UTILITY SYSTEM OPTIMIZATION UNDER AIR QUALITY CONSIDERATIONS

A Thesis

by

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ABSTRACT

Air pollution is a primary concern, and one of its major contributors is industry. Optimization of emissions from industrial facilities is well established in publications and reports. However, it does not extend beyond the stack or exhaust level i.e., emissions released to the atmosphere.

This work aspires to develop and test a methodology to optimize the operational scheme of a utility system considering air quality in the area around the facility by combining Process Design with Air Dispersion Modelling. The concept of this work is to investigate if atmospheric dispersion modeling can be used to improve pollution prevention/control by observing ground level concentration in the surrounding area of the unit at various operating scenarios and in different weather conditions. The methodology has been implemented in MATLAB following the coupling of a simple Gaussian dispersion model with a process model, both supplied with real meteorological and process data.

The case study used to test the methodology is a High Pressure Steam (HPS) generation unit. It consists of three identical boilers where the operational strategy is to operate two boilers, and the third is stand-by. The boilers accept two types of fuels: gas and liquid. Two separate optimization goals were studied. The first is to improve air quality in the surrounding area, i.e., minimize the ground level concentration, by changing the operating scheme of the three boilers. The second optimization goal is

to reduce the operating costs by optimizing the ratio of the two fuels while keeping the resulting ground level concentration just below the regulations limit.

Finally, the methodology allowed to derive and assess the different operational strategies. The first goal improved the overall air quality and reached up to 46% reduction of the maximum concentration exceedances. The second goal proved that facilities can reduce operational costs and still be in compliance with environmental regulations. On the other hand, this cost reduction does lead to a decrease of overall air quality, since the average ground level concentration is increased. In the future, this methodology could be applied to more case studies and at the industrial city level to improve air quality and to assist on more appropriate environmental policies.

DEDICATION

I dedicate this thesis to my family, my husband Khalil and my friends who kept encouraging me to achieve my goal. I am truly grateful for having you in my life.

To my son Ibrahim. Always be great!

ACKNOWLEDGMENTS

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All the work conducted for the thesis was completed by the student independently.

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1. INTRODUCTION

Sustainability of human life and the resources of planet earth has been a concern in the last few decades mainly to meet the increasing demand and preserve the resources of the planet for the next generations. This is a challenge especially in the industrial sector as it is the major consumer of the natural resources (El-Halwagi, 2012). Optimization techniques have been successfully implemented in industrial facilities and plants to optimize mass, energy, utilities and power consumption. Optimization is studied extensively with different objectives. Minimizing cost (capital or operational) and minimizing power consumption are excellent examples of optimization objectives. An example of optimization by minimizing cost is addressing reliability and availability of utility plants by focusing on optimization of design and operational parameters to determine the most cost-effective elements of redundancy as explained by Aguilar, Kim, Perry, &Smith (2008). Another example is Velasco-Garcia, Varbanov, Arellano-Garcia, & Wozny (2011) when they developed an optimization model in plants where optimal operational procedures are derived while considering associated costs. Ahmad, Zhang, & Jobson (2010) analyzed multi-period design to account for varying operating conditions and obtain the impact of these changes on operation and performance of utility network. A good example of optimizing both power and cost is the work done by Harkin, Hoadley, & Hooper (2012). They worked on optimization of utility rates by combining heat integration, cost estimation, and multi-objective optimization.

While in the past optimization efforts have been focused on saving cost and energy, nowadays greater attention is raised to the sustainability of the environment. Many efforts have been spent to accomplish environmental sustainability. One of the efforts is a set of methodologies called the Green Engineering principles. Green Engineering is a type of engineering optimization wherein the individual components must be integrated in the most efficient way. The systematic integration of these principles is a key towards achieving genuine sustainability in the design of industrial processes and systems to benefit the environment, economy, and society ("Green Engineering", 2018). The second principle of green engineering [19] is that preventing waste is better than treating it after it had formed. Therefore, the impact of air emissions at the design stage of the project is addressed to protect health, safety and environment. Many articles have addressesd the impact of air emissions and how it can be reduced by process optimizination. One example is the optimizing of process efficiency and emissions simultaneously by Heikkinen et al.(2009). He demonstrated optimization and process modelling system that has three applications: process state determination, optimization and emission reporting. His work represet a new type of service business. Liu, Huang, Fuller, Chakma, & Guo(2000) were interested in Non Renewable Energy (NRE) resource management optimisation with an objective to maximize economic return under constraint of NRE resource availability and environmental regulation. Sweetapple, Fu, & Butler (2014) did a multi objective optimisation of control strategy to reduce of operational Green House Gases emission from Waste Water Treatment plant in a cost effective manner. Henning, Amiri, &Holmgren (2006) studied process optimization and its effect on air pollution. He used emission limits to choose the type of fuel and illustrates the framework of the energy system optimization model.

All the aforementioned articles addressed emissions but does not extend beyond the stack level. However , pollutants disperse in air and are transported along way before they do their damage (Nevers, 2010). It depends on the meteorological conditions that affects the dispersion of the pollutants and how far it can reach. There are many publications that studied improving air quality at the receptor zones using dispersion modeling. Zelinski, Konieczynski, & Mateja-Losa (2004), for example, used a traditional Gaussian model to calculate the mean annual aggregate concentrations to optimize the air protection expenditures on a municipal scale by using alternative fuel. They have performed a case study on an industrial town established that only marginally increased the cost of alternative fuel can make a substantial improvement to the ambient air condition. Lu, Huang, &He (2010) proposed two-phase optimization model for regional air pollution control that can predict contaminant concentration at receptor zones and identify factors that affect output and thus help decision maker to adjust sources in real time using the state of the art pollution control systems. According to Skiba, Para-Guevara, & Belitskaya (2005), mathematical modeling of atmospheric dispersion is not only developed to predict concentrations of various pollutants, but rather to come up with methods to avoid the situations when these concentrations reach dangerous levels. They suggest a few methods to control the emission rates of enterprises. As part of their work, they described a method of determining an optimal position for a new enterprise in the region. Alvarez-Vázqueza, García-Chan, Martínez & Vázquez-Méndez (2015) proposed multi-objective programming interactive methods to solve the problem of air pollution control using the ecological and economic cost functions as objectives to obtain the optimal management of a set of industrial plants.

Following the second principle of green engineering (Anastas, 2003), this research aspires to develop and test a methodology by which the adverse air quality effects at receptor zones away from emission sources are minimized/mitigated through process optimization. This aspiration is enabled through adopting operational changes in the process while certain weather conditions prevail. Process operation is altered to to achieve better air quality (lower environmental impact). The plan is to intertwine two models: the process model and the air dispersion model and introduce optimization to achieve the optimum operation based on the effect on the surrounding air quality.

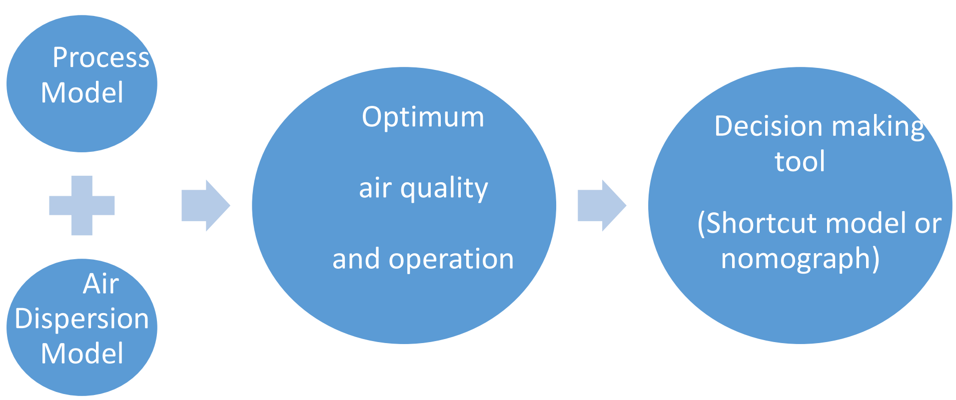

Figure 1.1 - Aim of Study

It should be noted that, the use of conventional pollution control techniques by lowering the pollutant concentration exiting the process such as adding new equipment to the process (absorbers, cyclones, etc.) is not the objective of the study. This means that the study objective is not to reduce the emission flow rate for a particular pollutant from a particular process. However, the intent is to optimize the process operation with multiple emission sources so that the ground level concentration of the studied pollutant is less (or is within regulations) in the area specified in a certain period of time.

The objectives of the study are outlined in Section Two. A comprehensive literature review was done on the different aspects of interest and detailed in Section Three. Section Four describes the methodology produced and adopted to ensure that the objectives of the study are met. Model construction is detailed in Section Five. The results are populated in Section Six. Finally, the research concludes with discussion and recommendations for future work.

2. RESEARCH OBJECTIVES

The study considers the optimization of a process operation considering air quality in the surrounding area of a utility unit. The work demonstrates the holistic application of engineering science and time management. Using effective computational tools, process modeling and atmospheric dispersion modeling are intertwined to meet the following objectives:

- Select a representative case study where operational changes can be applied
- Develop a system with different components. This is done by developing a simplified analytical model that can be used as a screening tool under optimization scheme:
    - Optimize process with an objective of lowering cost, satisfying demand or operation scheme
    - Optimize air quality with an objective of minimizing concentration at receptor, subside health impact, comply with regulations or minimizing the toxic load
- Perform sensitivity analysis to investigate effect of variable conditions
- Ensure that user interface is simple and it has the potential to be launched as a prototype with further modest development to develop an operational strategy or decision making tools.

3. LITERATURE REVIEW

3.1. Process Optimization

Process facilities are keen to meet the stringent regulations from international agencies and to improve the quality of their products. Thus, there are evolving businesses based on process optimization taking the environmental requirements as a key factor in their work. Many consultants now are relied on to improve the performance of the process by increasing the capacity of the facility and/or reducing the emissions. These objectives are met by either operational or physical changes in the process. A review was conducted to explore if there is work done to study the use of optimization in process operations and extend to air dispersion and whether this combination of the two fields was investigated before. Most of the work found stops at the emissions from the stacks and does not exceeds it to the dispersion of emissions or the air quality away from the facilities.

At the early design stages of a process, air dispersion models have been used to make consideration of the contributing factors. Some factors have an immense effect on the air quality in the region/area where a project (not necessarily a production facility) will take place. Gallagher, Gill, & McNabola (2011) investigated potential percentage reduction of pedestrian exposure to pollutants in streets. He considered the impact of parking configurations, car space occupancy and wind speed and direction. The study highlights the optimum parking layout and urban street canyon layout in different wind conditions. The novel configuration is to achieve maximum pollutant reduction in the hope for the results to be implemented by urban planning and public policy makers to improve air quality.

A direct relation between changing the operating conditions of a facility and the resulting impact on the surrounding air quality was found in the work done by Kakosimos (2015). He developed a framework where process design and pollutant transfer is considered simultaneously. New brute-force type optimization algorithm manipulated the operation cycle to improve air quality.

3.1.1. Case Study Selection

A survey was conducted to provide a case study. It is important to start with a simple case where complexity and assumptions are minimum. A utility systems is used a case study in this research because there are no reactions and no separation processes taking place. Utility units are a vital section of any plant where all utilities are produced and distributed plant-wide. Thus, there is an increased interest in optimizing utility system using various approaches to serve different goals.

The purpose was to obtain a simple utility system to represent the process side with features that help to achieve the objectives. A long time was consumed on finding real case study with no success. Finally, data for a fixed use utility plant used to generate High Pressure Steam (HPS) in an industrial city was used. The data is obtained through personal communication with approval to use without disclosure of the source.

Steam production, in particular, is a straightforward case where water is heated in boilers to produce steam at different pressures (high, medium and low depending on the process demand). Burning fuel is the traditional way to heat water. The output consists of pressured steam and the flue gasses resulting from combusting the fuel.

In our case study, HPS is required to fulfill the needs of a particular process/plant. The focus will be only on a system comprised of three boilers that produce HPS. Following the widely practiced N+1 (N =operating unit and 1=standby) sparing philosophy for multiple units, two boilers are considered operating, and one is standby. The capacity of each boiler is assumed 110,000kg/hr. The design demand of HPS is 220,000 kg/hr. Each boiler is fitted with a dedicated stack to emit flue gas produced from combustion. The three boilers are identical as well as their stacks.

The boilers are assumed to be fitted with dual fuel burners, which means it can accept two different types of fuel: fuel gas as well as liquid fuel. The characteristics of the fuels available for the process are as seen in Table 3.1. The final product is HPS at 370 C and 45 bar. Refer to the schematic representation of the system in Figure 3.1 below.

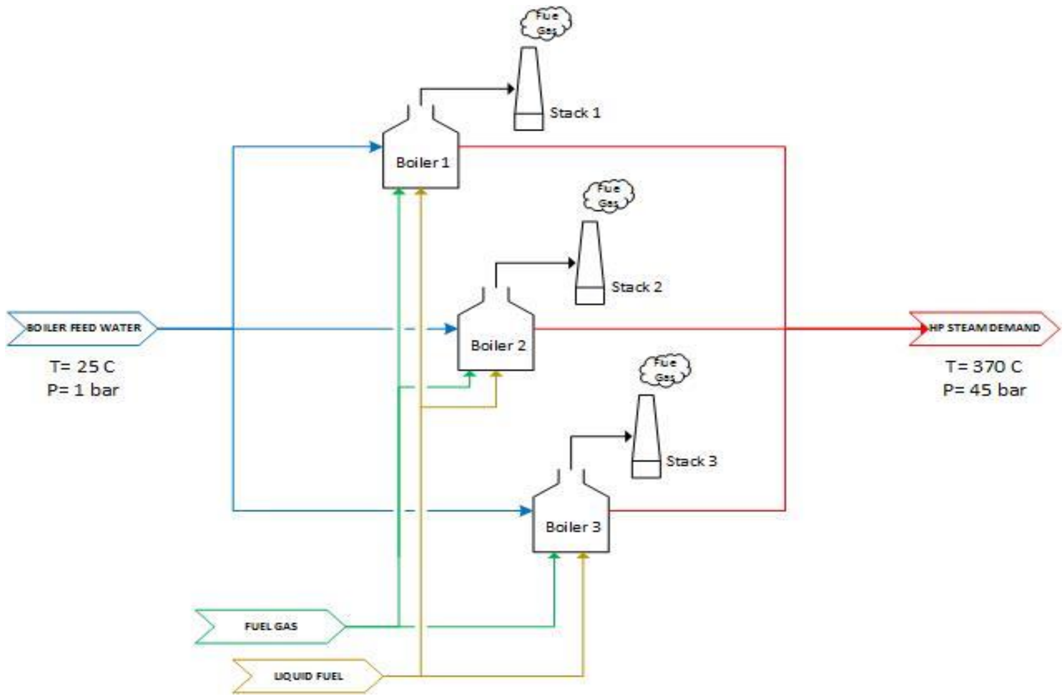

Figure 3.1 - Schematic Representation of the HPS Production System

There are different types of boilers available that have different performances. When selecting a boiler, it has to provide the steam demand but must do so energy efficiently. To ensure higher energy efficiency, the boilers are assumed of a new type that has a high turndown ratio. This way the efficiency will not drop with lower steam demand, and thus calculations are straight forward and exclude any complications. Appendix D explains the difference in performance between boilers with high and low turndown ratio using the design parameters set for the case study.

The fuel type or energy source used to produce steam will affect not only the boilers annual operation costs but also its size and energy efficiency. In some refinery/petrochemical plants and as a result of some reactions or separations some fuel types are produced within the process. The quantity of fuel produced might be less than could be sold. Instead of incineration and wasting this fuel, it is advisable and preferable to use it in the plant to generate energy.

Different types of fuel have different emission factors and thus different emissions rates associated with firing. In this case study, the effect of fuel type on the dispersion process and different percentage of fuel where allowable (clean vs. dirty) will be studied.

The process data collected for the fixed use HPS generation unit spans for six months presumably from June 1st to Nov 30th, 2013. The unit comprises of three boilers, and the daily data covers the following for each boiler:

- HPS flow produced (in kg/hr). Refer to Figure 3.2 below.
- Fuel gas consumption (in kg/hr)
- Fuel gas concentrations for Nitrogen oxides (NOx) and carbon monoxide (CO) (in ppm and mg/Nm^3)
- Stack flue gas flow (in kdscfh)
- Stack flue gas temperature (in ^{o}C)

The main design parameters for the process model are listed in Table 3.1 below.

Table 3.1 - Technical Design Data

Description	Value
Stack Diameter	2 m
Stack Height	30 m
No. of Unit Operations	3
Fuel Gas HHV	11408 kcal/kg
Liquid Fuel HHV	10900 kcal/kg
Product HPS Temperature	370 C
Product HPS Pressure	45 bar
Design capacity of one boiler	110,000 kg/hr

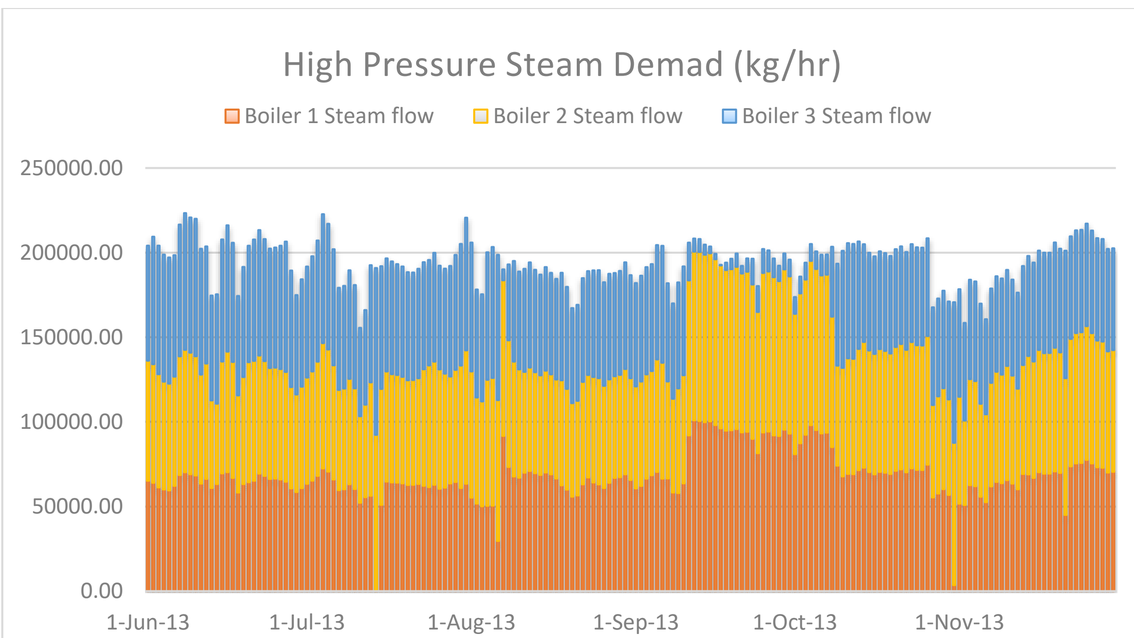

Figure 3.2 - HPS Produced from June to November 2013

3.2.Air Dispersion

According to the nature of the atmosphere which consists of mixtures of different types of particles, its gas molecules are in constant random motion, and due to the intermolecular distance, it allows mixing. If gas is introduced into the atmosphere, its molecules will gradually spread out and diffuse within the air molecules. In the case of gas emitted from stacks, the gas cloud disperses so that the concentration of the gas cloud decreases. As a result, the gas cloud density will approach that of air. Therefore, as a gas cloud disperses its behavior changes and finally the plume will completely vanish, and its contents become neutral with air. Eventually, when diluted, gas can never be separated from air.

Sometimes gas plume can travel long distances before it is totally dispersed in the atmosphere. Long dispersion distances create risk on the adjacent inhabited areas near to industrial sources. Several factors influence the dispersion of the gas namely by the gas process characteristics or thermodynamics (i.e., pressure, temperature, velocity, etc.) and by the ambient conditions (i.e., wind speed, terrain, temperature, etc.). The gas dispersion cannot be modeled based on density differences only because of the number of variables acting upon the released gas. Even on a calm day, the very low wind velocity that can hardly be felt can be enough to displace gases.

3.2.1. Air Dispersion Modeling

There are many types of dispersion models. According to the mathematical approach used to develop the model, it can be classified to empirical models, Lagrangian models and Eulerian models. The latter two are based on the transport phenomena, but each uses different reference system. While Eulerian models use a fixed spatial reference point set by the user, the reference point in Lagrangian models moves along with pollution plume parcel.

On the other hand, Empirical models are not entirely based on mathematical analysis. It considers steady-state dispersion of emissions from a continuous point source in an infinite medium. Empirical models include Gaussian models and Box models which are the most employed models in environmental control.

Box-models are the simplest as it assumes that pollutants are homogeneously distributed in a box shape to calculate the average concentration in the box area. It has been employed for the dispersion of heavy gasses from particular industries. Due to the assumptions in the model, it cannot be used to calculate the concentrations accurately.

On the other hand, there are many models of the Gaussian type. They have a great advantage over other models because of their simplicity and the short computing times. It can be used to simulate the dispersion of stable gas or aerosol with a particle diameter smaller than 20μm and remains airborne for a long time. Most of the national environmental agencies adopt Gaussian models. For the cases where simple atmospheric conditions with sufficient wind and normal topography, these models are the most adequate. Gaussian model is selected to model NOx dispersion in this research because of the following main reasons (Assael & Kakosimos, 2010):

- The results produced by the Gaussian model agree with experimental data as well as other similarity function's results,
- Mathematical calculation of the Gaussian equation are relatively easy,
- It is consistent with the random nature of turbulence,
- Though the model is empirical in nature, it uses a much lower degree of empiricism if compared to other similarity functions.

Accurate determination of ground level concentration is dependent on the atmospheric dispersion model used. According to Hystad et al. (2011) dispersion models have been used extensively in Canada. National air pollution model for several pollutants in seven cities was created to assess the population exposure and to inform surveillance, policy, and regulation. The environmental protection agencies often regulate the use and applicability of the available atmospheric dispersion models. For example, the United States Environmental Protection Agency (EPA) provides a list of models and guidance documents for different applications on its website ("SCRAM", 2018). Many dispersion models have been beneficial in many studies for achieving different objectives. Particularly the Gaussian models which are known for its simplicity and small computing time. Its accuracy was tested by Price (2004) by back calculating emission rates from industrial source when samples of ammonia and particulate matter are collected at sampling points.

3.2.2. Nitrogen Oxides (NOx)

Emissions of oxides of nitrogen, commonly referred collectively as NOx, are regulated because of their adverse effects on health and the environment. They play a major role in acid rain, the formation of harmful ozone and photochemical smog in the lower atmosphere and the depletion of the beneficial ozone in the upper atmosphere. NOx is chosen as the pollutant of interest in this research.

Over 90% of the NO_x from a typical flame is in the form of nitrogen monoxide (NO), and the remainder is nitrogen dioxide (NO_2). However, since NO eventually converted to NO_2 in the atmosphere, most regulations treat all of the NO_x as NO_2.

3.2.2.1. Regulations

Because of the adverse effects of air pollutants, international and local bodies all over the world have set standards for ambient air quality. The US EPA. (2016) standards for NO_2 are listed in Table 3.2

Table 3.2 - EPA Ambient Air Quality Standards

Criteria Concentration Limit(Ppb)	Averaging Period
100	1 hour (98^{th} percentile of 1-hour daily maximum concentrations, averaged over three years)
53	One year (annual mean)

The standards for NO_2 set by the European Union (European Commission, 2017) are listed in Table 3.3 below.

Table 3.3 - EU Ambient Air Quality Criteria

Criteria Concentration Limit (µg/m^3)	Averaging Period
200	1 hour (18 Permitted exceedances each year)
40	One year**

***Under the new Directive the member State can apply for an extension of up to five years (i.e. maximum up to 2015) in a specific zone. Request is subject to assessment by the Commission. In such cases, within the time extension period, the limit value applies at the level of the limit value + maximum margin of tolerance (* 48 µg/m^3 for annual NO2 limit value).

In Qatar, the criteria for NO_2 is a bit less stringent. The standards followed in industrial cities are as follows (SCENR, 2002):

Table 3.4 - Qatar Ambient Air Quality Criteria

Criteria Concentration Limit (µg/m^3)	Averaging Period
400	1 hour (99.9% of all hourly records in one calendar year)
150	24 hours (99.7% of all daily average in one calendar year)
100	Annual average (of all daily records in one calendar year)

The nitrogen oxides (NOx) emission limit from industrial boilers and furnaces with heat input capacity higher than 25MW is 55 mg/m^3 (SCENR, 2002).

3.2.3. Meteorological Data

For convenience and since the research is done in Qatar, it is assumed that the system studied is located in Qatar as well and hence meteorological data of the country will suffice. Meteorological data were extracted from historical climate data available in the National Climate Data Center (NCDC) website via the Climate Data Online (CDO) feature. The archive data are collected from fixed weather stations. The file supplied contains hourly observations of the various weather parameters for the period from 2011 to 2013 in two stations in Qatar which are Doha International Airport (DIA) and Mesaieed Industrial City. The file provided includes an extensive range of meteorological data. However, the data of interest for the air dispersion model are:

- Cloud coverage (CC)
- Wind speed
- Wind direction
- Ambient temperature (Ta)

The provision is that hourly data is going to be used for the research work. The existing weather station in Mesaieed Industrial City reported data in long intervals (every 6 hours) thus it was decided to use the meteorological data for DIA as it covers 24 hours of the day. Since data is collected hourly throughout the year, the possibility of error is present. After validation, some data were missing. It is important to fix this problem before exporting and using the data. Missing values of ambient temperature, wind speed or direction are filled by the average calculated between the two values before and after the missing value. For cloud coverage, all missing data are filled with 0 which denotes clear sky.

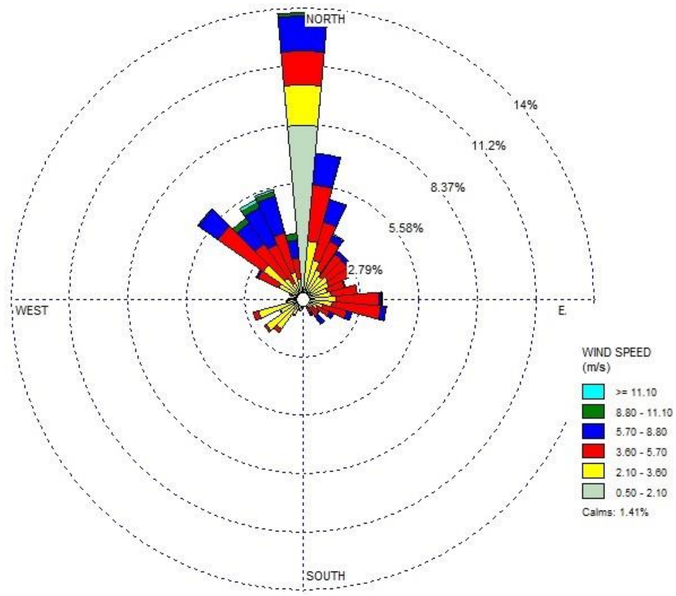

Figure 3.3 - Wind Rose Generated For the Collected Data

4. RESEARCH METHODOLOGY

4.1. Overall Research Methodology

The hypothesis behind this research is to integrate environmental science –air dispersion modelling in particular- and process optimization together in the hope of finding a new innovative solution to improve the air quality in the urban areas near industrial facilities. Figure 4.1 below outlines the methodology of this research.

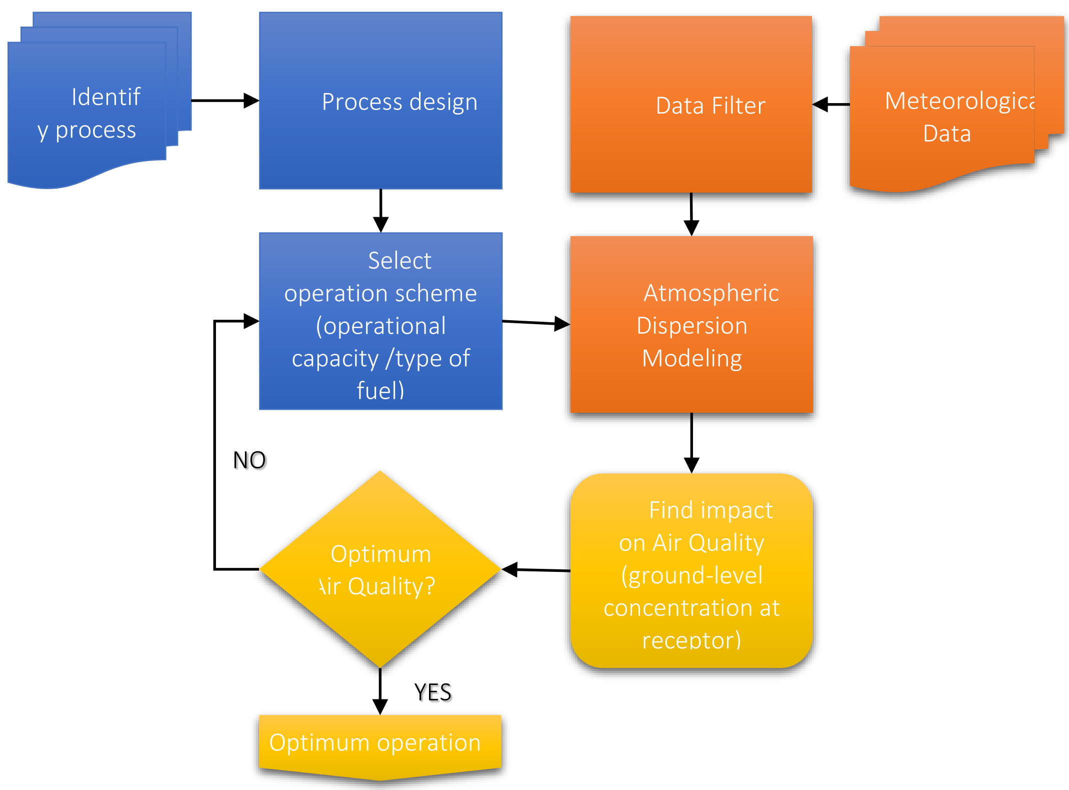

Figure 4.1 - Research Methodology Workflow. Adapted with permission from Kakosimos (2015).

The blue part of the diagram represents process modeling. A case study is built by gathering operational data for a process (Section 3.1.1). A process model is developed by relating available process parameters (e.g., production rate, fuel flow) to calculate the pollutants emission conditions resulting from the process and needed as an input to the dispersion model.

The orange part of the diagram represents the atmospheric dispersion modeling. Rea-time hourly meteorological data along with emissions conditions from the process model are supplied to the atmospheric dispersion model to calculate the ground-level concentration in the area surrounding the selected process.

This is considered as the base case. The output from the process model is used as an input to the dispersion model. The basecase scenario shows the performance of the original process and measures the ground level concentrations and give an insight of how the process is affecting the air quality in the surrounding area.

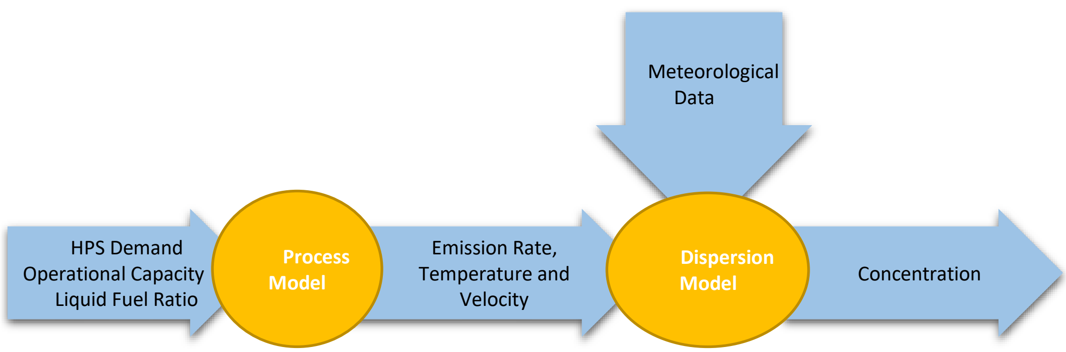

Figure 4.2 – Bas Case Flowchart

The hypothesis is to introduce a change in the process model to see if it generates a better air quality (lower ground level concentrations) in the surroundings. Thus, an investigation is performed to figure whether this is the optimum air quality that can be achieved. This is done through optimization. Operational parameters are changed in the process model, calculations are repeated to observe the resulting ground-level concentrations. When the ground-level concentration in the surrounding area is minimum, then the process operation is considered the optimum.

4.2. Optimization Goals

According to the nature of the case study selected, the following was set as the optimization goals:

- Goal 1: Optimize the **operating capacity**. Many operations constitute of multiple operating units (usually identical) that provide the product demand. The objective is to find the optimum operating capacity of each unit that can be applied to meet the required process output and at the same time result in minimum concentration of pollutants.

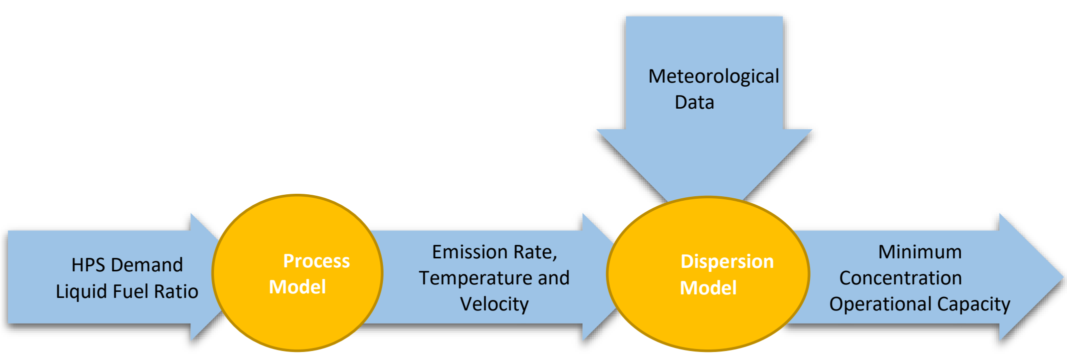

Figure 4.3 - Optimization Goal 1 Flowchart

- Goal 2: Optimize the **energy source**. A wide range of fuels can be used as an energy source in the combustion process. The amount of pollutants produced depends on the type of fuel used. If the process design allows the use of different types of fuels to meet the energy demand, then the objective is to optimize the ratio of one fuel to another keeping the air quality in compliance with the regulation of the region.

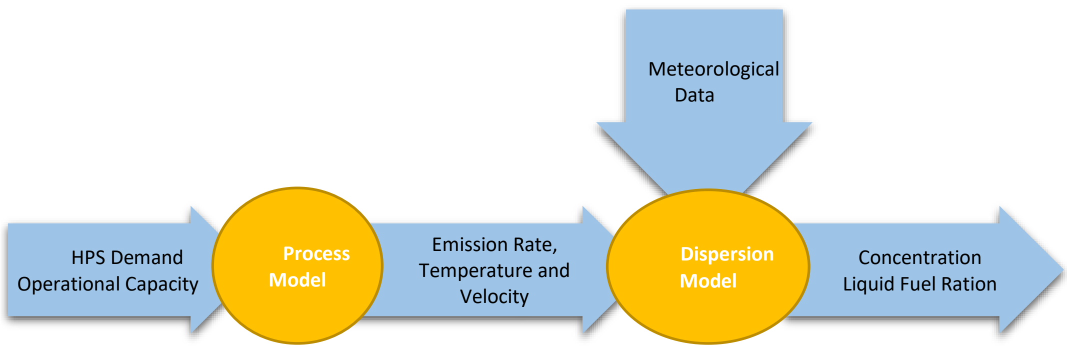

Figure 4.4 - Optimization Goal 2 Flowchart

5. MODEL SETTING

5.1. Process Model

The process model was built using the data collected for the fixed use HPS generation unit. Several dependencies were established between the different process variables. The final correlations were used as input to the air dispersion model. The objective of establishing these dependencies was to limit the input to the optimization model to the HPS demand only. All other variables are to be calculated within the process model such as fuel flow required and total emission flow. The output of the process model is NOx emission rate, temperature and velocity.

5.1.1. Assumptions

The following assumptions were used in the calculation to set the correlations representing the process model:

1) Emission factor for NOx from fuel gas burning = 60 g/GJ for process boilers (EEA, 2009)
2) Emission factor for NOx from liquid fuel burning =125 g/GJ. (EEA, 2009)
3) Reduction percent of 60% was applied to NOx emission rate to get a more accurate model.
4) When both fuels are used, NOx emissions are calculated as the sum of flue gas emitted from burning Fuel Gas and Liquid Fuel based on the emission factor for each.

5) 10% of the fuel fed to the boilers is liquid fuel while the balance is fuel gas (mainly methane) unless specified in the case.

6) Complete combustion takes place in the boiler.

7) Air consists of 79% Nitrogen and 21% oxygen.

8) Air molecular weight is 28.97 g/mol

9) Liquid fuel molecular weight is assumed 170 g/mol compared to known fuels with relatively close High Heating Value (HHV).

10) Air humidity is assumed 0.045 kg moisture/kg air

11) Boiler feed water is supplied at 25^{o}C and 1 bar.

12) Air is available with 15% excess to the boilers. If liquid fuel percentage provided to the boiler is higher than 40%, then the following formula is used to calculate excess air

$$Excess\ Air = \frac{(50 \times Liquid\ Fuel\% - 5)}{100}\%$$

5.1.2. Correlations

The established relations are as follows:

1- Steam demand - Fuel flow

The approach uses the HPS production rate to quantify the energy demand of the process and back calculates the fuel needed. Starting from the theoretical principles of boiler design:

$$Boiler\ Duty = Steam\ flow \times \Delta H\ (water + steam)$$

Assuming boiler feed water is fed at 25°C and 1 bar, and the resulting steam is at 370°C and 45 bar. Refer to the indicative temperature/enthalpy diagram in Figure 5.1 of water below to see the break down of enthapy. The following steps were followed in the calculation of enthalpy (ΔH):

$$\Delta H = \Delta H_{water}(\text{from } 25°C\ \&\ 1\ bar\ to\ 100°C\ \&\ 1\ bar)$$
$$+\ \Delta H_{vap}(Saurated\ water\ to\ saturated\ vapor\ at\ 100°C\ \&\ 1\ bar)$$
$$+\ \Delta H_{steam}\ (\text{from } 100\ °C\ \&1\ bar\ to\ 370°\text{C}\ \&45\text{bar})$$

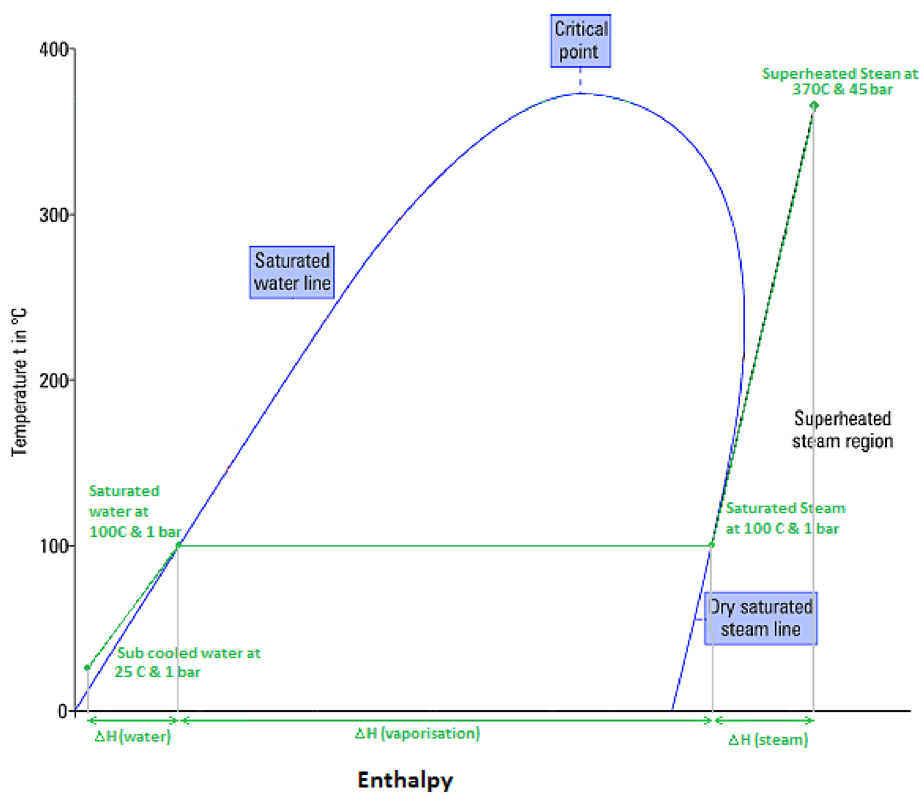

Figure 5.1 - Temperature / Enthalpy Diagram for Water

$$\Delta H_{water} = Cp \times \Delta T = \frac{75.4}{18.016}(100 - 25) = 313.88\,\frac{kJ}{kg}$$

$$\Delta H_{vap} = 2257\,\frac{kJ}{kg}$$ (Felder & Rousseau, 2005)

$$\Delta H_{steam} = 462\,\frac{kJ}{kg}$$ (Felder & Rousseau, 2005)

$$\Delta H = \Delta H_{water} + \Delta H_{vap} + \Delta H_{steam} = 3033\,\frac{kJ}{kg}$$

The boilers are fitted with dual fuel burners that can accept fuel gas as well as liquid fuel, therefore:

$$Fuel\ flow = Fuel\ Gas\ flow + Liquid\ Fuel\ flow$$

$$Liquid\ Fuel\ Fraction\ (P) = \frac{Liquid\ Fuel\ flow}{Fuel\ flow}$$

$$Boiler\ Duty = Fuel\ gas\ flow * FG\ HHV + Liquid\ Fuel\ flow * LF\ HHV$$

After incorporating all the above equations together with some unit conversions, the final fuel flow correlation below is established:

$$Fuel\ flow(kg/hr) = \frac{3033\ \times Steam\ flow}{4.18\ (11408 - 508\ P)}$$

The provided fuel flow data from the case study were compared to the correlation results, and it was found that there is a good agreement between the correlation established and the real data with an average error of 3%. Refer to the Figure 5.2 below for visual presentation.

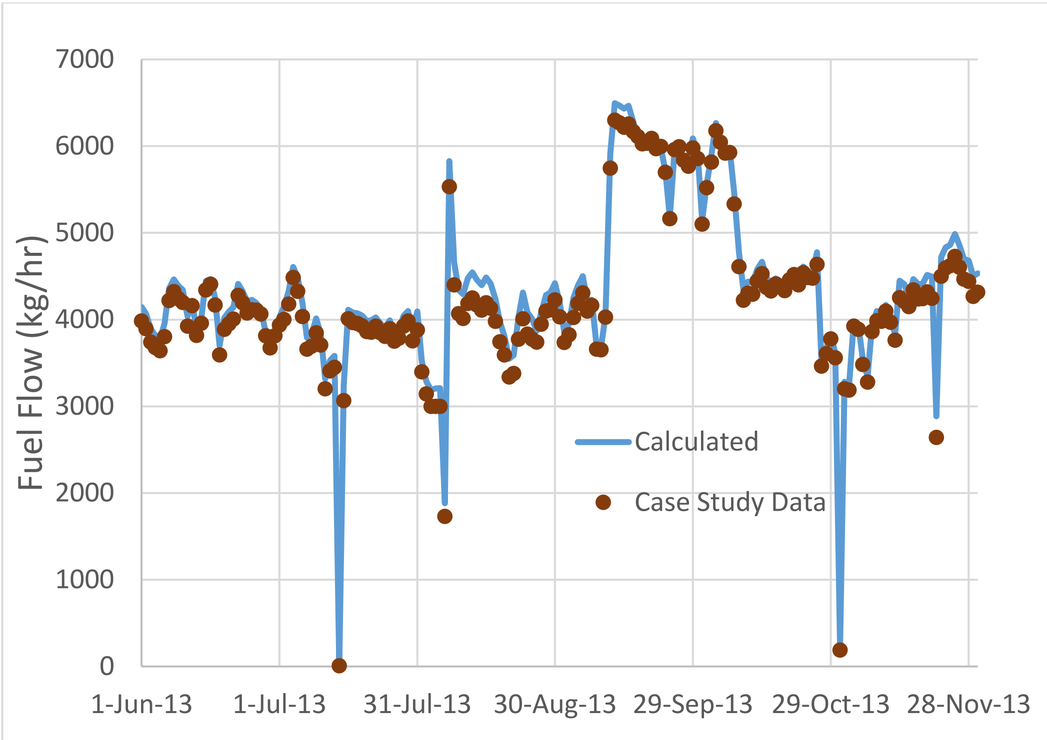

Figure 5.2 - Fuel Flow Correlation Fit

2- Fuel gas flow - NO_2 emission rate:

Emission factors are used to estimate the emission rate of certain pollutant. An emissions factor is a representative value that attempts to relate the quantity of a pollutant released to the atmosphere with an activity associated with the release of that pollutant. Emission factors for NOx are extracted from the EMEP/EEA Air Pollutant Emission Inventory Guidebook-2009 (EEA, 2009) issued by the European Monitoring and Evaluation Programme (EMEP)/ European Environment Agency (EEA).

In Part B, Chapter 1.A.1- Combustion in Energy and Transformation Industries, EMEP describes the methods and data needed to estimate emissions from Energy industries.

In Section 4 – Petroleum refining, the emission factor for process boilers using natural gas (US EPA Table 4-8, 2018) used is 60 g/GJ.

The emission factor from industrial boilers that uses residual oil given in the same section (US EPA Table 4-5, 2018) is 125 g/GJ. High Heating Values (HHV) of the fuels (Refer to Table 3.1) were used to obtain the emission factor for the fuel gas and liquid fuel assumed in the case study. Emission factors for NOx are defined in terms of NO_2 in the referenced chapter of the EMEP/EEA Air Pollutant Emission Inventory Guidebook-2009 (EEA, 2009). NOx emission rates obtained from the calculation gave the same trend as that of the case study but with higher values. When a reduction percent was introduced to the calculated rates, a closer fit was obtained. The estimated emission rates were minimized by 60% to reach that of the case study data. This huge percentage implies that the burners used in the boilers have excellent quality and reliability and might be Ultra Low NOx burners.

Figure 5.3 below shows the resultant fit compared to the provided NOx emission rate.

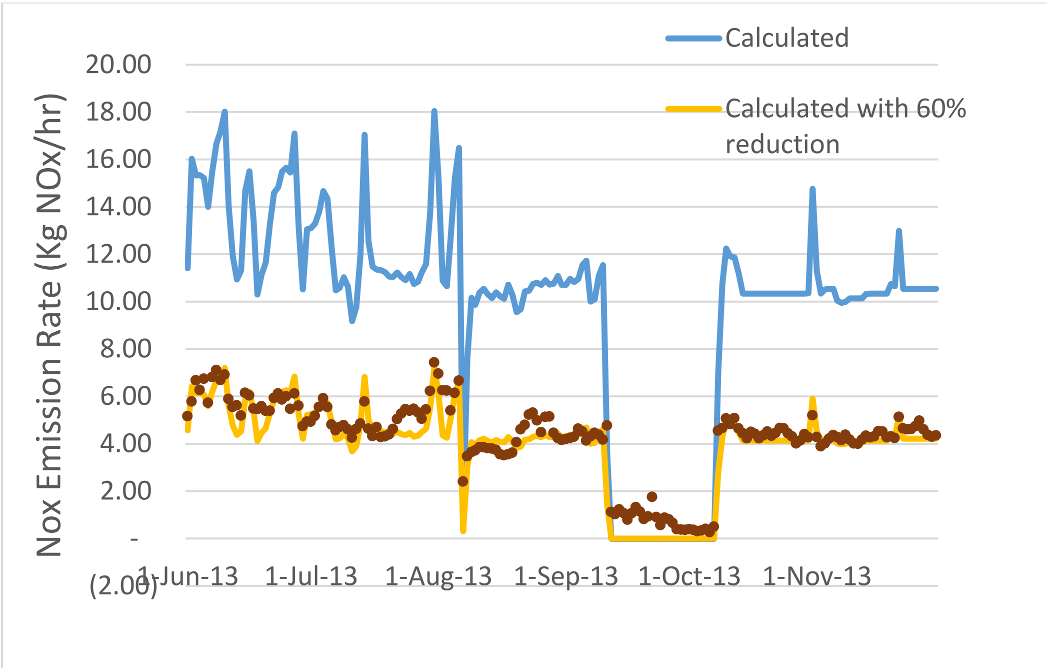

Figure 5.3 - NOx Emission Correlation Fit

3- Flue gas flow – Fuel Flow:

Assuming complete combustion takes place in the boiler where all fuel is burnt in the presence of oxygen to produce water and CO_2. Stoichiometric calculation is done to balance the components entering and exiting the "combustor" boiler (Nevers, 2010). Figure 5.4 demonstrates the consistency between the calculated flue gas flow and the provided data.

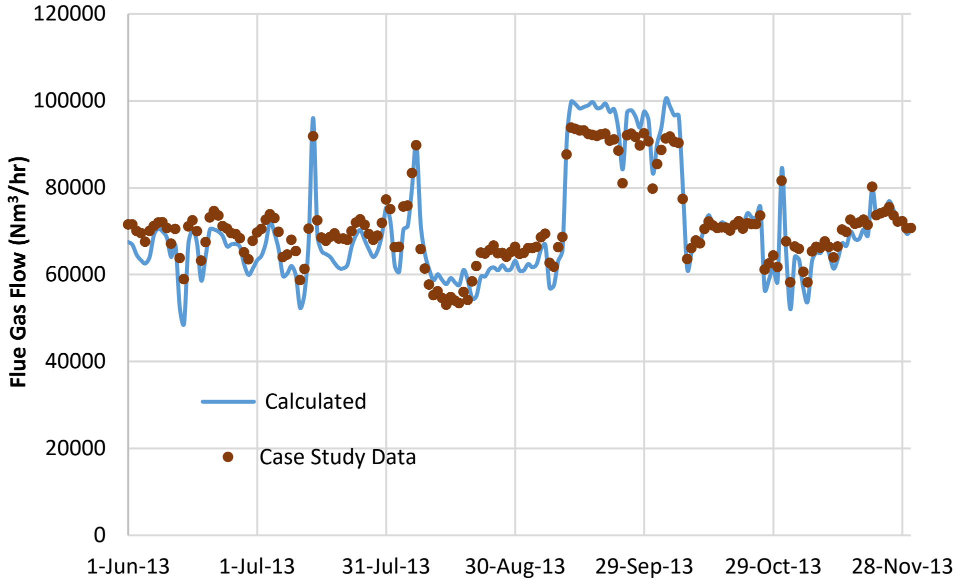

Figure 5.4 - Flue Gas Flow Correlation Fit

4- Flue gas flow – flue gas velocity

A simple calculation for flue gas velocity exiting the stack is done by dividing the daily volumetric flue gas flow over the cross-sectional area of the stack.

$A_{cs} = \frac{\pi}{4} d^2$, where A_{cs} is the cross sectional area of the stack and d is the diameter

5.1.3. Derived Correlations

5- Flue gas flow – flue gas temperature

In order to establish the dependency between the flue gas flow and temperature, an energy balance must be done for the process. Such exercise will require a lot of factors and data that are not available. Therefore, to establish this link, the two variables were fed to excel where data was sorted in ascending order (by steam flow), and then a chart of "x-y scatter" type was graphed to see the nature of the dependency.

A scatter chart combines steam flow (x-axis) and flue gas temperature (y-axis) values into single data points and shows them in intervals. Scatter charts are typically used for showing and comparing numeric values, in this case, the temperature measurements. As expected the relation between the two process variables is linear, but three regions were observed as can be seen in Figure 5.5 below:

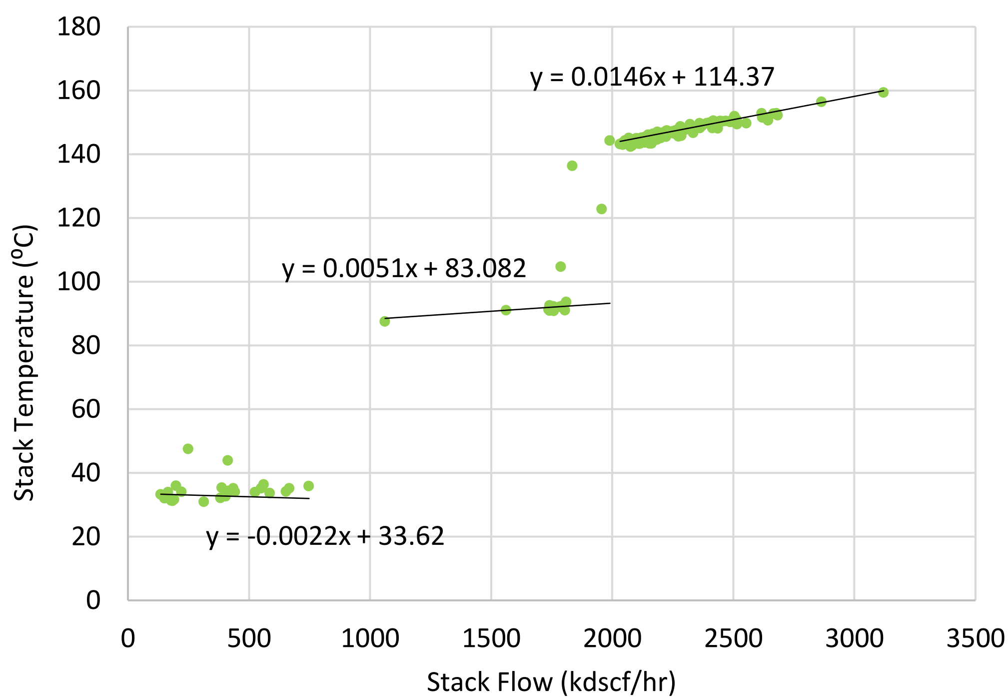

Figure 5.5 - Flue Gas Temperature Fit

Another feature in Excel charts is the ability to add a trend line which shows data trends or moving averages in a chart. Three trend lines were established for the three sets of data in each region and the following conditional functions where used in the model:

a) For flue gas flow < 1000 Kg/hr:

$$T_s = -0.0022 \times Flue\ Gas\ Flow + 33.62$$

b) For 1000 < Flue Gas Flow < 2000:

$$T_s = 0.0051 \times Flue\ Gas\ Flow + 83.082$$

c) For 2000 < Flue gas flow:

$$T_s = 0.0146 \times Flue\ Gas\ Flow + 114.37$$

Only steam flow was used as input to the model; all other process variables are calculated within the model as explained above. The steam data are daily data while the provision is to use hourly data as an input to the model. Thus the demand for the day was divided over 24 hours with normal distribution approach taking into consideration that the maximum demand for any hour should not exceed the design capacity of the three boilers.

5.2.Atmospheric Dispersion Model

For the aforementioned advantages -in Section 3.2.1- of the Gaussian model, it is found the most suitable for the purpose of the study to model light gas dispersion.

Input required to the simplified Gaussian plume model includes the meteorological conditions and the process characteristics of the emitted gas.

- Meteorological conditions are assumed to be stable in one hour time on average as covered in Section 3.2.3. It covers:
    - wind speed and direction considered stable with height
    - ambient temperature
    - cloud coverage
    - Time (day/night)
    - Terrain (rural/urban)

Thermal characteristics differ from rural to urban terrain due to different thermal characteristics and surface roughness. Anthropogenic heat sources and the thermal diffusivity of pavement and concrete increase temperature of urban areas compared to rural ones especially during the night. In many cases, this causes instability of meteorological conditions in urban areas during night time. Nevertheless rural is assumed for the model as most industrial cities are built away from cities and population concentrations.

- Process characteristics include the design of the emission source as well as the thermodynamic conditions of the emitted gas
    - Process design (as set in Section 3.1.1):
        - Number of stacks
        - Stack height
        - Stack diameter

- Gas conditions (calculated in the process model)
  - Gas exit velocity
  - Gas exit temperature
  - Emission –mass release- rate: continuous and stable with time

The final expected output from the Gaussian model is to calculate the concentration of the pollutant (NOx) at a certain point (relative to the stack position). However, there are other outputs which can be extracted along the way:

- Atmospheric Stability Class
- Prevalent forces (Buoyancy or momentum)
- Effective stack height
- Final Plume rise
- Distance of maximum plume rise

The final concentration equation adopted is as follows:

$$C = \frac{Q}{U} \cdot \frac{10^9}{2\pi\sigma_y} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \frac{1}{\sigma_z} \left\{ exp\left[-\frac{(h_e - z)^2}{2\sigma_z^2}\right] + exp\left[-\frac{(h_e + z)^2}{2\sigma_z^2}\right] \right\}$$

where,

C concentration of the gas pollutant (μg/m^3)

Q source pollutant emission rate (kg/s)

U horizontal wind speed along the plume centerline (m/s)

σ_y lateral dispersion coefficient (m)

σ_z vertical dispersion coefficient (m)

h_e plume rise (m)

y crosswind distance from the emission plume centerline

z height above ground level (assumed 2m)

The model is based on nine major assumptions mentioned by Assael & Kakosimos (2010). Concentration is calculated downwind of the emission source. Therefore for each source, the coordinated system was adjusted to cover all the area around the emission source taking into consideration the wind direction and the location of the stacks on the map. After choosing the extent of the map (x_{mesh}, y_{mesh}), coordinates of each point on the map is transformed as follows:

$$x_{grid} = x_{mesh} - x_{stack}$$

$$y_{grid} = y_{mesh} - y_{stack}$$

$$x_{cal} = x_{grid} \times \cos(dir) + y_{grid} \times \sin(dir)$$

$$y_{cal} = y_{grid} \times \cos(dir) - x_{grid} \times \sin(dir)$$

where,

dir wind direction

x_{mesh}, y_{mesh} coordinates that represent the size of the map

x_{grid}, y_{grid} coordinates shown on the map

x_{stack}, y_{stack} coordinates of the emission source

x_{cal}, y_{cal} coordinates used in the calculation

5.2.1. Assumptions

The following assumptions are used for building the air dispersion model. Wherever applicable, the assumptions are constructed so that it considers Qatar as the area of interest.

13) "z" the height above ground level where the concentrations are calculated is assumed 2m to give a closer representation of the air quality which is used by the population.
14) Meteorological data filtered to match the period for the collected process data (i.e., from June 1st to Nov 30th, 2013)
15) Rural terrain is assumed
16) Concentrations are calculated in the range of 20x20 square kilometers area around the emission sources which are located in the middle of the map
17) For faster computation, resolution of the calculation was 41x41 (every 500m) for the base case model and all subsequent codes.
18) The total concentration at a point with coordinates (x, y, z) is the summation of emission concentrations from all emission sources (3 stacks).

19) Average concentration is the average of the total concentration in the range of the mesh specified.

20) Anemometer height assumed 10 meters where meteorological data was recorded (Zref in the model).

21) Stacks are aligned along the x-axis and separated by 50 m.

5.3. Combining Models

At the early stages of the model development when the air dispersion model was calculating the concentration at only one point and from one emission source, an excel sheet was developed and used to double check the results of the calculations. Process model relations were validated against the original case study data as shown in the graphs illustrated in Section 5.1. After setting the correlations between variables and adjusting the inputs, the process model and the air dispersion model were ready to be integrated into one model.

5.3.1. Constraints

The following constraints were taken into taking into consideration in the model:

1- The maximum production capability of one boiler is 110,000 kg/hr

2- Maximum steam demand used is 330,000 kg/hr while the minimum is 40,000kg/hr.

3- The total steam demand input to the model must be met 100%

The steam demand flow exiting the utility unit, SD, is split between the three boilers. The sum of the operating capacity of the boilers OC_i must supply the steam demand.

$$SD = \sum_{i=1}^{n} OC_i$$

The split fraction of the boilers operating capacity is expressed as x_i for each boiler; the sum of these fractions must come to unity, meaning that all values must be between 0 and 1.

$$\sum_{i=1}^{n} x_i = 1$$

As such, the operating capacity of each boiler, OC_i, is equal to the split fraction x_i, multiplied by the steam demand.

$$OC_i = x_i * SD$$

5.3.2. Objective Function

After setting and running the base case, the code is reconfigured to be able to find the optimum operation. As stated in the objectives the optimum target in Optimization Goal 1 is the operational capacity distribution -that is the share of each unit (boiler) of the required steam demand. The objective function minimizes the concentration of NOx. The minimized variables in the study are the hourly maximum concentration or the hourly average concentration.

Minimize (Cavg or Cmax)

The optimum target in Optimization Goal 2 is the ratio of the liquid fuel used. The objective function is to keep the concentration of NOx below the selected limit (75µg/m3).

Minimize (|Cmax-75|)

NOx concentration is function of the steam demand, operating capacity, fuel ratio and meteorological conditions are stated earlier in Section 4.

5.3.3. Implementation

MATLAB® is a high-level language and interactive environment for numerical computation, visualization, and programming. MATLAB can be used to analyze data, develop algorithms, and create models and applications.

MATLAB is used by scientists and engineers in industry and academia. It supersedes spreadsheets and traditional programming languages, such as C/C++ or Java™ as it has tools and built-in math functions that enable faster numeric computation. Its capabilities include visualization tools that allow data modeling for easier analysis. Algorithms can be developed and optimized using a high-level language and development tools. Applications developed in MATLAB can be shared either as an application, code, executables, or software components (MathWorks, n.d.)

Because of the capabilities mentioned above, MATLAB was chosen as an engine for analysis of the model developed for the study. The following are some information about the software used.

Company: The MathWorks, Inc.

Version: R2013a (8.1.0.604)

Release Date: February 15, 2013

License Number: 263745

The Gaussian air dispersion model, as well as the process correlations obtained, were written as a comprehensive MATLAB code. Since hourly data for six months (4392 points) were input to the code and thus 4392 result points as output, a user-friendly interface, to extract input data from and export results to, was required. All required inputs (metrological and process data) were arranged in an excel sheet. MATLAB would read from the excel file and perform calculations then write the results back to the same file.

To address the model simplicity, the input was confined to hourly steam demand, operating capacity, liquid fuel ratio and metrological data as illustrated in the flowcharts in Section 4. Other process variables needed for the atmospheric dispersion calculation such as the flue gas velocity, flue gas temperature, and NOx emission rate are calculated within the MATLAB model. The model is upgraded to perform the two-dimensional concentration calculation at each coordinate (x, y) to cover a range of 20 x 20 kilometers around the utility unit. The model is integrated to run for multiple emission sources (three stacks in our case). The total concentration at each point is the summation of the emissions from the three stacks. Then the average concentration for the area around the emission sources is calculated and recorded. The maximum concentration as well as how many times selected limit were exceeded in the studied area each hour are also recorded.

The results sent to output file each hour are the average concentration, the maximum concentration and the count of exceedances above the selected criteria.

Since the input data are hourly data, the excel sheet is set so that the daily average concentration, maximum daily concentration and the count of concentrations above criteria in one day (every 24 hours) are automatically calculated as soon as the hourly results are exported from the code and written into the respective cells.

Later in the research excel was replaced by input and output text files.

An optimization function “FMINCON”, which finds a constrained minimum of an objective function, is utilized to optimize one/several variables of the model. FMINCON as other Optimization Toolbox solvers in MATLAB finds the local minimum in the basin of attraction of the starting point. To return a global minimum “MultiStart” solver was incorporated in the code from the Global Optimization Toolbox in MATLAB. The starting point (initial guess) in Optimization Goal 1 is the operating capacity used in the base case.

In Optimization Goal 2, the starting point is P=0.1 which indicates 10% of the fuel used is liquid fuel.

The built codes are provided in Appendix A as detailed in the Table 5.1 below

Table 5.1 - Appendix A Contents

Appendix	Code
A.1	Base Case
A.2	Optimization Goal 1
A.3	Optimization Goal 2
A.4	“gaussplume66” Function which represent the air dispersion model

6. RESULTS

6.1.Base Case

A baseline model (reference case) is established as per the case study conditions. It uses the case study's hourly data over the period of six months to simulate the operating conditions. Steam demand, operating capacity of each boiler and meteorological data are all input to the model. This model serves as the Base Case. For every hour (set of input data) the ground level concentrations are calculated in the 20 square kilometers area around the system. The emitting stacks are at the center of the maps produced, which gives the concentrations up to 10 kilometers in every direction around the utility system. 80μg/m^3 is used as a threshold in this research to allow comparison between different cases. It represent 20% of the regulation adopted in Qatar for the hourly ambient air quality criteria for NOx (refer to Section 3.2.2). Since one unit is studied it was assumed that it should not contribute to higher than 20% of the allowable criteria.

The average and maximum concentrations as well as how many times the concentration exceedes the selected limit (80μg/m^3) are all recorded for each hour (over the six months period) in the results text files produces from the MATLAB code. To establish a comparison between the base case and other future cases, the maximum concentration reached (over the six months period), the average concentration (over the whole area studied and within the plume) and the count of exceedances are all recorded in Table 6.1 below.

Then the average concentration of the six months period (4392 hours) is calculated at each point of the 20 x 20 km area around the utility system. The calculated values are used to produce a contour map as in Figure 6.1 below.

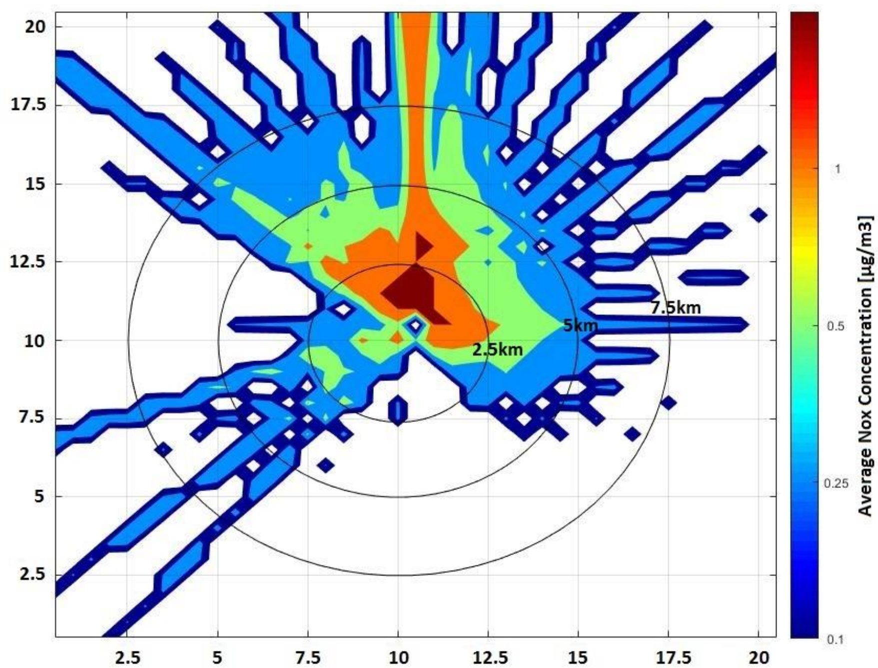

Figure 6.1 - Average Concentration Map - Base Case

Figure 6.1 shows the cumulative effect concentration on the area around the system over six months. In general the average concentration is very small and irrelevant.

The same approach is used with the maximum concentration. Maximum concentration in the six months period is also recorded at each point of the 20 x 20 km area around the utility system. The values are then used to produce a contour map as in Figure 6.2 below.

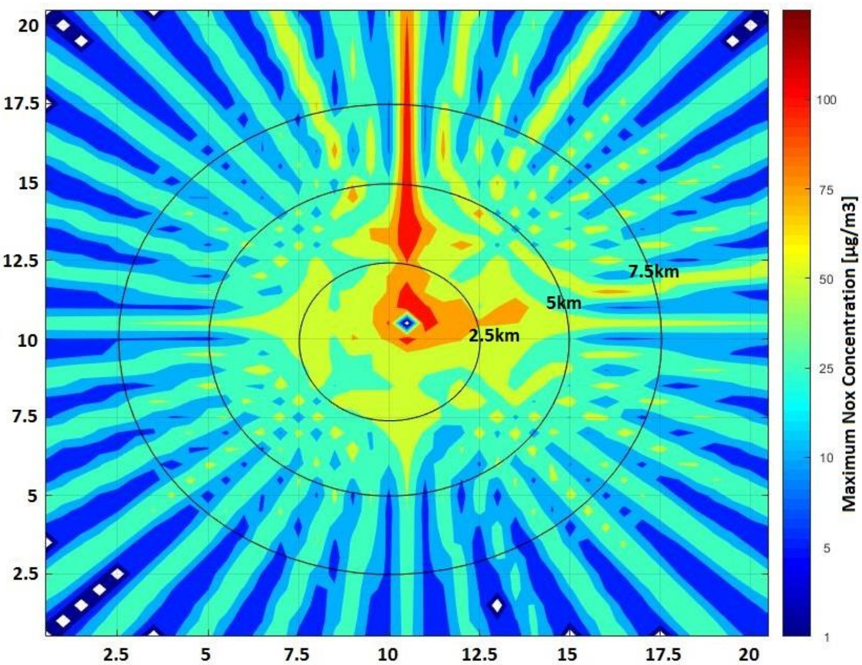

Figure 6.2 - Maximum Concentration Map - Base Case

It can be seen from the graph that the maximum concentrations exist to the north of the stacks, which is natural as most of the prevailed wind direction input data are to that direction. The red color represent the maximum concentration above 80µg/m^3.

6.2.Optimizing Goal 1 – Operational Configuration

In the base case, the steam demand was met most of the period by operating the three boilers. As can be seen in Figure 3.2. The optimization function was introduced to the MATLAB file with an objective of minimizing the resulting ground level concentration by changing the operational capacity distribution (the share produced from each boiler of the required steam demand). In the optimization files, the baseline model is modified to accept the total steam demand of the plant and the meteorological conditions only. The operational capacity distribution of the boilers is calculated for each hour by the optimization function. This step was done twice, once by minimizing the **average** concentration (Cavg) in each hour and another time by minimizing the **maximum** concentration (Cmax) in each hour.

6.2.1. Optimization by Minimizing Cavg

Firstly, the model was run with an objective of minimizing the average concentration in the specified area. The same contour map done for the base case was produced for the average concentration at each point (coordinates), and the result is as in Figure6.3 below:

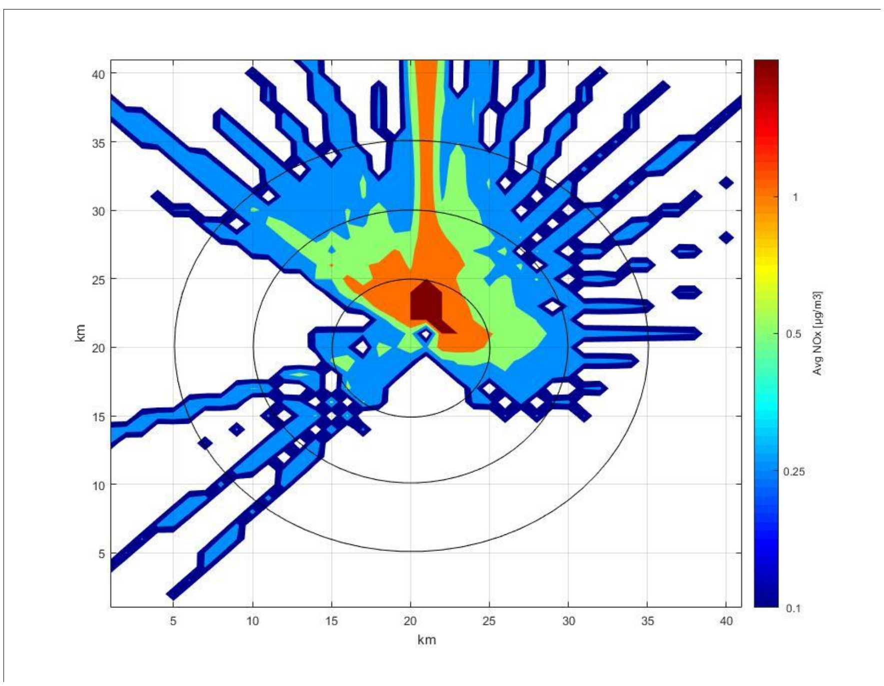

Figure 6.3 - Average Concentration Map – Minimizing Cavg

The resulting maximum concentration at each point (coordinate) are illustrated in Figure6.4 below. The results are in Table 6.1.

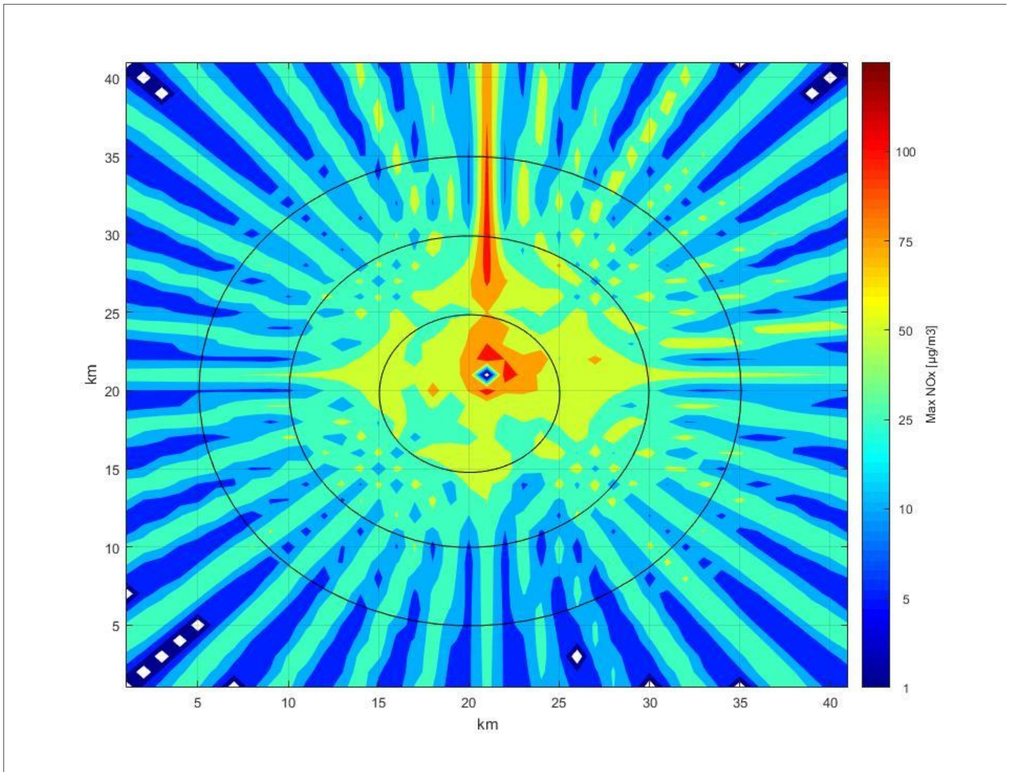

Figure 6.4 - Maximum Concentration Map – Minimizing Cavg

When comparing the resulting maps to that of the base case, there is an improvement seen in Figure 6.4 as the red area representing the concentration exceeding the regulation is notably smaller when minimizing Cavg. A percent of change map is illustrated in Figure 6.5. The percent change of the maximum concentrations between the base case and this case is calculated at each point. The figure shows that there is a reduction of the concentration in some points however in general there is an increase in concentrations in the studied area.

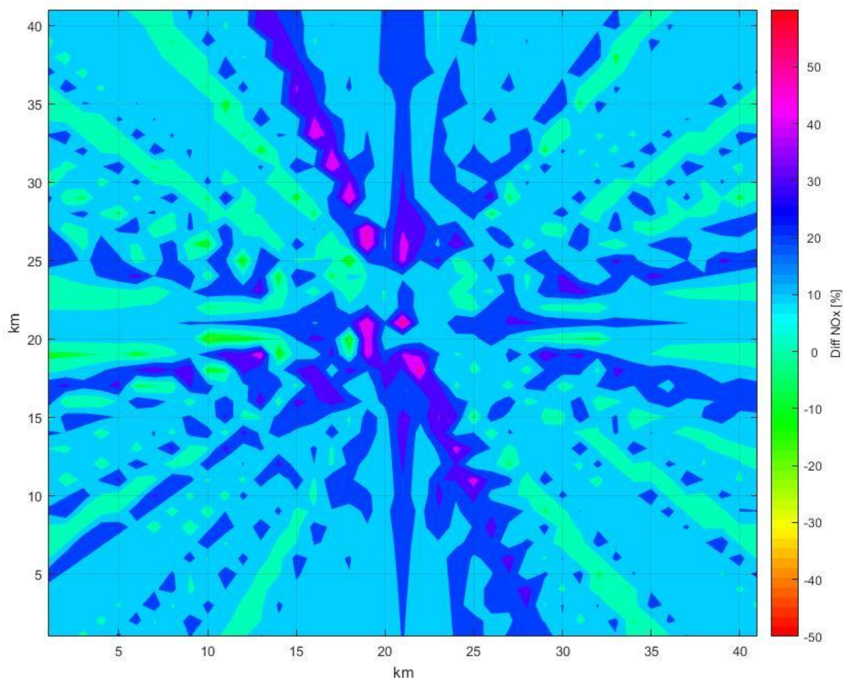

Figure 6.5 – Percentage Change Map - Minimizing Cavg

6.2.2. Optimization by Minimizing Cmax

Secondly, the model was run with an objective of minimizing the maximum concentration each hour in the specified area. The resulting contour map for the average concentration of the six months period at each point is illustrated in Figure6.6 below:

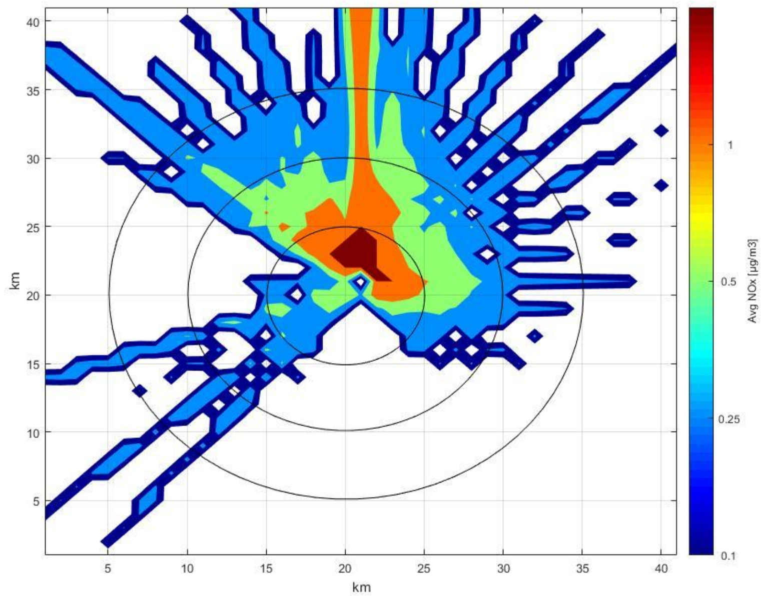

Figure 6.6 - Average Concentration Map – Minimizing Cmax

The maximum concentration is shown in Figure6.7 below:

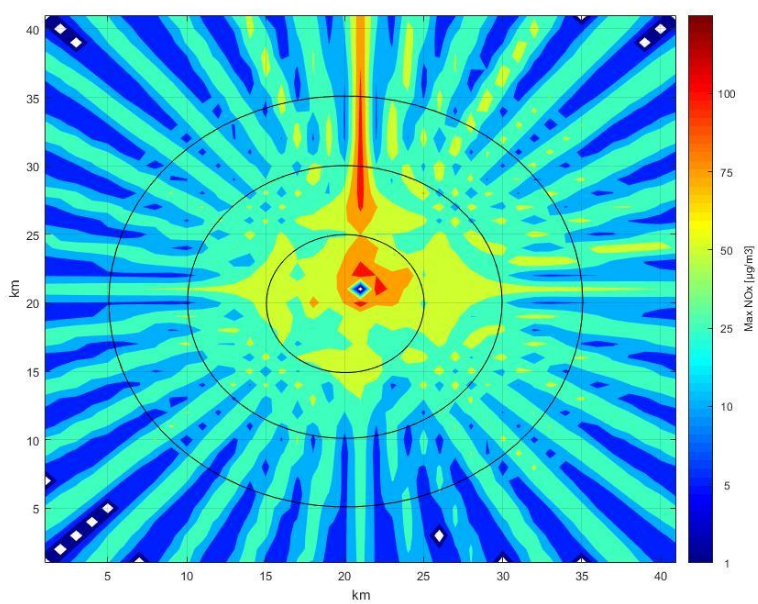

Figure 6.7 - Maximum Concentration Map – Minimizing Cmax

Both the average and the maximum concentrations are lower than that of the base case, and there is an improvement seen in the smaller areas of concentrations. The result concentration are recorded in Table 6.1. A percent of change map is represented in Figure 6.8. The percent change of the maximum concentrations between the base case and this case is calculated at each point. The figure shows a decrease of the concentrations where it reaches to 46% reduction at some points.

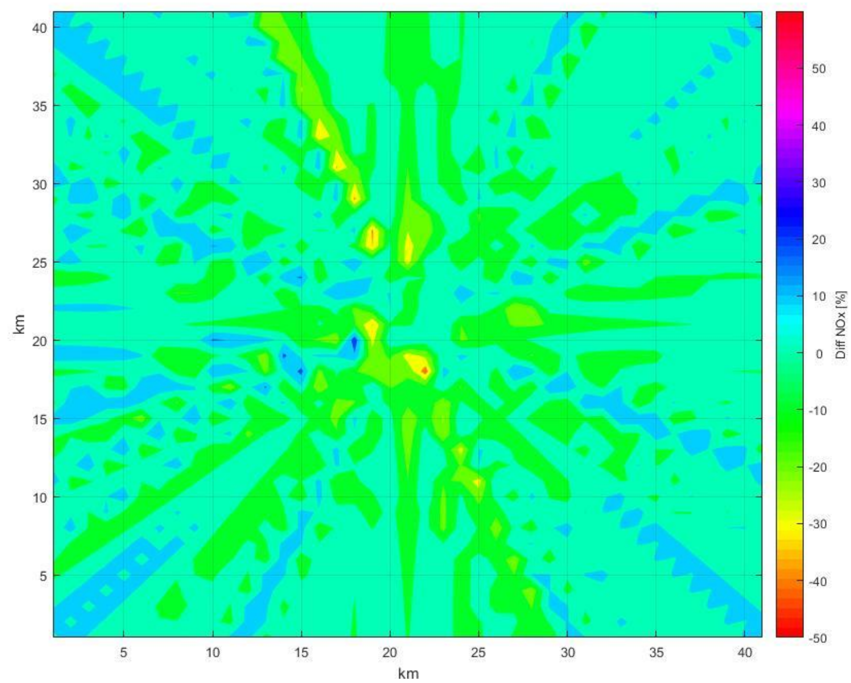

Figure 6.8 - Percentage Change Map - Minimizing Cmax

6.2.3. Summary of Results

Analysing the results from the above cases and taking into consideration that various parameters are affecting the dispersion process for each set of data (each hour). It is necessary that scenarios are set, and individual cases are run to find out the most affecting parameters on choosing the optimum operation distribution between the three boilers. Analyzing the base base versus the optimization results, some trends were discovered. To investigate further, sensitivity analysis was carried out.

Table 6.1 - Comparison between Base Case and Optimization Cases

	Base Case	Optimization by minimizing Cavg	Optimization by minimizing Cmax
Maximum Concentration	148	128	128
Average concentration over the whole area	1.1	0.9	0.9
Average concentration within the plume	3.831	3.1	3.1
Number of exceedances (concentration > 80 $\mu g/m^3$)	274	96	94

6.2.4. Sensitivity Analysis (Pre-Defined Cases)

Scenarios were set so that all the variables are kept constant while changing only one at a time. The effect of the variable on the dispersion process is studied without any effect from the other variables. The variables studied are:

1. Steam demand
2. Ambient temperature
3. Wind velocity
4. Cloud coverage

The direction of the wind is set to 45 degrees, and the emission sources are shifted to the bottom left of km area studied which now has been reduced to 10 square kilometers. The concentrations are calculated every 250 meter. This way there should be more space that allows seeing the plume of pollutants (NOx here) more clearly. The three boilers are sharing the load equally, i.e., each boiler is producing the third of the steam demand.

Firstly, varying steam demand, the understanding is that more steam demand means more burning fuel and thus higher pollutant concentrations. Higher steam demand also results in higher exit velocity of the pollutant which enhances the dispersion and takes pollutants further. As can be observed in the resulted simulation Figures 6.9 below, the plume is dispersing on a larger area when the steam demand is higher. The summary of the variables and results for this scenario is summarized in Table 6.2. As expected the concentration has increased noticeably when increasing the steam demand.

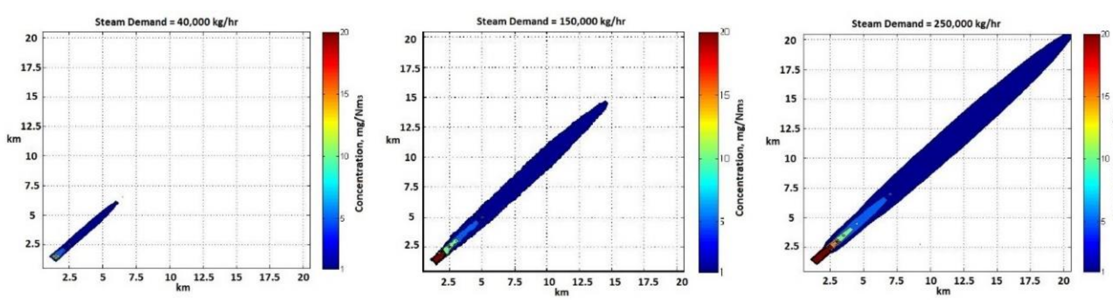

Figure 6.9 - Effect of Steam Demand on Dispersion. a) 40,000kg/hr, b) 150,000kg/hr, c)250,000kg/hr

Secondly, varying ambient temperature, the effect on the dispersion also depends on the exit temperature of the pollutants. Atmosphere or pollutants, whichever has the higher temperature will go upwards according to the simple physical properties. Within the full range of ambient temperature experienced in the region from June to November, the pollutant's temperature is always much higher than that of the ambient temperature. Thus, the effect of changing ambient temperature is not expected to affect the dispersion process. The result of simulating the effect of ambient temperature is as follows.the plumes can be said identical as well as the reulting concentration. Thus ambient temperature is not considered in future analysis.

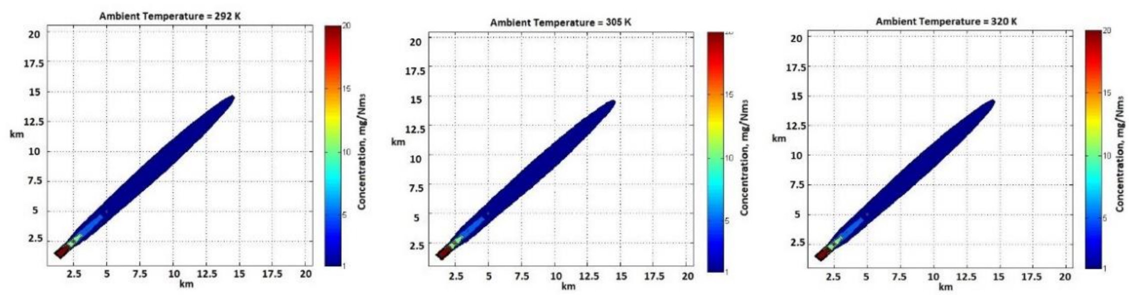

Figure 6.10 - Effect of Ambient Temperature on Dispersion. a) 292K, b) 305K, c)320K

Thirdly, varying wind velocity has a great effect on the dispersion process however when stability of the atmosphere (refer to Appendix B) is different, the effect of wind velocity is different. Because of that, test of wind velocity was done twice. One case assuming daytime and another assuming nighttime. This guarantees change in atmospheric stability class. Looking at the plumes in Figures 6.11 and 6.12, in daytime, dispersion is less and resulting concentration are lower too. On the other hand, higher concentration are recorded at nighttime although dispersion is enhanced. In general higher velocities resulted in lower pollutant concentrations. However these findings cannot be generalized without a thorough study of the atmospheric stability.

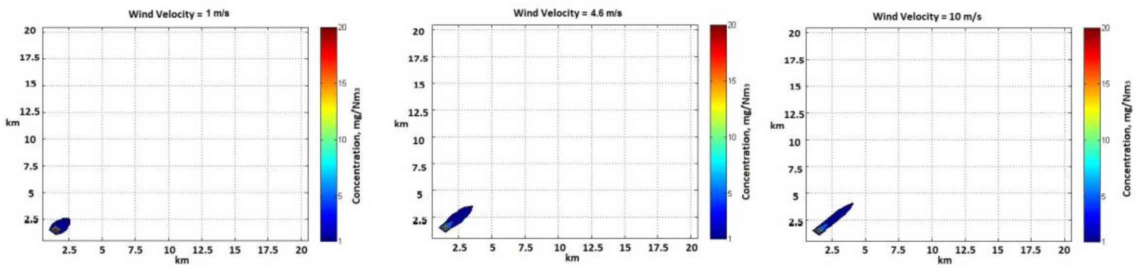

Figure 6.11 - Effect of Wind Velocity on Dispersion at Daytime. a) 1m/s, b) 4.6m/s, c)10m/s

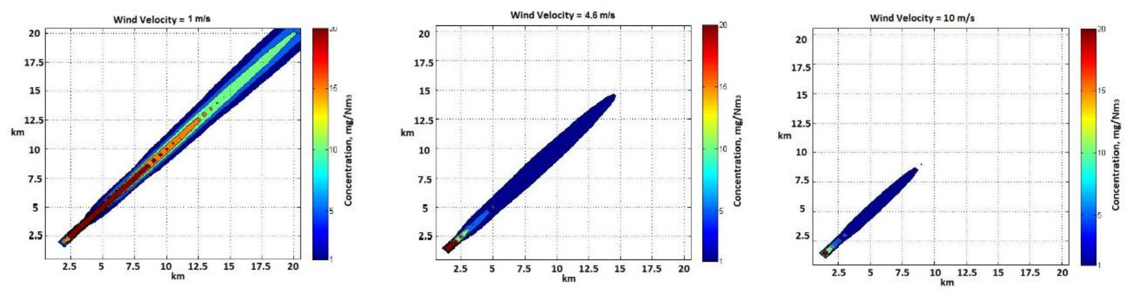

Figure 6.12 - Effect of Wind Velocity on Dispersion at Nighttime. a) 1m/s, b) 4.6m/s, c)10m/s

Finally, cloud coverage is a factor that directly affects the stability of the atmosphere. Comparing the extreme conditions of clear sky (0 cloud coverage) versus low sun radiation (7/8 cloud coverage) the resulting plumes can be seen in Figure 6.13 and variables are populated in Table 6.2 below.

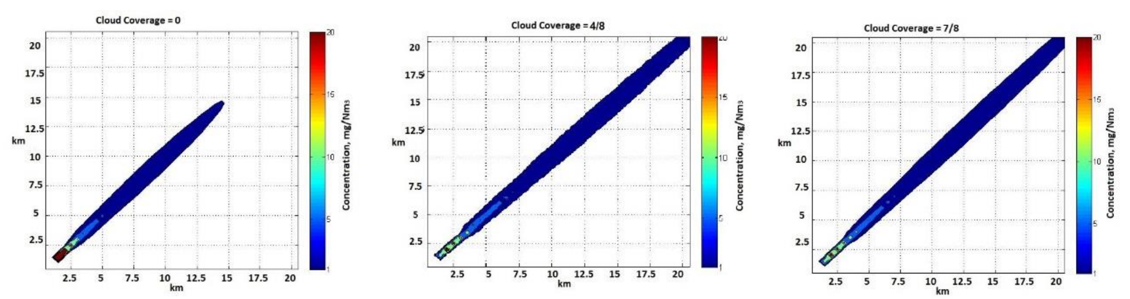

Figure 6.13 - Effect of Cloud Coverage on Dispersion. a) 0, b) 4/8, c)7/8

As atmospheric stability is directly identified by wind velocity, cloud coverage and time, it can be concluded from the analysis above that the major contributors towards the dispersion process are steam demand and atmospheric stability whether it is the breadth of the plume or the resulting ground level concentrations. Explanation of atmospheric stability and the stability classes is provided in Appendix B.

Table 6.2 - Results of the Variables Sensitivity Analysis

Variable changed	Wind direction	Wind velocity (m/s)	Ambient temperature (C)	Cloud Coverage	HPS demand (kg/hr)	Cmax (µg/m3)	Cavg (µg/m3)	Stability Class
HPS demand	45	4.6	32	0	40,000	20.5	0.07	D
	45	4.6	32	0	150,000	56.1	0.26	D
	45	4.6	32	0	250,000	66.2	0.41	D
Ambient temperature	45	4.6	19	0	150,000	56.1	0.26	D
	45	4.6	32	0	150,000	56.1	0.26	D
	45	4.6	47	0	150,000	56.1	0.26	D
Wind velocity (daytime)	45	1	32	0	150,000	28.1	0.03	A
	45	4.6	32	0	150,000	22.3	0.05	B
	45	10	32	0	150,000	21.7	0.05	C
Wind velocity (nighttime)	45	1	32	0	150,000	52.6	1.14	F
	45	4.6	32	0	150,000	56.1	0.26	D
	45	10	32	0	150,000	32.8	0.13	D
Cloud coverage	45	4.6	32	0	150,000	56.1	0.26	D
	45	4.6	32	4/8	150,000	28.5	0.28	E
	45	4.6	32	7/8	150,000	28.5	0.28	E

6.2.5. Stability Class Analysis

The Analysis of the variables showed that the major variables affecting the dispersion process are Steam Demand and Stability. To further explore the driver for using one operating scheme over another, six predefined cases (one for each stability class) are configured so that the full ranges of steam demand as well as the wind velocity are plugged in a matrix.

New input files were prepared so that all other variables are fixed (i.e., wind direction, ambient temperature, and cloud coverage). Steam demand is varied from 40,000 kg/hr to 250,000 kg/hr with 7000kg/hr increment. Wind velocity is varied from 1 m/s to 10.2 m/s with 0.4 m/s increment.

Stability is defined by cloud coverage, time of the day and wind velocity (refer to Appendix B - Pasquill Stability Classes). Since the cloud coverage in the area studied is 0 (which denotes clear) sky almost all the time (86% of the data points supplied for the studied period from June 1st to November 30th), it has been set to 0 in the analysis. Although MATLAB still reads cloud coverage and time, it will not affect the calculations as it is only used in the algorithm to determine the stability and since stability is fixed in the MATLAB code, all the calculations will be valid.

The same MATLAB algorithm used to find the optimum operating configuration of the three operating units by minimizing the maximum concentration (Cmax) in the surrounding area is applied. For each stability class, optimization file was run and the resulting operating configurations (one for each point [steam demand vs. wind speed]) were illustrated in a surface chart. Every operating scheme is represented by a certain color as shown in Figure 6.14.

Starting with stability class A, this stability class represents very unstable conditions and the only region of the graph of interest is below wind velocity of 3 m/s – assuming daytime with low cloud coverage (refer to Appendix B). Analyzing the data, it was found that for steam demand less than 110,000 kg/hr (which is the maximum capacity of one boiler), all the demand is met by one boiler and the pollutant is sent to its dedicated stack. For higher steam demand, one boiler is using its full capacity (110,000kg/hr), and the balance is met by another boiler – which is represented by the orange area in Figure 6.14. For steam demand higher than 220,000 kg/hr, two boilers are using their full capacity, and the remainder is met by the third boiler.

Stability class B represents unstable conditions. The only region of the graph of interest is wind velocity below 5 m/s – assuming daytime (refer to Appendix B). The same trend was found as that of Stability Class A.

Stability class C represents slightly unstable conditions (Refer to Appendix B), the only region of the graph of interest is wind velocity higher than 2 m/s – assuming daytime and depending on cloud coverage. At lower wind velocities, the trend is not clear. Sometimes it is desirable to use the minimum number of boilers possible to meet the demand, and in some instances, the load is shared between 2 or 3, even if fewer boilers can handle the demand. In the condition of higher wind velocity (higher than 3.8m/s), it is preferred to use the minimum number of boilers at full capacity to meet the steam demand.

Stability class D represents Neutral conditions (Refer to Appendix B), it covers a wide range of wind velocity (higher than 3 m/s) depending on the time (day/night) and cloud coverage. It's clear from the figure that other configurations are giving better air quality results. It is no longer ideal/necessary to use the full capacity of boilers. For lower wind velocities it is better to split the demand on two boilers even if can be met by one and on three even it can be met by two. On the contrary, for higher wind velocities (higher than 5m/s) it is still desirable to use the full capacity of the boiler with the minimum number of boilers to meet the steam demand.

Stability class E represents slightly stable conditions (Refer to Appendix B), the only region of the graph of interest is wind velocity between 2 to 5 m/s – assuming nighttime. The dominant configuration is to use:

1- One boiler for demand lower than 110,000 kg/hr represented by the red area in Figure 6.14.

2- Two boilers (1 running full capacity) for demands from 110,000 to 220,000 kg/hr, represented by the orange area in Figure 6.14.

3- Three boilers (2 running full capacity) for demands higher than 220,000 kg/hr, represented by the yellow area in Figure 6.14.

Finally, Stability class F represents stable conditions (Refer to Appendix B), the only region of the graph of interest is wind velocity less than 3 m/s – assuming nighttime. The dominant configuration is to use is the same in Stability E.

It can be seen from the surface charts in Figure 6.14 produced by excel that at unstable conditions classes A & B and Stable conditions classes E&F, in the condition of low steam demand, the operating scheme preferred would be operating only one boiler. If steam demand exceeds the operating capacity of one boiler, then a second is utilized to produce the balance. Once the demand is higher than the design capacity of two boilers, the third is utilized to produce the balance. Thus the preferred operating philosophy is to use the boiler to its full capacity with the minimum number of boilers to cover the steam demand.

Only 2 points in stability A, 3 points in stability B, 5 in stability E and 4 in stability F deviated from that conclusion and is not recommending to utilize the boiler's full capacity. This is attributed to truncation errors as the model is full of conditional functions. These errors could not be traced. While for slightly unstable conditions (class C) and neutral conditions (class D), it tends to operate two boilers even if one boiler can satisfy the demand. These conditions (Classes C & D) covers a wider range of wind velocity. However, at higher wind velocities it follows the results of stable and unstable conditions of using the minimum number of boilers to their full capacities.

The resulting concentrations for the different stability classes from A to F are compared in Table 6.3, the following was concluded:

- The maximum concentration of the studied area around the plant is mostly the highest in unstable conditions and the lowest in stable conditions
- The average concentration of the studied area around the plant is generally the lowest in unstable conditions and the highest in stable conditions
- For all stability classes, Cmax and Cavg are higher in conditions of lower wind velocities and higher steam demands

Table 6.3 – Results of the Stability Sensitivity Analysis

Stability Class	A	B	C	D	E	F
Maximum concentration	120	104	105	83	98	68
Average concentration	0.22	0.92	1.59	2.76	3.32	2.59
Exceeding 80µg/m^3	27	14	42	3	23	0

Further investigation resulted that the operational configurations tends most of the cases to operate the first or third boiler to supplement the required amount of steam. This is due to the fact that the produced plumes are less intersected and thus lower concentration is expected than to operate the second boiler. As the second boiler is located in the middle, it contributes to higher concentration as the plume intersects with those of the first and the third boilers.

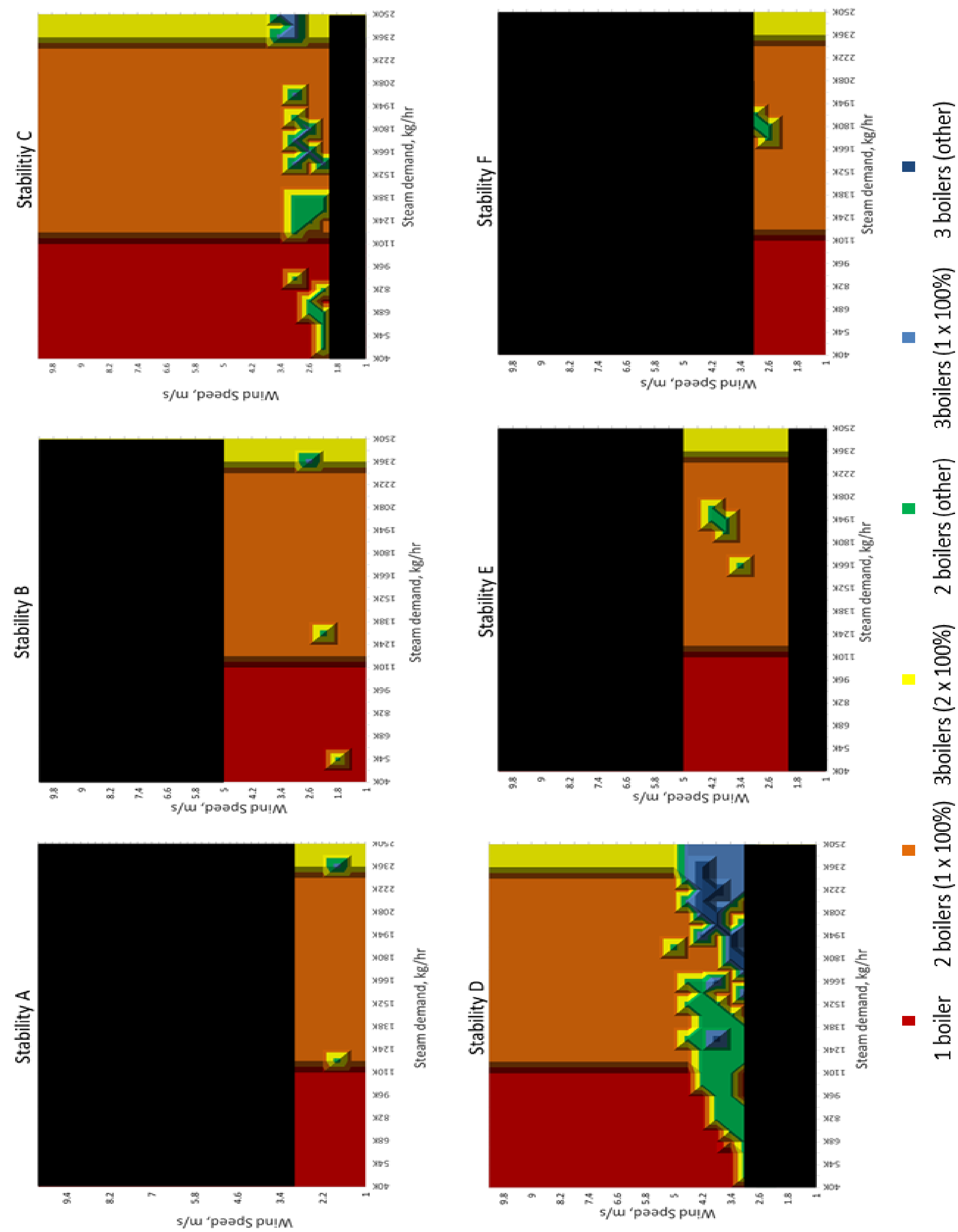

Figure 6.14 - Surface Charts Illustrating the Optimum Operating Configuration at Different Steam Demands and Wind Velocities for All Stability Classes

6.3.Optimizing Goal 2 - Fuel Type

This Section investigates the result of switching between different types of fuel which are fuel gas and liquid fuel as introduced in Section 3.1.1. The operational capacities of the three boilers used are the result of the optimization by minimizing Cmax.

6.3.1. All Fuel Gas Case

Firstly, the base case model is set to run assuming fuel gas only (i.e. P=0) is introduced to the boilers. The results are represented in following maps:

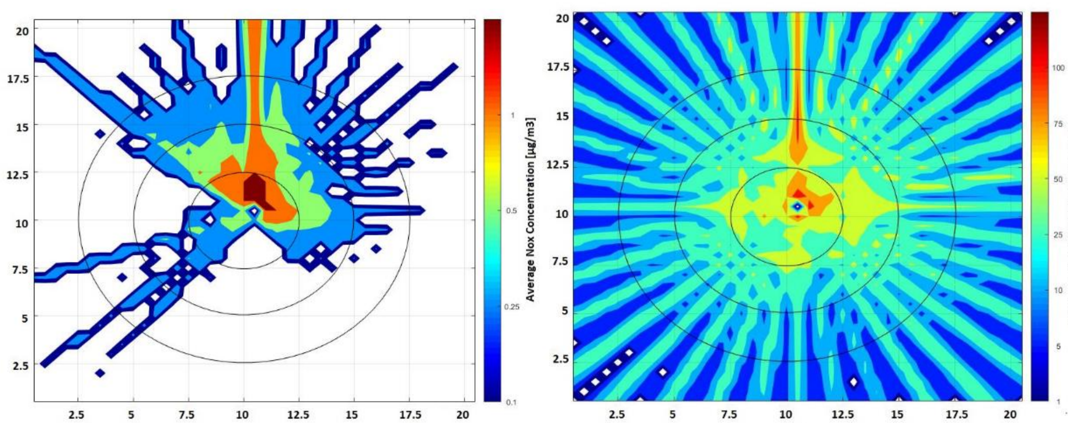

Figure 6.15 - Concentration Maps - Fuel Gas Case

6.3.2. All Liquid Fuel Case

Then the model is set to run assuming liquid fuel only (i.e. P=1) is introduced to the boilers. The results are represented in following maps:

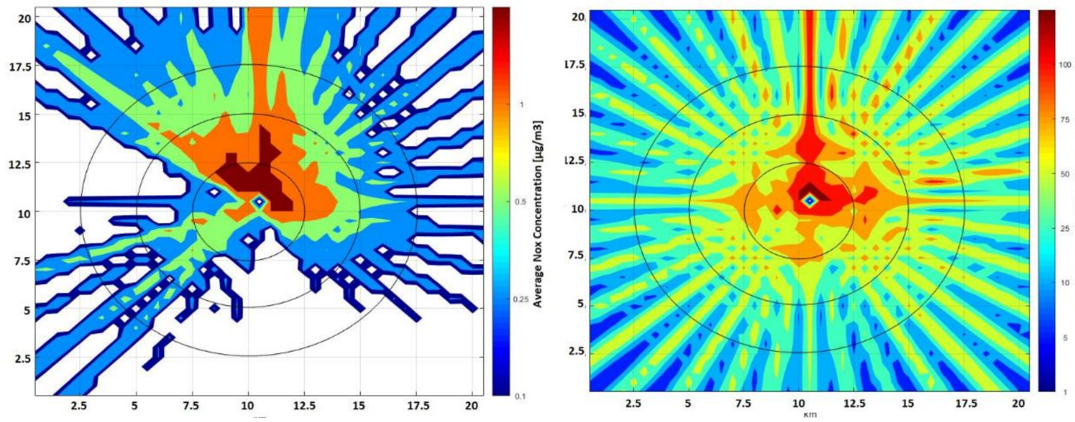

Figure 6.16 - Concentration Maps - Liquid Fuel Case

6.3.3. Optimization Results

The optimization file is modified so that the operating capacities for the three boilers resulting from minimizing Cmax is read from the excel file. The objective function is set to minimize |Cmax – 75|. Which means optimization function will find the liquid fuel fraction (P) that does not exceed 75µg/m^3 which is just below the selected limit (80µg/m^3).

If the objective function used is to minimize Cmax by changing P, then the expected result would be P=0 for all data points. The contour maps produced are in Figure 6.17 below.

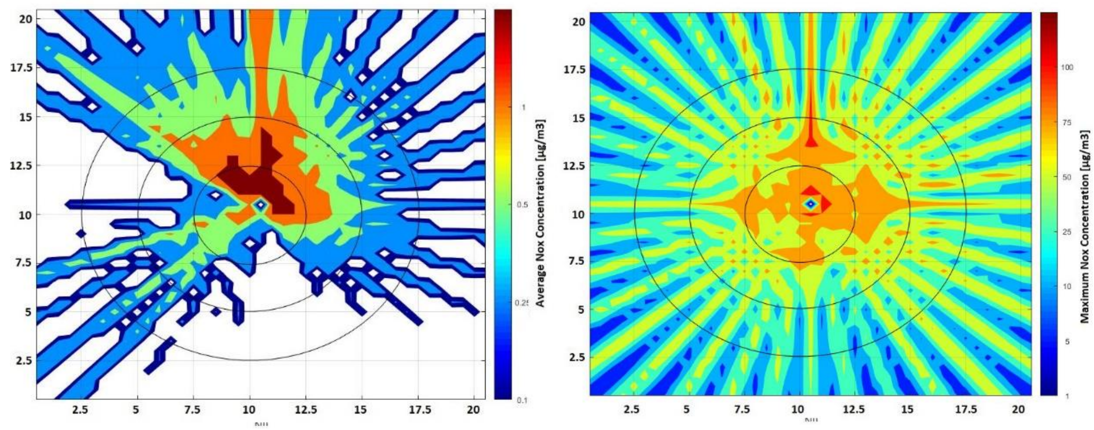

Figure 6.17 - Concentration Maps - Fuel Optimization Case

Comparing the maximum concentration contour maps of the base case and the fuel optimization case, we can see a reduction in the red area which represents exceedance of the regulations. However the orange area is bigger. This is due to firing more liquid fuel. Nevertheless, the concentration is still compliant with the regulations. Figure 6.18 represents a percent difference map that shows the percent change in maximum concentration between the base case and the fuel optimization case. There is a noticeable decrease in the concentration where it was exceeding the regulations. Reduction reaches 33% at some points. However, in other parts od the map there is an in increase in the concentration.

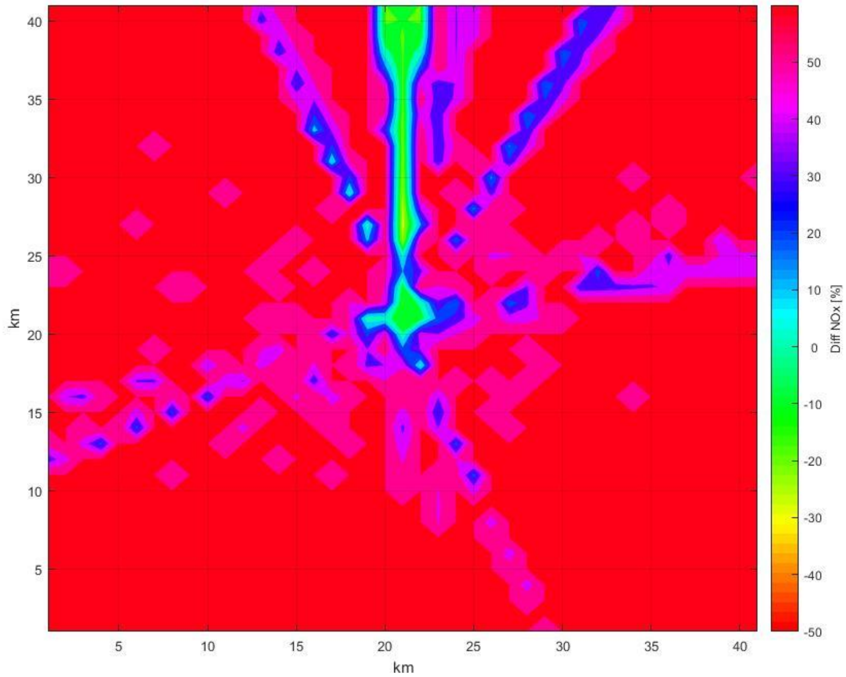

Figure 6.18 - Percentage Change Map - Fuel optimization

The following Figure 6.19 is comparing the concentrations resulting from the different cases for 100 data points. For the case when P is equal to 0 the maximum concentration exceeded 80µg/m^3 then by default the optimum P is 0. There is not a better case. On the other hand, when P is equal to 1 and the maximum concentration is less than 80µg/m^3, then MATLAB will choose P=1 as the optimum value.

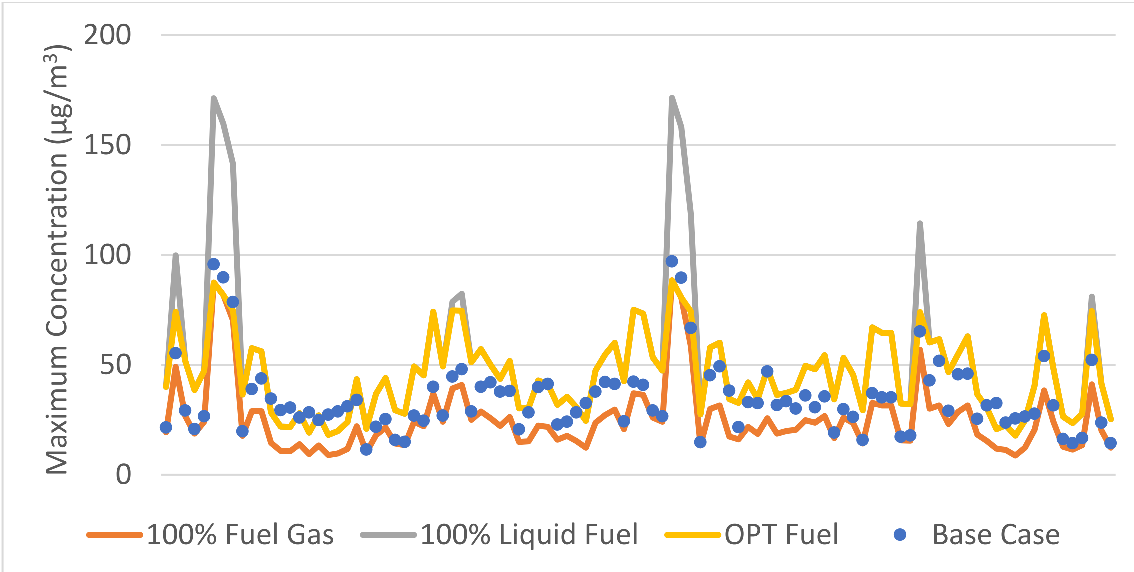

Figure 6.19 - Maximum Concentration for the Different Fuel Cases for 100 Data Points

Type of fuel has a direct effect on the pollutant concentration as can be seen from the results above and Table 6.4.

Table 6.4 – Results of the Fuel Cases

	Max Concentration	Exceeding 80µg/m^3
Base Case	148	274
All Fuel Gas (P=0)	118	40
All Liquid Fuel (P=1)	211	1193
Optimization P	118	40

Since the operational configuration of the three boiler was already optimized, it can be seen that there is still room for improvement from the fuel optimization case. Most of the exceedances were avoided. The same sensitivity analysis applied for the first optimization goal (operational configuration) was applied for the fuel optimization. In this sensitivity analysis the goal was to find the optimum P for different conditions of steam demand and atmospheric stability. Figure 6.20 shows the surface charts produced for stability A, D and F.

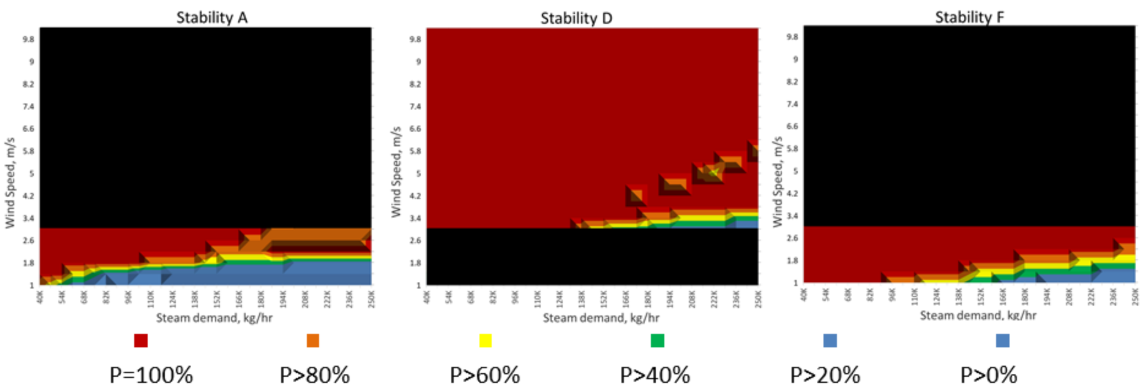

Figure 6.20 - Surface Charts Illustrating the Optimum Liquid Fuel Ratio at Different Steam Demands and Wind Velocities for Stability Classes A, D and F

The general conclusion is that more liquid fuel can be used at higher wind velocity and lower steam demand. In the opposite conditions fuel gas must be used. These surface charts can be applied as operational procedure for this case study. But the approach can be applied to other cases where similar charts can be produced. This helps a facility to be compliant with the regulations and in some favorable cases cut in the operational costs. Liquid fuel is cheaper than fuel gas in normal situations and in our case study there was 28% reduction in the fuel cost when using prices that goes back to 2014 - as supplied with the case study. However, nowadays natural gas is cheaper and in such cases it becomes more economically and environmentally superior.

7. DISCUSSION, CONCLUSIONS AND FUTURE WORK

The average concentration was not a very good indicator of the emissions however maximum concentration gave a very good comparison method to measure the improvement between the developed cases. The variables in the model that have major effect on the output of dispersion are steam demand and atmospheric Stability. Thus, it is very important in some cases to switch to other operating configuration.

When it comes to optimize operational configuration, the recommendation for Stability classes A, B, E and F is to use the minimum number of boilers to produce the HPS demand using the boilers to their maximum design capacity. There was a reduction that reached 46% in concentrations as a result of optimization. This recommendations allows maximization of the pollutants velocity exiting the stacks so that it will be carried away quickly.

For stability classes C and D, at low wind velocities it tends to use more boilers with load less that their design capacities. A more representative case with more emission sources should be studied to further explore the possibility of producing an operational procedure. For each atmospheric stability class.

When a facility accepts different type of fuels and the concentration is not permitted to go above certain limit in certain area around the facility, it is possible to use optimization of the fuel type so that ground level concentrations are within regulation. The use of fuel optimization allowed 33% reduction in concentrations at some points and a total saving 28% in operational cost. The same approach can be used on different facilities. The surface charts for stability classes will give a good reference for operators to make sure they are within regulation with the possibility of reduction in operational costs. In general, it can be said that in the conditions of low steam demand and high wind velocities liquid fuel can be used. On the other hand it shows for regulatory authorities that their method of regulating emissions can be manipulated because the regulation will be met however the overall air quality will be much worse.

7.1.Future Work

Although the results presented here have demonstrated the effectiveness of using process optimization to control the air quality in the very early stages of a project, this effort could be further developed in a number of ways:

1- Expand the study to larger scale

Though in the selected case study the point sources (stacks) were congested in one location, expanding the study over a full plant operation using the same methodology will be more reflective when emission sources are scattered and distant from each other within the plant area. Such model can expand to cover full industrial city and address the affected areas around it.

2- Apply energy losses for low turn down ratio boilers

One way to move forward is to upgrade the model to consider conventional boilers with lower turndown ratio. In this condition as the steam demand decreases or operating capacity of one boiler drops, the burning rate will drop causing a drop of the efficiency and an increase in the fuel consumption. Below certain firing capacity, the burner will cycle off causing valuable energy to be wasted. To account for this conventional type of boilers it is necessary to establish a relation of the burning rate and efficiency to predict the additional fuel required. Also the energy needed to start the burners after cycling off has to be estimated and considered in the calculations.

As the operational capacity drops, it is expected that lower fuel will be required. However and due to efficiency drop and wasting energy due to the cycle off below the minimum turndown, the situation is more complicated and requires more analysis to decide on the optimum capacity.

3- Apply design modifications

If the facility is in the design phase, then introducing design changes to the process would also affect the dispersion process. Design of the stack (diameter or height) can contribute to reduce concentrations at receptors.

Instead of dedicating a stack for each boiler the emission balance can be optimized between multiple emission sources (stacks). i.e. flue gas from different operations can be merged prior to emitting to the atmosphere. The assumption that each unit operation is sending emissions to its respective stack no longer applies at this point and different allocations will represent different scenarios. The effect of shifting the emission rate produced from different unit operation between the different stacks must consider the capacity and design of the stack and study the effect on emissions velocity and flow rate.

4- Use more advanced dispersion model where accuracy matters and for larger areas. Its not recommended to used plume models beyond ten kilometers as the metrology differs with distance. Advanced models produce more accurate results and address more potential effects but comes with more computational time burden. In specific areas it might be needed because it represents an important receptor say an urban residential area near plant of interest. This will narrow down the area and produce results that are more indicative.

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APPENDIX A

CODE

A1 – Base Case Code

```
function [success, Ctot] = ComputeAverage(Cmaxh)

TotSteam=dlmread('TotSteam.txt');
Hour = dlmread('Time.txt');
Steam1 = dlmread('Steam1.txt');
Steam2 = dlmread('Steam2.txt');
Steam3 = dlmread('Steam3.txt');
dir = dlmread('dir.txt');
Us = dlmread('Us.txt');
Ta = dlmread('Ta.txt');
CC = dlmread('CC.txt');

    CXYmax=zeros(41,41);
    CXYavg=zeros(41,41);

    Nboilers=3;
    P=0.1;

    for i=1:4392 %Met conditions   %%
        for k=1:Nboilers
            xstack(k)  = 9900+k*50;
            if k==1
                Steam(k)=Steam1(i);
            else if k==2
                    Steam(k)=Steam2(i);
                else Steam(k)=Steam3(i);
                end
            end

        SteamFlow=Steam*TotSteam(i);
        Fuel= 3032.89*SteamFlow/(4.184*(11408-508*P));
        LF= P*Fuel;
        FG= (1-P)*Fuel;
        Q=(1-0.6)/1000/3600*(FG*2.86386+LF*5.70070);

        %Emission rate calc:
        ER=(0.7282*FG+0.81098*LF)*22.414; %Nm3/hr

        end
        CtotXY=zeros(41,41);
        counth(i)=0;
        counta(i)=0;     %%
        Csum(i)=0;       %%
```

```
        xi=0;
        for xmesh = 1:500:20001;
            yi=0;
            xi=xi+1;
            for ymesh = 1:500:20001;
                yi=yi+1;

[C1(i,xi,yi),stability]=gaussplume66(xmesh,ymesh,Q(1),ER(1),Us(i),Ta(i)
,CC(i),Hour(i),xstack(1),dir(i));

[C2(i,xi,yi)]=gaussplume66(xmesh,ymesh,Q(2),ER(2),Us(i),Ta(i),CC(i),Hou
r(i),xstack(2),dir(i));

[C3(i,xi,yi)]=gaussplume66(xmesh,ymesh,Q(3),ER(3),Us(i),Ta(i),CC(i),Hou
r(i),xstack(3),dir(i));

                Ctot(i,xi,yi)= C1(i,xi,yi)+C2(i,xi,yi)+C3(i,xi,yi);
                if Ctot(i,xi,yi)>80;
                    counth(i)=counth(i)+1;
                end
                if Ctot(i,xi,yi)>0;      %%
                    counta(i)=counta(i)+1;       %%
                end           %%

                CtotXY(xi,yi)=CtotXY(xi,yi)+Ctot(i,xi,yi);
                Csum(i)=Csum(i)+CtotXY(xi,yi);

                CXYmax(xi,yi)=max(Ctot(i,xi,yi),CXYmax(xi,yi));
                CXYavg(xi,yi)=CXYavg(xi,yi)+Ctot(i,xi,yi);
            end
        end

        %temp=squeeze(Ctot(i,:,:));
        %Cavgh(i)=mean(mean(temp));

        Cavgh(i)=Csum(i)/1681;
        CavgN(i)=Csum(i)/counta(i);    %%
        Cmaxh(i)=max(max(Ctot(i,:,:)));

        S(:,i)=stability;
        disp(i/4392*100)
    end

    CXYavg=CXYavg/i;
    save CXY.mat CXYmax CXYavg CtotXY;

    %Enter the Results to separate files
    dlmwrite('Cmax.txt',Cmaxh);
    dlmwrite('Cavg.txt',Cavgh);
    dlmwrite('CavgN.txt',CavgN);    %%
    dlmwrite('CountH.txt',counth);
    dlmwrite('Stability.txt',S);
```

```
        success = true;
```

A2 – Optimization Goal 1 Code

```
function optim
 %% Read the input files:

 TotSteam1 = dlmread('TotSteam1.txt'); %%Total Steam flow
 BCSteam1 = dlmread('BCSteam1.txt'); %%Base Case Steam 1 flow
 BCSteam2 = dlmread('BCSteam2.txt'); %%Base Case Steam 2 flow
 BCSteam3 = dlmread('BCSteam3.txt'); %%Base Case Steam 3 flow
 Time = dlmread('Time.txt'); %%Time (Hour)
 dir1 = dlmread('dir1.txt'); %%Wind Direction with North axes
 Us1 = dlmread('Us1.txt'); %%Wind Speed
 Ta1 = dlmread('Ta1.txt'); %%Ambient Temperature
 CC1 = dlmread('CC1.txt'); %%Cloud Coverage

  Cavg=zeros;
  Cmax=zeros;
  CountH=zeros;
  Steam=zeros(3,1);

  parpool(24);

    parfor i=1:4392
      [Cavgh,Cmaxh,counth,Steam123,S]=
myfunc1(i,TotSteam1,Us1,BCSteam1,BCSteam2,BCSteam3,Time,dir1,Ta1,CC1);

        Cavg(:,i)=Cavgh;
        Cmax(:,i)=Cmaxh;
        CountH(:,i)=counth;
        Steam(:,i)=Steam123;
        Stability(:,i)=S;

        disp(i)
    end

  %Enter the Results
  dlmwrite('Cmax.txt',Cmax);
  dlmwrite('Cavg.txt',Cavg);
  dlmwrite('CountH.txt',CountH);
  %dlmwrite('Stability.txt',Stability);
  dlmwrite('Stability.txt',Stability,'delimiter',''); %%

  dlmwrite('Steam.txt',Steam);

end

function Cavg=ObjFun(xq)
```

```
  Steam(1)=xq(1);Steam(2)=xq(2); Steam(3)=xq(3);
  [sucess,Cavg]=ComputeAverage(Steam);

  end

  function                                [Cavgh,Cmaxh,counth,Steam,S]=
myfunc1(i,TotSteam1,Us1,BCSteam1,BCSteam2,BCSteam3,Time,dir1,Ta1,CC1)
  global TotSteam Us Ta dir CC Cavgh counth Cmaxh Hour S

        TotSteam=TotSteam1(i);
        dir=dir1(i);
        Us=Us1(i);
        CC=CC1(i);
        Ta=Ta1(i);
        Hour=Time(i);

        Aeq=[1,1,1];
        beq=1;
        A=[TotSteam 0 0;
            0 TotSteam 0;
            0 0 TotSteam];
        b=[110000; 110000; 110000];

        Steam0=[BCSteam1(i),BCSteam2(i),BCSteam3(i)];

        MultiStartIteration=25;
          %minimise @ObjFun to find optimum Steam configuration
        O=optimset('Algorithm','sqp','TolCon',1e-4);

problem=createOptimProblem('fmincon','objective',@ObjFun,'Aeq',Aeq,'beq
',beq,'Aineq',A,'bineq',b,'x0',Steam0,'lb',[0,0,0],'ub',[1,1,1],'nonlco
n',[],'options',O);
        ms=MultiStart;
        [Steam,fMs,FlagMS]=run(ms,problem,MultiStartIteration);

          %%[Steam,fval]                                                  =
fmincon(@ObjFun,Steam0,A,b,Aeq,beq,[0,0,0],[1,1,1]);
  end

  function [success, CavgOF] = ComputeAverage(Steam)
  global TotSteam Us Ta dir CC Cavgh counth Cmaxh Hour S

      P=0.1;
      Nboilers=3;
      for k=1:Nboilers
          xstack(k)=9900+k*50;

          SteamFlow=Steam*TotSteam; %kg/hr
          Fuel= 3032.89*SteamFlow/(4.184*(11408-508*P)); %kg/hr
          LF= P*Fuel; %kg/hr
```

```
            FG= (1-P)*Fuel; %kg/hr
            Q=(1-0.6)/3600/1000*(FG*2.86386+LF*5.70070); %kg NOx/sec %0.6
reductin

            %Emission rate calc:
            ER=(0.7282*FG+0.81098*LF)*22.414; %Nm3/hr
        end

            counth=0;
            xi=0;
            for xmesh = 1:500:20001;
                yi=0;
                xi=xi+1;
                for ymesh = 1:500:20001;
                    yi=yi+1;

[C1(xi,yi),stability]=gaussplume66(xmesh,ymesh,Q(1),ER(1),Us,Ta,CC,Hour
,xstack(1),dir);

[C2(xi,yi)]=gaussplume66(xmesh,ymesh,Q(2),ER(2),Us,Ta,CC,Hour,xstack(2)
,dir);

[C3(xi,yi)]=gaussplume66(xmesh,ymesh,Q(3),ER(3),Us,Ta,CC,Hour,xstack(3)
,dir);

                    Ctot(xi,yi)= C1(xi,yi)+C2(xi,yi)+C3(xi,yi);
                    if Ctot(xi,yi)>80;
                        counth=counth+1;
                    end
                end
            end

            temp=squeeze(Ctot(:,:));
            Cavgh=mean(mean(temp));

            Cmaxh=max(max(Ctot(:,:)));

            CavgOF=Cavgh;
            S=stability;
        success = true;
    end
```

A3 – Optimization Goal 2 Code

```
function optim
 %% Read the input files:

 TotSteam1 = dlmread('TotSteam1.txt'); %%Total Steam flow
 Steam1 = dlmread('Steam1.txt'); %%Steam 1 flow
 Steam2 = dlmread('Steam2.txt'); %%Steam 2 flow
 Steam3 = dlmread('Steam3.txt'); %%Steam 3 flow
```

```
    Time = dlmread('Time.txt'); %%Time (Hour)
    dir1 = dlmread('dir1.txt'); %%Wind Direction with North axes
    Us1 = dlmread('Us1.txt'); %%Wind Speed
    Ta1 = dlmread('Ta1.txt'); %%Ambient Temperature
    CC1 = dlmread('CC1.txt'); %%Cloud Coverage

     Cavg=zeros;
     Cmax=zeros;
     CountH=zeros;
     %Steam=zeros(3,1);

    delete matlabpool;
    matlabpool(24);%%

    parfor i=1:4392
     [Cavgh,Cmaxh,counth,S,P]=
myfunc1(i,TotSteam1,Us1,Steam1,Steam2,Steam3,Time,dir1,Ta1,CC1);

           Cavg(:,i)=Cavgh;
           Cmax(:,i)=Cmaxh;
           CountH(:,i)=counth;
           %Steam(:,i)=Steam123;
           p(:,i)=P; %%%
           Stability(:,i)=S;

           disp(i)
     end

     %Enter the Results
     dlmwrite('Cmax.txt',Cmax);
     dlmwrite('Cavg.txt',Cavg);
     dlmwrite('CountH.txt',CountH);
     %dlmwrite('Stability.txt',Stability);
     dlmwrite('Stability.txt',Stability,'delimiter',''); %%added to fix
Stability text file

     dlmwrite('P.txt',p); %%%

     matlabpool close

   end

   function Cmax=ObjFun(xq)

   P(1)=xq(1);
   [sucess,Cmax]=ComputeAverage(P);

   end

   function                                    [Cavgh,Cmaxh,counth,S,P]=
myfunc1(i,TotSteam1,Us1,Steam1,Steam2,Steam3,Time,dir1,Ta1,CC1)
```

```
  global TotSteam Us Ta dir CC Cavgh counth Cmaxh Hour S steam1 steam2
steam3

         TotSteam=TotSteam1(i);
         dir=dir1(i);
         Us=Us1(i);
         CC=CC1(i);
         Ta=Ta1(i);
         Hour=Time(i);
         steam1=Steam1(i);
         steam2=Steam2(i);
         steam3=Steam3(i);

         Aeq=[];
         beq=[];
         A=[];
         b=[];
         P0=[0.1];

         MultiStartIteration=25;
           %minimise @ObjFun to find optimum liquid fuel percent (P)
         O=optimset('Algorithm','sqp','TolCon',1e-4);

problem=createOptimProblem('fmincon','objective',@ObjFun,'Aeq',Aeq,'beq
',beq,'Aineq',A,'bineq',b,'x0',P0,'lb',0,'ub',1,'nonlcon',[],'options',
O);
         ms=MultiStart;
         [P,fMs,FlagMS]=run(ms,problem,MultiStartIteration);

  end

  function [success, CmaxOF] = ComputeAverage(P)
  global TotSteam Us Ta dir CC Cavgh counth Cmaxh Hour S steam1 steam2
steam3

       Nboilers=3;

       for k=1:Nboilers
               xstack(k)=9900+k*50;
                   if k==1
                       Steam(k)=steam1;
                   else if k==2
                           Steam(k)=steam2;
                       else Steam(k)=steam3;
                       end
                   end

           SteamFlow=Steam*TotSteam; %kg/hr
           Fuel= 3032.89*SteamFlow/(4.184*(11408-508*P)); %kg/hr
           LF= P*Fuel; %kg/hr
           FG= (1-P)*Fuel; %kg/hr
```

```
          Q=(1-0.6)/1000/3600*(FG*2.86386+LF*5.70070);  %kg  NOx/sec  ,
60% total reductin

          %Emission rate calc:
          X=0.045*28.97/18;
          if P<0.4
              E=0.15;
          else
              E=(50*P-5)/100;
          end

          ERFG=FG/17.09*(9.23*(X+X*E+E)+10.2917);
          ERLF=LF/170*(83.91439*(X+X*E+E)+91.2937);
          ER=(ERFG+ERLF)*22.414; %Nm3/hr

      end

      counth=0;
      xi=0;
      for xmesh = 1:500:20001;
          yi=0;
          xi=xi+1;
              for ymesh = 1:500:20001;
                  yi=yi+1;

                  [C1(xi,yi),stability]=gaussplume66(      xmesh,ymesh,
Q(1), ER(1), Us,Ta,CC,Hour,xstack(1),dir);
                  [C2(xi,yi)]=gaussplume66(  xmesh,ymesh,  Q(2),  ER(2),
Us,Ta,CC,Hour,xstack(2),dir);
                  [C3(xi,yi)]=gaussplume66(  xmesh,ymesh,  Q(3),  ER(3),
Us,Ta,CC,Hour,xstack(3),dir);

          Ctot(xi,yi)= C1(xi,yi)+C2(xi,yi)+C3(xi,yi);
              if Ctot(xi,yi)>80;
                      counth=counth+1;
                  end
              end
      end

      temp=squeeze(Ctot(:,:));
      Cavgh=mean(mean(temp));

      Cmaxh=max(max(Ctot(:,:)));

      CmaxOF=abs(Cmaxh-75);
      S=stability;

      success = true;
  end
```

A4 – "gaussplume66" Function (Air Dispersion Model)

```
function [C,stability] = gaussplume66(xmesh,ymesh, Q, ER,Us,Ta,CC,Time,xstack,dir)

ystack = 10000;
xgrid = xmesh - xstack;
ygrid = ymesh - ystack;

%coordinates transformation
x=xgrid*cosd(dir)+ygrid*sind(dir);
y=-xgrid*sind(dir)+ygrid*cosd(dir);

H=30;
D=1.992;
V=4*ER/pi/D^2/3600;

FlueGas=ER*37.326/1.04712/1000;
if FlueGas<1000
    Ts=-0.0022*(FlueGas)+ 33.62;
elseif FlueGas<2000
    Ts=0.0051*(FlueGas)+ 83.082;
else
    Ts=0.0146*(FlueGas)+ 114.37;
end


if (500<=Time)&&(Time<1700);
    time = 'day';
else
    time='night';
end

terrain = 'rural';
z=2;

switch (time)
    case 'day'
        if Us<2
            if CC<4/8
                stability = 'A';
            else stability = 'B';
            end
        elseif Us<=3
            if CC<=1/8
                 stability= 'A';
            elseif CC<=5/8
                 stability= 'B';
            else stability ='C';
```

```
            end

        elseif Us<=5
            if CC<=4/8
                stability= 'B';
            elseif CC<=5/8
                stability= 'C';
            else stability ='D';
            end
        elseif Us<=6
            if CC<=4/8
                stability= 'C';
            else stability ='D';
            end
        else
            if CC<=2/8
              stability= 'C';
            else stability ='D';
            end
        end

    case 'night'

        if Us<2
            stability = 'F'; %%
        elseif Us<=3
            if CC<=3/8
                stability ='E';
            else stability='F';
            end
        elseif Us <=5
            if CC<=3/8
                stability = 'D';
            else stability='E';
            end
        else stability='D';
        end
end

% Compute the dispersion coefficients
switch(terrain)
    case 'rural'
        % Pasquill-Gifford curves
        switch(stability)
            case 'A'
                 P = 0.07;
                % [c, d] coefficients
                coeffs_y=[24.1670, 2.5334];
                % [x a b] matrix
                coeffs_z=[0.10 122.800 0.94470;
                          0.15 158.080 1.05420;
                          0.20 170.220 1.09320;
                          0.25 179.520 1.12620;
```

```
                    0.30 217.410 1.26440;
                    0.40 258.890 1.40940;
                    0.50 346.750 1.72830;
                    3.11 453.850 2.11660;
                    inf  nan     nan];

        case 'B'
            P= 0.07;
            coeffs_y=[18.3330, 1.8096];
            coeffs_z=[0.20 90.673 0.93198;
                    0.40 98.483 0.98332;
                    inf  109.300 1.09710];
        case 'C'
            P=0.10;
            coeffs_y=[12.5000, 1.0857];
            coeffs_z=[inf 61.141 0.91465];
        case 'D'
            P=0.15;
            coeffs_y=[8.3330, 0.72382];
            coeffs_z=[0.30 34.459 0.86974;
                    1.00 32.093 0.81066;
                    3.00 32.093 0.64403;
                    30.00 36.650 0.56589;
                    inf   44.053 0.51179];
        case 'E'
            P=0.35;
            coeffs_y=[6.2500, 0.54287];
            coeffs_z=[0.10 24.260 0.83660;
                    0.30 23.331 0.81956;
                    1.00 21.628 0.75660;
                    2.00 21.628 0.63077;
                    4.00 22.534 0.57154;
                    10.00 24.703 0.50527;
                    20.00 26.970 0.46713;
                    40.00 35.420 0.37615;
                    inf 47.618 0.29592];
        case 'F'
            P=0.55;
            coeffs_y=[4.1667, 0.36191];
            coeffs_z=[0.20 15.209 0.81558;
                    0.70 14.457 0.78407;
                    1.0 13.953 0.68465;
                    2.0 13.953 0.63227;
                    3.0 14.823 0.54503;
                    7.0 16.187 0.46490;
                    15.0 17.836 0.41507;
                    30.0 22.651 0.32681;
                    60.00 27.074 0.27436;
                    inf   34.219 0.21716];
        otherwise
            error('gaussianPlume:stability', ['Unknown stability
class ', stability]);
    end
```

```
        % Construct sigmay vector along the x-axis
        prev_boundary=0;
        TH = 0.017453 *( coeffs_y(1) - coeffs_y(2)*log(0.001*x));
        sigmay = 0.4651*x* tan(TH);
        % Construct sigmaz vector along the x-axis
        % Pre-allocate (should be same size as x since all tables end
        % with 'inf')
        sigmaz=nan(size(x));
        for section=1:size(coeffs_z, 1)
            idx=find(prev_boundary<=(x/1e3)                          &
(x/1e3)<coeffs_z(section, 1));
            sigmaz(idx)=coeffs_z(section,
2).*(x(idx)./1e3).^coeffs_z(section, 3);
            prev_boundary=coeffs_z(section, 1);
        end

    case 'urban'
        % Pasquill-Gifford with urban fit (McElroy-Pooler)
        switch(stability)
            case 'A'
                P=0.15;
                coeffs_y=0.32;
                coeffs_z=[0.24 1 0.001 0.5];
            case 'B'
                P=0.15;
                coeffs_y=0.32;
                coeffs_z=[0.24 1 0.001 0.5];
            case 'C'
                P=0.20;
                coeffs_y=0.22;
                coeffs_z=[0.20 1 0 0];
            case 'D'
                P=0.25;
                coeffs_y=0.16;
                coeffs_z=[0.14 1 0.0003 -0.05];
            case 'E'
                P=0.30;
                coeffs_y=0.11;
                coeffs_z=[0.08 1 0.0015 -0.05];
            case 'F'
                P=0.30;
                coeffs_y=0.11;
                coeffs_z=[0.08 1 0.0015 -0.05];
            otherwise
                error('gaussianPlume:stability',       ['Unrecognized
stability class ', stability]);
        end
        % Construct sigmay along x-axis
        sigmay=coeffs_y(1).*x.*(1+0.0004.*x).^(-0.5);
        % Construct sigmaz along x-axis
        sigmaz=coeffs_z(1).*x.*(1+coeffs_z(2).*x).^coeffs_z(3);
    otherwise
```

```
            error('gaussianPlume:terrain', ['Unrecognized terrain option
', terrain]);
    end

    % wind velocity at stack height
    Zref = 10;
    U=Us*(H/Zref)^P;

    % Actual Stack Height calculation
    if V/U <1.5
        Hs=H+2*D*(V/U-1.5);
    else Hs=H;
    end

    Fm= V^2*D^2*(Ta/4/Ts);
    Bj=(1/3)+(U/V);
    Fb=9.81*V*D^2*((Ts-Ta)/4/Ts);

    if stability == 'E'
        s=9.81/Ta*0.02;
    else s=9.81/Ta*0.035;
    end

    if stability == 'E'|| stability=='F'
        dTc=0.019582*Ts*V*sqrt(s);
    else
        if Fb<55
            dTc=0.0297*Ts*V^(1/3)/D^(2/3);
        else dTc=0.00575*Ts*V^(1/3)/D^(2/3);
        end
    end

    if (Ts-Ta)>dTc
        % buoyancy prevails case
        if stability == 'E'|| stability=='F'
            xf=2.0715*U/sqrt(s);
            if  xf > x
                He=Hs+1.6*((Fb^(1/3)*x^(2/3))/U);
            else He=Hs+2.6*(Fb/U/s)^(1/3);
            end
        else
            if Fb<55
                xf=49*Fb^(5/8);
            else xf=119*Fb^(2/5);
            end
            if xf > x
                He = Hs+1.6*(Fb^(1/3)*x^(2/3)/U);
            else
                if Fb<55
                    He=Hs+21.425*Fb^(3/4)/U;
                else He=Hs+38.71*Fb^(3/5)/U;
                end
```

```
            end
        end
    else % momentum prevails case with unstable conditions
        if stability == 'E'|| stability=='F'
            xf=0.5*22/7*U/sqrt(s);
            if xf > x
                He=Hs+(3*Fm*sin(x*sqrt(s)/U)/Bj^2/U/sqrt(s))^(1/3);
            else
                He=Hs+1.5*(Fm/U/sqrt(s))^(1/3);
            end
        else
            xf=4*D*(V+3*U)^2/V/U;

            if xf > x
                He = Hs+1.6*(3*Fm*x/(Bj*U)^2)^(1/3);
            else He=Hs+3*D*V/U;
            end
        end
    end

    C  = Q *10^9./ (2*pi*U*sigmay.*sigmaz) .* exp( -0.5*y.^2./sigmay.^2 )
.* ...
          (    exp(    -0.5*(z-He).^2./sigmaz.^2     )     +     exp(     -
0.5*(z+He).^2./sigmaz.^2 ) );
      ii = find(isnan(C) | isinf(C));
      C(ii) = 0;   % Set all NaN or inf values to zero.

    End
```

APPENDIX B

ATMOSPHERIC STABILITY

Table C5.2. Pasquill Atmospheric Stability Classes.

Surface Wind Speed[a] (m/s)	Relative Cloud Coverage Day 0/8 - 2/8	Day 3/8 - 5/8	Day 6/8 - 8/8	Night < 3/8	Night > 4/8
< 2	A	A - B	B	F	F
2 - 3	A - B	B	C	E	F
3 - 5	B	B - C	D	D	E
5 - 6	C	C - D	D	D	D
> 6	C	D	D	D	D

[a] At a height of 10 m.

<u>Neutral conditions</u>, denoted by atmospheric stability class D, exist when the velocity of the moving air mass (wind speed) is large or there are clouds.

<u>Unstable conditions</u> can be categorized in three classes:

1) Very unstable, stability class A.
2) Unstable, stability class B.
3) Slightly unstable, stability class C.

<u>Stable conditions</u> can be separated into the following classes:

1) Slightly stable, stability class E.
2) Stable, stability class F.
3) Very stable, stability class G (also denoted as "-").

Unstable condition is when the atmosphere enhances the vertical motions due to temperature differences between atmosphere layers. When the higher layer is cooler than the lower, convective currents will cause it to overturn and turbulent eddies is produced and pollutants are spread. As a result in unstable conditions the configuration used is mostly using the lowest number of boilers to produce the steam demand. This will limit mixing.

Stable condition is when lower layer of the atmosphere is cooler than the one on top. Atmosphere resists the vertical motion thus vertical exchange is minimal. In this case the pollutant will be carried away by the air above certain height and will not be mixed with the lower level where the concentration is being calculated and thus away from inhabited areas. (Assael & Kakosimos, 2010)

APPENDIX C

NOMENCLATURE

Units of measurements

The following units were used in the context and calculations:

Temperature	ºC	Degree Celsius
	K	Kelven
Mass Flow	Kg/hr	Kilogram per hour
Volumetric Flow	Kdscfh	Kilo standard* cubic feet per hour (dry basis)
	Nm^3/hr	Normal** cubic meter per hour
Concentration	ppm	Part per million
	mg/Nm^3	Milli gram per normal** cubic meter
	µg/m^3	Micro gram per cubic meter
Power	MW	Mega Watt
Length	m	Meter
	Km	Kilo meter
Velocity	m/s	Meter per second

* Standard Conditions for Gas

Standard conditions for gas measured in cubic feet are 60 ºF and 14.696 pounds per square inch absolute.

** Normal Conditions for Gas

Normal conditions for gas measured in cubic meter are 0 ºC and 1.0333 kilograms per square centimetre absolute.

Abbreviations & Acronyms

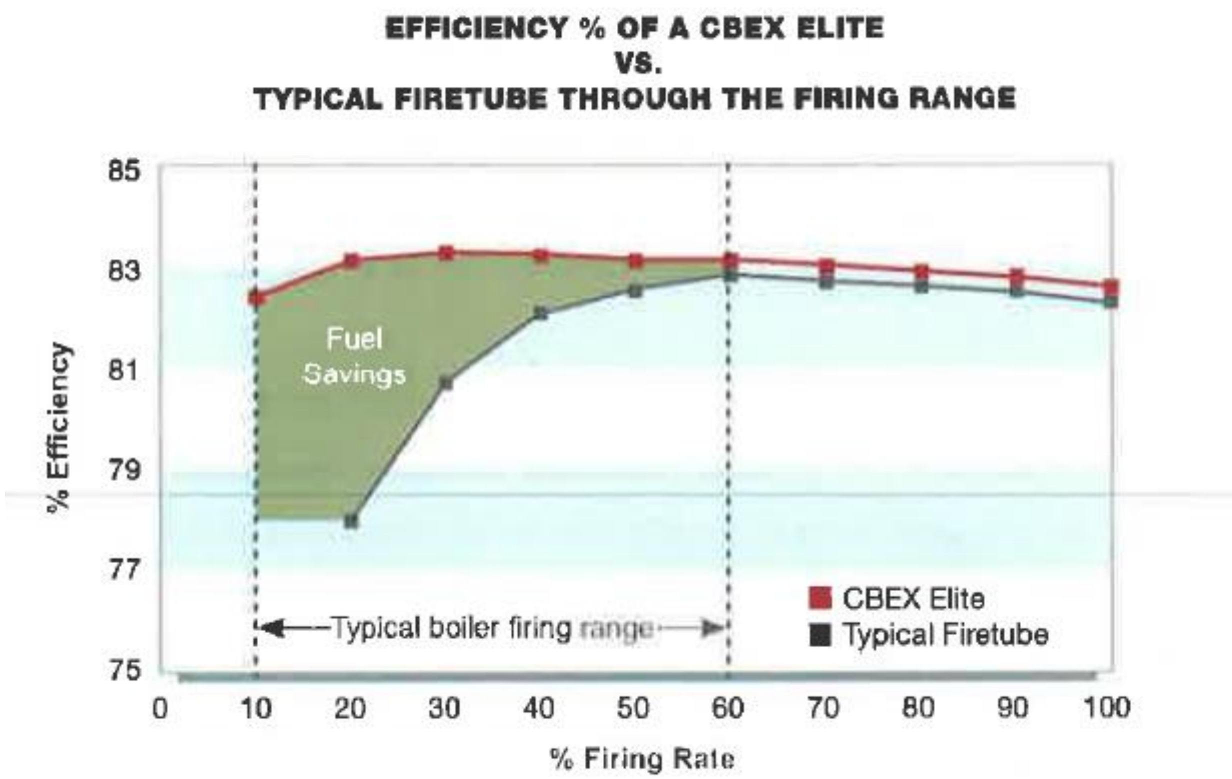
Cavg Average Concentration

CC Cloud Coverage

Cmax	Maximum Concentration
EEA	European Environment Agency
EIA	Environmental Impact Assessment
EMEP	European Monitoring and Evaluation Programme
FG	Fuel Gas
HHV	High Heating Value
HPS	High Pressure Steam
LF	Liquid Fuel
NCDC	National Climate Data Center
P	Liquid Fuel Fraction in Fuel Used
SCENR	Supreme Council for the Environment and Natural Reserves
SNCR	Selective Non Catalytic Reduction
T_a	Ambient Temperature
T_s	Flue Gas Temperature
US EPA	United States Environmental Protection Agency

APPENDIX D

TURN DOWN RATION EXPLANATION



In the case of increased HP steam demand within the plant above the design capacity of 220,000 kg/hr due to changing process efficiency or reliability of the utility system, operation with 3 boilers at times and circumstance is a possibility. This is done by using the three boilers in the same time however the third boiler is originally kept for redundancy, to kick in when one of the other two shutdowns for any reason. This flexibility of operation can impact differently on the surrounding under different meteorological conditions. But looking at the figure above and operating with boilers with high or low turn down ratio as the efficiency is not affected by increasing the firing rate.

Graph 3.x shows the difference between the two types. High turn down ratio (1:10) is represented by the red line while the low turn down ratio (1:4) is represented by the green.

At the other extreme, at minimum load when the process demand falls, the firing rate must also decrease. For low turn down ratio (say 1:4) the efficiency drops with decreasing the firing rate which means more fuel required.

All burners within the boiler have a specific turndown below which the boiler cycles off, purges and loses heat. This requires more firing is restarted to recover the heat loss and go beyond to supply the demand. Thus the fuel spend is higher and therefore the emissions. It is assumed that at cycle off the 3rd boiler will be stopped and the 2 running boilers will load share, to until the capacity and requirement needs the 3 boiler again. For low turn down ratio (1:4) the boiler cycles off at 25% firing rate while the high turn down ratio boiler (say 1:10) will go down to 10%firing rate before cycling off.

For the purpose of this study, it is assumed that the boilers are new and integrated for better performance with high turndown ratio (1:10). As the steam demand decreases the boiler can turndown up to 10% capacity without cycling and thus saving energy due to relatively constant efficiency and prolonged operation before cycling off. This will eliminate a lot of complexity in the calculations.

The target is to use different combinations of loads with up to 3 boilers so that the plant steam demand is met with an optimum running combination to minimize the fuel consumption and eventually achieve less emission, which contributes towards better air quality.

In other words, boiler operation at high efficiency with load sharing of multiple units will save fuel and is recommended. Also, optimizing the operating capacity of the boiler by enhancing its turn-down ability for minimum load operation will improve the emission balance at the stacks for a given type of fuel. For such case the ground level concentration will be an indicator of the air quality achieved.

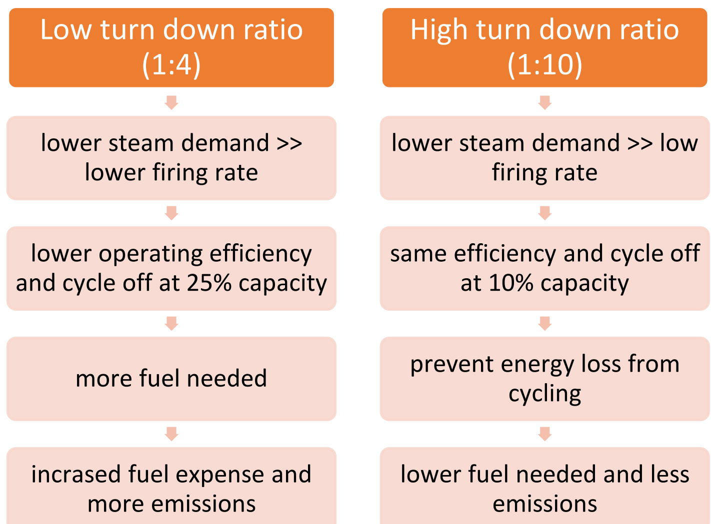


Figure – Comparison between boilers with low and high turn down ratios

From the analysis above, if the objectives in chapter 2 are to be applied on this case study then:

Varying the operational capacities of three boilers to meet the total demand of a plant of HP steam, will result in different firing rate in each boiler. As long as the operating capacity is higher than 10% of the design capacity of one boiler (110,000kg/hr) then varying (decreasing) firing rate is not an issue throughout the study as it is not affecting the efficiency.