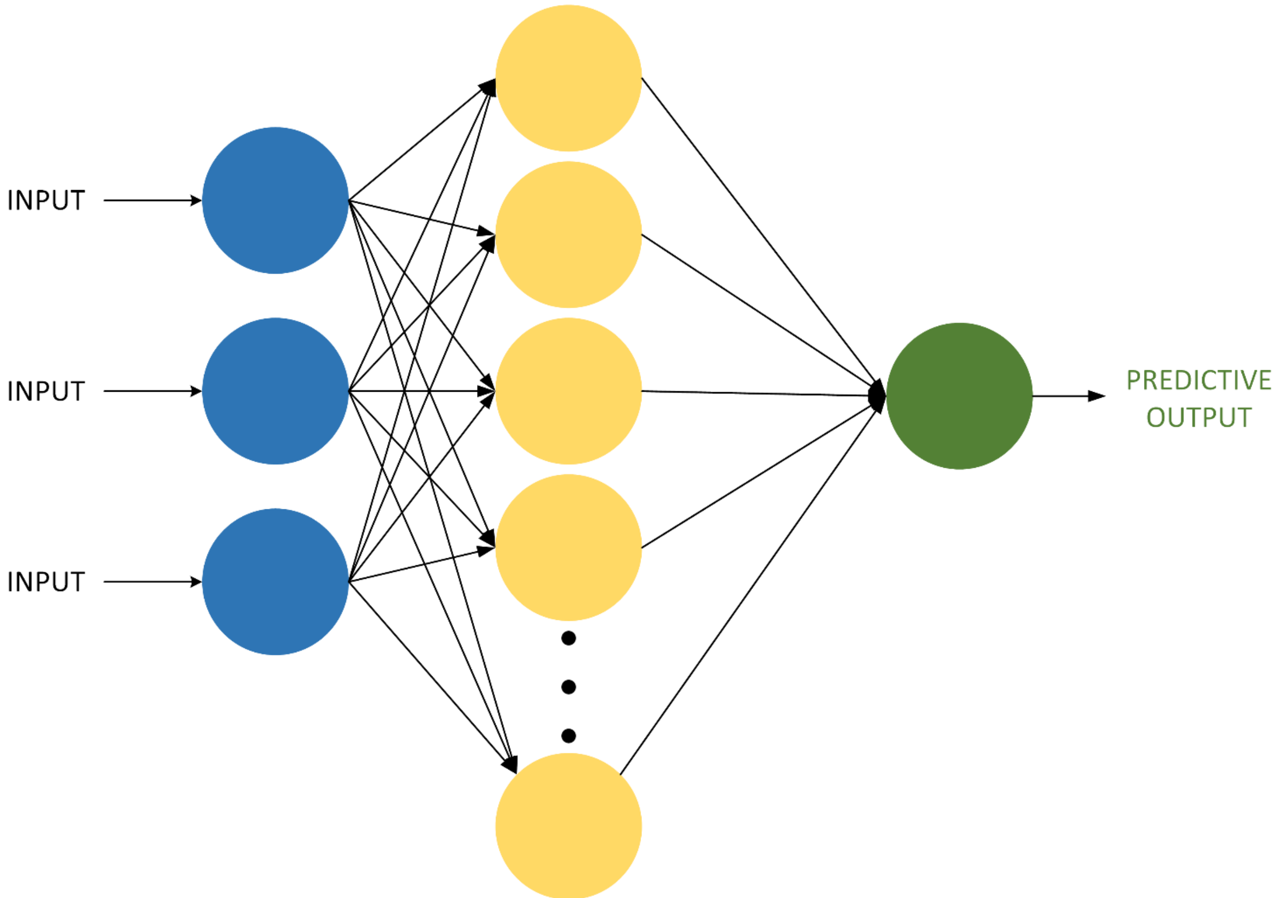

Utilizing Neural Networks to Minimize NOx-Emissions in a Steam Cracking Furnace

Investigating the viability of using real-time data for training of the neural networks for NO_x, CO and temperature of cracking

Master of Science Thesis in the Master's Degree Program Sustainable Energy Systems

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CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2020
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Cover:
Schematic of a simplified artificial neural network, showing the neuron layers as circles, and the connectors as arrows.

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Thank you,
Emelie Gierow

Abstract

Emissions of nitrogen oxides (NO_x) is detrimental to human health and the environment. The industrial sector is the second largest emitter of NO_x emissions in Sweden. NO_x is formed through complex processes during combustion, but formation can be reduced through optimizing the combustion process, which often is a cost-effective method to reduce emissions. The combustion process is however highly integrated with the main process in the steam cracking furnace, making the product quality the primary target for the combustion optimization.

NO_x formation is complex and difficult to predict. Reliable methods for predicting NO_x emissions depending on operational modes for the combustion chamber is therefore vital to minimize NO_x emissions. One method is to use artificial neural networks to create models for NO_x formation depending on the process control variables. Artificial neural networks is a type of machine learning that are created to predict the outputs of a specific process using data collected for the process in question.

This thesis presents a method for find operational modes of a cracking furnace that would reduce NO_x while not affecting the main purpose of the furnace i.e. maintaining the product quality. The furnace in question is a steam cracking furnace operated by Borealis AG in Stenungssund. The process of finding optimal operational modes where started with collecting real-time data for all parameters that was available and identified as important, followed by data cleaning. Multiple networks were trained to account for three parameters of interest, i.e. emissions of NO_x and carbon monoxide (CO), as well as temperature of cracking. The trained networks were then incorporated into a genetic algorithm to find operational modes that would minimize NO_x emissions while keeping CO low and the temperature of cracking within an acceptable range.

Two operational modes where proposed, which would reduce emissions by 10% and 50% compared to current levels, respectively. The operational mode with 50 % reduction carries the risk of leaving the furnace too cold and should be further tested before implemented. Using real-time data for training neural networks to predict NO_x proved comparable to other methods, with a correlation coefficient of 0.927. Using neural networks to predict CO emissions and temperature of cracking was not as successful. Especially the networks for CO predictions showed poor performance.

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Nomenclature

Abbreviations

BPNN	Back-Propagating Neural Network
COT	Coil Outlet Temperature (temperature of cracking)
GC	Gas Chromatograph
GRNN	Generalized Regression Neural Network
HP	High Pressure (referring to steam)
LP	Low Pressure (referring to steam)
mae	Mean Absolute Error
MP	Medium Pressure (referring to steam)
RMSE	Root Mean Square Error
SSE	Sum of Squared Errors

Chemical formulas

CH_4	Methane
CO	Carbon monoxide
H_2	Hydrogen gas
NO	Nitrogen (mon)oxide
NO_x	Nitrogen oxide (compound name)
O_2	Oxygen gas

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1. Introduction

High concentrations of nitrogen oxides (NO_x) is detrimental to human health and the surrounding environment. When NO_x resides in the troposphere and reacts with sunlight and volatile organic compounds, ground level ozone is formed which is damaging to the lungs and can have severe effects on health (van Zelm, Preiss, van Goethem, Van Dingenen, & Huijbregts, 2016). Nitrogen oxides in the atmosphere also contribute to acidification and eutrophication of the natural environment. Limiting NO_x emissions to the atmosphere is therefore of importance. The main source of NO_x emissions in Sweden is, by far, road transport, with the industrial sector being the second largest contributor with 22% in 2017 (Naturvårdsverket, 2018).

The harmful consequences of NO_x emissions have led to the implementation of several policies aiming to decrease emissions. In 1992 “The NO_x charge” was introduced in Sweden. It is an economic instrument aimed at reducing emissions of NOx from large combustion plants and was the biggest reason why NO_x reduction measures were implemented in large boilers during the 1990s (Naturvårdsverket, 2006). In 2016 an EU directive was issued which details that by 2030 Sweden is expected to have a reduced NO_x emissions by 66% compared to the levels of 2005 (European Parliament and Council, 2016).

Increasingly restrictive emission limits leads to increased interest for new methods that reduce formation of NO_x in combustion processes. Some common reduction measures used today are introducing low NO_x burners, flue gas cleaning, air and/or fuel staging and optimization of operational parameters. Introducing such measures is often coupled with an economic cost, but in 2006 Naturvårdsverket reported that half of the time boilers that had optimized the combustion efficiency through changing of process parameters had implemented those changes at zero cost (Naturvårdsverket, 2006). In order to efficiently optimize the operational parameters, having a good model of the process is imperative. However, creating an analytical model for NO_x formation has been challenging as the process is very complex with many coupled parameters (K. Li, Peng, Irwin, Piroddi, & Spinelli, 2005). Models utilizing Computational Fluid Dynamics (CFD) has seen some success (Stopford, 2002), but requires significant investments in time and computational power (K. Li et al., 2005).

In 1998 Booth and Roland used artificial neural networks to model process parameter in boilers in order to optimize operational parameters in order to reduce NO_x emissions and improve performance (Booth & Roland, 1998). The authors reported reductions of NO_x emissions between 10-60% using their method. Artificial neural networks is a set of algorithms used in machine learning for data modelling which can be used to create predictive models, often referred to simply as neural networks. The networks created are black-boxes which only takes inputs and outputs into account, which works well with the complexity of NO_x formation (Frank, 2013). The simplest version of neural networks is a shallow feed forward neural network which is almost always coupled with a back-propagating algorithm, often called back propagating neural network (BPNN) for short. BPNNs has been used successfully in many applications in the energy section, ranging from modelling of a single boiler (Rusinowski & Stanek, 2007) to an entire combined heat and power plant (De, Kaiadi, Fast, & Assadi, 2007).

Using neural networks to predict NO_x emissions from boilers has been previously researched by many different teams. In 2008 Zheng et.al. (Zheng, Yu, & Yu, 2008) modelled the emissions of NO_x through two types of networks; BPNN and a generalized regression neural network (GRNN) and found that while both networks performed well, the GRNN had greater performance and faster computational time. Other examples of networks investigated for NO_x emission prediction is eng-genes neural networks (K. Li et al., 2005) and a bidirectional learning machine(G.-Q. Li, Qi, Chan, & Chen, 2017). Ilamathi et.al (Ilamathi, Selladurai, Balamurugan, & Sathyanathan, 2013) and Zhou et al(Zhou, Cen, & Fan, 2004) coupled their predictive neural networks with an optimization algorithm in order to optimize the operational parameters with the aim of reducing NO_x emissions. Both showed promising results and concluded that neural networks coupled with an optimization algorithm could be used to reduce NO_x emissions.

The most common method applied in previous works using neural networks was to identify the operational parameters of importance, and then change the values of one operational paramter at a time to previously decided upon setpoints. This ensures that the network has all combination of parameters that is of interest. In this thesis real-time data from a steam cracking furnace was used to produce neural networks. With using real-values the hope is to achieve similar results, but without having to disturb the production of the furnace during data collection.

The networks created was then coupled with an optimization algorithm in order to find the optimal combination of operational parameter values that produces the least NO_x emissions. To ensure that the suggested optimization takes the efficiency of combustion into account, the output of carbon monoxide (CO) is taken into consideration. A high level of CO in the flue gas is usually an indicator of inefficient and incomplete combustion. Optimziation of a steam cracking furnace is different from optimizing a boiler, which aims to produce as much heat as possible. In a steam cracking furnace the product quality from the cracking of feedstock is governing instaed. The composition of the product flow after cracking is heavily dependent on the temperature of the cracking process, meaning that the aim of the combustion process is to achieve a specific temperature as efficiently as possible. The optimization therefore needs to take this temperature into account. The temperature of cracking in this work is denoted as coil outlet temperature (COT) due to it’s location in the furnace.

1.1 Aim and Scope

The aim of this thesis is to develop and evaluate a method for optimizing NO_x emissions without compromising the main purposes of the furnace i.e. cracking of feedstock and efficient combustion. Using real time data, models were developed by training BPNNs, for predicting NO_x emissions, temperature of cracking (COT) and CO emissions. The networks trained to predict NO_x emissions was then run through an optimization algorithm as a fitness function to minimize NO_x formation while keeping within the constraints of COT and CO.

Several previous studies have used neural networks to predict the emissions of NO_x, often using more complicated models than a basic BPNN. The focus in this thesis is, however, not the optimization of the models, but, 1) to investigate the viability of using real-time data, which differs from the more commonly applied method of carefully controlling the parameter values to give optimal training conditions. 2) To explore the possibility of using neural networks for predicting emissions of CO and temperature of cracking and 3) To suggest optimal process conditions for running the furnace that minimizes the emissions of NO_x.

2. Background

NO_x formation in a furnace is a complex process, of which a short background is presented in this chapter. Theory on the basic structure and creation process involved in training neural networks is also included. The networks described are the more basic type as those are the types utilized in this work. The world of neural networks is heavy in nomenclature and a basic understanding of the creation process is imperative to understanding the created networks.

2.1 NO_X-Formation and Reduction in Furnaces

The process of formation of NO_x in combustion is complex and therefore difficult to predict. The three main pathways for NO_x formation in a combustion chamber is from fuel, through prompt formation and through thermal formation. Depending on the combustion conditions and fuel, one of those pathways are dominating the formation. NO_x formed from fuels are the main source of NO_x when liquid and solid fuels are used, the source is nitrogen bound in the fuel, which is released and oxidized during combustion. Thermal formation of NO_x occurs when nitrogen in air reacts with oxygen at high temperatures and is the main source of NO_x when combusting gaseous fuel that contains no nitrogen. Nitrogen is almost always present in combustion in the form of air, which means that completely eliminating the formation of NO_x is impossible. Prompt NO_x is formed when nitrogen in air reacts when CH_i radicals are present and is the dominating pathway when the ratio of oxygen-to-fuel is low. Prompt NO_x formation is often disregarded when doing calculations as its influence is limited.

The methods for reducing emissions of NO_x from combustion can often be divided into two separate categories: altering the process and changing the design of the combustion chamber. Methods that change the design includes flue gas cleaning devices such as SNCR or SCR, low- NO_x burners, reburning and recirculation. Altering the combustion process could mean choosing a new fuel or changing the process parameters of combustion such as reducing oxygen intake.

In combustion in furnaces it is standard to use more air than what is stoichiometrically necessary as more oxygen generally leads to a better and more even combustion. However, when there is too much air the efficiency is lowered again. Adding more oxygen also means more nitrogen which absorbs heat and limits the temperature in the furnace, as well as resulting in an increase in NOx formation. Finding the optimal air intake is therefore a balance that is important to strike.

2.2 Artificial Neural Networks

Artificial neural networks are a form of machine learning that tries to mimic the way our brain works to recognize patterns. Neural networks can be used in several settings e.g. for medical diagnoses, text-to speech applications and image recognition, to mention a few. Depending on the purpose of the created network, the construction can vary significantly, but the basic components will always be the same.

The basic structure of a neural network consists of neurons and the connections between them, as depicted in Figure 1, where the circles are neurons and the arrows are the connections. The black inputs to the left are input values which when run through a working network produces the green predictive output on the right. The inputs are added to the first layer of neurons, which produces outputs depending on parameters contained in the connections and neurons themselves. Each layer of neurons receives the output of the previous layers as inputs and produces outputs which the next layer receives. This process repeats for all the layers until it reaches the output layer, where the predictive output of the network is calculated. This process of moving forward in the network is called forward propagation.

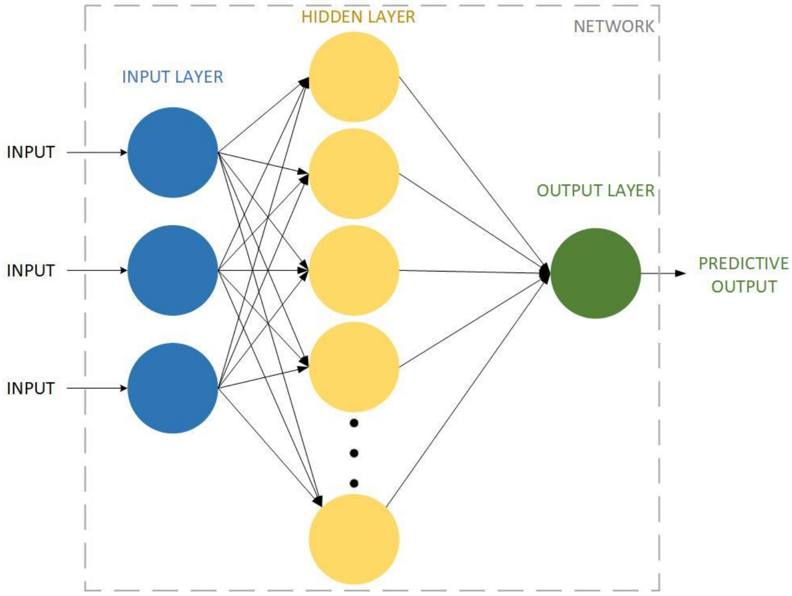

Figure 2: The basic structure of an artificial neural network, circles represent neurons and arrows represents the connections between them.

Before a network can be used to properly predict an output it requires training, which changes the values of the parameters in the connections and neurons in such a way that the network accurately predicts the outputs. In Figure 2 the internal parameters of the connections and neurons are depicted. Each connection between neurons contains a weight that represents the relative importance of that input to the output of the neuron. The neuron itself contains two parameters: a bias and an activation function. The activation function, *f*, is the function that is used to calculate the output of the neuron. It takes all the inputs to the neuron and produces the output or "activation" of the neuron. Each layer of neurons utilizes the same activation function, but different layers can have different activation functions.

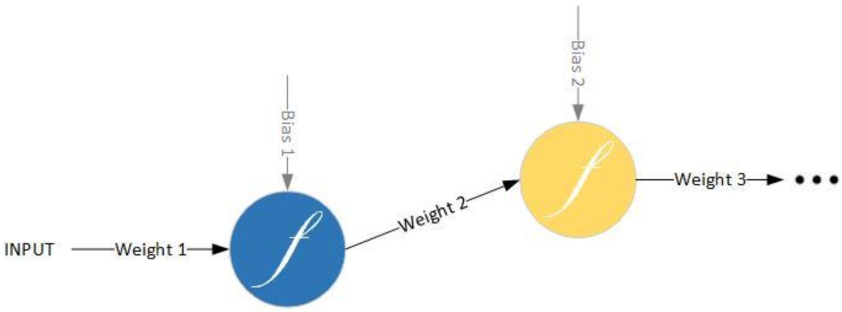

Figure 1: The internal parameters of neurons and connections i.e. weights, biases and activation functions.

The training of the network is based on changing the weights and biases of the network to minimize a cost function of the programmers choosing. Networks trained through supervised learning is given real inputs and the real corresponding outputs. In such cases, the cost function is often the sum of squares (SSE) of the networks errors of the prediction compared to the real value.

The network training starts with random values for the weights as real inputs are fed to the network and predictive values are calculated. The predictive values are then compared to the real values, and the error is calculated. The network then starts the back-propagating process, as depicted in Figure 3. The error is then moved backwards, and individual errors are calculated for each neuron using the same values on weights as during forward propagation. This gives the network information on which neurons gives the largest errors, and the weights and biases can be readjusted accordingly. Readjustments are made by the program by using a training function which locates the weights which produces the minimum error. This is how a standard Back-Propagating-Feedforward neural network is structured and trained to accurately predict the output values. The trained network then consists of the optimal weights and biases which can model the outcomes of certain inputs.

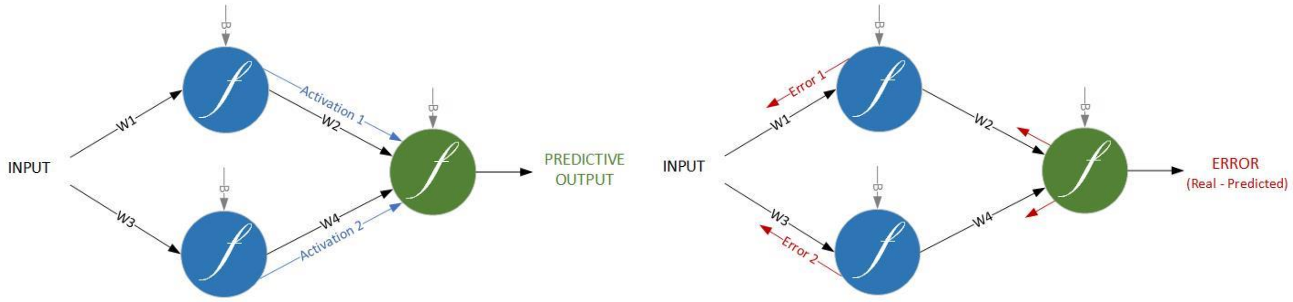

Figure 3: Showing forward and backwards propogation respectivley.
Insprired by Figures created by Tony Yiu [https://towardsdatascience.com/understanding-neural-networks-19020b758230]

There are multiple options for customization of the training and structure of the network to give a better performance. Deep neural networks for example utilizes multiple hidden layers and the number of neurons in layers can range from tens to hundreds. It is also possible to optimize the network by using different activation, cost and training functions.

In minimizing the cost function, there is always the risk of the network learning the dataset, rather than creating a generalized model i.e. the risk of overfitting. A risk which is especially high when training is conducted on small data sets. Two of the more common methods to ensure that the model is not overfitted to the data is through Regularization and Early Stopping. Regularization changes the cost function to also incorporate the mean of sum of squares for the network's weights and biases, which gives a smoother response. Early stopping uses additional data that is not part of the training set to ensure that the model is not overfitted. Before training, the dataset is divided into three separate sets, a testing, validation and training set respectively. The testing set is never used during training, and not seen by the model, but is instead used to evaluate the network when training is complete. The training set is used for creating the network, while the validation set is used to determine when training is finished. During training the networks performance is evaluated based on the training set, and parallel to the training the performance of the network on the validation set is continuously calculated. When the network begins training the results are usually quite bad for both the training and validation sets but begins to slowly improve as training continues. At some point the networks performance on the validation set will stop improving, even though the performance of the training set keeps getting better. Early stopping then ensures that the training stops when performance on the validation set no longer improves, as at that point any improvements on performance on the training set can be attributed to overfitting.

3. The Steam Cracking Furnace

The steam cracking takes place in the furnace and is the process of thermally breaking down larger saturated hydrocarbons into smaller components. Which components that are formed during cracking depend on the composition of the feed, ratio of hydrocarbon to steam, residence time in the furnace and the temperature. The main purpose of the combustion in the furnace is thus to keep the cracking temperature at a level which properly produces the desired components.

In this chapter the steam cracking furnace investigated is described in detail. Initially the processes involved in cracking and combustion is described. This is followed by a review of the operational parameters in the furnace that is of interest when training the neural networks.

3.1 Process description

The furnace which is investigated in this thesis is schematically represented in Figure 4, where the parameters that is of importance to this work is marked and labeled from 1-6. The parameters are divided into three categories; set, measured and process parameters. Set parameters are operational parameters that is set to be a chosen value and is kept stable. These parameters are denoted by diamond shaped markers in Figure 4. The circular markers denote process parameters, which are flexible in value and is changed by the control system to ensure that the set parameters are kept at the desired level. Measured parameters are the measured result of set and process parameters. The square marker with the 6 notation is where the gas chromatograph (GC) is located and contains parameters of all types.

The feedstock for cracking enters the furnace at the top of the convection section at marker 1 and consists solely of naphtha. After mixing with medium pressure (MP; 8.8 bar) steam, the naphtha/steam mixture is heated in the convection section of the furnace to 590-670°C. The flow is looped out of the furnace before entering the radiation section at the bottom of the furnace. The feedstock mixture is then heated in the tubes to temperatures over 800°C at which point the cracking starts. Cracking then occurs for approximately 0.1-0.12 seconds in the coil shaped pipes. The products of cracking then exit the furnace at position 2 in Figure 4, this is where the temperature of cracking, denoted as Coil Outlet Temperature (COT) is measured. The flow is then quickly cooled in the primary quench exchanger which is situated as close as possible to the exit of the furnace. Rapid cooling of the feed is important to ensure that the cracking stops as desired.

The combustion in the furnace is fueled by waste products from other processes that takes place at the plant. It consists of a mixture of methane (CH_4) and hydrogen (H_2), with a smaller share of longer hydrocarbons. When the supply of waste products is compromised due to trouble with the other processes the combustion is supplemented with natural gas. Because the fuel is a waste product the composition changes during the day. The fuel is fed to the burners, which are situated on the floor near the wall on either side of the furnace in rows of 20. The burners have two fuel nozzles, a pilot burner and a steam nozzle. The pilot burners have ignition and utilizes the same fuel as the rest of the burner. Low pressure (LP; 1.8 bars) steam is added through the steam nozzle in order to reduce the formation of NO_x through reducing the flame temperature. Air enters each burner through an individual air inlet, which is powered by an induced draft from a fan in the stack.

In the convection section, process streams are heated from excess heat in the flue gases. Process flows includes preheating of naphtha mixture, heating of feedwater and overheating steam to produce high pressure (HP; 85 bars) steam. This results in flue gas exiting temperature at approximately 200°C. Flue gases exit through the stack at position 6, where a gas chromatograph (GC) measure the composition of the flue gas.

During day-to-day operation of the furnace unburnt coke accumulates in the naphtha tubes. This affects the flow profile, impacts the heating of the feedstock and increases wear on the tubes. Cleaning of the tubes therefore takes place regularly in a process called de-coking. During the de-coking the feedstock flow is replaced by a mixture of air and steam where oxygen in the air burns away the coke buildup and the steam ensure an even flow. This cleaning process is conducted approximately once a month to ensure build-up is limited.

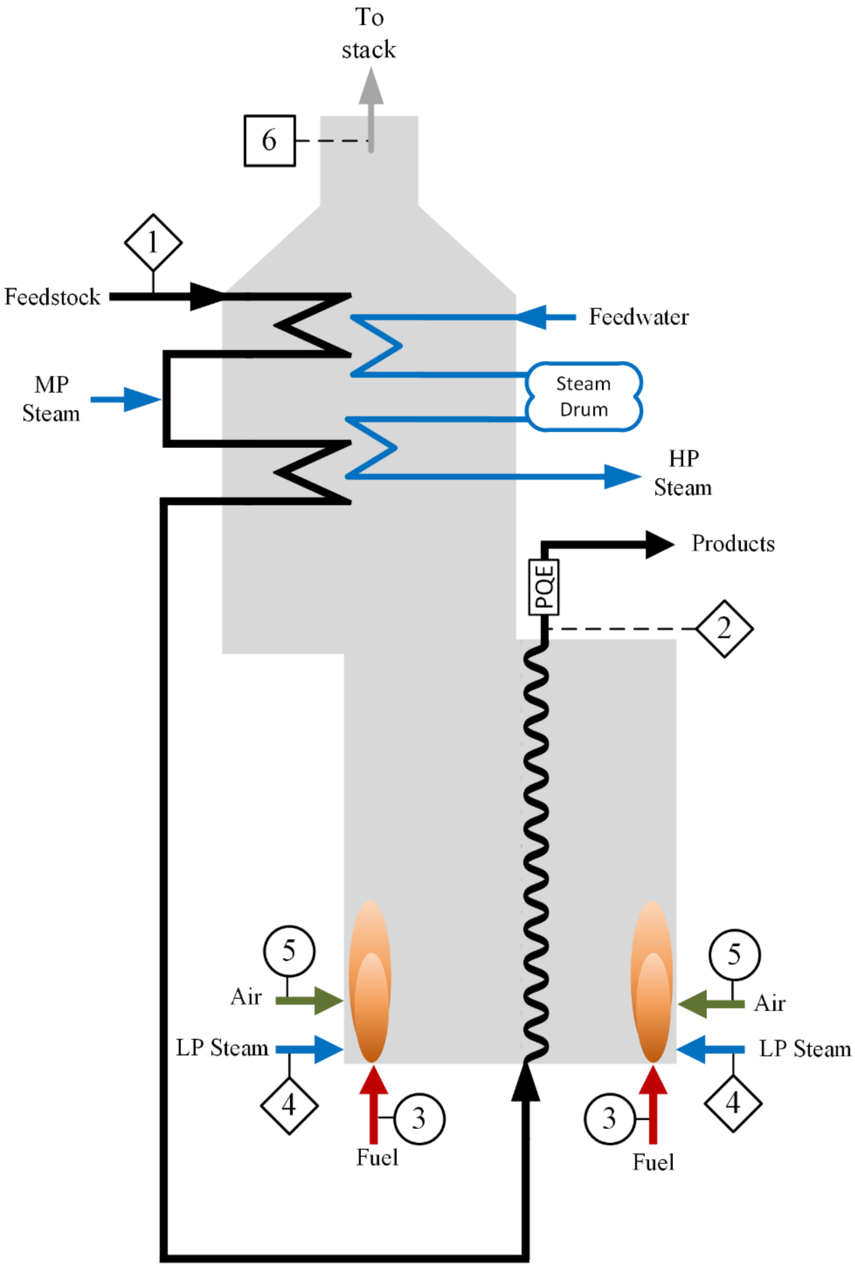

Figure 4: The steam cracking furnace. The markers denote locations that are of importance to this work. Circular markers are process parameters, diamond shapes are set parameters and the square marker is the GC which contains multiple types of parameters.
Marker 1: *Flow of Naphtha*, Marker 2: *Temperature of Cracking (COT)*, Marker 3: *Flow of Fuel Gas*, Marker 4: *LP steam to burners*, Marker 5: *Air inlet to burners*, Marker 6: *GC measuring CO, NOx and* O_2 *concentrations.*

3.2 Operational parameters

The operational parameters of the furnace are logged every minute, by an automatic system in the furnace. The operational parameters of the furnace of interest to this work is presented in Table 1.

Flow of Naphtha, ratio of LP steam to burners and COT are set values that is chosen by operators. The feedstock flow of naphtha is measured in tons per hour and the measurement is taken before steam is added. This flow is set to a value chosen based on the availability of naphtha and demand on products and does not have any dependence on any other parameters. The quantity of LP steam to the burners is measured as the ratio of LP steam to fuel to the burners and is often relatively stable at around 0.4-0.5. Neither the set value for Naphtha flow or LP ratio to fuel has any impact on the control system for other parameters.

The COT is the focal point of the combustion and is the main parameter that the control system is regulated around. This is set to be at a temperature that produces the desired components after cracking and is measured just before the quench exchanger at position 2 in the schematic. The fuel flow is a process parameter that is controlled to ensure that COT is kept at the desired level.

Table 1: Operational parameters in the furnace of interest in this work

Name	Type	In Fig. 4	Mean value	Unit
Naphtha flow	Set	(1)	27.99	ton/h
Fuel flow	Process	(3)	3.52	ton/h
LP steam in burners	Set	(4)	0.47	Ratio of Steam to fuel
O_2 conc. in stack	Process/Set	(6)	3.08	% (dry)
NO_x concentration	Measured	(6)	49.18	ppm_{mole} (dry)
CO concentration	Measured	(6)	12.55	ppm_{mole} (dry)
COT	Set	(2)	820.20	°C

The concentration of NO_x and CO are measured in ppm_{mole} in dry flue gas in the GC. The GC does not measure the actual NO_x concentration, but rather the concentration of nitrogen oxide (NO) which is 96-98% of total NO_x emissions in this furnace. Since the mechanics of creation is similar the NO concentration is a good indicator of the total NO_x emissions and will from here on be referred to as NO_x. The NO_x parameter is not used to regulate the control system in the furnace, measurements are taken mainly for reporting purposes.

The flow of air to the burners (position 5) is not a parameter that is logged, the only measurement of Oxygen (O_2) in the furnace is the oxygen concentration measured in the stack by the GC. The concentration of O_2 in the stack is categorized in this thesis both as a process and set parameter. It is a value set by operators that is regulating the intake of air. If too much CO is formed, then operators increase the set value of desired oxygen concentration in the stack. This change in set value increases the air intake in position 5 until the chosen concentration is achieved. In this way it is both a set value that is chosen by operators and kept stable over a long period of time, and a process parameter that can flexibly be changed to ensure that CO is kept at a desired level.

Calculations from engineers at Borealis has estimated that approximately 2% oxygen in the stack is enough to ensure efficient combustion. However, operational experience is that when the GC reports the oxygen concentration at 2% in the stack, there is significant emissions of CO, which indicates that there is not enough oxygen in the radiation section to ensure complete combustion. This mismatch between calculations and operational experience is suspected to be due to leakage of air into the convection section. Air leakage would mean that when the concentration is 2% in the top, it is less in the radiation part of the furnace. The oxygen concentration in the stack is therefore set at a higher level than 2%.

The composition of the fuel influences emission formation and the amount of fuel necessary to reach the set temperature of COT. For example, the lower heating value of methane is more than 3 times higher than the lower heating value for hydrogen, but the carbon atom means that methane can cause CO emissions. The composition of fuel is relatively constant over a period of a few hours, and as such is measured only once every 24 hours by the on-site lab. Over the past year the composition has ranged from 45% H_2 with 55% CH_4 to 60% H_2 with 39% CH_4 with the remaining percentage consisting of longer hydrocarbons. The mean composition of fuel during the past year has been 54% hydrogen, 45% methane and 1% longer hydrocarbons.

4. Methodology

In this section the methodology implemented in the thesis is described. A schematic of the methodology is shown in Figure 5. The first step is collecting the data from the furnace, any data that is faulty is then removed in the cleaning step. The cleaned data is the basis for the modelling using neural networks and networks for the three relevant outputs are then created: NO_x, CO and COT. Next the optimization model is created, choosing fitness functions and implementing limits to data. Lastly the process is evaluated by using the networks and optimization model in conjunction to produce suggestions of an operation mode to minimize NO_x emissions while keeping CO low and COT stable.

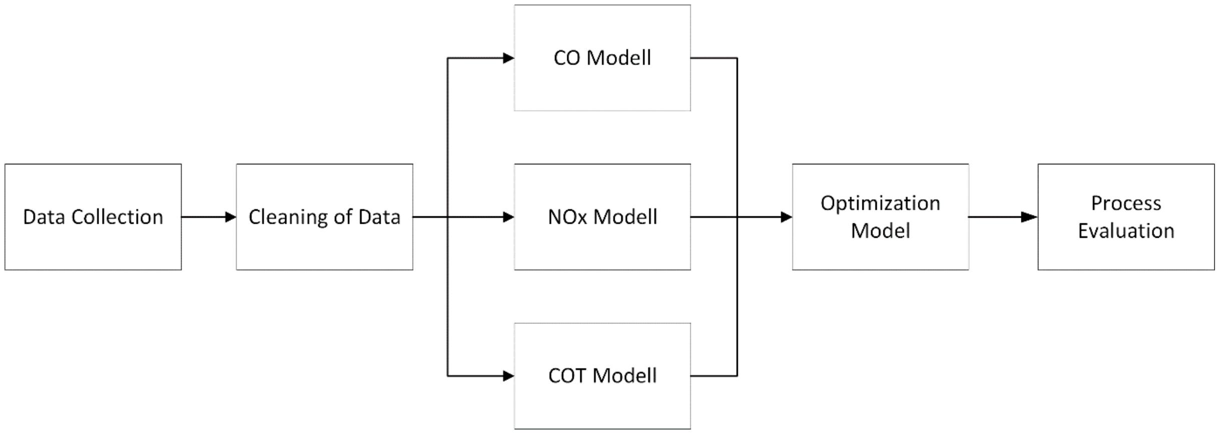

Figure 5: Overview of the methodology applied in this work

4.1 Data Collection

The data was collected from Borealis steam cracking furnace, which has records of minute-based process data. Data representative for the present outlay of the process were taken from the first of October 2018 to the last of September 2019, i.e. a year's worth of data points for a total of 525600 data points. Data was collected for all the available parameters that was identified as being important for modelling.

Data collected were split into two categories for the purpose of the training of the networks: inputs and outputs. Inputs are the flows that enters the furnace, e.g. flow of fuel, naphtha and steam. Outputs are parameters whose values depend on the inputs e.g. NO_x emissions. The inputs and outputs to the furnace that was identified as relevant to this works is presented in Table 2. In this work three outputs are of interest: NO_x and CO concentration and COT.

Table 2: Parameters of interest to the modelling in this thesis

Name	In Fig. 4	Type
Naphtha flow	(1)	Input
Fuel flow	(3)	Input
LP steam in burners	(4)	Input
O_2 conc. in stack	(6)	Input
% of H_2 in fuel	-	Input
% of CH4 in fuel	-	Input
NO_x concentration	(6)	Output
CO concentration	(6)	Output
COT	(2)	Output

4.2 Data Cleaning

Data was divided into three sets: one each for the three outputs. Each set consisted of data for one of the outputs i.e. NO_x, CO and COT as well as the data for all the inputs. The sets were then cleaned by removing faulty data and as there had been issues with production in the furnace and problems with storing of data a thorough data cleaning was necessary. Removal of data was identical for the sets containing data for NO_x and COT as any issues the furnace had affected both equally. However, for the dataset used for modelling CO there were additional problems affecting only that set, therefore cleaning was done separately.

A total of 63519 data points was removed due to being faulty from the sets of NO_x and COT, which corresponds to 12.09% of original data extracted. Faulty data that had to be removed was due to production problems, problem with storing of data and times when the GC was recalibrating. In Figure 6a data for NO_x concentration for June 2019 is shown, wherein the calibration of GC can clearly be seen by the dips to zero. The spike in emissions at the end is an example of what happens to the concentration of NO_x during de-coking. Figure 6b depicts when the program storing the data was having issues, and no data was stored. When this happened the program that stored data often extrapolated the missing values as a straight line between the last correct value and first new correct value.

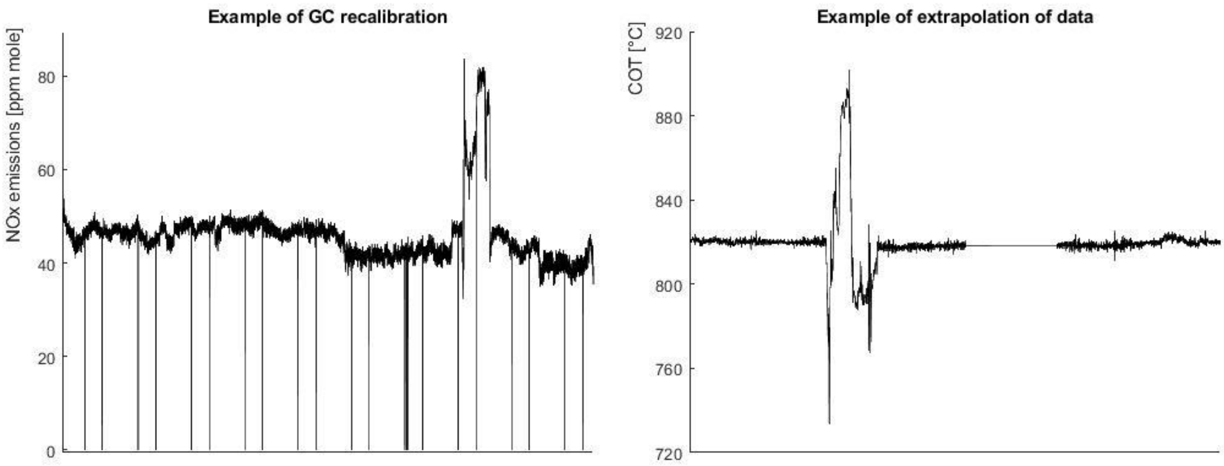

Figure 6: a) Raw data for NO_x concentration for June 2019 b) Raw data for COT from November 2018

Finding strict rules for data to be removed proved difficult, mainly due to the data collected during de-coking where the parameters often take on values that is outside the usual range. Any general rule for cleaning then risks removing data that is correct and might skew the following optimization. Because of this data cleaning was done individually for each month, but following the same prioritization order. The first step was to remove data that was recorded during the calibration of the GC, followed by the removal of any clearly extrapolated data. Lastly Borealis was consulted as to any known troubles in the furnace the past year and any data identified in the consultation was removed.

No values for NO_x emissions where found to be less than 30 ppm outside of when the GC is calibrating, and so all data corresponding to a NO_x value of less than 30 ppm were removed. Next each month was inspected for any data that was extrapolated by the system and any such data found was manually removed. Two periods when the production was having problems were identified when consulting with Borealis. From the middle of December to the end of January when the furnace was down and a couple of days in August when the GC was having trouble. This removal due to production problems corresponds to slightly over half of all data removed.

The program storing data was having issues when the concentration of CO was too high. During such periods as CO was more than 420 ppm the system marked the data as bad and put the values to zero. This resulted in plots looking like Figure 7, where the values changed from zero to 400 and back to zero in the course of three minutes. It is not possible to know what the actual values were so in order to be certain that all the data used is true data, more data was removed compared to the other sets.

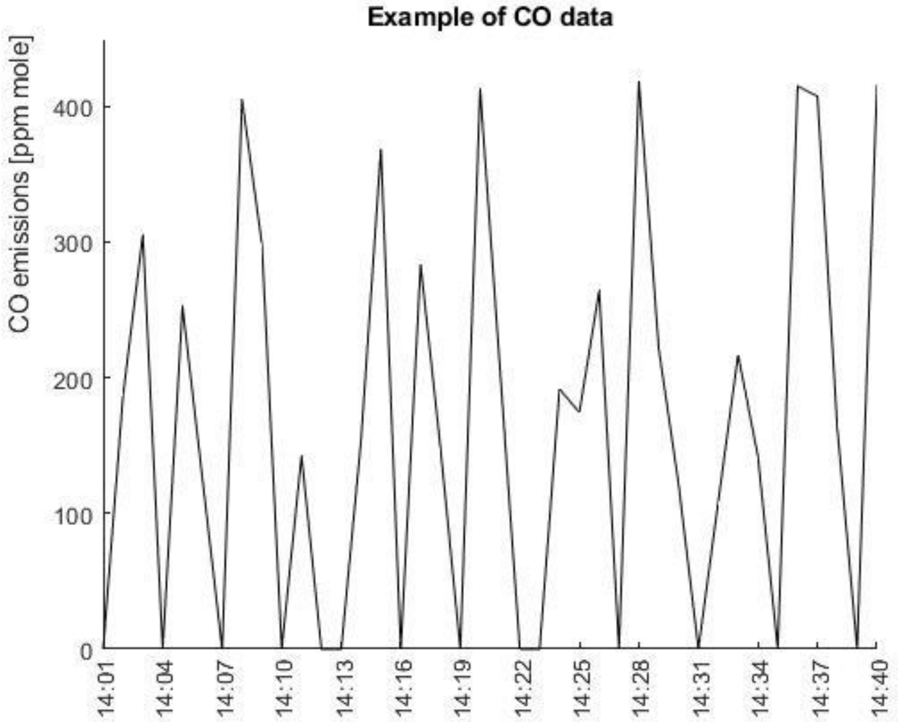

Figure 7: CO concentration showing values that are likely over 420 ppm but set to zero by the data storing program.

Faulty data was firstly removed from the set using the same methods as for the NO_x and COT sets. At the advice from Borealis all remaining data from January was removed from the set due to the production issues that month. To ensure that all influence from the bad data was removed, all data that was close to any peak over 350 ppm where removed. All data that was exactly equal to 0 was removed as well. The cleaned data for CO consists of 217005 datapoints, a bit over 40% of the original data collected.

4.3 Training of Neural Networks

Neural networks were trained using the MatLab software, which has built in functions for this purpose. The networks for each output were each trained separately but following the same method.

The cleaned dataset for the output of interest was loaded into MatLab where it was separated into training, validation and testing sets with a 70-15-15 distribution. Which data that was separated into which category was completely random to ensure that no bias in results exists. This was done so that early stopping could be used to limit the risks of overfitting. The networks structure has two layers, a hidden layer and an output layer. The hidden layer has a sigmoid activation function, while the output layer has a linear activation function. The networks utilize a Levenberg-Marquardt backpropagation training function for training purposes. This is a standard algorithm used in training of neural networks and is one of the fastest back-propagating algorithms offered in MatLab. The speed is essential due to the large datasets that was used for training in this thesis as it allowed time for several iterations of training as well as production of multiple networks for each output. The number of neurons that provide the best fit depends on the output, amount of data input and starting point of training. To find the optimal number of neurons for each output several networks were created, each with a different number of neurons. The number of neurons tested were 30, 40, 60, 80,100 and 140 respectively.

The set up for the algorithm was to begin by dividing the data into separate categories, followed by initiating training on the training data. 10 networks where then created for each tested number of neurons. The networks were then evaluated using the sum of squared errors (SSE) as a cost function and the best performing network on the validation set was saved and its performance on the testing set were investigated.

4.4 Optimization

A genetic algorithm (GA) was used for the optimization, which is a heuristic search algorithm that mimics natural selection in order to find an optimum. The networks crated for predicting NO_x emissions were used as the fitness function which the optimization is to find the minimum of. A built-in function in the MatLab software where used for the GA. Exploring the structure of how the networks predicting the three outputs were incorporated into the GA was the first step. This is followed by an investigation of two ranges of restrictions that were put on the input parameter values.

The networks are trained to accurately predict the emissions of NO_x and CO and COT on inputs that are normal for the furnace. Care therefore must be taken when optimizing the inputs to reduce emissions. If no limits are placed on the input values during optimization, the GA could suggest combinations that are far outside of the normal range for the furnace. For the networks to properly predict emissions they must have seen similar combinations of values before. The network for example has no data on what happens when the O_2 concentration reaches 0 while the furnace is still running. Any predictions made by the network for such extreme values will therefore be guesses at best. Restrictions were therefore placed on the input values, one more lenient range where the network might have some experience, and one where the networks has a lot of experience on all combinations.

Running the optimization on the lenient restrictions has a higher risk of the results not being general as some of the combinations might be more extreme. Any optimal composition of inputs using this range of inputs therefore has a higher risk of being false minimums that exists due to the networks being less precise in those ranges. To investigate this the optimization was run twice on the two best performing networks for NO_x while using the best networks for CO and COT. If the two optimizations using the different networks find different minimums, then there is no good way of deciding which one, if any, is correct. If the two networks finds the same minimum however, the risk of the minimum being due to extreme cases is less.

4.4.1 Incorporation of Neural Networks

To ensure that the suggested optimal parameters would not result in values of COT and CO outside of the viable range, the networks predicting those outputs were incorporated into the GA as well as the network for NO_x. This process is described in Figure 8, where it is shown how the neural networks are used with the genetic algorithm. The GA then suggests input values and uses the neural network for NO_x as a fitness function and calculates the predicted NO_x emissions. Thereafter the values of CO and COT networks were also calculated by their respective network using the same suggested input values. If COT and CO is within the viable limits, then the NO_x value is kept as is. However, when COT or CO was non-viable then the calculated NO_x value is increased by an arbitrary large number, in this case 200. It was found that the size of this number had no bearing on the results as long as it is sufficiently larger than the expected minimum of NO_x. In this way the GA received the information that any suggested parameters composition that resulted in COT and CO being too high or too low resulted in very high NO_x emissions as well. This ensured that the solutions that are un-feasible were

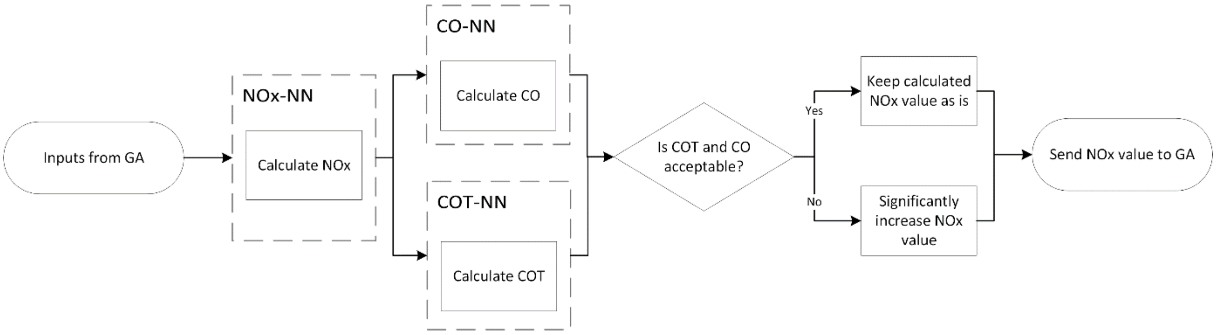

Figure 8: Schematic representation of how the optimization incorporates the networks for NO_x, CO and COT.

not suggested as optimal. GA then suggests new inputs based on the results of the networks, and this process is repeated until a minimum is found.

4.4.2 Limiting parameter range

The networks predictive ability is lessened when faced with extreme input values that the networks has little or no experience on. Placing limits on the values the input parameters can take is therefore imperative. Attempts to generalize and use networks on data that is not part of the basis of training should therefore be done with caution. As no thorough investigation of exactly which combinations of parameter values that is part of the base data has been conducted, it is unclear if the network has experience on some combinations of inputs. Two different levels of restrictions were therefore tested, with one range being a bit more lenient with the risk of extreme combinations and one range being more limited where it was certain that all combinations had been a part of the training.

The restriction imposed on the inputs i.e. O_2 concentration, steam to burners and flows of feedstock and fuel are presented in Table 3. Range 1 has a larger range in viable values in comparison to Range 2. The hope is that if the input data is not extreme and the suggested inputs are viable, then using Range 1 for optimization could lead to the finding of operational modes that is not currently in operation in the furnace. This has a larger risk of finding false minimums however, as the networks might not have experience on those exact compositions. Restriction 2 of parameters is stricter, but the risks of the suggested compositions being unviable is a lot smaller.

The restrictions were determined based on what values the parameters has taken on the last year. Range 1 is values that is close to the maximum and minimum values of that parameter while Range 2s limits where determined based on what levels where the most used. No investigation has been made to look for combinations of input values available in the training set.

The composition of fuel was logged on a 24h basis, as compared to the other parameters which was logged every minute. This limited the availability of different compositions more compared to other parameters. Coupled with fuel composition being difficult to regulate on a day to day basis it was decided that it would not be part of parameters to be optimized. The fuel composition is therefore set to always be the mean of the data used for modelling at 54% hydrogen, 45% methane and 1% larger hydrocarbons.

Table 3: Restrictions on input values for optimization

Parameter	Range 1	Range 2
Naphtha flow	25-30 ton/h	27-29 ton/h
Fuel flow	2.6-3.9 ton/h	3.45-3.9 ton/h
Steam to burners	0.4-0.51 ratio	0.44-0.51 ratio
O_2 conc. in stack	2.23-4.26 %	2.7-3.5 %
% of H_2 in fuel	54 %	54 %
% of CH_4 in fuel	45 %	45 %

The restriction for COT is 820±2°C, as this is the temperature range in the furnace that produces the desired components. For CO there is no clear limit of what is deemed a good level of emissions, but rather the aim is to emit as little as possible. Due to the lack of precision of the neural network predicting CO this restriction is set at 10 ppm. The actual restrictions placed by Borealis is slightly more lenient, but has been made stricter in the optimization due to the impreciseness of the networks predicting COT and CO.

5. Model and Method Evaluation

In this section the neural network models and the methodology followed is evaluated. Neural networks are discussed and evaluated based on their ability to accurately and consistently predict the correct outputs. The two best performing networks for predicting NO_x is examined more closely and utilized in the optimization algorithm. The results of the optimization are then presented and examined. Lastly a discussion on the pros and cons of using real-time data is had.

5.1 Neural Networks

For each output, several networks were created, and the results of the best performing networks are presented in this chapter. The performance of the networks was evaluated based on comparing the results of running the networks in the training sets inputs and the corresponding real values. Evaluation is presented as R-value i.e. a correlation coefficient, mean absolute error (mae) and root mean square error (RMSE). The two best performing networks for NO_x prediction are presented in greater detail where SSE and number of neurons is presented in addition to R-value, mae and RMSE. The networks predictive ability is also graphically presented, comparing real values to predicted values.

5.1.1 Result of modelling

The performance of the best performing networks for each output is shown in Table 4. The errors are calculated on the test set, where the real outputs are compared to the predicted outputs. The R-value is a mean of R-values for training, validation and test set results and is calculated directly by the MatLab neural network application.

Table 4: Evaluation of performance for neural networks

Performance	NOx	CO	COT
R-value	0.927	0.731	0.850
mae	1.75 ppm_{mole}	2.51 ppm_{mole}	2.63 $°C$
RMSE	2.33 ppm_{mole}	7.20 ppm_{mole}	4.68 $°C$

The mean concentration of NO_x emissions in the furnace is 49.18 ppm, meaning that the mean absolute error of 1.75 ppm is a deviation of 3.5% from the mean. For COT the mean absolute error of 2.63 °C for a mean temperature of 820.2 °C corresponds to a deviation of just 0.3%. For CO prediction, however, the deviation is at 20% compared to the mean value of 12.55 ppm. RMSE squares the errors before averaging, which means that a large weight is given to large errors. The difference between mae and RMSE for CO is a lot higher than for NO_x and COT which indicates that the errors for the network are larger for CO.

In Table 5 the performance values for the two networks that had the highest R-value and SSE for NO_x prediction are presented. The difference in performance is marginal in all parameters, with a SSE difference of 0.019 and mean absolute error of 0.0019. The R-value and RMSE also has almost identical values, the same number of neurons were also used in the structure, performance of the two should therefore be similar.

Table 5: Comparing the performance of the two best networks for NO_x prediction

Performance	Network A	Network B
SSE	4.9070	4.8878
R-value	0.93635	0.93256
Mae	1.7002	1.6983
RMSE	2.3051	2.2801
Neurons	140	140

In Figures 9-11 the predictive ability of the best networks for NO_x, CO and COT are presented graphically. In these figures the real values that were given to the network is plotted together with the networks predicted value.

In Figure 9 the two best NO_x networks are presented. Both network A and B has been presented here to better visualize any differences and similarity between the two. The first 20000 datapoints that remained after cleaning was used for easier visualization. In general, the models show predicted values are close to the real values. Both networks show very similar results, but closer inspection shows that there are spikes in Network B that does not exist for Network A and vice versa.

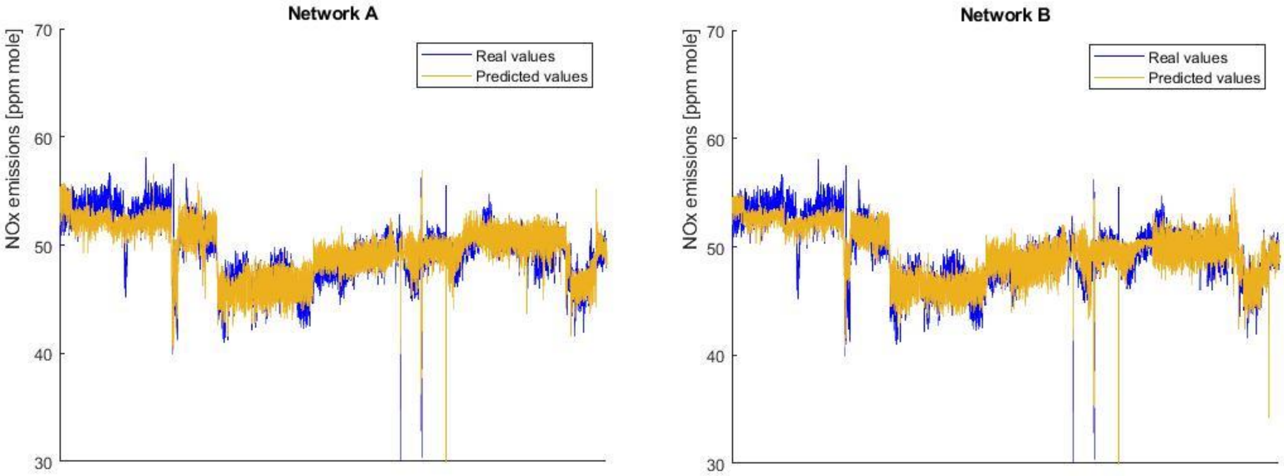

Figure 9: Comparison between real and predicted values for Network A and B for NO_x emissions

For both networks there are times when the predicted value is significantly off compared to the real value. The values around two thirds into the graph has a real value of approximately 55 ppm, but both networks predict it to be less than 30 ppm. An inspection of the inputs show that the input data consists of values that are far outside of the usual range of data extracted.

Figure 10 shows the graph where the real values and predicted values for COT is compared. The predictive values are calculated using the best performing network for COT, with 80 neurons and a R-value of 0.889. Comparing to predictions for NO_x in Figure 9, The predictions for COT is slightly worse, with the start predicting a value that is almost 5 degrees cooler than the real values.

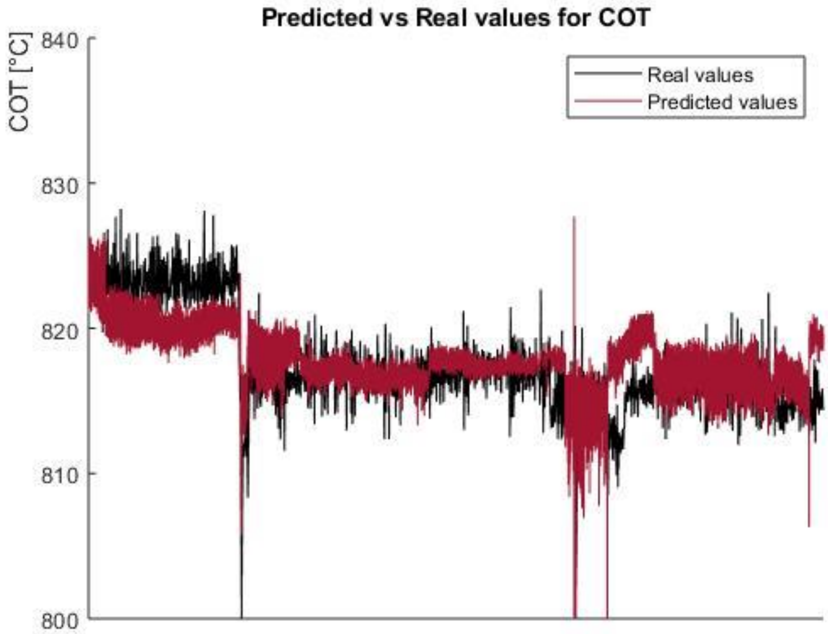

Figure 10: Plot of the real vs predicted values for COT

In Figure 11 the graph for predicting CO emissions using the best network with an R-value of 0.755 and RMSE of 7.12 is shown. It is evident that the prediction is a lot worse compared to the networks predicting NO_x and COT. The network has problem with predicting values that are close to zero, and often predicts negative emissions. The peaks of predictive values also do not reach as high as the real values.

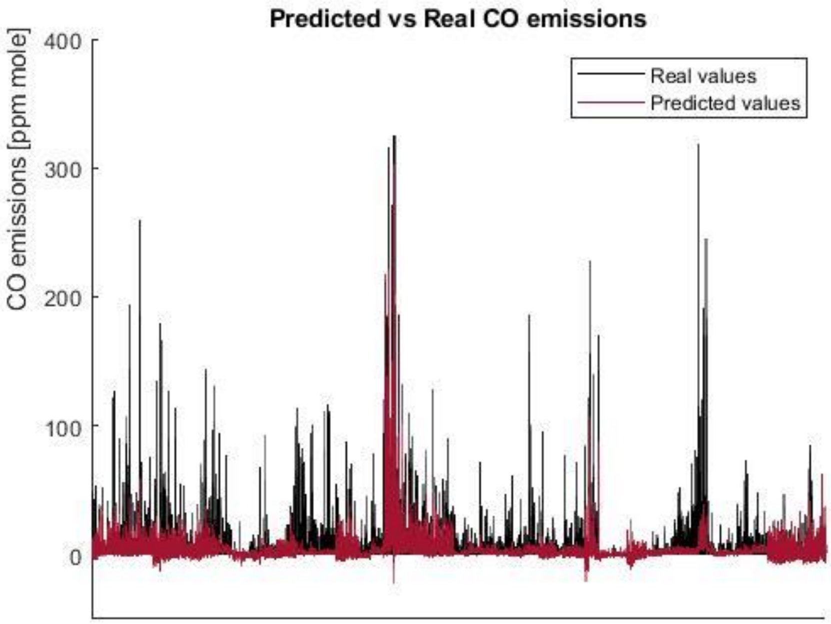

Figure 11: Visualizing the difference between real and predictive values for CO emissions

The difference in Figure 9 for network A and B is difficult to assess at a glance, the difference is therefore visualized in Figure 12 by a histogram over the difference in predictions for the networks. The difference in prediction is shown to usually be within 3 ppm_{mole}, there are times when the differences are higher, but they are so few that they are not visible in the graph. This is further indication that the difference between the two networks is limited.

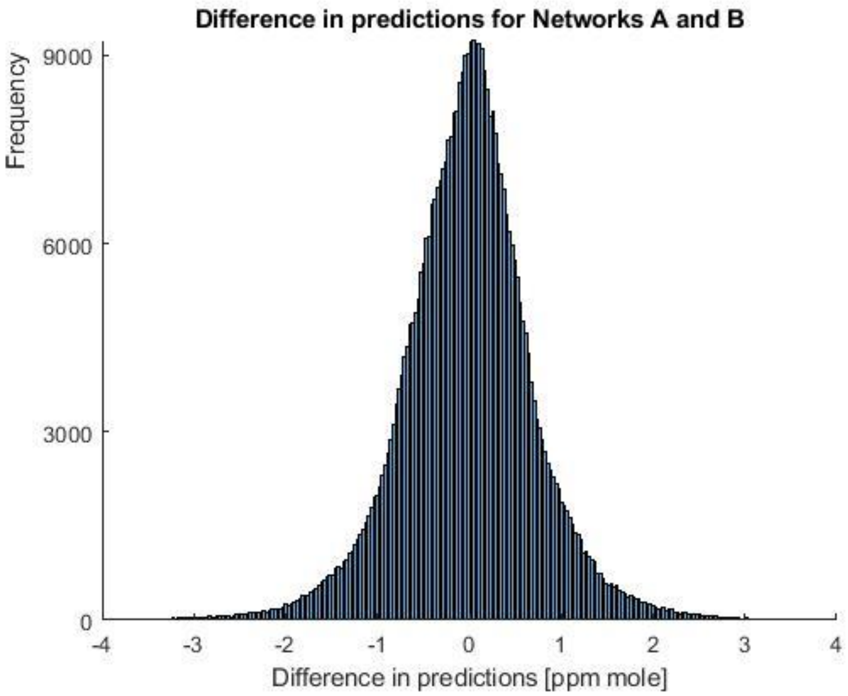

Figure 12: Histogram of the difference in predictions for networks A and B

5.1.2 Discussion on modelling

The performance of the NO_x models outperforms those of COT and CO, regardless of which performance parameter that is evaluated. COT in turn outperforms the network predicting CO in all categories. For the purpose of optimization, the model that needs to be the most precise is the NO_x model as that is the main fitness function used. The mae and RMSE are lower than the natural variance in the NO_x emissions data, which indicates that it is a viable method for predicting NO_x. The R-value of COT is lower, at a mean of 0.850 which indicates a worse predictive ability. The errors are however small, with an average deviation of just 0.3% from the mean temperature. It is possible that COT could have been better predicted using other parameters but based on the small errors the networks should be functional as a limiting factor in the optimization. Combining the error with the restriction placed on COT during optimization suggests that the mean temperature of suggested operational mode is between 815.37-824.63°C.

As discussed in data cleaning of CO in section 4.2.2 there were issues with the data storing for CO emissions which resulted in a data set for modelling that was half the size of the sets for NO_x and COT. The network struggled with accurately predicting outputs and has a mean RMSE of 7.20 ppm. The R-value is the worst of the networks tested at only 0.756. The graph in Figure 11 also shows that the networks predict values that are less than zero, which is impossible.

The impreciseness of the CO model could be a sign that there are other inputs than those used in this thesis that affects the CO emissions. If that is the case, then the model could be improved by additional points of measurements installed. Formation of carbon monoxide is generally very tightly tied to the O_2 input, so the imprecise measurement of oxygen inputs could also be a contributing factor to the uncertainty of the model. The network predicting CO performs badly, with high errors and predictions that are not physically possible. This indicates that neural networks as they are applied in this work is not the optimal method for predicting CO in the furnace.

The biggest difference between real and predictive values for the NO_x models are consistently found when the input data is far outside the normal range. For example, if the input data all take on their mean value, except for flow of fuel which is set to 0, then the networks predictions are a lot different compared to real values. When this happens, predictions are often as much as 40 ppm off compared to real values. Such data is not removed in the cleaning step described in section 4.1 as it is within the critera. The occurrence of such extreme spikes is not common, with just a few hundred in total. It is difficult to tell if it had determinantal effect on the training, as such data represents less than 0.1% of all data used for training. However, the occurrence of such spikes indicates that the method for cleaning should be revisited and the rules made more rigorous.

5.2 Optimization

Running the optimization as suggested in section 4.4 results in suggestions for input values that would minimize NO_x while keeping COT within 820 ± 2°C and CO less than 10ppm. The most precise method of validating that the results of the optimization would be to test the suggested operational mode on the furnace and observe if output behaves as predicted. Testing on the furnace was however not an option during this work due to time constraints, so an alternative method is suggested in this chapter.

The two best performing networks for NO_x performed very similar on R-value, mae, SSE and RMSE. The networks where therefore both used as fitness function in the optimization structure and the results were compared. In theory using both networks for optimization should result in similar suggestions for operational mode which would cause the least amount of emissions. When that is not the case and the networks suggest different inputs and/or emissions there are two options: there are different operating modes that both reduce emissions an equal amount, or one or both networks are finding false minimums. Such false minimums might be due to a combination of values that are far outside of the normal operating mode, and thus the networks have little experience on them.

If the networks have found different compositions of parameters that result in a minimum, and both options are viable, then the results should in theory be general. That is; if optimizations using network A suggests a certain composition that is optimal, then using network B to predict the NO_x emission of those inputs should result in a similar level of emissions. If not, then one or both networks are likely wrong in their optimization. Which one, or if it's both are difficult to assess with this method.

The furnace is often run at different loads, which is defined by the flow of feedstock. Different load levels have a large effect on the size of the other inputs to ensure the desired cracking process takes place. Therefore, the optimal running conditions is expected to be heavily dependent on the level of naphtha flow and because of this the optimization is run for different flows of feedstock.

In Figure 13 the predicted emissions of the suggested operational mode for network A and B when inputs were restricted to Range 1 is presented. For each load different operational modes where found to be optimal. Using those optimal operational modes suggested, the expected NO_x emissions are presented, represented by a solid line for the corresponding network that was used for the optimization. The network that was not used in the optimization process was then used to predict the NO_x emission using the suggested operational modes, this is represented by the dashed line.

It was investigated how both networks perform on the suggested optimal values suggested by the other network. Network A was used as the neural network for NO_x predictions in the optimization, which produces suggested values for the input parameters that would minimize the emissions of NO_x. Network B was then used on the inputs suggested, predicting how high the NO_x emissions would be for the suggested operational mode. The result of this process is plotted in Figure 13. Figure 13a is optimization and prediction for network A, with the dashed line representing predictions of using network B on the suggested inputs. Figure 13b is the other way around, with the solid line representing where network B is used to produce optimal parameter values. Those values where later used to predict NO_x using network A. The optimal emissions suggested by Network A range from 30-18 ppm, and 27-20 ppm for Network B. This is significantly lower compared to the emissions of the normal running conditions which produces emissions between 40-60 ppm.

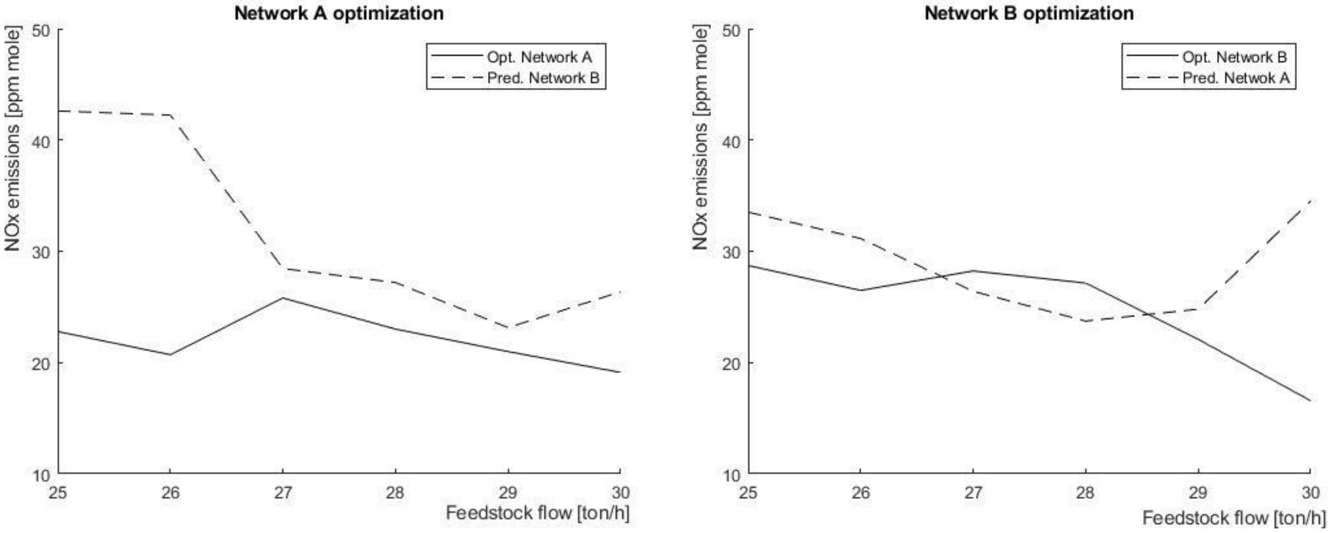

Figure 13: Results of running the optimization for the two different networks and using the other network on the suggested operational mode to predict NOx emissions. Inputs limited in accordance with Range 1.

Both versions show decent generalization when the flow of feedstock is between 27-29, where the difference is just a few ppm. This difference of a few ppm could be compared to the difference in the histogram of Figure 12 where the predictions of the two networks were compared. The difference between the two networks in that figure is usually less than 3 ppm, which could be the difference seen in Figure 13 for the medium loads.

For high and low loads of 25,26 and 30 tons per hour for restrictions on inputs for Range 1, there is a stark difference between the network's predictions on the suggested running conditions. The difference in Figure 13 differs between 7 and 20 ppm. The difference in predicted emissions could be due to the network having little to no experience on how those suggested input values interact with each other. It is possible that the data used during training has feedstock flow of 25 that is only paired with very low flows of fuel, the networks could then have trouble accurately predicting what happens when a low feedstock flow is paired with a high flow of fuel. As there is no convergence in predicted emissions for the suggested operational values for high and low loads, it is probable that either one or both are false minimums. The suggested operational modes for loads of 25,26 and 30 tons per hour will therefore not be presented in the process evaluation in section 6.

The same operation as applied in Figure 13 where done for the more restricted values for inputs limited by Range 2 and the difference between the two networks were marginal. The biggest difference was about 4 ppm, for a feedstock flow of 27 tons per hour, with the mean difference of 0.96 ppm for all three. The optimal NO_x emissions suggested when restriction 2 was used range from 40-47.5 ppm, which is in line with expected emissions during the daily running. There is no suspicion of those being false minimums, partly due to convergence in predictions, and partly due to the networks having more experience on those combinations. All three loads optimized will therefore be presented in section 6.

5.3 Discussing the use of real-time data

Usage of real time data for the modelling of neural networks has the advantage of not requiring the process to be stopped for a few weeks to gather data. However, if the models trained on real-time data is not viable, then the method needs to be adjusted.

The R-values of the neural networks predicting NO_x with a mean of 0.927 is comparable to the R-values found by Zheng et al. (Zheng et al., 2008) of 0.928 for the test and training set. Zheng et al. conducted their research on a coal-fired boiler, which is different from the gaseous fuel used for this steam cracking furnace. Generally, it is harder to create models predicting NO_x formation when solid fuel is used. This indicates that it is possible to use real-time data without suffering a significant loss in performance, but performance could have been better. No studies have been located which predicts a temperature of cracking or emissions of CO using neural networks, so no comparisons on performance can be made for those networks.

Two big drawbacks of using real-time data is the limited knowledge of the data and the limited combinations of values on the operational parameters. The limited knowledge increases the risk of incorporating faulty data into the set used for modeling as there is no information if there was a small error in a measuring instrument for an hour or two. If detailed records existed of any minor production errors in the past year, then this would not be a problem. For the training of neural networks, the influence of those errors is likely to be limited due to the sheer number of data points utilized but might have consequences for the optimization as it searches for a minimum. The faulty data that escaped cleaning is however often outside of the restrictions placed on the inputs and should therefore have limited influence on the optimization.

The furnace is often run using similar input values from day to day with no significant differences in operation. This limits the combinations of values of the operational parameters that is incorporated in the training of the network. The consequences of this can be seen in Figure 13. The networks have little experience on feedstock flows of 25 tons per hour and the predictions vary wildly between the two networks. Combinations where the networks have more experience i.e. the more common loads of 27-29 tons have very similar predictions.

The training of the networks incorporated data that was outside of the range of what was common for the running. Utilizing this type of data was done to investigate the possibility of finding optimal running conditions that was outside of the normal range. When the optimization algorithm tried to find the minimum while allowing the data to have a large range of values, the resulting optimization risked being unviable. This was shown when the optimizations did not converge for high and low loads when inputs were restricted in accordance with Range 1, and it is doubtful that the suggested operating modes are viable. When the input range was more restricted, the optimization converged and had believable values. This indicates that with the method used in this thesis, the additional data did not harm the optimization, but probably did not contribute either.

6. Process Evaluation

In Table 6 the optimal input values suggested by running the optimization in 4.4 for the larger range of restrictions on inputs is shown. Only the values suggested using the medium loads are presented, as other loads investigated showed to be unreliable in section 5.2.

The suggested operational mode for the furnace is very similar for the two networks. With a suggested fuel flow at 2.8-2.9 tons/hour and a high ratio of LP steam of 0.51-0.49. The biggest difference is found in the oxygen concentrations, which varies between 2.8-3.1 % for network A, while being stable around 2.8 %

For optimization on network A the LP steam to burners is always at the absolute maximum, while the O_2 concentration is the highest for a load of 28 tons naphtha per hour. The optimal fuel gas flow suggested is relatively stable at 2.8-2.9 tons per hour. Suggested input values for Network B shows relatively stable values regardless of level of load, with the exception being the O_2 concentration which is lowered for a high load.

Table 6: Values of operational parameter that is suggested for Range 1

	Network A				Network B			
Feedstock Flow [ton/h]	NO_x emissions [ppm_{mole}]	Fuel flow [ton/h]	LP steam [-]	O_2 conc. [%]	NO_x emissions [ppm_{mole}]	Fuel flow [ton/h]	LP steam [-]	O_2 conc. [%]
27	25.78	2.79	0.51	2.86	28.42	2.78	0.51	2.84
28	24.37	2.90	0.51	3.16	27.14	2.84	0.50	2.88
29	20.80	2.88	0.51	3.09	22.08	2.90	0.49	2.78

The optimization for both network A and B results in values that are outside of the current range of NO_x emissions. The data that was extracted rarely goes below 40 moles ppm while the suggested minimums from optimization ranges from 20-28 ppm. The largest difference in the suggested operational parameters compared to the current values is in fuel flow, which is reduced by 20% compared to current values. Oxygen concentration and LP steam to burners are at levels that is consistent with current levels in the furnace. If this reduction of fuel flow is viable, and doesn't lead to the furnace being too cold, then it would halve the emissions of NO_x compared to current levels.

When the limits on the inputs were set closer to those of the standard running conditions in accordance with Range 2, the results are more cohesive. In Table 7 the suggested optimal input values and resulting NO_x emissions are stated. The suggested running conditions for flows of 27 and 29 are almost identical for optimizations on both network A and B. For a flow of 28, optimization on network A suggests having as low flow of fuel as possible, while keeping O_2 concentration high. Optimization on network B however, suggests keeping a high amount of fuel and low O_2 concentration. Emissions range between 47 and 40 ppm, which is in the lower range of the current emissions in the furnace. The emissions could then be reduced by 10% compared to current levels.

Table 7: Suggested operational parameters using limited values

	Network A				Network B			
Feedstock Flow [ton/h]	NO_x emissions [ppm_{mole}]	Fuel flow [ton/h]	LP steam [-]	O_2 conc. [%]	NO_x emissions [ppm_{mole}]	Fuel flow [ton/h]	LP steam [-]	O_2 conc. [%]
27	40.03	3.90	0.46	2.83	43.46	3.90	0.44	2.78
28	47.57	3.45	0.46	3.45	47.52	3.90	0.44	2.48
29	44.88	3.45	0.49	2.70	44.15	3.45	0.49	2.70

7. Conclusion

This master thesis has investigated the possibility of optimizing the NO_x emissions from a steam cracking furnace by using real-time data to create simple artificial neural networks, which was then coupled with a genetic algorithm. Input parameters of importance to were decided upon and data was extracted from a steam cracking furnace operated by Borealis. The extracted data was then cleaned and used as a basis for training of the networks. Networks where created for the three outputs deemed relevant for the running of the furnace: emissions of NO_x and CO, and the temperature of cracking (COT). The optimization algorithm utilized the networks to find inputs which would limit the emissions of NO_x while keeping the values of CO emissions and COT at acceptable levels.

The networks created for prediction of NO_x emissions performed very well, with R-values around 0.927, which is comparable to those in literature. This indicates that usage of real-time data is a viable method for modeling emissions of $NO_{x.}$ Networks created for COT performed slightly worse, with R-values of 0.850. Creating networks for CO predictions was more difficult due to problems in data collection limiting data availability and the lack of the important control variable of air intake to the furnace. The models for CO also had trouble with data close to zero, and often predicted negative emissions. This indicates that neural networks are a viable strategy for predicting NO_x emissions in a furnace but doesn't work as well on predicting other outputs tested in this work. This might be due to the values of the other outputs being dependent on parameters that are not logged, and therefore not available for modelling. It is also possible to customize a neural network in a way which might make modelling of CO more consistent.

When the networks were combined with the optimization algorithm the viability of the optimization depends on the restrictions placed on the input values. Using the method described in this work, two suggestions for possible running conditions were made. It was found that the running conditions which allowed the operational parameters to take on values outside of normal values sometimes resulted in suggestions that was deemed unviable.

When the possible values of the operational parameters were more restricted, the suggested running conditions and predicted emissions are more in range with what is currently in operation in the furnace. This implies that the method used in this thesis is viable with finding optimal process conditions that is part of the normal running of the furnace. If optimization with large range of parameter values are true, then emissions could be reduced by up to 50%. The optimization suggested when more restricted inputs were used would result in a reduction of emissions of 10% compared to current levels.

8. Suggested future work

For future work alternative methods for the modelling of CO would have to be investigated. The predictive ability of the network used in this thesis is not great and could hopefully be improved by finding alternative parameters that influence the formation of CO.

There are many more complicated ways to create a neural network than the methods employed in this thesis. A GRNN has shown good performance on the prediction of NO_x for example and it would be interesting to see what improvements could be made to the neural networks predicting COT and CO as well.

Extracting data with the aim of trying to make as many combinations of parameters available might result in more precise networks over the interval tested for. The aim of using a large data set was to have the option of finding optimal parameter compositions that is outside of the normal values of the operational parameters. This would be possible only if the data contained many combinations of parameter values. Actively looking for as many combinations as possible would be time consuming, and the development of a more automated process would be imperative.

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