity of industries is compelling firms to seek for alternatives that would make the production processes more efficient. Though the uses of steam boilers are not limited to large industries, their different application, such as in the mobile steam engine, is largely to enhance performance or productivity (Waldner et al., 2013). A steam boiler basically generates steam through the application of heat energy to water. The operations of the steam boiler vary and are also dependent on the kind of fuels used. In this regard, the combustion facilitated by different fuels such as petrol or diesel generates a varied concentration of gases. In a plant, nitrogen oxides (NOx) are some of the gases emitted in a substantial proportion. It is therefore important to understand the processes that take place in steam boilers, the formation of NOx as well as the environmental considerations that are associated with NOx emissions (Waldner et al., 2013).

Steam Boiler Process in Natural Gas Plant

A steam boiler involves uncomplicated principles applied in the process of operations where heat is the foundation. A boiler produces high pressure on the premise that a single volume in a unit mass of steam is far greater than that of water (pressure tends to rise where water is transformed to steam in an enclosed vessel). Steam Boiler designed according to the requirement of combustion process, this process transfers the large amount heat possible if the combustion to water by using different process such as convection, radiation and conduction etc. It is important for maintaining the efficiency of heat transfer because fuel burn is maximum and generate cost effective outcomes.

Depending on the type, a boiler includes a furnace chamber for the purpose of burning the fuel as well as generating the required heat. As part of creating the ideal combustion characteristics of the fire, there is a need for air to be conveyed through the grate, as well as over the fire. It is worth noting that, majority of boilers now rely on mechanical draft equipment instead of natural draught. The heat generated at the initial stages is transmitted to water in order to create steam in what is referred to as the boiling process. The boiling process results in the production of saturated steam at a degree or rate that can differ in keeping with the pressure beyond the boiling water. High-speed diesel (HSD) and low sulphur heavy stock (LSHS) are some of the fuels used in gas-fired boilers (Ranjan, 2015). The greater the temperature in the furnace, the quicker the production of steam.

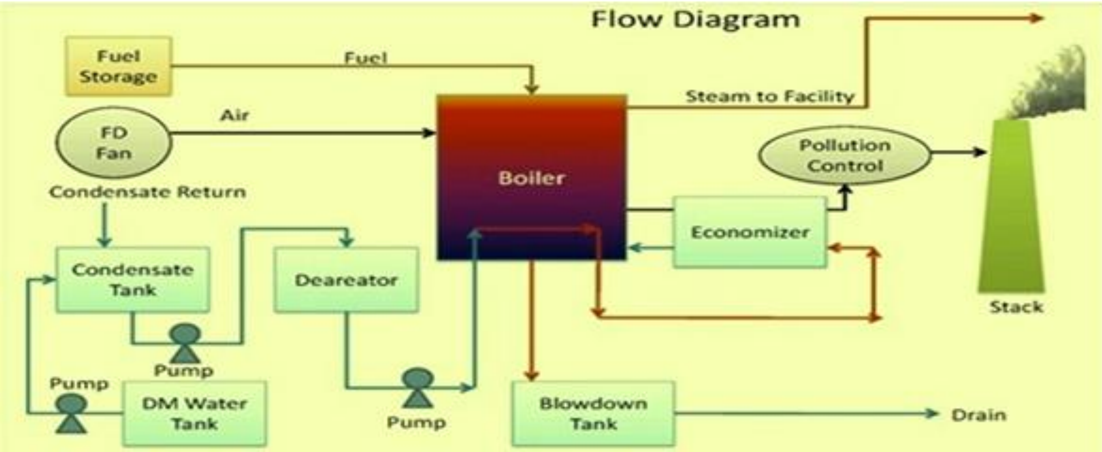

Figure 2. Boiler process flow diagram

During the process, the saturated steam made can then be used instantly to generate power through a dedicated alternator and turbine. Also, the saturated steam might be superheated more to a greater degree of temperature. Super-heater provides more energy to the boiler’s exit steam (Ganapathy, 2003). The extra energy increases the temperature, therefore, heating the content of the steam beyond the saturation point.

The superheating lowers the content of the suspended water thus producing a particular volume of steam in addition to creating a higher temperature gradient that assists in reducing the likelihood of condensation in any form. Should there be any heat remaining, then it may either be removed or made to go through a system called an economizer (Merritt, 2015). The economizer is basically a set of coils that are made from steel tubes situated towards the broiler's end and whose function is warming the feed water it before reaching the boiler. Feed water refers to the water delivered to the boiler that is turned into steam. The feed water sources are condensed steam that is returned from the process as well as the makeup water generated from the water treatment plant. The temperatures of the final re-heater are usually between 560 to 600 °C. Re-heaters are comparable in design and structure to the super-heaters but vary due to the fact that they function at lower pressures.

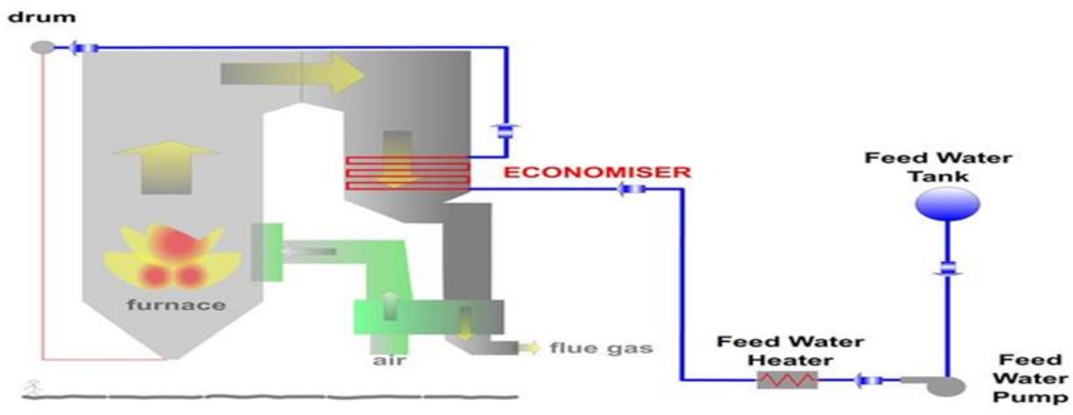

Figure 3. Economizer process flow diagram

According to (Amin & Talebian, 2018) There are some components like heat exchanger, burner, controls and combustion chambers etc. these are main components which help in controlling the entire process of steam boiler in natural gas plant. The burner can mix with the fuel and oxygen together to generate combustion platform. This combustion take place in the chamber and also useful for transferring heat. This is also playing role as a heat exchanger. Heating generating process is also managed the air supply, water temperature, rate of burner, boiler pressure, steam pressure and fuel supply and exhaust draft etc. boiled water produced with the help of boiler through pipes and also delivered the equipment by using building. This is an efficient process to manage the entire functionality of steam boiler in natural gas plant.

According to (Basso & Cumo, 2017) there are some advantage of natural gas steam boiler. Natural gas steam boiler follows to generate power in the system and their processes. It is a high quality and powerful boiler to increase the productivity of organization and plant. This process is reduced energy cost because most of plant uses this process to generating high energy. Natural gas is powerful as compare to electricity and fuel due to less cost and price. This is beneficial of industry to increase their profitability and production with the help of this process. There are many factories or industries uses this process to generate excess amount of energy. This process will reliable for company as well as stakeholders.

Factors Affecting Steam Boiler Efficiency

According to (Pambudi and Handogo, 2017) there are important factors that affects the steam boiler efficiency:

Fuel gas temperature: Fuel gas temperature is called stack temperature because this will help for measuring the hot gas combustion which is exit in the boiler.

Sometimes, fuel gases increase their temperature and it also produced more heat energy. Boiler is applicable in industry for maintaining the heat and their temperature. It will not use for generating steam. Time to time, maintenance required for plant to manage their operations and functions. Heat can be loss through gas temperature and involves for installing the combustion air heater and economizer in the steam boiler system.

Fuel specification: It is not surprising but fuel specification can impact on the efficiency of steam boiler. This issue is generated when it is establishing the right fuel specification. It is important for maintain the actual fuel which is required for processes. Natural gas plant mainly concerns about the fuel specification. Hydrogen content highly essential for generating steam. Sometimes, this gas is inevitably through water at the time of combustion. It can create monopolizes energy on the other hand. it also uses the combustion process for industrial activities. There are important combustible components in natural gases such as methane CH_4, Propane C_3H_8, pentane C_5H_{12}, ethane C_2H_{12} etc. Hydrogen content is burned quickly and produced more water by using combustion process.

Excess air: Some of the boilers are burned which required to excess air because the combustion process required rich fuel. It is an inevitably that absorb the combustion heat and also reducing the heat transferred efficiency. This is also major issue that could be addressed by calibrating boiler because they always monitoring the different level of firing.

Ambient temperature: Ambient temperature is a process that enter in the boiler through combustion air. Accordingly, the temperature can be impelled through the forced draft fan. It is determined that steam boiler in natural gas effect the both efficiency calculation and boiler efficiency. According to (Masum, 2013); It is directly affecting the net stack temperature. This is the most important difference between the fuel gas temperature and ambient temperature. Nitric oxide and carbon monoxide gases are trying to reduce the ambient temperature and also decrease the temperature. It is important for industries to balance the energy combustion in the processes. According to calculation, the ambient temperature of steam boiler is 70 to 80 degree Fahrenheit.

Radiation and convection losses: Radiation and Convection losses is major factor that affecting the efficiency of boiler steam in natural gas plant. There are two strategies helps for reducing convection and radiation losses. They also useful to control the airflow over the steam boiler surface. The external surface of steam boiler high and they generate high temperature water as compare to its surroundings. Sometimes, it is difficult for measure the actual loss because it is complex process. Radiation and convection losses is proportional to external surface area of unit.

Formation of NOx in Steam Boilers

The formation of NOx is complex and is influenced by several aspects that are specific to the boiler used (Reddy, 2013). However, fuel NOx and thermal NOx are predominantly used in the formation of NOx. Thermal nitrogen oxides are byproducts of the combustion process which are generated by industrial plant boilers as well as process heaters in the course of burning natural gas. In a very high-temperature combustion processes with the use of air as an oxidizing agent, the mixture of both atmospheric nitrogen as well as oxygen leads to the nitric oxide (NO) formation. Even though nitric oxide is not stable thermodynamically especially at reduced temperatures, the rate of decomposition is quite slow that upon formation, the concentration continues to be the same as the heat is eliminated from the combustion gases.

Reaction kinetics point to increased formation of nitric oxide with increased excess air, the temperature of the flame, as well as time at temperature. Small quantities of NO undergo an oxidation process form nitrogen II oxide (NO2) with the combustion gases cooling. The emission, in this case, is the sum of the two substances and is known as NOx. During the process, the NOx formation rate rises considerably above 2,800°F flame temperature.

The emissions of NOx from boilers are incumbent upon a number of factors. The most important aspects are the quantity of nitrogen in the fuel, the temperature of the flame, excess air level as well as the combustion air temperature. In addition, an extended residence time at higher temperatures leads to increased amounts of NOx. Whereas temperature of the flame mainly affects the formation of thermal NOx, the quantity of nitrogen in the fuel used influences the level or the rate of fuel NOx emissions. For that reason, the fuel that contains more nitrogen leads to the generation of greater levels of NOx emissions. Among the common fuels used, coal is to a large extent the major producer of NOx as a result of the nitrogen that is contained in the fuel itself.

As stated, the formation of NOx in industry has been a long-standing problem for many businesses. In the simplest terms, however, NOx is mainly formed during combustion activities as they relate to industrialized, factory-based processes (Singh & Lou, 2017). Again, this formation requires a specific fuel, usually gas, coal or sometimes other biomass substances that are used to produce various products like plastic or in the creation of energy for public or industrial usage. Overall it has been the conversion of nitrogen that basically forms NOx and the subsequent poisonous gas released.

It has generally been through these industry-based processes within specific business activities that emissions of NOx are thus introduced into the environment through various means. Factory boilers, burners, kilns, and the like, have a tendency to be the most common producers of these types of NOx emissions (Singh & Lou, 2017). Therefore, such activities, due to the potential for harm to the environment, living creatures, and the overall living conditions of the entire planet, should be accounted for by regulatory frameworks more thoroughly.

Environmental Considerations related to NOx Emissions

Due to a variety of factors, the formation, accidental exposure, and subsequent consequences of the common chemical nitrogen (NOx), many industries across the globe are in need of changing the way they deal with this dangerous emission. In addition, there have been several drastic environmental concerns raised because of the proliferation of noxious deadly gases from increased NOx formation. Therefore, the need to better understand this phenomenon, as well as a construction of possible control factors, will be vitally important moving forward for industrial activities that cause the release of NOx during any and all operations.

NOx is a common, yet extremely deadly, gas that is created from industrial processes such as factory activities. Generally speaking, the formation of NOx occurs when the combustion process takes place, most notably during when coal is used as a fuel and high-temperature air as an oxidant (Singh & Lou, 2017). Thus, since this gas can so easily be created through the industrial processes taking place each and every day, it would be valuable to understand its various properties therein; as well as its actual formation (Tian et al., 2013).

The emission of NOx to the atmosphere raises important environmental issues that ought to be given significant consideration. Anthropogenic nitrogen oxides (NOx = NO + NO2) emissions, according to (Tian et al., 2013), are linked with substantial effects on human health as well as ecosystems. These impacts extend to include the ozone layer due to the reactions that take place. In addition, (Tian et al., 2013) noted that the anthropogenic nitrogen oxides lead to fine particle formation as well as regional acid deposition. The biggest amount of nitrogen oxides emissions is released as NO (monoxide) and are oxidized in the atmosphere to NO2

The ozone forms a protective shield on the stratosphere of the earth from harmful radiation emitted by the sun. Pollution of air in the form of Nitrogen oxides (NOx) has the potential to affect the ozone layer when there are huge quantities of the gases in the atmosphere. Volatile ozone compounds (VOCs) and react with the sun's rays and heat as the catalyst to form smog or ground-level Ozone (Calhoun & Seideman, 2005). Wind currents can transport ozone and lead to lasting health effects far from the original bases (Calhoun & Seideman, 2005). NOx also reacts freely with some of the common organic chemicals to form a broad spectrum of toxic products such as nitrosamines and radicals of the nitrate (Gupta, 2012). A number of these resulting compounds can lead to mutations of DNA. NOx gases react with ammonia (NH3+), water particles, as well as other elements to form nitric acid vapor and associated particles (Singh & Lou, 2017). The resulting tiny particles can enter deep into sensitive tissues of the lung thus causing damage it. Also, acid rain affects the ecological environments such as soil and water thus leading to more harm in the ecosystem (Gupta, 2012). The concentration of nitrogen oxides at a particular threshold negatively affects the environment. Considering various direct as well as indirect impacts, NOx emissions also contribute negatively to global warming (Singh & Lou, 2017).

NOx Possible Harm

The potential harm done in many situations that relate to production industries like oil and gas plants has been ongoing, studied within certain academic fields, and exists within a myriad of circumstances. For example, the amount of NOx in the environment itself (i.e. air, water, and products consumed by humans and other animals) can be substantial when power plants, industrial boilers, and cement kilns are active, NOx can be spilled into the environment) which produces smog in large urban areas (Nitrogen oxides (NOx) control regulations, 2019). Such environmentally negative impact can thus pose a grave threat to the atmospheric environment.

Poor air quality can lead to ongoing health problems for many human populations where large factories are present that produce high levels of NOx. In turn, these high levels of NOx found in the air can also wreak havoc when combined with other potentially harmful gases. For instance, due to the volatile nature of NOx, when it is released through the chemical processes described, it can also produce additional noxious fumes when introduced into the air (Nitrogen oxides (NOx) control regulations, 2019). Obviously, difficulty in breathing for many people can be experienced, as well as tainted water supplies.

Therefore, the negative impact NOx formation might have on related industries such as agriculture can also be quite harmful. This harm can take several forms. One harmful consequences of NOx creation due to industry has been related to how NOx reacts to organic compounds, some found in soil used to grow food, and thus can contribute to negative yields and chemical laden crops (Nitrogen oxides (NOx) control regulations, 2019). Understanding the specific formation of NOx can thus lead to possible solutions to reduction.

Previous Studies

Many studies have addressed various aspects of NOx emissions in steam boiler and data mining role in predicting the factors affecting the formation. However, most of these studies are related to coal-fired boilers rather than gas-fired boilers that are commonly used in countries rich in natural gases such as Qatar. The following are some of the previous researches that have discussed the NOx emissions:

1. (Chongwatpol, 2016) illustrated the importance of building a data mining framework to form a neural network model to address the NOx high emissions in a coal-fired boiler in power generation plant in Thailand. The study followed a

comprehensive framework of 10 steps to run a data mining project at a power generation plant to resolve the NOx emission issue.

The researcher also demonstrated the role of big data analytics in resolving business problems. Although the study was rich in technical matters, it was conducted within the context of power generation plant and examined the NOx formation in a specific coal-fired boiler. (Chongwatpol, 2016) used only one data mining technique in deriving the most important factors influencing the NOx formation.

Additionally, the results of (Chongwatpol, 2016) showed that the coal chemical properties are mainly the most vital factors contributing to NOx emission; this makes the study tighter to the used source of fuel (i.e. coal) and cannot be generalized to other steam boilers that uses other types of fuel such as gas.

2. (Zhou et al., 1998) showed the significance of decreasing toxin emissions and increasing the combustion efficiency on both environment and energy conservation in a Chinese power generation plant. This study was one of the earliest research dealing with data analytics and big data.

One of the challenges faced the researchers was to develop an algorithm model that overcomes the limitation in the traditional intelligent algorithms to deal with the big data. Another challenge confronted (Zhou et al., 1998) was to build a mode that can reduce the NOx emissions while increasing the boiler combustion efficiency, hence, the multi-objective optimization was used.

In this study, the distributed Particle Swarm Optimization (PSO) algorithm and the Extreme Learning Machine (ELM) based on an application called (MapReduce) were used to build the model.

The results of this research showed that the optimization of power plant boiler combustion was achieved by using the suggested techniques.

3. (Ding et al., 2007) built a mode to predict a coal-fired boiler efficiency and pollutant emissions using neural network method based on secondary data. The study implemented an inherited algorithm constructed on the neural network model in order to obtain real-time solution every 30 seconds.

   The developed algorithm has been connected to the process distributed control system (DCS) in order to form a closed-loop supervisory control to attain real-time optimization for the boiler.

   In fact, the research has provided two modes of supervisory control: (1) adviser mode and (2) closed-loop mode. In the adviser mode, the plant operators receive the results of the supervisory control and then they input it in the DCS via HMI. In the closed-loop mode, the supervisory control writes the results directly in the DCS for real-time correction.

   (Ding et al., 2007) proved that the supervisory control enhanced the boiler efficiency by 0.7% without compromising the safety of the boiler. Additionally, they showed that the NN model decreased NOx emissions by approximately 14 ppm.

   Although this study contains many strong bases such as the supervisory control and closed loop correction in the DCS, it has a number of weaknesses. Firstly, the model was built based on the use of experimental data rather than real data which raise a question about the validity and reliability of the data to mimic the actual steam boiler characteristic. Secondly, the researchers used a limited number of process parameters and excluded important variables such as steam pressure and temperature, flue gas flow and temperature and excess air percentage. Finally, the closed-loop supervisory control was only proposed for improving the boiler efficiency not aimed for decreasing the NOx emissions.

4. One of the most recent studies that aimed to predict the NOx emissions using

artificial neural network technique was (Stamenkovic et al., 2017). Accordingly, data represented 11 process, sustainability, industrial, and economical variables were used as models' inputs. Then, the artificial neural network models tested with online data from various European countries, USA, Japan and other countries.

The researchers successfully reduced the number of the models' input variables by applying correlation and variance inflation factor analysis. The researchers created the artificial neural network using general regression neural network (GRNN) architecture and some indicators as input variables. These indicators represent sustainability, economical, industrial, and agricultural benchmarks.

One of the drawbacks of this research is that it did not mention how the used input variables were quantified or measured. Secondly, the study tried to build a general model that can be applied in any country, on any source of NOx emission, and covering all pollution aspects.

CHAPTER 3: RESEARCH METHODOLOGY

In this research, two types of data miming techniques are used in order to develop a model that predicts the boiler NOx emission (target variable) from process data. Data mining explores for hidden patterns, correlations, and interdependencies in dataset that traditional data gathering approaches such as report creation, pie and bar charts, decision support systems (DSS) cannot oversee (Gargano & Raggad, 1999). Data mining uses a diversified toolkit of innovative algorithmic models that help to automatically answer user specific questions (Gargano & Raggad, 1999).

The used data mining techniques are Neural Network and Decision Tree methods. It is very challenging to build theoretical models for boiler NOx emissions because of their complicated formation process. Therefore, a data-driven model is more efficient and practical in examining boiler operations. In other words, since the mechanism of forming the NOx emission is difficult to be determined theoretically, building a supervised model using historical data is a smart way to predict the target variable.

Data Mining Techniques

In this research, the used data mining techniques are Neural Network and Decision Tree. The reasons behind selecting these two techniques are due to the fact that the creation of the combustion emission in the steam boiler is a nonlinear and dynamic process, and also the NOx emission (target variable) is categorical (Normal or Alarm); neural network technique is a powerful tool for developing an effective complex nonlinear models, especially when the mechanism of the system is ambiguous or hard to identify. Similarly, decision tree can model data that has nonlinear relationships between variables, and both can handle interactions between variables.

Techniques Comparison

In the following table, the two chosen techniques are compared against multiple data science factors (Lin et al., 2017; Jackson, 2002; Wu et al., 2014):

Table 1. Comparison between The Used Techniques

Factors	Neural network	Decision Tree
Model Complexity	It is sophisticated and complex model. It is based on solid scientific foundation.	Easy to follow natural flow, easy to program for computer systems (IF, THEN, ELSE)
Results Complexity	Output is complex to explain or to interrupt	Easier to understand, to interpret and to explain
Target Variable	• Can handle continuous or categorical target variable • Can handle multiple targets	• Can only handle categorical target variable • Cannot handle more than one target
Parametric or Non-parametric	Non-parametric, they make judgments without assuming a distribution	Non-parametric, they do not have assumptions about the distribution or classifier structure
Linearity	It deals with linear or nonlinear relationships	It handles only linear relationships
Data Mining Tasks	It is a multi-task technique; considered as classification and estimation model	It performs classification and estimation tasks
Handling Noise	It is robust when handling noisy data	It is sensitive to noise (especially If signal to noise ratio in the data is low)
Handling Errors and Missing Data	For some extent, it tolerates errors, noise and missing data	It requires efforts for data preparation
Overfitting	Overfitting error is more common to occur with NN	It can happen, but less to occur compared to NN
Processing Time	It requires more processing time	Less processing time compared to NN
Visual Representation of Data	It does not provide visual data representation	Provides clear visual data representation

Research Data Collection

Real primary data representing 27 process parameters from company's steam boiler is used in the research to develop the method. Historical data for the past 4 years is collected from the company's historian system, known as Process Information (PI) System and from the distributed control system (DCS), which represent various independent variables that contribute in the boiler process along with the NOx emission outcomes.

Data Preparation

The collected data set has some missing values and errors. Thus, it needs to be cleaned prior to analyzing them. In the following sections, handling missing data will be practiced. In addition to the missing data, the multicollinearity will be examined in order to reach a conclusion about the included and excluded variables from the model. At the end, a discussion about oversampling technique and its importance in creating a balanced model will take a place.

Missing Data

Several approaches are used for handling missing data. For example, we could simply eliminate the records that contain the missing data, impute or estimate reasonable values for missing observations, such as the mean or median, or use a data mining procedure to deal with them (Jackson, 2002; Marvin et al., 2003). In this project, the mean is going to be used as a reasonable value to handle the missing values. The complete list of the correlation analysis on the independent variables is given in Appendix C.

Multicollinearity

The correlation analysis will be applied to the variables in order to identify the highly correlated variables and then to exclude them from the data mining models. The idea behind excluding highly correlated variables is to avoid multicollinearity. Some experts suggest that correlations between variables exceeding an absolute value of 0.7 may indicate multicollinearity (Jackson, 2002; Wu, et.al., 2014).

Oversampling

The oversampling technique will be used on the data set to balance the categories (Normal and Alarm) in the target variable (Phillips-Wren et al., 2015). Before using the oversampling, 95% of NOx alarm data is classified as category 0 which indicates normal value and 5% belongs to category 1 which indicates alarm value.

Data Mining Software Packages

Three different software packages will be used in performing data mining statistical analysis such as neural network and decision tree on the dataset. These software packages are *SPSS, Modeler* and *XLMiner*.

Table 2. Used Software Applications

	SPSS	**SPSS Modeler**	**XLMiner**
Developer	IBM Corporation	IBM Corporation	Analytic Solver
Software Release	Version 25.0	Version 18.1	Version 2018

CHAPTER 4: RESEARCH FINDINGS

In this section, the research findings from applying the data mining techniques on the collected dataset will be presented. Data mining involves discovering new, meaningful information, so that decision makers can learn as much as they can from their precious source of information (Gargano & Raggad, 1999).

Business and Data Understanding

The NOx emission from the steam boiler combustion reaction has been chosen to be the subject of the testing, and hence, to develop the best model to predict it. Steam boiler encompasses a high level of NOx releases that are emitted as a result of combustion reaction. Historical data for the past 4 years has been collected for 27 process parameters which represent meaningful information about the boiler process, NOx emissions and combustion data. The following table lists the independent and dependent variables that will be used in the model:

Table 3. List of Dependent and Independent Variables

Variable	Description	Unit	Type	Role
TI1111D	Steam Drum Temperature No. 1	°C	Continuous	IV
LY1110D	Steam Tank Level	%	Continuous	IV
TI1110D	Steam Tank Temperature	°C	Continuous	IV
PI1110D	Steam Tank Pressure	bar	Continuous	IV
TI0403D	Burner Furnace Temperature	°C	Continuous	IV
TI1112D	Steam Drum Temperature No. 2	°C	Continuous	IV
TI0405DC	Stage 3 HHP Steam Temperature	°C	Continuous	IV
TI0405DD	Stage 4 HHP Steam Temperature	°C	Continuous	IV
TI1113D	Steam Drum Temperature No. 3	°C	Continuous	IV
TI0405DA	Stage 1 HHP Steam Temperature	°C	Continuous	IV
TI0405DB	Stage 2 HHP Steam Temperature	°C	Continuous	IV
TI0400D	Feed Water Temperature	°C	Continuous	IV
FC0401D	Feed Water Flow Control	m^3/h	Continuous	IV
FI0405D	HHP Steam Output Flow	t/h	Continuous	IV
AI0401D1	NOx resulted from Combustion	PPMV	Continuous	IV
AI0401D2	CO resulted from Combustion	PPMV	Continuous	IV
AC0400D	O_2 resulted from Combustion	MOL%	Continuous	IV

Variable	Description	Unit	Type	Role
PI0405D	HHP Steam Output Pressure	bar	Continuous	IV
TC0406D	HHP Steam Output Temperature	°C	Continuous	IV
EXCESS_AIR	Excess Air Percentage in Boiler	%	Continuous	IV
CO_2_RATE	CO_2 Emission Rate	g/sec	Continuous	IV
B0400D_FLUE	Flue Gas Output Flow	kg/h	Continuous	IV
FT0402D	Combustion Air Flow	Nm^3/h	Continuous	IV
PT0403D	Furnace Pressure	mbar	Continuous	IV
PT1313D	Fuel Gas Input Pressure	bar	Continuous	IV
B0400D_RNST	Boiler Run/Stop Status	-	Categorical	IV
NOX-Alarm	NOx Emission Alarm (50 mg/Nm^3)	-	Categorical	DV

It is worth to start with examining the descriptive characteristic of the data set. It helps describe, display and summarize data in a meaningful matter, for instance, patterns may be arisen from the raw data (Lee & Siau, 2001).

Descriptive Analysis

The importance of the descriptive analysis is that it simply presents the raw data in an informative way, and in most cases it would be hard to visualize big data (Lee & Siau, 2001). The next table provides descriptive statistics of the dataset:

Table 4. Descriptive Characteristics of Input Variables:

Input Variable	Mean	Median	STD	Skewness	Kurtosis	Min	Max	Corr. W/ NOx
TI1111D	213.14	248.06	82.82	-1.76	1.16	15.28	281.51	0.13
LY1110D	53.25	59.96	20.07	-1.98	3.18	-2.82	104.90	0.08
TI1110D	217.34	254.62	83.24	-1.80	1.27	16.30	257.01	0.18
PI1110D	35.97	42.96	16.08	-1.77	1.13	0.00	45.98	0.20
TI0403D	298.52	352.11	120.39	-1.77	1.15	15.90	379.88	0.32
TI1112D	217.03	254.14	83.46	-1.80	1.27	16.02	260.35	0.21
TI0405DC	284.37	334.88	114.51	-1.77	1.16	0.00	365.34	0.17

Input Variable	Mean	Median	STD	Skewness	Kurtosis	Min	Max	Corr. W/ NOx
TI0405DD	291.79	345.30	118.15	-1.77	1.15	11.99	363.99	0.41
TI1113D	219.70	255.02	86.17	-1.75	1.14	14.46	290.34	0.22
TI0405DA	316.87	375.14	129.37	-1.77	1.14	12.46	391.44	0.54
TI0405DB	321.41	381.25	131.64	-1.76	1.14	11.92	393.50	0.31
TI0400D	107.86	121.51	35.82	-1.84	1.48	15.64	126.77	0.19
FC0401D	118.25	130.32	57.00	-1.23	0.30	0.00	220.07	0.24
FI0405D	114.20	125.14	54.89	-1.22	0.42	0.00	256.56	0.55
AI0401D1	21.12	21.99	5.68	-0.52	11.85	0.00	82.84	0.30
AI0401D2	8.45	1.68	38.88	16.82	329.79	0.00	840.00	0.02
AC0400D	3.39	1.97	5.19	3.20	8.33	0.07	21.68	0.65
PI0405D	34.81	41.89	15.70	-1.76	1.09	0.01	53.57	0.16
TC0406D	323.11	384.13	132.89	-1.77	1.13	13.38	390.20	0.26
EXCESS_AIR	41.82	43.06	8.69	-1.22	6.51	0.00	100.00	0.66
CO_2_RATE	3799	5040.38	2766	-0.50	-1.45	0.00	9553.15	0.49
B0400_FLUE	138791	139758	155829	7.50	68.05	0.00	1750449	0.53
FT0402D	72514	87131	32304	-1.77	1.17	0.00	87214	0.24
PT0403D	8.04	8.52	4.68	-0.20	-0.41	0.00	27.12	0.30
PT1313D	0.93	0.07	2.06	37.07	2212	0.00	125.18	0.00

Cluster Analysis

Cluster analysis is a technique that seeks to group a collection of records into clusters (or subsets), such that those within each cluster are more closely related to one another than records assigned to different clusters. The records within a cluster should exhibit a high amount of similarity. Unlike many other data mining techniques, cluster analysis is mainly descriptive, so we cannot draw statistical conclusion about sample using it (Lee & Siau, 2001; Jackson, 2002).

In this section, cluster analysis will be applied on our data using *SPSS software*. The K-means clustering method is used to create 3 clusters using the *SPSS software*. The size of each of the 3 clusters is given in the following table:

Table 5. Size of Each Cluster

	Cluster1	Cluster2	Cluster3
Absolute Size	3035	1004	1926
Percentage	51%	17%	32%

From the above table, it is clear that cluster1 is the largest with 3,035 records out of 5,965 (51% of total cases), whereas cluster2 is the smallest with 1004 records out of 5,965 (17% of total cases).

The *SPSS* has used 10 iterations to produce the clusters. Iterations stopped because the maximum number of iterations was performed:

Table 6. Distance between Final Cluster Centers

	Cluster1	Cluster2	Cluster3
Cluster1		171,700.68	1,414,808.72
Cluster2	171,700.68		1,570,283.97
Cluster3	1,414,808.72	1,570,283.97	

As illustrated, the distance between cluster2 and cluster3 centers is the longest and the distance between cluster1 and cluster2 centers is the shortest.

The clusters identifiers are unique and dependent on the specific procedure used. Therefore, it does not result in a definitive answer but only provide new ways of looking at data. Nevertheless, it is widely used technique in data mining.

In order to study the impact of the cluster analysis on the determination of the NOx emissions, the average of the NOx value in each cluster is calculated in the following table:

Table 7. NOx Average Values of Different Clusters

	Cluster1	Cluster2	Cluster3
Average of NOx Emission	39.792	41.806	42.401

Since the average values of the NOx among the three clusters are almost similar to each other, the cluster analysis has not resulted in a conclusive answer about which cluster group contributes more to NOx emission levels.

Moreover, the following graph shows clearly the high similarity within each cluster and the dissimilarity of records assigned to different clusters when 2 variables are plotted (AC0400D and FI0405D):

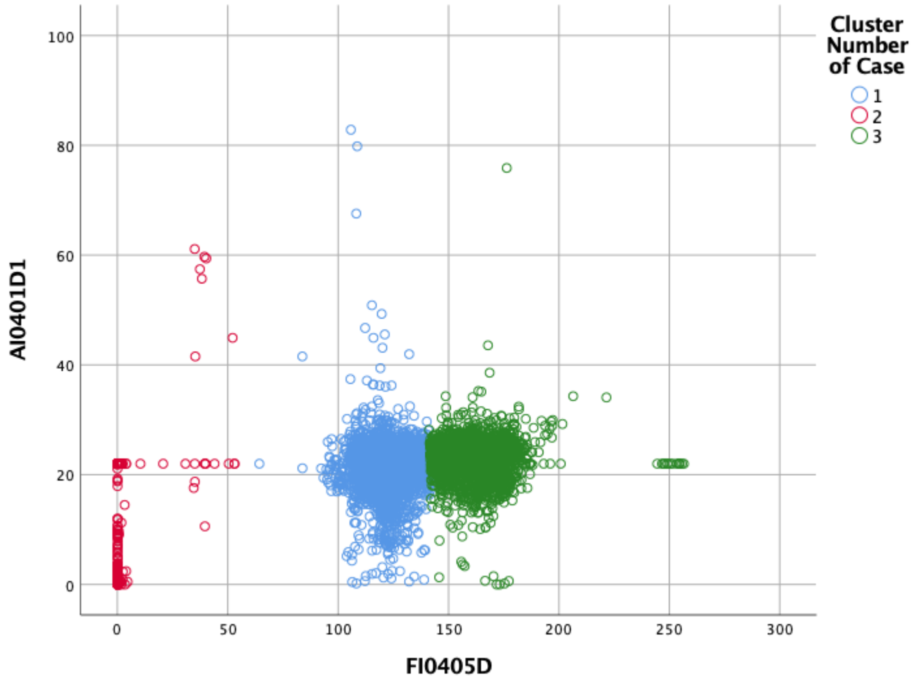

Figure 4. Clusters' similarities and dissimilarities

Modeling

Neural Network Model

In this section, the neural network technique will be applied on boiler data to build a model that can predict the dependent variable, NOx Alarm. The multilayer perception technique in *Modeler Software* has been used to build the model. The neural network has the ability to handle continuous or categorical target variable as well as to handle multiple target variables (Lee & Siau, 2001). The neural network results are presented in the following section.

The classification table (confusion matrix) of the neural network model obtained by the software is given by the below table:

Table 8. Classification Table Using Neural Network

Observed	Predicted	
	0	1
0	5,021	149
1	257	538

From the classification table of the neural network model, we can see that the count of true negative is 5,021 (which indicates a correct prediction of 0, Normal); the count of true positive is 538 (which indicates a correct prediction of 1, Alarm); the count of false negative is 149 (which indicates a wrong prediction of 0, Normal); the count of false positive is 257 (which indicates a wrong prediction of 1, Alarm).

The neural network achieved a high accuracy of 93.2%. The accuracy can be also computed manually from the confusion matrix as follows:

$$Accuracy\% = \frac{TP + TN}{TP + TN + FP + FN} \times 100\%$$

$$= \frac{5{,}021 + 538}{5{,}021 + 538 + 149 + 257} \times 100\% = 93.2\%$$

The neural network model complexity is explained by the generated number of layers and nodes within each layer. In general, the model consists of 1 input layer, 7 hidden layers and 1 output layer. The following table and graph illustrate the model complexity:

Table 9. Neural Network Complexity

Network Layers	Number of Nodes
Input Layer	11 Nodes (10 Neurons + 1 Bias)
Hidden Layer	7 (6 Neurons + 1 Bias)
Output Layer	1

The neural network generated by the software is shown in the below figure:

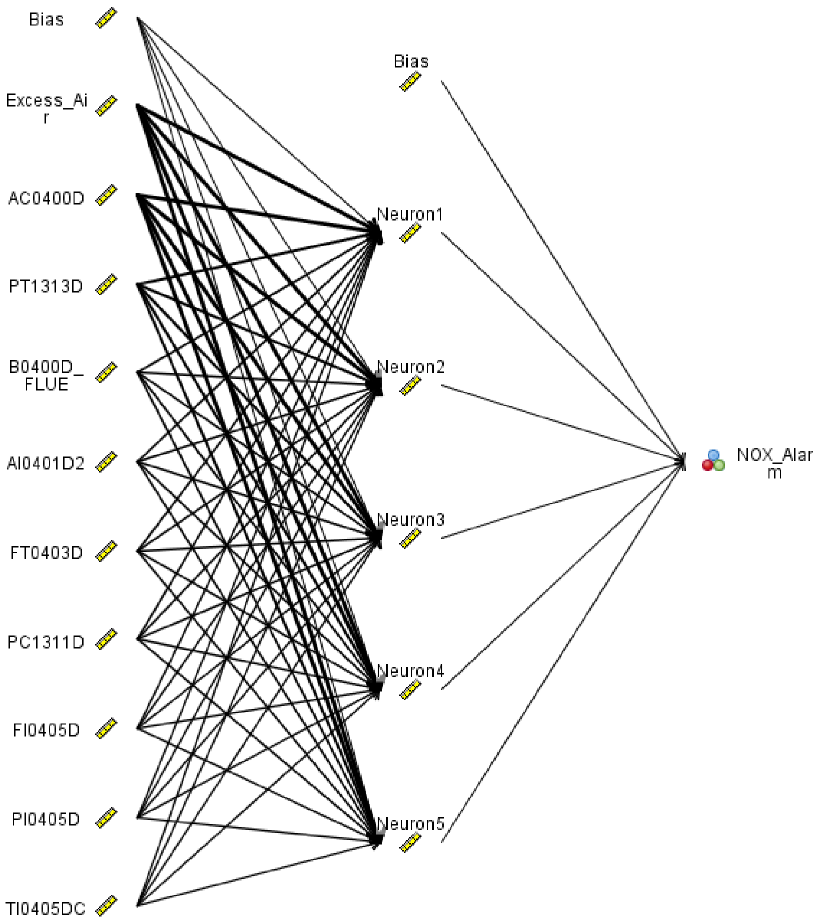

Figure 5. Neural network model for NOx emission prediction

The model has provided the order of the variables' importance. In fact, 10 inputs have been used by the model as nodes in the input layer. In the next table the variables are ordered based on their importance:

Table 10. Neural Network Predictor Importance

Rank	Nodes in Input Layer	Description	Importance
1	AC0400D	O_2 resulted from Combustion	0.19
2	Excess_Air	Excess Air Percentage in Boiler	0.16
3	B0400D_FLUE	Flue Gas Output Flow	0.08
4	FC0402D	Combustion Air Flow	0.06
5	PC1313D	Fuel Gas Input Pressure	0.05
6	PI0405D	HHP Steam Output Pressure	0.04
7	TI0405DA	Stage 1 HHP Steam Temperature	0.04
8	CO_2_RATE	CO_2 Emission Rate	0.04
9	FI0405D	HHP Steam Output Flow	0.04
10	TC0406D	HHP Steam Output Temperature	0.03

From the neural network results, the most important variable of the neural network model in determining the NOx emission is tag: AC0400D "O_2 resulted from Combustion" of the boiler with importance factor of 0.19. The second important variable is tag: EXCESS_AIR "Excess Air Percentage in Boiler" of the boiler with importance factor of 0.16. The "Flue Gas Output Flow" and the "Combustion Air Flow" have importance values of 0.08 and 0.06 in the third and fourth places, respectively. In the next chapter, the implications of these results will be discussed. Appendix B provides the output of the *Modeler Software* neural network models.

Decision Tree Model

The decision tree method will also be applied on the process parameters of the steam boiler using *Modeler Software* in order to build a model that can predict the dependent variable, NOx emission alarm. The decision tree is a non-parametric method which does not have assumptions about the distribution or classifier structure (Lee & Siau, 2001). The decision tree result is displayed in the following section:

The accuracy of the decision tree model is 94.6% which indicates a high accuracy in predicting correctly the target variable, NOx Alarm.

The decision tree model's complexity is described by the number of nodes and the number of rules (or leafs). In the generated decision tree, there are 11 rules (or leafs) and 21 nodes (including the parent node) arranged in 7 levels (height), which are:

Table 11. Output Rules of Decosion Tree Model

Rule No.	Node No.	Rule Algorithm (Normal = 0 and Alarm = 1)	Confidence
1	3	IF EXCESS_AIR <= 47.949 AND EXCESS_AIR <= 46.168 AND AC0400D <= 24.870 THEN 0.0	99.4%
2	5	IF EXCESS_AIR <= 47.949 AND EXCESS_AIR <= 46.168 AND AC0400D > 24.870 AND AC0400D <= 1.974 THEN 0.0	100%
3	6	IF EXCESS_AIR <= 47.949 AND EXCESS_AIR <= 46.168 AND AC0400D > 24.870 AND AC0400D > 1.974 THEN 1.0	100%
4	7	IF EXCESS_AIR <= 47.949 AND EXCESS_AIR > 46.168 THEN 0.0	91.2%
5	9	IF EXCESS_AIR > 47.949 AND CO_2_RATE <= 0.005 THEN 0.0	96.4%
6	11	IF EXCESS_AIR > 47.949 AND CO_2_RATE > 0.005 AND EXCESS_AIR <= 49.233 THEN 0.0	64.7%

7	14	IF EXCESS_AIR > 47.949 AND CO_2_RATE > 0.005 AND EXCESS_AIR > 49.233 AND AC0400D <= 27.825 AND TI0403D <= 354.397 THEN 1.0	78.7%
8	17	IF EXCESS_AIR > 47.949 AND CO_2_RATE > 0.005 AND EXCESS_AIR > 49.233 AND AC0400D <= 27.825 AND TI0403D > 354.397 AND B0400D_FLUE <= 853,517 AND TI0405DD <= 345.540 THEN 0.0	60.5%
9	18	IF EXCESS_AIR > 47.949 AND CO_2_RATE > 0.005 AND EXCESS_AIR > 49.233 AND AC0400D <= 27.825 AND TI0403D > 354.397 AND B0400D_FLUE <= 853,517 AND TI0405DD > 345.540 THEN 1.0	78%
10	19	IF EXCESS_AIR > 47.949 AND CO_2_RATE > 0.005 AND EXCESS_AIR > 49.233 AND AC0400D <= 27.825 AND TI0403D > 354.397 AND B0400D_FLUE > 853,517 THEN 0.0	100%
11	20	IF EXCESS_AIR > 47.949 AND CO_2_RATE > 0.005 AND EXCESS_AIR > 49.233 AND AC0400D > 27.825 THEN 1.0	93.1%

The decision tree model has provided the order of the variables' importance. The *Modeler Software* has ordered the 10 variables based on their importance:

Table 12. Decision Tree Predictor Importance

Rank	Nodes in Input Layer	Description	Importance
1	AC0400D	O_2 resulted from Combustion	0.37
2	EXCESS_AIR	Excess Air Percentage in Boiler	0.32
3	CO_2_RATE	CO_2 Emission Rate	0.09
4	FC0402D	Combustion Air Flow	0.06
5	TC0406D	HHP Steam Output Temperature	0.05
6	B0400D_FLUE	Flue Gas Output Flow	0.05

Rank	Nodes in Input Layer	Description	Importance
7	PC1313D	Fuel Gas Input Pressure	0.05

The most important variable as indicated by the decision tree model is tag: AC0400D “O_2 resulted from Combustion” of the boiler with importance factor of 0.37. The second important variable is tag: EXCESS_AIR “Excess Air Percentage in Boiler” with importance factor of 0.32. The third factor is “CO_2 Emission Rate” with importance factor of 0.09. The “Combustion Air Flow” is in the fourth place with importance factor of 0.06. In the next chapter, the implications of these results will be discussed. Appendix A provides the output of the *Modeler Software* decision tree models.

Comparison between Model Results

In the previous sections, results from neural network and decision tree models have been provided. Both of neural network and decision tree models have been perfect in predicting the NOx prediction from the dataset with accuracy of 93.2% and 94.6%, respectively.

Additionally, the utmost factors in determining the models’ target variables have been also determined. The importance of models’ predictors has been almost close among the two techniques. The top two important factors obtained by the models were similar which indicates the importance of these two variables.

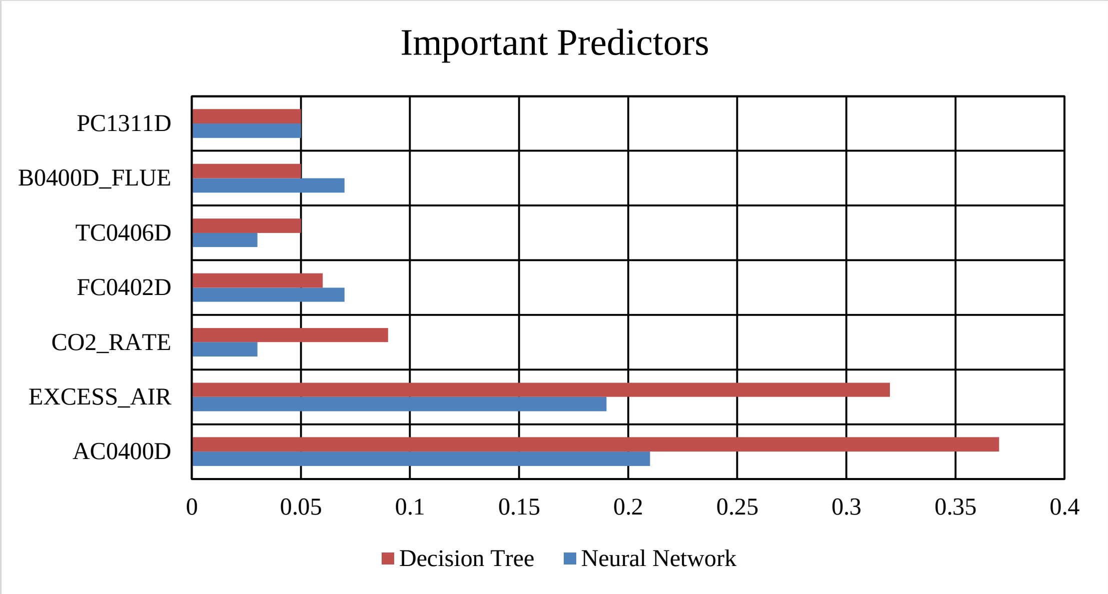

Figure 6. Comparison between neural network and decision tree models' predictors

CHAPTER 5: DISCUSSION AND IMPLICATIONS

The results of neural network and decision tree techniques obtained in the previous chapter have shown that the NOx emissions of the steam boiler is highly affected by the air flow parameters which are, the amount of O_2 in the boiler, the amount of excess air, the flow quantity of the flue gas and the amount of the combustion air. The results of the important factors are matching with the literature review which showed that the relation between the NOx emission and the O_2 amount as well as the excess air is directly proportional.

Effect of Excess O_2 on NOx Emission

As an initiative toward NOx emission reduction, the company has tuned the O_2 controller as well as the excess air level to the minimum in order to influence the availability of oxygen for the NOx formation. In fact, this approach is a traditional technique that is widely adopted by numerous gas processing plants which aims to reduce the excess air flow in the boiler, and then reduces the available oxygen for the NOx reaction (Bullin & Wilkerson, 2010). The O_2 level controller of the boiler is set to 2 MOL% by the Operation team which is by far less than the desired O_2 levels. Similarly, the excess air percentage is almost fixed by the Operation team at 10%.

The company followed exactly the publication of American Petroleum Institute (API) which states that as the level of oxygen increases in the fuel gas burners, the NOx concentrations will also increase (API, 2006).

In order to compare the current actual O_2 set by the Operation team and the corresponding excess air with the theoretical calculated levels, the desired O_2 amount and the percentage excess air will be calculated as follows:

$$Stoichiometeric\ Air$$
$$= \frac{2CH4 + 3C2H4 + 3.5C2H6 + 5C3H8 + 6.5C4H10 + 0.5H2 + 0.5CO + C}{O2\ in\ Oxidant\ Air\ \%}$$

where, the stoichiometric air represents the exact amount of air in the boiler requires to burn the complete amount of the fuel (Liu et al., 2013).

The hydro-carbon volume specifications of the company's natural gas are given by the following table:

Table 13. Volume Specs of Natural Gas Components

Component	Volume %	Component	Volume %
CH4	93.74	H_2	0.001
C2H4	0	CO	0.002
C2H6	1.31	CO_2	0.52
C3H8	0.12	N_2	4.24
C4H10	0.07	C	0.0001

By substituting the hydro-carbon volume specs in the above equation:

$$Stoichiometeric\ Air = \frac{193.12\%}{21\%} = 9.2$$

Where, $O2\ in\ Oxidant\ Air\ \% = 21\%$

The desired air flow and stoichiometric air can be calculated as follows:

$$Desired\ Air\ Flow = Stoichiometeric\ Air \times Actual\ Fuel\ Gas = 9.2 \times 9{,}303$$

$$= 85{,}552\ Nm^3/h$$

$$Stoichiometeric\ Ratio = \frac{Actual\ Air\ Flow}{Desired\ Air\ Flow} = \frac{114{,}807}{85{,}552} = 1.34$$

where, the actual fuel gas and the actual air flow to burner is the mean value obtained from the plant historical data. The excess air% can be determined by the following equation:

$$Excess\ Air\ \% = (Stoichiometeric\ Ratio - 1) \times 100\% = (1.34 - 1) \times 100\%$$
$$= 34\%$$

The relation between the excess air% and the calculated O_2 MOL% can be obtained by the following characteristic graph (Liu et al., 2013):

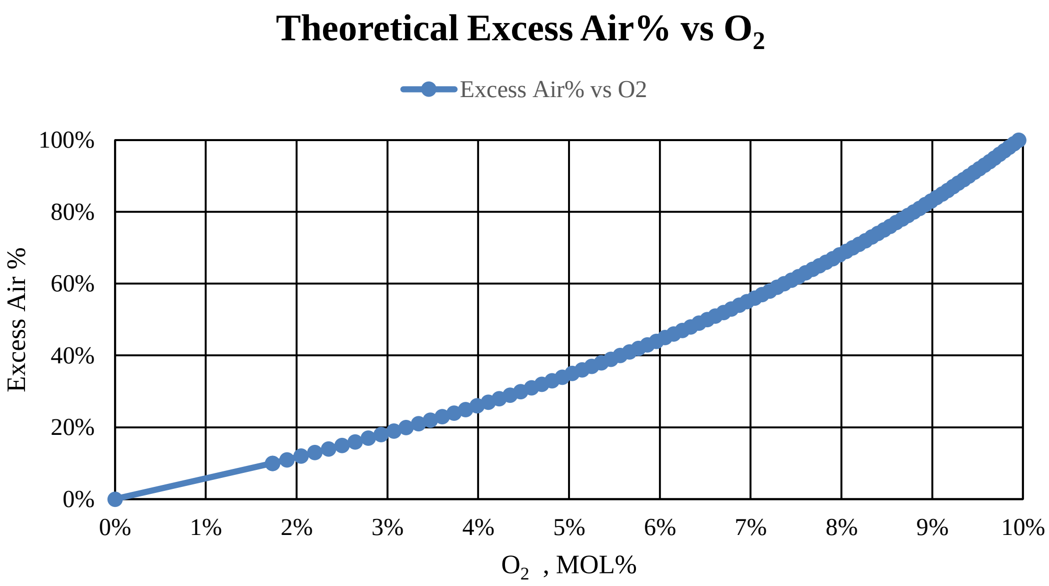

Figure 7. Relationship between oxygen level and excess air

From the graph and the calculations, the O_2 corresponding to excess air of 34% equals 4.9% which is approximately 2.5 times larger than the O_2 level set by the company which is 2%, and the excess air set by the company at 10% is much smaller than the theoretical calculated figure which is 34%. According to (Bullin & Wilkerson,

2010) boiler operations become unstable and the control becomes harder when the operators pursue to run their boilers with low excess air. However, most operators choose the use of lower excess air to reduce the availability of O_2 for NOx formation.

The following graph compares the actual O_2 level in the boiler with the theoretical calculated O_2 at different boiler load.

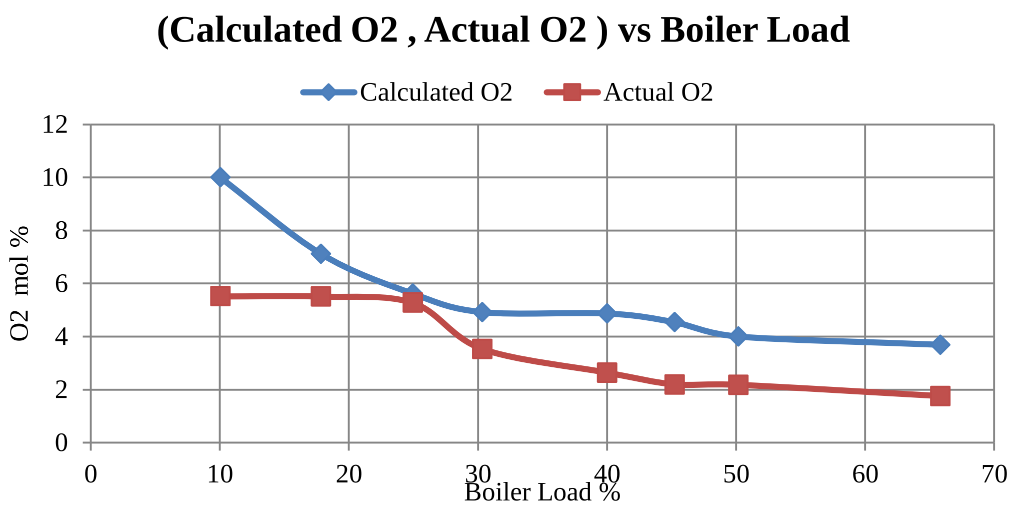

Figure 8. Comparison between actual and calculated O_2

The graph illustrates the fact that the company operates the boiler under low levels of oxygen below the theoretical calculated O_2 in order to reduce the chances of high NOx formation.

Furthermore, results showed that the relation between the O_2 and the NOx in the steam boiler is directly proportional until the boiler load reaches 40% of its operational steam capacity. When the boiler load exceeds the 40%, the NOx increases despite the reduction in the O_2 level as illustrated in the below graph:

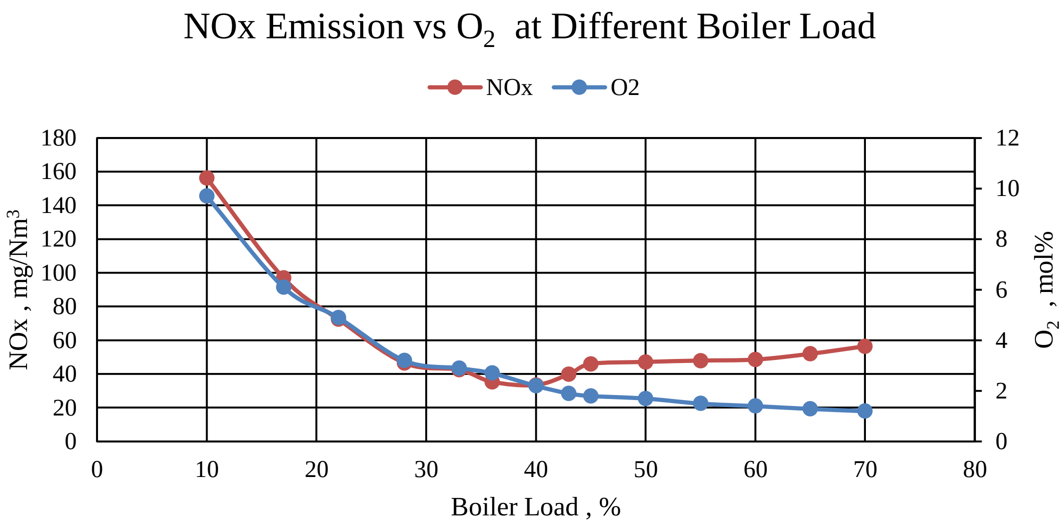

Figure 9. NOx and O_2 relationship at different boiler load

Adiabatic Flame Temperature (AFT) Effect

Although the company has been following the reduction of the O_2 level approach for the last couple of years, the NOx emission levels have not been noticeably decreased. This is because of the existence of other factors that still induce the NOx formation; one of these factors is the effect of the adiabatic flame temperature (AFT) on the boiler (Masum, 2013). The AFT phenomena states that when the O_2 level decreases below the theoretical desired level, the heat index of the burner flame will drastically increase causing a stimulation in the NOx formation, hence, the reduction in the NOx is not achieved (Masum, 2013). It has been shown in an article that NOx concentration will increase exponentially with the increase of the AFT temperature (Zhang, 2010; Liu et al., 2013). Moreover, the reduction in the O_2 has a serious impact on the boiler's burners performance on the long run. It compromises the safety of the boiler as the low level of the oxygen inside the boiler increases the flame temperature and can cause a physical damage in the internal tubes which might lead to boiler explosion (Venkatesh et al., 2012; Liu et al., 2013).

The AFT has been calculated for the collected plant data in order to show the relation between the AFT and the change in the excess air amount. The following graph illustrates clearly this relationship:

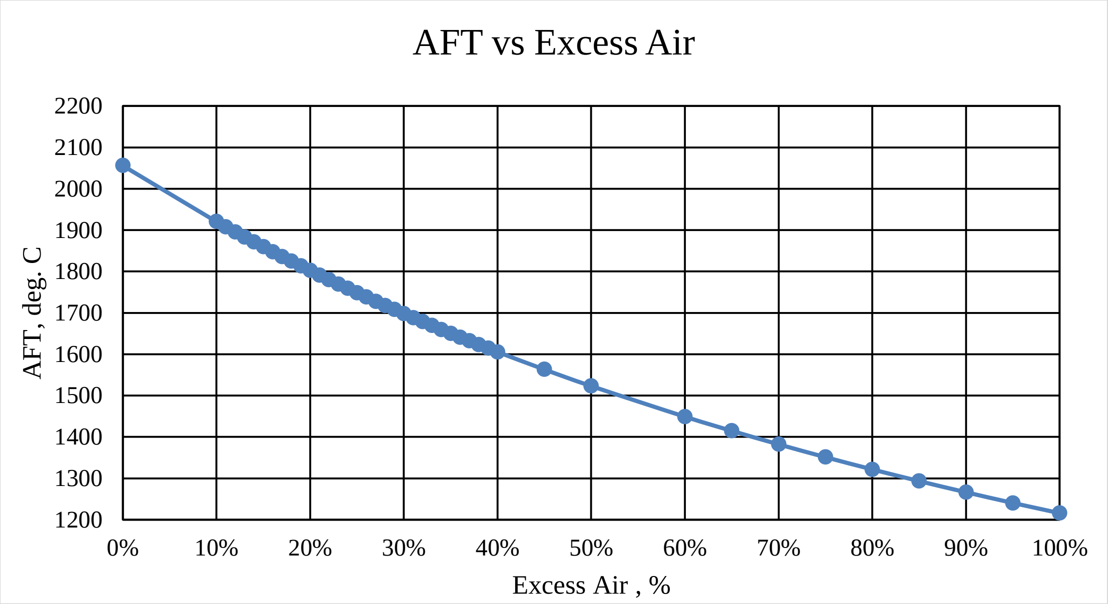

Figure 10. Relationship between AFT and excess air percentage

From the previous figure, it is obvious that the relation between the AFT and the excess air is inversely proportional which indicates that as the Operation team decreases the excess air in order to reduce the oxygen levels, the AFT increases. A decrease in the excess air from 34% to 10% will lead to an increase in the flame heat index by 261 °C.

Flue Gas Recirculation

One of the most effective methods that normally used to address the O_2 reduction and AFT dilemma, is the implementation of the Flue Gas Recirculation

(FGR) at the outlet of the flue gas line using a giant recirculation fan. The idea behind this modification, is to send the flue gas, that is rich in NOx and low in O_2, back to the boiler (Masum, 2013). This method can achieve two advantages:

1. It will decrease the O_2 level in the boiler by reducing the need for the excess air that is high in oxygen and substituting it with the circulated flue gas that is low in oxygen. This will intensely reduce the O_2 level in the boiler (Masum, 2013).
2. It will limit the effect of the adiabatic flame temperature (AFT) on the burner flame by purging the recirculated flue gas that was cooled by the FGR fan in the boiler. This will decrease the temperature of the burner flame and will accordingly reduce the NOx formation. It has been proven in an article that increasing the circulation of the flue gas from 60% to 80% will decrease the AFT from 3,000 K (1,727 °C) to below 2,000 K (2,726 °C) (Venkatesh et al., 2012; Kobayashi & Bool, 2011).

Though the adoption of the FGR technique looks a great idea, its implementation requires an extensive detailed engineering to study the impact of thermodynamics on all the process parameters (Venkatesh et al., 2012; Masum, 2013).

Effect of NOx and Other Emissions on Boiler Efficiency

According to (Ganapathy, 2003), steam boiler efficiency is defined as the percentage of the total absorption heating value of output steam in the total supply heating value. It is calculated as:

$$Boiler\ Efficiency\% = \frac{(Steam\ value\ per\ hour) \times (x1 - x2) \times 100\%}{(Fuel\ Consumption/hr)\ \times (Fuel\ low\ calorific\ heating\ value)}$$

where, $x2 = \ The\ ratio\ enthalpy\ of\ feed\ water\ (kJ/kg)$ and

$x1$: $The\ ratio\ enthalpy\ of\ steam\ (kJ/kg)$

From the collected data, the mean value of the plant boiler efficiency is 94% which indicates a high boiler performance in generating heated steam from the feed water and the input mixture of fuel gas and air. According to the literature, efficiency below 88% indicates a low boiler performance. Whereas, a value equals or exceeds 88%, indicates a high boiler performance (Ganapathy, 2003; Basso & Cumo, 2017).

The impact of the released toxin emissions from the boiler combustion process including NOx, H_2S, CO_2 and CO has been studied using the collected data. The aim of this study is to indicate the influence of the environmental gas releases on the overall boiler efficiency (BE%). Therefore, a model based on artificial neural network was developed to study the effect of the emissions on the target variable, boiler efficiency flag (0 if BE% < 88% and 1 if BE% ≥ 88%).

The results did not show a strong relation between the target variable and the independent variables. In fact, the model has a very low performance in predicting category 0 of the target variable i.e. the false negative error was very high.

Therefore, we conclude that there is no strong relationship between the boiler efficiency and the toxin emissions (NOx, H_2S, CO_2 and CO) from the boiler combustion process.

CHAPTER 6: RECOMMENDATIONS

In the previous chapters, the most important factors influencing the high NOx levels in the steam boiler have been identified using data mining techniques. The results showed that these factors are mainly related to the air flow parameters which includes, O_2 amount in the boiler, percentage of excess air in the boiler and the flue gas escaping from the boiler's outlet

In this section, some recommendations will be given to the company in order to help reduce the NOx emissions and consequently avoid any authority's sanctions. These recommendations can be divided into two categories, short-term and long-term, based on their adoption period.

Short-Term Recommendations

The research recommends the company to assign a team from Operation Department or Environmental HSE Department to closely monitor on daily basis the air flow parameters in the steam boiler unit which are O_2 amount (AC0400D), excess air in the boiler (EXCESS_AIR) and the flue gas flow (B0400D_FLUE).

That is, the findings from the data mining models can help the company prioritize the important factors associated with the NOx emissions, and then, more attention to these factors can be promptly given in order to reduce the NOx emission levels and to adhere with QP environmental regulations. After the adoption of the monitoring process of the air flow factors, evaluation of the NOx emission levels has to be conducted in order to examine the results.

Long-Term Recommendations

The research also recommends the adoption of the flue gas recirculation (FGR) technique in the steam boiler as a long-term solution because it has two advantages. Firstly, it achieves good results in reducing the NOx concentration through the recirculation of the flue gas that is low in oxygen back to boiler. This can achieve 40%

to 50% reduction in the NOx formation according to the literature (Bullin & Wilkerson, 2010; Masum, 2013). Secondly, it reduces the flame heat index as well as the adiabatic flame temperature (AFT) which leads to lower NOx formation (Masum, 2013).

CHAPTER 7: CONCLUSION

Data mining has become a very important and a rapid growing field due to the availability of a great amount of data in the applications involved in several domains. In this research, the data mining techniques have been applied on real plant data representing 27 boiler's process parameters in order to identify the factors that directly contribute to the NOx emission in the gas fired boiler. Models based on artificial neural networks and the decision trees were developed using various data mining applications such as *SPSS, Modeler* and *XLMiner*. The neural network models achieved 93.2% of accuracy and the decision tree models achieved 94.6% of accuracy in predicting the target variable precisely. The results indicate that the most important factors influencing the NOx emissions are those related to the air flow parameters which include O_2 amount, percentage of excess air in the boiler, the flue gas flow and the combustion air flow, followed by some process control parameters such as the temperature of the fuel gas input and the pressure of the fuel gas inlet.

It was shown that the company operates its steam boiler at low levels of oxygen concentration in order to reduce the amount of oxygen available for the NOx formation. However, this approach was verified by the research to be sufficient only under certain threshold of boiler load that does not exceed 40% due to other important factors such as the adiabatic flame temperature (AFT) which induces the formation of NOx emissions.

Furthermore, the research did not find any strong relationship between the overall steam boiler efficiency and the toxin emissions from the combustion process such as NOx, H_2S, CO_2 and CO.

The research recommends monitoring carefully and on daily basis the resulted research's most important factors that influencing the NOx formation by a dedicated team assigned by the company who has to promptly apply corrective actions to keep these factors within their desired levels. Consecutively, the monitoring process of the important factors have to be evaluated by the company to examine its impact on the NOx levels.

It is also recommended to adopt the implementation of the flue gas recirculation (FGR) technique in the steam boiler as a long-term solution because it has two advantages. Firstly, it achieves good results in reducing the NOx concentration according to the literature via the recirculation of the flue gas that is low in oxygen. Secondly, it reduces the flame heat index as well as the adiabatic flame temperature (AFT) which leads to lower NOx emissions.

CHAPTER 8: RESEARCH LIMITATIONS

The research suffered from the insufficient availability of references that discuss the NOx emissions in gas fired steam boilers. Most of the available articles were conducted in the context of NOx formation in coal-fired boilers. In fact, there are many differences between the two types of boilers in term of operating temperatures, types of emissions, levels of oxygen and design of burners which indeed affect the NOx emission results.

Moreover, the study experienced lack of information about the chemical compositions of the fuel gas that is used as a burning medium in the steam boiler due to the technical difficulties of collecting data from the plant laboratory samples. This has resulted in excluding of the fuel gas compositions from the models' input variables.

CHAPTER 9: FUTURE WORK

The research can form the foundation for further work involving other gas processing plants operating in Qatar. Since this research is built within the context of a specific gas fired steam boiler, a more generic study can be conducted which examines the formation of NOx pollutant in other process units, rather than steam boiler unit, where combustion reactions exist.

Furthermore, the study can include other environmental toxic emissions such as SOx, H_2S and CO_2 which are also rich topics that deserve to be studied. Additionally, since the research recommended the use of flue gas recirculation (FGR) technique to reduce the NOx emissions in the steam boiler, a comprehensive study of adopting the FGR, the expected benefits and references of successful implementations in oil and gas industry can be studied.

Last but not least, a supervisory closed loop control can be programmed based on the developed models and connected back to the plant DCS system in order to adjust and optimize the boiler process to reduce the NOx emissions.

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APPENDIX

Appendix A: Decision Tree Outputs

The results of the Decision Tree model obtained by the *SPSS Modeler* are:

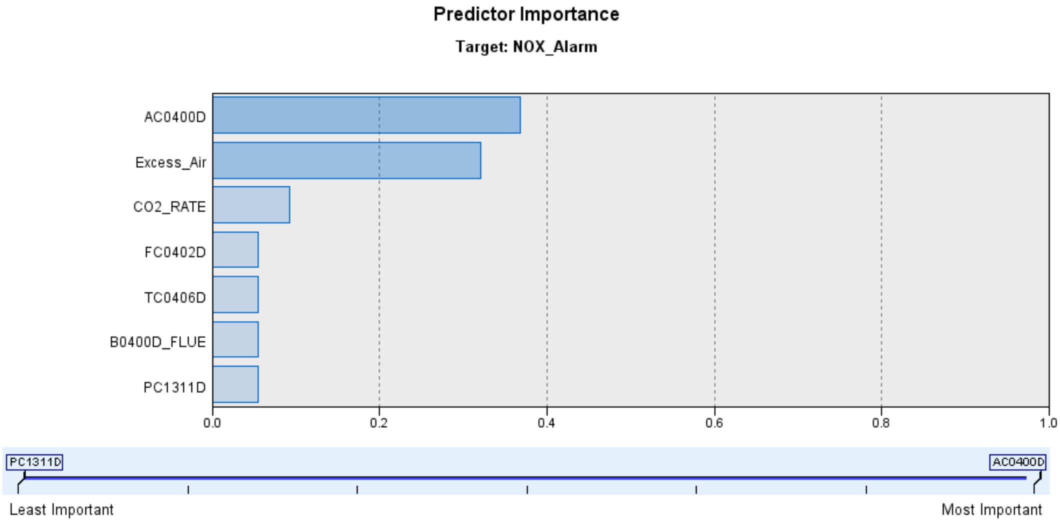
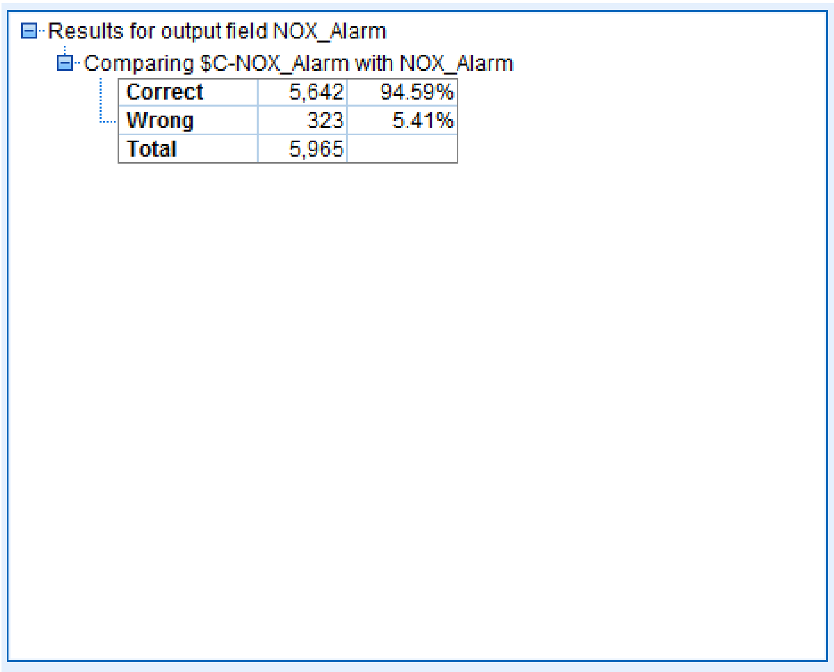


Figure 11. Decision tree's predictor importance


Results for output field NOX_Alarm
Comparing $C-NOX_Alarm with NOX_Alarm

Correct	5,642	94.59%
Wrong	323	5.41%
Total	5,965	

Figure 12. Decision tree model's performance

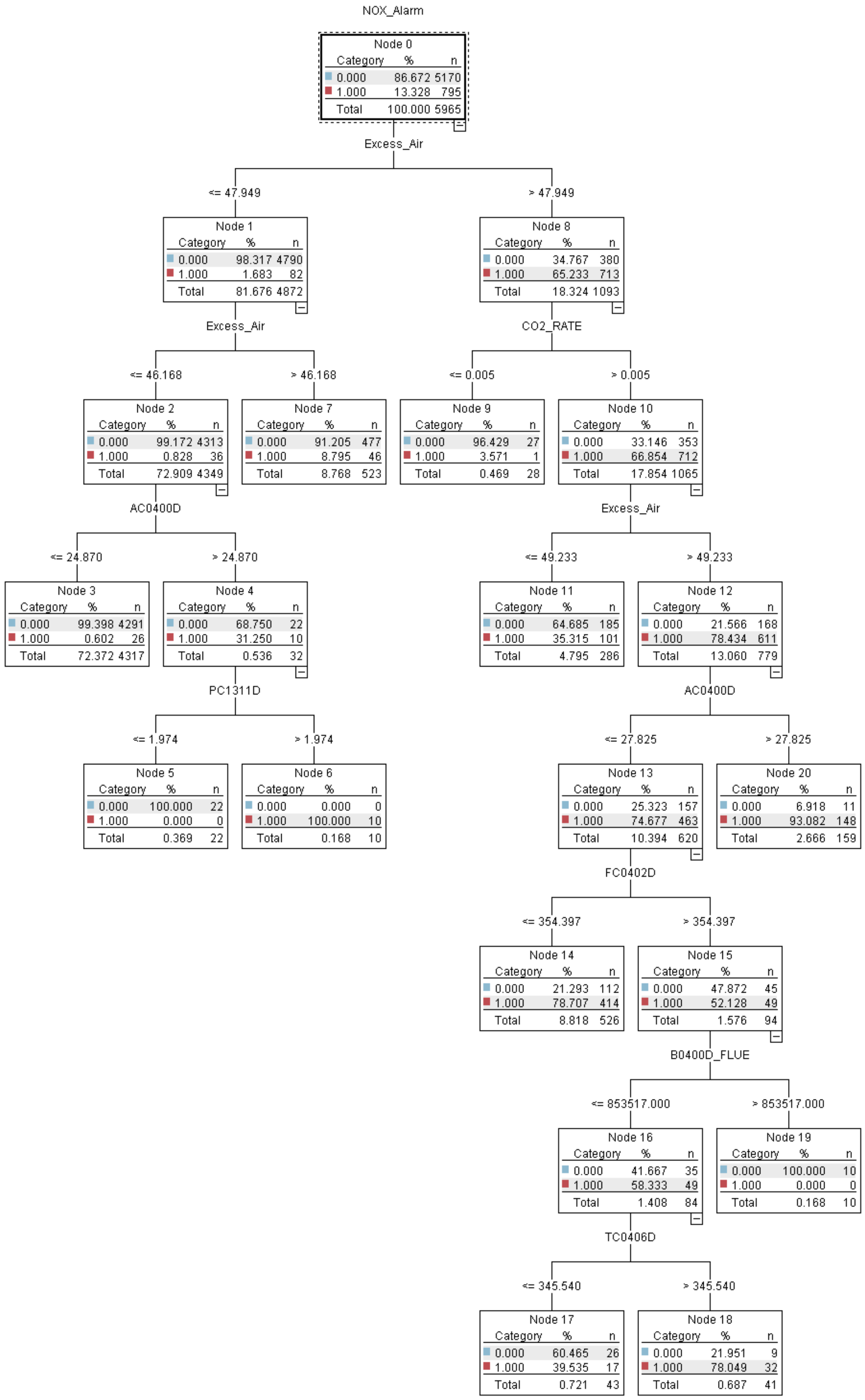


Figure 13. Decision tree model

Appendix B: Neural Network Outputs

The results of the Neural Network model obtained by the *SPSS Modeler* are:

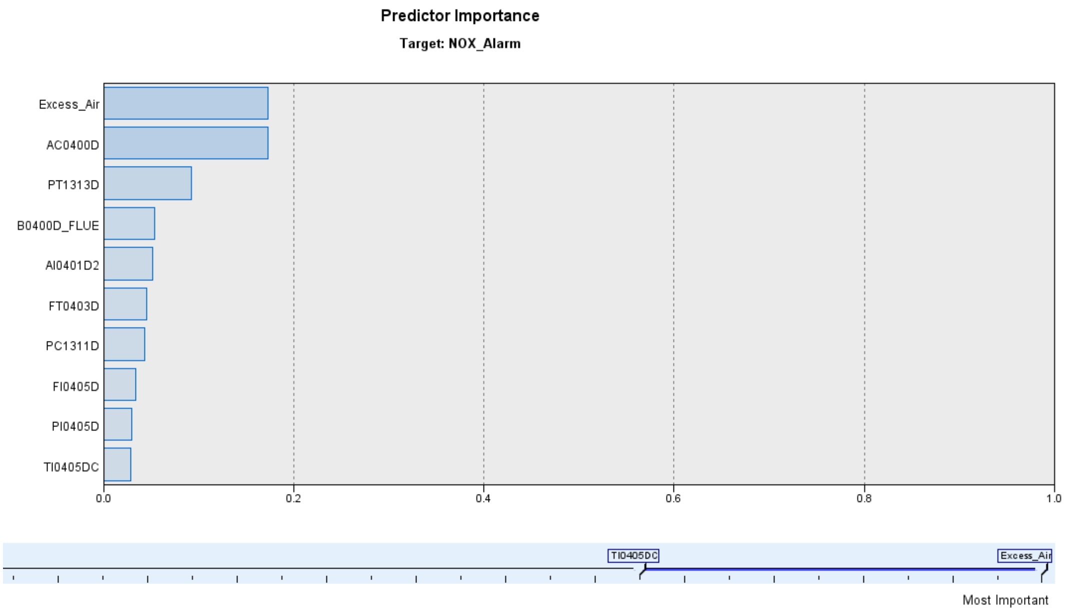


Figure 14. Neural network's predictor importance

Results for output field NOX_Alarm

Comparing $N-NOX_Alarm with NOX_Alarm

Correct	5,559	93.19%
Wrong	406	6.81%
Total	5,965	

Figure 15. Neural network model's performance

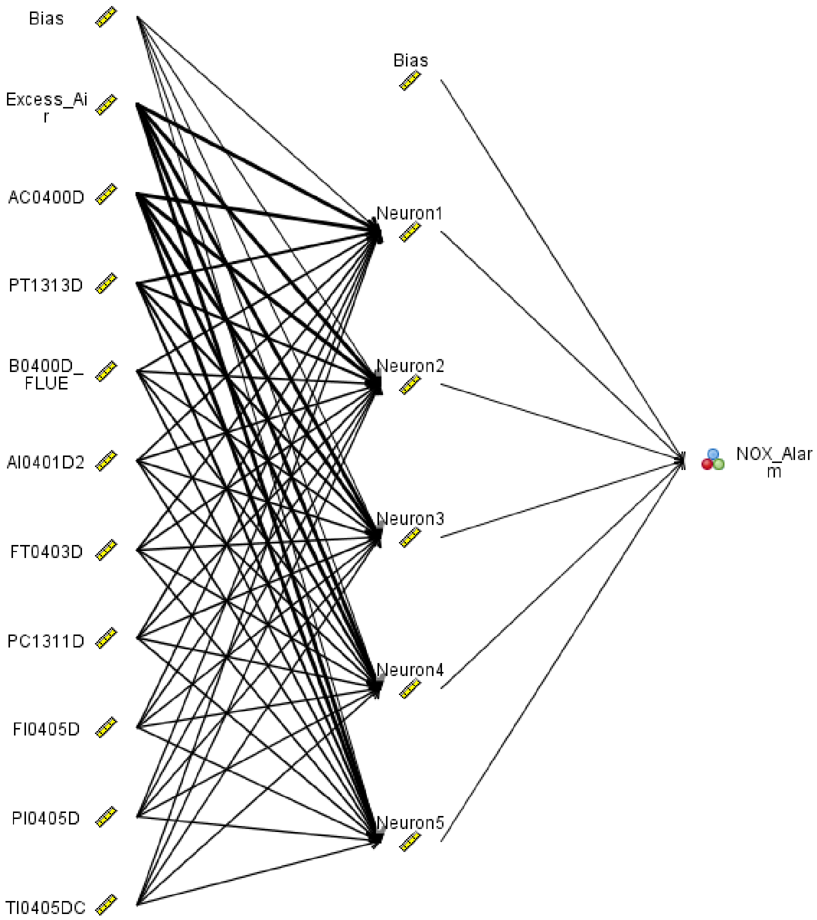


Figure 16. Neutal network model

Appendix C: Correlation between Process Variable

Table 14. Correlation between Independent Variables

	TI1111D	LY1110D	TI1110D	PI1110D	TI0403D	TI1112D	TI0405DC	TI0405DD	TI1113D	TI0405DA	TI0405DB	TI0400D	FC0401D	FI0405D	AI0401D1	AI0401D2	AC0400D	PI0405D	TC0406D	EXCESS_AIR	CO2_RATE	B0400D_FLUE	FT0403D	PT0403D	PT1313D
TI1111D																									
LY1110D	0.8																								
TI1110D	0.6	0.3																							
PI1110D	0.6	0.7	0.2																						
TI0403D	0.7	0.7	0.2	0.4																					
TI1112D	0.7	0.8	0.5	0.4	0.4																				
TI0405DC	0.6	0.5	0.2	0.5	0.6	0.8																			
TI0405DD	0.7	0.8	0.6	0.6	0.2	0.6	0.5																		
TI1113D	0.7	0.5	0.5	0.5	0.2	0.2	0.8	0.2																	
TI0405DA	0.7	0.8	0.4	0.7	0.2	0.2	0.6	0.2	0.6																
TI0405DB	0.8	0.5	0.4	0.8	0.7	0.2	0.6	0.2	0.6	0.9															
TI0400D	0.6	0.8	0.2	0.7	0.7	0.6	0.6	0.6	0.6	0.6	0.6														
FC0401D	0.7	0.7	0.9	0.7	0.6	0.7	0.6	0.6	0.7	0.7	0.7	0.8													
FI0405D	0.6	0.7	0.6	0.7	0.6	0.7	0.7	0.9	0.6	0.6	0.6	0.8	0.5												
AI0401D1	0.2	0.1	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.3	0.3											
AI0401D2	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1										
AC0400D	-0.6	-0.3	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.6	-0.5	-0.6	-0.5	-0.4	-0.1									
PI0405D	0.2	0.7	0.7	0.6	0.7	0.7	0.6	0.8	0.6	0.8	0.8	1.0	0.7	0.8	0.2	0.1	-0.6								
TC0406D	0.6	0.8	0.7	0.6	0.6	0.8	0.8	0.4	0.4	0.4	0.6	0.4	0.9	0.7	0.2	0.1	-0.6	0.5							
EXCESS_AIR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.1	0.7	0.0	0.8	0.0	0.0						
CO2_RATE	0.6	0.5	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.3	0.1	-0.4	0.6	0.6	0.2					
B0400_FLUE	0.4	0.3	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.5	0.5	0.1	0.1	-0.3	0.4	0.4	0.1	0.2				
FT0403D	0.7	0.8	0.7	0.7	0.7	0.6	0.5	0.5	0.5	0.6	0.7	0.7	0.7	0.8	0.2	0.1	-0.6	0.2	0.2	0.0	0.6	0.4			
PT0403D	0.8	0.6	0.7	0.8	0.7	0.6	0.8	0.8	0.6	0.5	0.8	0.7	0.6	0.6	0.2	0.1	-0.5	0.7	0.8	0.0	0.4	0.5	0.7		
PT1313D	0.2	0.1	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.1	0.1	-0.1	0.0	-0.1	0.2	0.2	-0.1	0.0	0.0	0.2	0.1	